การสร้างแบบจำลองและการจำลองการลดขนาดของเชื้อเพลิงภายในเตาเผาฟลูอิไดซ์เบดแบบหมุนเวียนโดยพิจารณาแอตทริชันและแฟรกเมนเทชัน

นายณัฐพงศ์ งามประดิษฐ์

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรดุษฎีบัณฑิต
สาขาวิชาเคมีเทคนิค ภาควิชาเคมีเทคนิค
คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย
ปีการศึกษา 2547
ISBN 974-17-7072-3

MODELING AND SIMULATION OF SIZE REDUCTION OF FUELS IN CIRCULATING FLUIDIZED BED COMBUSTOR BY CONSIDERING ATTRITION AND FRAGMENTATION

Mr. Natthapong Ngampradit

A Dissertation Submitted in Partial Fulfillment of the Requirements
for the Degree of Doctor of Philosophy in Chemical Technology

Department of Chemical Technology
Faculty of Science
Chulalongkorn University

Academic year 2004

ISBN 974-17-7072-3

Thesis Title	MODELING AND SIMULATION OF SIZE REDUCTION OF FUELS IN CIRCULATING FLUIDIZED BED COMBUSTOR BY CONSIDERING ATTRITION AND FRAGMENTATION
By	Mr. Natthapong Ngampradit
Filed of study	Chemical Technology
Thesis Advisor	Associate Professor Pornpote Piumsomboon, Ph.D.
Thesis Co-advisor	Boonrod Sajjakulnukit, Ph.D.

Accepted by the Faculty of Science, Chulalongkorn University in Partial Fulfillment of the Requirements for the Doctor's Degree

..... Dean of the Faculty of Science

(Professor Piamsak Menasveta, Ph.D.)

THESIS COMMITTEE

..... Chairman

(Professor Pattarapan Prasassarakich, Ph.D.)

..... Thesis Advisor

(Associate Professor Pornpote Piumsomboon, Ph.D.)

..... Thesis Co-advisor

(Boonrod Sajjakulnukit, Ph.D.)

..... Member

(Professor Somsak Damronglerd, Dr. Ing.)

..... Member

(Associate Professor Lursuang Mekasut, Dr. Ing.)

..... Member

(Associate Professor Sunun Limtrakul, Ph.D.)

ณัฐพงศ์ งามประดิษฐ์ : การสร้างแบบจำลองและการจำลองการลดขนาดของเชื้อเพลิงภายในเตาเผาฟลูอิไดซ์เบดแบบหมุนเวียน โดยพิจารณาแอตทริชันและแฟรกเมนเทชัน (MODELING AND SIMULATION OF SIZE REDUCTION OF FUELS IN CIRCULATING FLUIDIZED BED COMBUSTOR BY CONSIDERING ATTRITION AND FRAGMENTATION) อ. ที่ปรึกษา : รศ.ดร.พรพจน์ เปี่ยมสมบูรณ์, อ.ที่ปรึกษาร่วม : ดร.บุญรอด สัจจกุลนุกิจ 251 หน้า. ISBN 974-17-7072-3.

เตาเผาฟลูอิไดซ์เบดแบบหมุนเวียน เป็นเตาเผาที่มีประสิทธิภาพสูง และสามารถใช้กับเชื้อเพลิงได้หลายชนิด เช่น ถ่านหิน เชื้อเพลิงชีวมวล หรือเชื้อเพลิงผสม ถ่านหินและชีวมวลมักเป็นเชื้อเพลิงให้ความร้อนกับเตาเผาประเภทนี้เพื่อทำหน้าที่ผลิตไอน้ำในโรงงานอุตสาหกรรมหลายประเภท การกระจายตัวของขนาดอนุภาคในเตาเผาฟลูอิไดซ์เบดแบบหมุนเวียนมีผลต่ออุทกพลศาสตร์ และการถ่ายโอนความร้อนภายในเตาอันมีผลเกี่ยวเนื่องต่อประสิทธิภาพในการเผาไหม้ และการปล่อยแก๊สเสีย การทำความเข้าใจเรื่องการลดขนาดของอนุภาค จึงเป็นประโยชน์ต่อการทำนายการกระจายตัวของขนาดอนุภาค ในการทดลองนี้ได้ศึกษาการลดขนาดของถ่านหินและชานอ้อยในเตาเผาฟลูอิไดซ์เบดแบบหมุนเวียนขนาดเส้นผ่าศูนย์กลางภายใน 2.5 เซนติเมตร สูง 160 เซนติเมตร ผลการทดลองแสดงถึงกระจายตัวของขนาดอนุภาคอันเป็นผลเนื่องมาจากกระบวนการปล่อยสารระเหยง่าย และการเผาไหม้ โปรแกรมแอสเพนพลัส ถูกนำมาใช้ในการจำลองสภาวการณ์การกระจายตัวของขนาดอนุภาค โดยการเพิ่มแบบจำลองการแตกของอนุภาคที่ได้จากการทดลอง ผลปรากฏว่าการจำลองสภาวการณ์โดยใช้แบบจำลองนี้ให้ผลในการทำนายการกระจายตัวของขนาดอนุภาคได้ดีกว่าการใช้แบบจำลองการลดขนาดตามแนวแกน (Shrinking Particle Model) เพียงอย่างเดียว นอกจากนั้นในส่วนของการจำลองสภาวการณ์เชิงอุตสาหกรรม มีการเพิ่มแบบจำลองการปล่อยแก๊สเสีย เพื่อคำนวณจลศาสตร์ของแก๊สไนโตรเจนออกไซด์ และไนตรัสออกไซด์ และการเปลี่ยนแปลงของแก๊สซัลเฟอร์ไดออกไซด์ เพื่อทำนายการปล่อยแก๊สเสียสู่สิ่งแวดล้อม

ภาควิชา	เคมีเทคนิค	ลายมือชื่อนิสิต.....
สาขาวิชา	เคมีเทคนิค	ลายมือชื่ออาจารย์ที่ปรึกษา.....
ปีการศึกษา	2547	ลายมือชื่ออาจารย์ที่ปรึกษาร่วม.....

4373814023 : MAJOR CHEMICAL TECHNOLOGY

KEY WORD: ATTRITION / FRAGMENTATION / CFBC / SIMULATION / CIRCULATING FLUIDIZED BED COMBUSTOR / PARTICLE COMMUNITION

NATTHAPONG NGAMPRADIT : MODELING AND SIMULATION OF SIZE REDUCTION OF FUELS IN CIRCULATING FLUIDIZED BED COMBUSTOR BY CONSIDERING ATTRITION AND FRAGMENTATION. THESIS ADVISOR : ASSOC PROF. PORNPOTE PIUMSOMBOON, THESIS COADVISOR : BOONROD SAJJAKULNUKIT, Ph.D. 251 pp. ISBN 974-17-7072-3.

A Circulating Fluidized Bed Combustor (CFBC) is a high efficient combustor. It can handle various types of solid fuels such as coal, biomass or mixed fuels. Coal and biomass has been used as fuels to generate heat for a boiler in many industries. The particle size distribution (PSD) of the solid inventory in a CFBC affects the hydrodynamic and heat transfer leading to the changes of combustion efficiency and gas emission. The understanding of the particle comminution is useful for PSD prediction. The experiments of coal and bagasse comminution was studied in the 2.5 cm ID, and 160 cm height of the CFBC. The PSD resulted from the devolatilization and combustion processes were obtained. The ASPEN PLUS program was used to simulate the PSD of fuel particles by adding the fragmented particle models resulted from the experiment. The simulation result showed that by adding these models the prediction is better than those with only the shrinking particle model. Moreover, for the industrial-scale CFBC simulation, gas emission models were included to calculate the kinetic rates of NO, N_2O and the conversion of SO_2 to predict the gas emission to the environment.

Department	Chemical Technology	Student's signature Natthapong Ngampradit
Field of study	Chemical Technology	Advisor's signature
Academic year	2004	Co-advisor's signature Boonrod

ACKNOWLEDGEMENTS

The author would like to express his gratitude to his supervisor, Assoc.Prof. Pornpote Piumsomboon, and co-supervisor, Dr. Boonrod Sajjakulnukit for their great help and support. The help and advice from his supervisors are greatly appreciated, especially from Assoc.Prof. Pornpote Piumsomboon. The author also would like to acknowledge Prof. Pattarapan Prasassarakich, Prof. Somsak Damronglerd, Assoc. Prof. Lursuang Mekasut, and Assoc. Prof. Sunun Limtrakul for serving as chairman and members of thesis committee, respectively.

The author greatly indebted to Mr. Vitthawat Ngampradit for his helpful suggestions and assistance throughout the course of this study.

Many thanks are also extended to technicians and members of cybernetic group of the Department of Chemical Technology, Chulalongkorn University, especially Mr. Noppon Manggaranochai, Mr. Aungsuthorn Mahittikul and Miss Napida Hinchiranan for their assistance and helpfulness during the period of this research.

Thanks are forward to Petroleum and Petrochemical Technology Consortium, Ratchadaphisek Somphot Endowment, Energy policy and planning office of ministry of Thailand, and Graduate School of Chulalongkorn University for financial support of this research, and Siam Kraft Industry Co., Ltd. for the details of CFBC.

The words of thanks and appreciation cannot reward the people who sacrifice almost all their lives for the author, his parents. Their excellent support and patience enabled the author to reach the goal.

CONTENTS

PAGE

PAGE

LIST OF TABLES

LIST OF FIGURES

FIGURE PAGE

FIGURE PAGE

FIGURE PAGE

FIGURE PAGE

NOMENCLATURES

A	:	Bed cross section (m^2)
A_c	:	Cross section area of combustor (m^2)
Ar	:	Archimedes number (dimensionless)
a	:	Decay constant (dimensionless)
a_1	:	Parameter in eq. (3.58) (dimensionless)
b	:	Stiochiometric coefficient of gas in the combustion reaction (dimensionless)
C	:	Combustion gas concentration ($kmol \cdot m^{-3}$)
CCD	:	Charge Coupled Devices
CFB	:	Circulating Fluidized Bed
CFBC	:	Circulating Fluidized Bed Combustor
c_{Ag}	:	Concentration of A ($kmol \cdot m^{-3}$)
c_i	:	Oxygen concentrations in the inlet air ($mole \cdot m^{-3}$)
c_p	:	Oxygen concentrations in the particulate phase ($mole \cdot m^{-3}$)
DCW	:	Dual Cylindrical Wave
D_A	:	Diffusion coefficient of A ($m^2 \cdot s^{-1}$)
D_g	:	Oxygen diffusivity ($m^2 \cdot s^{-1}$)
D_i	:	Initial diameter (m)
DLS	:	Dynamic Light Scattering
D_p	:	Average sorbent surface particle diameter (cm)
D_r	:	Riser diameter (m)
d	:	Average particle diameter (m)
d_t	:	Diameter of the largest particle that would be elutriated at operating conditions (m)
E_a	:	Elutriation arising from attrition of particle surfaces ($kg \cdot s^{-1}$)
E_{a1}	:	Activation energy ($J \cdot kmol^{-1}$)
E_c	:	Elutriation of particles reduced in size by combustion ($kg \cdot s^{-1}$)
ECT	:	Electric Charge Transfer
E_f	:	Elutriation due to the original fines fraction in the coal feed ($kg \cdot s^{-1}$)

E_{fr} : Elutriation of fragmented particles ($kg \cdot s^{-1}$)

EGAT : Electricity Generating Authority of Thailand

E_t : Total elutriation rate of unburned carbon ($kg \cdot s^{-1}$)

FBC : Fluidized Bed Combustion

F_c : Feed rate of carbon entering the combustor ($kg \cdot s^{-1}$)

F_l : Mass flow rate of limestone in the feed ($kg \cdot s^{-1}$)

F_p : Specific surface area (m^{-1})

$F_{O_{2,v}}$: Oxygen molar flow rate required for combustion of volatiles in the particulate phase ($mole \cdot s^{-1}$)

F_t : Volumetric flow rate of solid ($m^3 \cdot s^{-1}$)

f : Fraction of gas for each component (dimensionless)

f_B : Size parameters (dimensionless)

f_i : Fraction of fuel particles with initial diameter (dimensionless)

G_s : Solid circulation rate ($kg \cdot m^{-2} \cdot s^{-1}$)

g : Acceleration due to gravity ($m \cdot s^{-2}$)

HGI : Hard Grove Index

ICFB : Internally Circulating Fluidized Bed

K : Rate constant (s^{-1})

K_v : Volumetric rate constant ($kmol \cdot m^{-3} \cdot s^{-1}$)

k : Free parameter in Weibull distribution (dimensionless)

k_0 : Frequency factor ($m \cdot s^{-1}$)

k_{Ag} : Mass transfer coefficient of A ($m \cdot s^{-1}$)

k_a : Attrition rate constant (m^{-1})

k'_a : Attrition rate constant (dimensionless)

k_{fr} : Fragmentation rate constant (s^{-1})

k_s : Carbon surface reaction rate constant ($m \cdot s^{-1}$)

k_{s1} : First order reaction rate constant base on unit surface ($m \cdot s^{-1}$)

L_1 : Height of dense bed (m)

LDV : Laser Doppeler Velocimeter

l	:	Diameter of particle (mm or μm)
M	:	Bed mass inventory (kg)
$M(<l)$	:	Cumulative mass of fragments of size less than l (g)
M_c	:	Carbon atomic weight (kg·mole^{-1})
MSW	:	Municipal Solid Waste
M_T	:	Total mass of fragments in the distribution (g)
NC	:	Non Conventional component
P	:	Bed pressure (atm)
PCS	:	Photon Correlation Spectroscopy
PIV	:	Particle Imaging Velocity
PSD	:	Particle Size Distribution
R	:	Radius of particle (m)
Re	:	Reynolds number (dimensionless)
Re_{mf}	:	Reynolds number at minimum fluidized condition (dimensionless)
R_g	:	Universal gas constant (kcal·kmol^{-1}·K^{-1})
R_{g1}	:	Universal gas constant (atm·cm^3·gmol^{-1}·K^{-1})
R_{g2}	:	Universal gas constant (J·kmol^{-1}·K^{-1})
R_s	:	Mean sorbent particle radius (cm)
$R_{SO_2,1}$	:	Rate SO_2 generate per unit volume of dense bed (kmol·m^{-3}·s^{-1})
Rt	:	Rate of reaction (kmol·m^{-3}·s^{-1})
Rt_A	:	Rate of NO formation (kmol·m^{-3}·s^{-1})
Rt_B	:	Rate of N_2O formation (kmol·m^{-3}·s^{-1})
Rt_C	:	Rate of NO reduction by char in the first reaction (kmol·m^{-3}·s^{-1})
Rt_D	:	Rate of NO reduction by char in the second reaction (kmol·m^{-3}·s^{-1})
Rt_E		Rate of N_2O reduction by char (kmol·m^{-3}·s^{-1})
Rt_F	:	Rate of homogeneous destruction of N_2O (kmol·m^{-3}·s^{-1})
Rt_G	:	Rate of thermal decomposition of N_2O (kmol·m^{-3}·s^{-1})
r_c	:	Residual radius (m)
Sc	:	Schmidt number (dimensionless)

Sh	:	Sherwood number (dimensionless)
SPC	:	Single Particle Counters
T	:	Temperature (K)
t	:	Time (s)
t_1	:	Mean residence of sorbent particles in dense bed (s)
t_i	:	Mean residence time of sorbent particles in i^{th} interval of the bed (s)
$\hat{t}$	:	Residence time (s)
U	:	Fluidization gas superficial velocity at bed temperature ($m \cdot s^{-1}$)
U_1	:	Superficial gas velocity in dense bed ($m \cdot s^{-1}$)
U_2	:	Superficial gas velocity in dilute bed ($m \cdot s^{-1}$)
U_{ch}	:	Choking velocity ($m \cdot s^{-1}$)
U_{mf}	:	Minimum fluidizing gas superficial velocity at bed temperature ($m \cdot s^{-1}$)
U_t	:	Terminal velocity ($m \cdot s^{-1}$)
V	:	Reactor volume (m^3)
V_{CaO}	:	Molar volume of CaO ($m^3\ kmol^{-1}$)
W_c	:	Carbon loading in the bed (kg)
W_s	:	sulfur weight fraction in dry-based coal (dimensionless)
$X_{CaO,i}$	:	Fractional conversion of CaO in the i^{th} interval (dimensionless)
x	:	Number of transfer units (dimensionless)
$Y_{SO_{2,i}}$	:	Mole fraction of SO_2 in the i^{th} interval (dimensionless)
Z_{ac}	:	Height of acceleration zone (m)
Z_{ni}	:	Distances for the ni^{th} above the lower region (m)
Z_{ni-1}	:	Distances for the $(ni - 1)^{th}$ above the lower region (m)
α	:	External mass transfer coefficient ($cm \cdot s^{-1}$)
ΔL	:	Height of the ni^{th} interval (m)
ε	:	Void fraction (dimensionless)
$\varepsilon_{d,avg}$	:	Mean voidage of the lower region (dimensionless)
ε_i	:	Porosity of particle after calcinations (dimensionless)
ε_u	:	Axial voidage in the dilute phase (dimensionless)

ε^* : Asymptotic voidage in the dilute phase (dimensionless)

γ : Adjustable parameter (dimensionless)

μ : Gas viscosity ($kg.m^{-1}.s^{-1}$)

Φ : Slip factor (dimensionless)

ϕ : Mechanism factor

σ : Size related to the average size (mm or μm)

σ_{sp} : Volume fraction occupied by sorbent particles (dimensionless)

ρ : Gas density ($kg \cdot m^{-3}$)

ρ_B : Solid molar density ($kmol \cdot m^{-3}$)

ρ_c : Bed carbon density ($kg \cdot m^{-3}$)

ρ_l : Limestone density ($kg \cdot m^{-3}$)

ρ_p : Particle density ($kg \cdot m^{-3}$)

τ : Complete conversion time (s)

ξ : Parameter in eq. (3.63) (dimensionless)

CHAPTER I

INTRODUCTION

Circulating Fluidized Bed Combustors (CFBCs) are widely used in many industries for steam production and power generation. The advantages of the CFBC are high combustion efficiency, high heat transfer rate, and fuel flexibility. Various kinds of fuels can be used such as coals, biomass and agricultural wastes. The process is also considered to be cleaner technology, since it has potentials to reduce NO_x and SO_2 emissions. In Thailand, the industries, that use such technology, are the ones that have large amount of agricultural wastes, such as pulp and paper, rice mill, and power plant. In order to improve its performance, the knowledge about its hydrodynamics, heat transfer, and fuel distribution is very essential. These factors are highly interacting. Thus, one factor change could affect the others. In this dissertation, the study was focused on fuel comminution since it has affected on combustion efficiency and pollution control. The comminution of fuels in the riser is a main phenomenon that affects the particle size distribution. The particle size affects the reaction rates and temperatures profile in the riser. This could lead to undersiable reactions those could increase emission. To study this phenomenon, the experiments were conducted to investigate the behavior of the attrition and fragmentation of particles in the CFBC. The knowledge of PSD can be employed for improving the design of the CFBC components such as cyclone for the pollution control, and the riser for heat transfer improvement.

This work will be described over experiment, modeling, and simulation on the CFBC. In this chapter describes the objectives of this research and covers the literature reviews about the circulating fluidized bed, the particles comminution, the particle sizing method, the CFBC emissions, and the CFBC simulation. The next chapter covers the laboratory scale experiment on the particles comminution in a CFBC. The experiment was divided into three parts: attrition, primary fragmentation, and secondary fragmentation. The fuels in this experiment are coal and bagasse. Chapter 3 is intended to describe the kinetic reaction, shrinking particle model, hydrodynamics, and emission

models for the simulation. Chapter 4 concerns the development of the CFBC simulation by Aspen Plus. The main four parts of the CFBC simulation are devolatilization and volatile combustion, char combustion, NO_x formation, and SO_2 absorption. Chapter 5 simulates an industrial scale CFBC by adding the model that described in chapter 3 to the subroutine. The simulation results show the rates of reactions, emission, and changing sizes of particles. In this simulation the shrinking particle model was added into the subroutine to calculate the particle size distribution. Chapter 6 was focused on the simulation of laboratory-scale CFBC. The models from chapter 2 were modified to fit with laboratory-scale CFBC. Two case studies were developed to study the particle size distribution when considering only shrinking particle model or considering both shrinking particle and comminution models. The last chapter provides the conclusion and recommendations for future work.

1.1 Research Objectives

- Study the comminution of local coal and biomass.
- Model and simulate a circulating fluidized bed combustor by including the condition of the comminution effect.

1.2 Circulating Fluidized Bed (CFB)

A Circulating Fluidized Bed Combustor (CFBC) is considered as an improvement over the traditional methods associated with coal combustion. Basu and Fraser (1991) described the definition of the CFB that the CFB is a device for generating steam by burning fossil in a furnace operated under a special hydrodynamic condition: where fine solids are transported through the furnace at a velocity exceeding the terminal settling velocity of average particles, yet there is a degree of refluxing of solids adequate to ensure uniformity of temperature in the furnace. Grace et al. (1997) show a typical configuration for a CFB reactor in Figure 1.1. High vessel are required, a means of introducing particles usually near the bottom, a sufficient upwards flow of gas to cause substantial entrainment of particles from the top of the vessel, and a means of capturing a substantial majority of these particles and returning them continuously to the bottom. The term ‘circulating’ signifies that the particle separation and return systems

are integral and essential components of the overall reactor configuration. The words 'fluidized bed' denote the fact that the particles are supported by the fluid, while there is still a substantial suspension density.

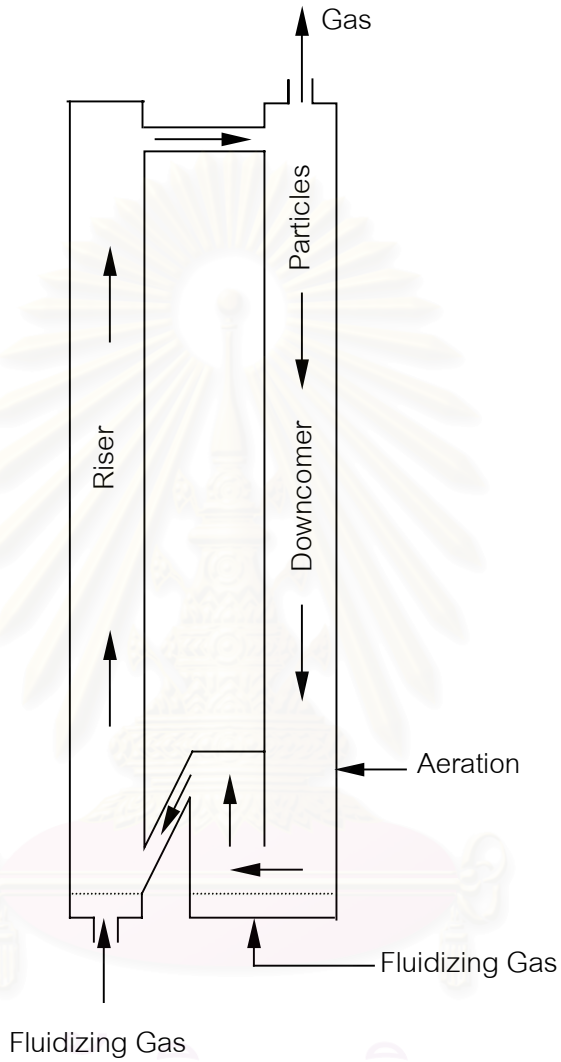


Figure 1.1 Typical configuration for circulating fluidized bed system (Grace et al., 1997).

The CFBC exhibits many advantages over conventional coal combustion methods but it shows some disadvantages. The following comparisons show the typical advantages and disadvantages of CFB reactors relative to conventional low velocity fluidized bed reactors without baffles (Grace et al., 1997).

Advantages:

1. Improved gas-solid contacting given the lack of bubbles.
2. Reduced axial dispersion of gas.
3. Reduced cross-sectional area given the higher superficial velocities.
4. Potentially more control over suspension-to-wall heat transfer because of the ability to use the solids circulation flux as an additional variable.
5. No region like the freeboard region of low-velocity beds where there can be substantial temperature gradients.
6. Less tendency to show particle segregation and agglomeration.
7. Recirculation loop providing a location where a separate operation (e.g. regeneration or heat transfer) can be carried out.
8. Easier to have staged processes.
9. Because of superior radial mixing, fewer solids feed-points needed.
10. Higher solids flux through the reactor.
11. Fuel flexibility, various kinds of fuels being used such as coals, biomass and agricultural wastes.
12. The process being also considered to be cleaner technology, since it has potentials to reduce NO_x and SO_2 emissions.

Disadvantages:

1. Increased overall reactor height.
2. Higher capital cost.
3. Decreased suspension-to-wall heat transfer coefficients for given particles.
4. Somewhat more restricted range of particle properties.
5. Do not lend themselves to horizontal surfaces due to erosion of in-bed surfaces.
6. Added complexity in designing and operating recirculating loop.
7. Increased particle attrition.

Although CFBC technology is becoming more common from these commercial applications, there are some significant uncertainties in predicting their performance in large-scale systems. This might be attributed to the fact that the combustion process occurring in a CFBC involves complex phenomena including chemical reactions, particle size reduction due to combustion, attrition, fragmentation and other mechanisms, and hydrodynamic properties.

1.3 The studies in comminution phenomena during combustion

Attrition is an inevitable phenomenon in the operation processes. It is carried out on the premise that comminution can be seen as the result of at least four phenomena occurring in series-parallel with each other and with combustion (Chirone, Massimilla et al., 1991). The comminution phenomena are shown in Figure 1.2.

1. Abrasive attrition is the phenomenon by which fines are abraded from the surface or the mother particle by wearing against bed solids and system walls and internals. The fines generally escape through the cyclone and constitute a major combustibles loss. Attrition is greatly enhanced by combustion. Macerals of varying reactivities are present in the char. This causes an uneven oxidation or combustion on the char surface. Thus, some parts of the char surface burn faster than others, leaving fine ridges on the surface. These ridge are broken loose by hydrodynamic forces exerted by other bed materials. This process of attrition of char particles is call combustion-assisted attrition by Basu and Fraser (1991).
2. Primary fragmentation occurs during devolatilization, as a consequence of the buildup of volatile pressure in the pore network of the combustible particles. Here, a coal particle is broken into several pieces that are smaller than the parent coal particle.
3. Secondary fragmentation would result from the weakening caused by combustion, with the breakup of bridges with connected the elements of a char particle, by particle collision.

4. Fragmentation by uniform percolation would take place in the last stage of burn off, when combustion was controlled by internal surface reactions, and the particle structural connectivity would suddenly collapse, by pore enlargement and coalescence.

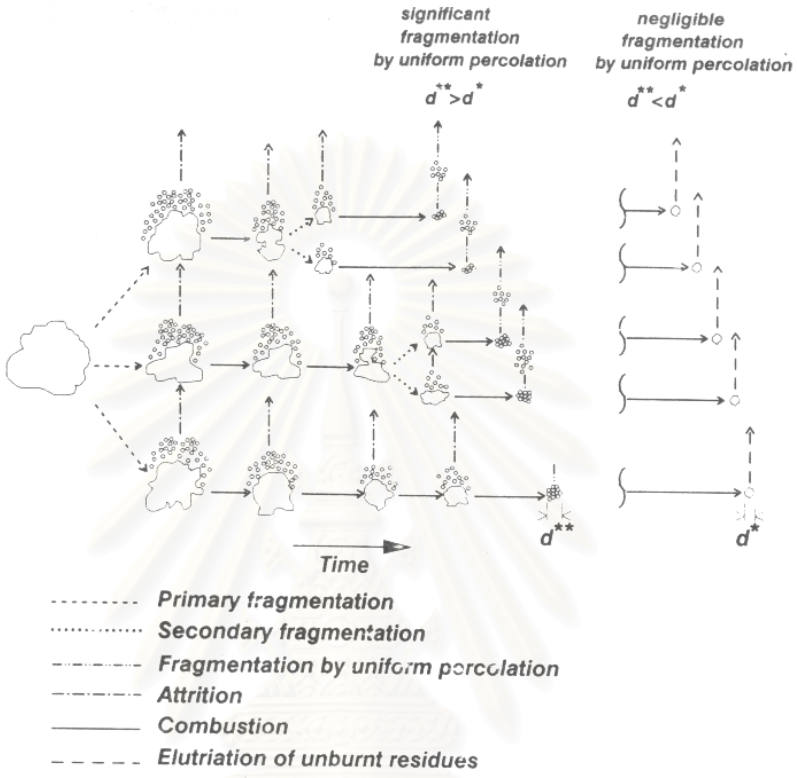


Figure 1.2 Series-parallel comminution phenomena (Chirone, Massimilla et al., 1991).

Combined combustion and comminution end up with particles which become sufficiently small to be elutriated as unburnt residues or with generation of swarms of fines depending on whether fragmentation by uniform percolation does not or does take place. Key variables of the series-parallel network of comminution phenomena and combustion are: d*, the size of unburnt residues, that is the size of particles whose terminal settling velocity is equal to superficial fluidizing velocity; d**, the size of particles at the point of uniform percolative fragmentation, that is the size at which transition from diffusion to chemical kinetic limited combustion takes place. A useful assumption is that attrition produces fine particles of sizes smaller than values of d* as evaluated at fluidizing velocities typical of bubbling bed operations. Particles of size > d* are generated by secondary fragmentation, while those of size < d* are

generated by attrition. Thus, neither primary nor secondary fragmentation participates in the generation of elutriable particles. The loss of carbon from the bed can be contributed by two mechanisms: attrition and uniform percolation. The unburnt particles of size d*, generated by attrition, will be entrained. For comparable carbon particle densities, if d** > d*, fragmented by uniform percolation will also enhance carbon loss. Nevertheless, primary and secondary fragmentations indirectly affect combustion efficiency by influencing the extent of carbon surface exposed to attrition and the number of particles, for each carbon particle charged into the bed, elutriated as unburnt residues or as fines generated by uniform percolation.

In the fluidized bed systems, particles are normally required to remain in the bed for considerable periods. Any attrition to smaller sizes may affect the fluidizing properties or the process operating conditions as well as causing loss of fine material by elutriation. In systems containing two different types of particle, for example sand and coal in fluidized bed boilers, attrition of the main bed material must be minimized, but attrition of the secondary particles (coal) is unimportant since these particles are being consumed in the process (Bemrose and Bridgwater, 1987). However, in a circulating fluidized bed combustor, the size distribution of the solid inventory affects fluidization characteristics and heat transfer that are the key parameters to determine the combustion efficiency and pollution control (Lee et al., 2003).

In the bubbling fluidized bed combustors, Chirone et al. (1991) showed three apparatus to investigate the carbon comminution (Figure 1.3).

- The Cyclone equipped combustor (A)
- Basket equipped combustor (B)
- Two-exit head combustor (C)

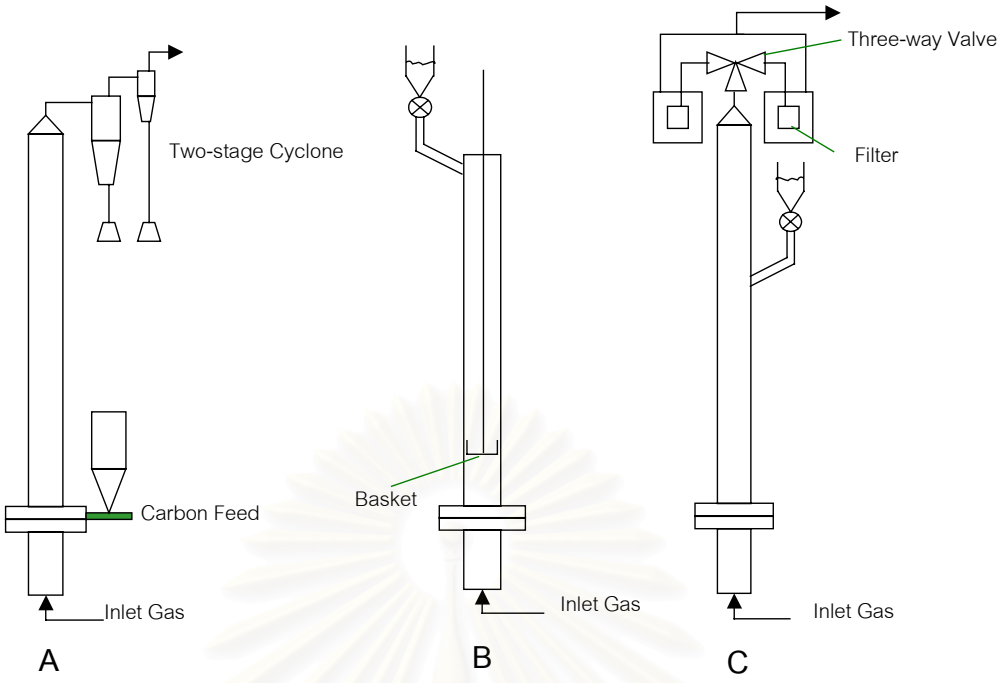


Figure 1.3 Fluidized bed combustors use in comminution experiments: *Continuously operated*, (A) cyclone equipped combustor, and *Batchwise operated*, (B) basket equipped combustor; (C) two-exit head combustor (Chirone, Massimilla et al., 1991).

The Cyclone equipped combustor had been used to investigate secondary fragmentation (Cambell and Davidson, 1975; Essenhigh et al., 1990 cited in Chirone et al., 1991). It was studied by comparing the actual particle size distribution of bed carbon with that expected, for given inlet size, from size population balance in absence of secondary fragmentation. The apparatus was also used to measure carbon attrition because the second stage cyclone collected the fine particles that were generated from the attrition.

Basket equipped combustor was a typical investigation on primary and secondary fragmentation because the basket that put into the bottom of the column is useful to measure the fragmented particle size from the primary fragmentation. Fragmented and unfragmented particles could be retrieved at any time after injection by means of the basket (Andrei, 1978; Andrei et al., 1985; Chirone et al., 1989 cite in Chirone et al., 1991). In a modified version of this apparatus, when secondary

fragmentation was investigated, the basket was replaced by a probe for continuous monitoring of CO_2 concentration in the exit gas (Sundback, 1984 cited in Chirone et al., 1991). Spikes in the CO_2 concentration profiles indicated the occurrence of a secondary fragmentation act. This apparatus was useful when time-resolution of phenomena leading to primary and secondary fragmentation was required.

Two-exit head combustor was used to characterize carbon attrition taking place under nonreactive and reactive conditions. After carbon particle injection, two filters were periodically inserted into the outlet flue gas line by means of a three-way valve. The amount of carbon fines collected at a given time by the filter not in operation divided by the collection time gives instantaneous elutriation rate. Considering that carbon burning in the freeboard was prevented by keeping this section at low temperature, carbon elutriation rates could be assumed to equal to carbon attrition rates. This apparatus proved to be particularly useful in experiments directed to time-resolving carbon attrition.

The research on particle attrition in fluidized beds has been considerably forwarded by the development of fluidized coal combustion systems. In 1983, Arena et al. studied the generation of carbon fines by attrition during the fluidized combustion of a bituminous coal in 140 mm. ID fluidized bed combustor. The variables in this experiment were excess air factor, bed temperature, fluidizing velocity, and size of bed sand and coal. The results indicated that rates of attrited fines were roughly proportional to excess of gas velocity above the minimum velocity for fluidization and bed carbon exposed surface. Attrition rate constant was affected by size of sand and, to a less extent, particularly with finer coal, by bed temperature. Moreover, they evaluated the attrition rate constants of char burning in laboratory scale fluidized beds combustor in 1986 (Arena et al., 1986).

Brown et al., (1992) experimented on the elutriation rates of unburned carbon from a 20 cm ID bubbling fluidized bed. They showed the expression of the total elutriation rate of unburned carbon from a fluidized bed combustor following the equation:

$$E_t = E_f + E_c + E_a + E_{fr} \tag{1.1}$$

where E_t is total elutriation rate of unburned carbon, E_f is elutriation due to the original fines fraction in the coal feed, E_c is elutriation of particles reduced in size by combustion, E_a is elutriation arising from attrition of particle surfaces, and E_{fr} is elutriation of fragmented particles.

The value of E_c can be estimated by using a shrinking particle model for burning spherical particles of coal (Donsi, 1981 cited in Brown et al., 1992).

$$E_c = F_c f_i \left(\frac{d_t}{D_i} \right)^3 \tag{1.2}$$

where F_c is the feed rate of carbon entering the combustor, f_i is fraction of fuel particles with initial diameter, d_t is diameter of the largest particle that would be elutriated at operating conditions, and D_i is initial diameter.

On the basis of the two phase theory of fluidization (Arena et al., 1983), assuming perfect mixing of gas in the particulate phase and plug flow of bubble phase (Campbell and Davidson, 1975 cited in Arena et al., 1983) with fast devolatilization of coal and burning of volatiles, the rate of shrinkage due to combustion is:

$$\left(-\frac{d(d)}{dt} \right) = c_p \frac{1}{\frac{d\rho_c}{2M_c ShD_g} + \frac{\rho_c}{2M_c k_s}} \tag{1.3}$$

$$\left(-\frac{d(d)}{dt} \right) = \left\{ c_i - \frac{F_{O_{2,v}} + (F_c - E_t)/M_c}{A\left[U - (U - U_{mf})e^{-x}\right]} \right\} \frac{1}{\frac{d\rho_c}{2M_c ShD_g} + \frac{\rho_c}{2M_c k_s}} \tag{1.4}$$

where c_p is oxygen concentrations in the particulate phase, d is average particle size, ρ_c is bed carbon density, M_c is carbon atomic weight, Sh is Sherwood number, D_g is oxygen diffusivity, k_s is carbon surface reaction rate constant, c_i is oxygen concentrations in the inlet air, $F_{O_{2,v}}$ is oxygen molar flow rate required for combustion of volatiles in the particulate phase, A is bed cross section, U is fluidization gas superficial

velocity at bed temperature, U_{mf} is minimum fluidizing gas superficial velocity at bed temperature, and x is number of transfer units.

Elutriation of carbon due to particle attrition (Merrick and Highley, 1974 cited in Brown et al., 1992) was described by

$$E_a = k_a \left(U - U_{mf}\right) W_c \qquad (1.5)$$

where k_a is attrition rate constant, W_c is carbon loading in the bed.

The above equation was the first elutriation rate of carbon attrition model to describe size reduction in a continuous BFB, developed by Merrick and Highley (Merrick and Highley, 1974 cited in Tardin et al., 2001). They assumed fines were generated only by abrasion and considered the rate of generation of a new superficial area to be proportional to the rate of inserted energy, according to Rittinger's law. Because the size distribution of fines in their tests was approximately constant, the rate of production of new surface was taken to be proportional to the mass rate of fines production. The rate of inserted energy was taken to be proportional to U-U_{mf}.

The rate of char elutriation due to primary fragmentation is expected to be proportional to the pressure increase within coal particles. For a given pore structure, this pressure was proportional to the volatile release rate, which was proportional to the heating rate experienced by the coal particles (Howard, 1981 cited in Brown et al., 1992). Accordingly, the elutriation rate due to primary fragmentation will depend on the total surface area of the coal particle in the bed. This relationship in term of carbon loading in the bed is:

$$E_{fr} = k_{fr} W_c \qquad (1.6)$$

where k_{fr} is fragmentation rate constant inversely proportion to particle diameter.

The results showed that the elutriation rates were well correlated with carbon loading in the bed, but there was no evidence that they depended on superficial

velocity. These results suggest that the fragmentation, rather than attrition, is primarily responsible for carbon loss during fluidized bed combustion.

The attrition in a turbulent fluidized bed was investigated in a 41 mm diameter and 1.2 m tall, open top, turbulent fluidized bed apparatus (Halder and Basu, 1992). The particles in this experiment were prepared by machining carbon rods of dry-cell batteries. The temperature of combustion was maintained at 1073 K using electrical controls. The attrition rate was characterized by vigorous motion of agglomerates and interconnected gas pockets. They assumed that the abrasion between the particle agglomerates and the particle would increase with the gas velocity. As the first approximation, they took the attrition to depend on the first power of gas velocity so that the attrition rate could be written for turbulent fluidization as

$$E_a = k_a' U \frac{M}{d} \tag{1.7}$$

where M is bed mass inventory.

The attrition rate constant, k_a' calculated under 1073 K ranged between 2.57×10^{-7} - 4.8×10^{-7} while that in absence of combustion was only 0.03×10^{-7} - 0.05×10^{-7}. They suggested that these constants were independent of the regime of fluidization when compared with available data on bubbling fluidized. Tardin et al. (2001) reported that the attrition constant depended on the type of particles. The attrition constant for coal in bubbling fluidized bed combustor was 9.81×10^{-3} m^{-1} (Merrick and Highley, 1974 cited in Tardin et al., 2001) and 1.3×10^{-3} m^{-1} for carbon particles (Donsi et al.,1981 cited in Tardin et al., 2001). In a cold fast fluidized bed Pécora et al., observed no particle attrition and obtained a fragmentation constant of 0.438×10^{-3} m^{-1} for reported shale particles (Pécora et al., 1988 cited in Tardin et al., 2001).

Walsk, P.M. and Li, T. (1994) tested the attrition of coal char particles in a furnace on a vibrating screen. Pittsburgh Seam chars initially 5 mm. in diameter was burned at temperatures of 900, 1000, and 1100 K in the presence of 2, 5, 10, and 21 mol % oxygen. By varying the vibration frequency and energy of collisions, the yield of fines was varied from 0 to 40 wt% of the fixed carbon in a batch feed. The yield of fines

decreased with increasing temperature, decreased with increasing oxygen, and increased with simultaneous increases in the energy and frequency of collisions. The data suggested a model based on two parallel routes for fines formation: (1) attrition at a rate depending only on the mass of particles and collision frequency and (2) fragmentation at a rate determined by the removal of the solid structure by combustion, occurring at a critical porosity which decreases with increasing collision energy. No fragments are formed if the critical porosity is greater than the porosity at complete burnout, when only the ash residue remains.

In 2001, the mechanical attrition and fragmentation of particles in the fast fluidized bed were studied in 0.3 m. ID vertical riser, 2.22 m. high, (Tardin et al., 2001). The tests were performed in the fast fluidized bed, working at ambient condition, to check the influence of operational conditions, namely, superficial gas velocity, particle diameter, test duration, and solids inventory, on the size reduction process of a friable material particle. Considering the different transport phenomena observed in bubbling fluidized beds and fast fluidized beds, one could imagine that size reduction in a fast fluidized beds would have its own characteristics in comparison to bubbling fluidized beds. Experimental observation, however, showed that the size reduction rate was proportional to the fluidization excess velocity and to mass inventory, as in bubbling fluidized beds.

The primary fragmentation of anthracites was studied by Chirone and Massimilla in 1991. The anthracites were Russian anthracite with low and a South Korean anthracite with high ash content. Irregular particles and spheres of size ranging between 1 and 15 mm. tested in a fluidized bed combustor of 40 mm. ID, equipped with a basket. The results showed that the fragmentation depended on the type of anthracite and the size of particles. Fragmentation occurred with different degrees of probability, with different ratios of the total number of particles after fragmentation to the number of feed particles and with generation of fragments different shapes (Figure 1.4): hemispheres, one or two base spherical segments, polyhedrals with curved surfaces. Hemispheres and spherical segments were prevalently found with the South Korean anthracite, where fragmentation took places along parallel, whereas deviant polyhedrals

were found with the Russian anthracite, where fragmentation occurred by random division of particles. The rate of devolatilization of various sizes of coal under fluidized bed conditions was estimated by Paul et al. (1992).

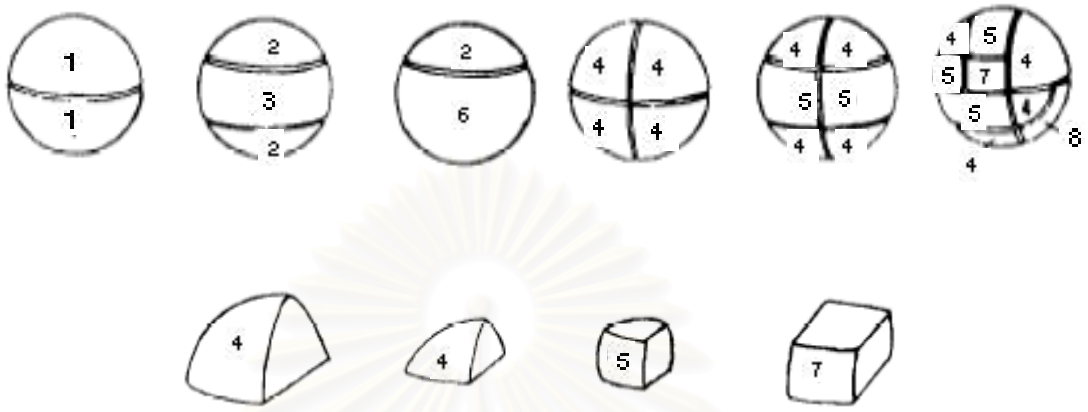


Figure 1.4 Types of fragments: (1) hemisphere; (2) one-base spherical segment; (3) two-base spherical segment; (4) one-base haft-spherical segment, deviant polyhedral; (5) two-base half-spherical segment, deviant polyhedral; (6) sphere without a one-base spherical segment; (7) core of two-base spherical segment, polyhedral; (8) spherical bowl deviant polyhedral type (Chirone and Massimilla, 1991).

The secondary fragmentation of char particles during combustion in a batchwise fluidized bed was studied in 1989 (Chirone et al., 1989). They investigated the different particle sizes and oxygen concentrations in inlet air of two char: one from a nonswelling and the other from a swelling coal. The experimental apparatus consisted of 40 mm. ID quartz combustor equipped with a basket made of a 0.6 mm. mesh to allow collection of char from the bed. Char particles were prepared by devolatilizing each coal in a fluidized bed under and inert atmosphere at 1173 K, The same temperature at which fragmentation experiments have been performed. Within the range of variables tested, both oxygen concentration and initial particle size exerted only a negligible influence upon the fragmentation patterns. The swelling coal was affected by particle breakup more than the nonswelling coal.

In 2003 the comminution characteristics of anthracite were studied in CFB reactor with 35 mm. ID and 2.3 m. height (Lee et al., 2003). With an increased of

operation temperature, the coal showed a high degree of fragmentation and generation of fine particles in the CFB reactor. The particle fragmentation occurred actively as its size and Hard Grove Index (HGI) increase. The attrition was also affected with particle size and HGI of the coal. Initial surface crack and fine particle clusters on the coal surface affected the degree of fragmentation and the generation of the fine particles during the early stage of the coal devolatilization and combustion. For the industrial scale, the coal comminution characteristics were investigated in 1 MW_{th}, 1.5 MW_{th}, and 12 MW_{th} respectively.

Scala, F., and Salatino, P. (2000) investigated the fluidized bed combustion of a biomass char (*Robinia pseudoacacia*). Different experimental techniques were adopted to characterize the combined role of combustion and comminution phenomena in determining fixed carbon conversion and the rate of carbon elutriation. Comparison of experimental results obtained under steadily oxidizing conditions an under alternating oxidizing/inert conditions suggested mechanistic aspects of the fluidized bed combustion of biomass char. Fixed carbon combustion was almost always complete. Conversion occurred to a large extent via the generation of carbon fines followed by post combustion during their residence time in the bed. Approximately half of the initial fixed carbon followed this pathway, the remainder being directly burnt as coarse char. The prevailing mechanism of carbon fines generation in the bed was percolative fragmentation rather than attrition by abrasion. In spite of the extensive generation of elutriable carbon fines, the combined effect of high fuel reactivity and of relatively long fines residence times in the reactor determined the large combustion efficiency. It is inferred from experimental results that char fines adhesion onto bed solids might be relevant to the observed phenomenology.

The interaction between fuel particles and incipiently bubbling gas fluidized beds during devolatilization was investigated by X-ray imaging in 2002 (Bruni et al., 2002). The fuel consisted of a ligneous biomass (*Robinia pseudoacacia*) reduced into millimeter-sized particles and doped with lead nitrate in order to make particles visible upon X-ray irradiation. A purposely designed single-particle-injector was used to impulsively introduce fuel particles one at a time at a given depth into the fluidized bed.

The significance of the study lies in that the role of hydrodynamic interaction between fuel particles and the emulsion phase in the course of devolatilization is high-lighted. Three main features of the phenomenology are: (a) the formation of (endogenous) volatile matter bubbles around devolatilizing fuel particles; (b) the uprise of endogenous bubbles; (c) the uprise of fuel particles closely associated to endogenous bubble motion.

1.4 Particle sizing methods

Particle-size measurements are important to researchers, scientists, and engineers in both the research-and-development and industrial communities working in a broad range of disciplines (Black et al., 1996). Table 1 describes some of many fields in which particle-size analysis is essential and lists some of the primary uses of particle-sizing methods in these areas. For example, particle size and number density are critical parameters in two-phase combustion experiments and modeling, since the particles or droplets represent the energy source in reacting two-phase flows. Thus, knowledge of the particle size distribution is a key parameter in modeling radiative heat transfer, as well as in characterizing other properties, such as droplet evaporation rates and total droplet/particle burnout.

As the first step in analyzing a particle system (Barrett, 2003), gather as much information as possible about the key process variables affecting the system, including operating temperatures, pressure, flowrates in pipes, mixing condition, etc. With this information, attempt to define the issue. Is the particulate process plagued by a filtration problem or reaction rate problem? Or is the final product quality or process efficiency not up to par?

In addition to the unit operation in question determine which upstream unit operations impact the particle system. For instance, as particles are transported between pieces of equipment, is attrition or aggregation occurring due to differences in temperature or flowrate? Next, identify how the particle systems impact process parameters (e.g., filtration rate, reaction rate or particle flowability) or the product parameter of concern (e.g., stability or particle strength). What aspect of the particle

system is key to controlling the problem or optimizing the solution? And, are the fine or large particles driving the process problem?

Table 1.1 Applications of particle-sizing technology (Black D.L. et al., 1996)

Uses of particle-size analysis	Applications in area
Combustion	Size and velocity measurements
Sprays	Characterizations and descriptions of nozzles
Medicine/pharmaceuticals	Control of manufacturing processes
Paints	Control of pigment size distribution
Metallic powders	Control of manufacturing processes
Agriculture	Control of pesticide application
Pollution control	Monitoring and analysis of emissions
Foods and consumer products	Control of taste and texture

Figure 1.5 shows a diagram outlining several broad methods of particle-size analysis, including those based on optical techniques and those mechanical in nature. Many specific techniques are also listed under their respective categories, although the list is not all inclusive. Due to the large number of methods available for sizing particles in many different fields, the information of the combustion systems has been restricted to methods using laser light to determine particle size. Because of the demanding nature of the environment (high temperature and sometimes pressure), special attention has been given to those methods that can be applied to combustion systems to determine the characteristics of the condensed phase before, during, or after combustion.

Laser diffraction instruments are designed for offline particle-size measurement of solids or liquids suspended in an other phase (i.e., a solid particle suspended in a liquid, a liquid suspended in another liquid, or a solid particle suspended in air). These instruments use a light-scattering phenomenon, coupled with mathematical algorithms, to calculate the volume-based distribution of spherical particles.

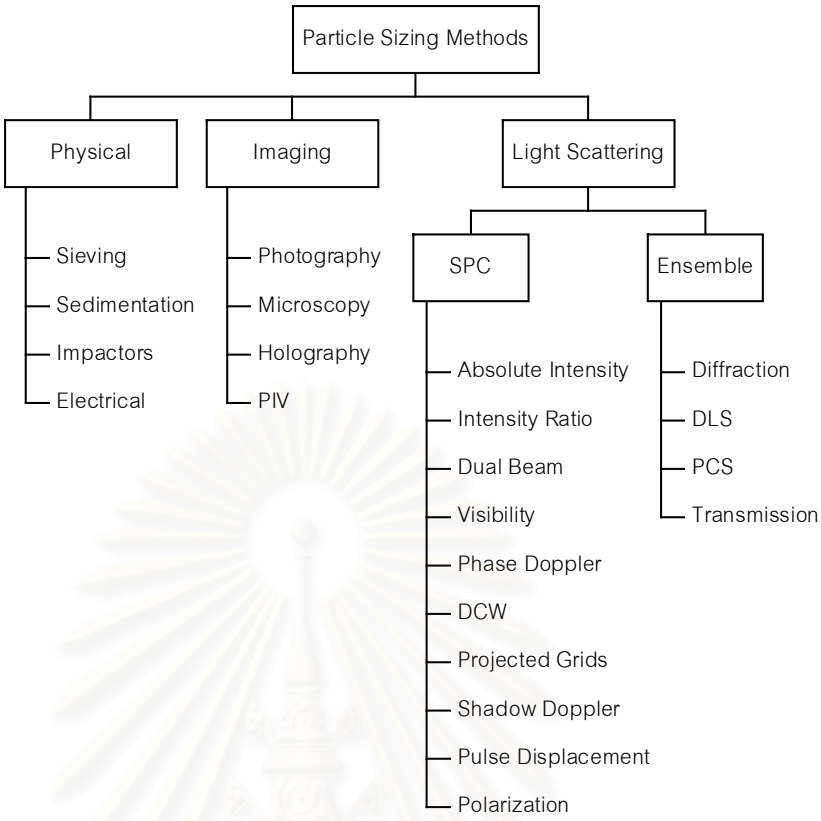


Figure 1.5 Various methods of particle-size analysis (Black et al., 1996).

Particle Imaging Velocimetry (PIV) is the one method for particle-size measurement. Kadambi et al. (1998) investigated the size distribution in a mixture of polydisperse particles flow. Components of a standard PIV system, a high resolution CCD (Charge Coupled Devices) camera and argon ion laser, were used to capture images of stationary particles. The image data were used to ascertain the limitations of estimating particle size. Zhang et al. (2003) used a Laser Doppeler Velocimeter (LDV) system to investigate the flow structure in CFB.

For the industrial CFBC, Foster Wheeler Energy Corporation used the ECT (Electric Charge Transfer) technology for particle size measurement (Laux et al., 2003). The patented technology measures the electric charges present in any two phase flow transport and uses the signals to determine the relative coal distribution between the conduits of one mill. In addition, the system can be configured to measure the flow velocity and the absolute flow in each conduit as show in Figure 1.6. The ECT system for the coal flow balance consists of three receiving antennas in each coal

conduit that is connected to a signal conditioning unit. This signal conditioning unit is in turn connected to a personal computer that is used for data processing and analysis.

The principle of this apparatus uses the movement of particles that generates electrostatic charge (Yan and Stewart, 2001). The electrification of particulate solids can be expected whenever a powder comes into contact with another surface, e.g. in pneumatic transportation, mixing, grinding, sieving, pouring and micronising. Although the amount of charge carried on particles is usually unpredictable, it can be detected by a screened and insulated electrode in conjunction with a suitable charge detection circuit, which derives useful signals from the fluctuations in the electric field caused by the passage of the charge particles. A number of different electrode configurations have been used in commercial or prototype electrostatic flow sensors. Figure 1.7 shows four such examples. The exact geometrical shape and dimensions of the electrode depend on the application and pipe size. For a given pipe size, the shape and axial dimension of the electrode are two crucial factors affecting the fundamental characteristics of the sensor, including spatial sensitivity, sensing volume, and spatial filtering effects (Yan, 1998 cited in Yan and Stewart, 2001).

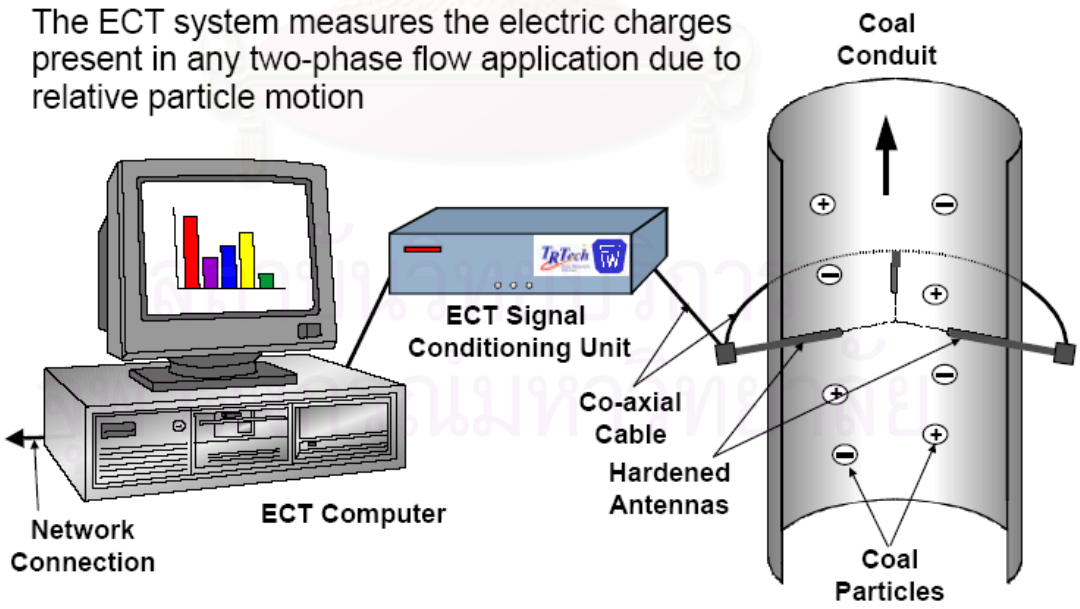


Figure 1.6 Major components of the electric charge transfer system (Laux et al., 2003).

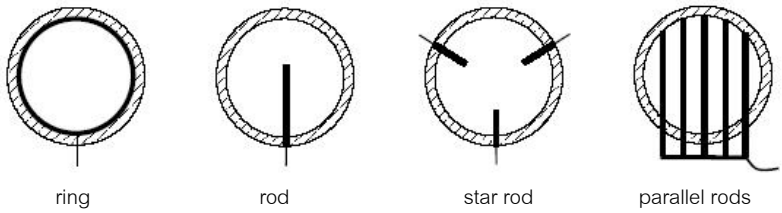


Figure 1.7 Common electrodes used in commercial electroststic flow sensors (Yan and Stewart, 2001).

1.5 Studies in CFBC emissions

The major gaseous effluents that affect the environment are sulfur dioxide, nitrogen oxide, greenhouse gases, and particulate matter. Furthermore, emissions of trace metals and toxic organic compounds provide significant potential for polluting the environment. The combustion of fossil fuels in stationary and transportation systems is the main source of air pollution. Many countries have established emissions limits for particulate matter, NO_x, and SO_2 from combustion plant, although these limits vary widely between and within countries, and also with size and type of plant. Then the scientists try to working on the emission reductions.

Although the CFBC is one type of clean coal technologies (Kamall, 2002), Many literatures try to present experimental results and modeling of the emissions both from combustion of coal and biomass fuels. In a CFBC, a char particle may take 1-10 s (depending upon the riser height) to pass through the furnace once (Basu, 1999). However, as the particle is likely to make many trips around the CFB loop, The total residence time could be as much as 10,000 s, depending on the solid inventory, feed rate, coal size, etc (Stenseng et al., 1997 cited in Basu, 1999). The emissions of CO and CO_2 are generated by the mechanism of combustion. Basu (1999) presented three models for this mechanism.

Model I: Oxygen diffuses to the carbon surface and oxidizes further to CO_2 in a gas-phase reaction so close to the carbon surface that carbon dioxide may be considered the primary combustion product. This model is predominant in a low Reynolds number flow, for large char particles (d > 1 mm.) or at high temperatures (900-1300 $^{\circ}$C)

Model II: Oxygen diffuses to the carbon surface and produces both CO and CO_2 on the carbon surface. Carbon monoxide and carbon dioxide diffuse away from the carbon surface. CO further meets in a gas-phase reaction with oxygen arriving from the bulk gas, and forms CO_2.

Surface reactions: $C + \frac{1}{2}O_2 \rightarrow CO$ ΔH_r = - 111 kJ/mol (1.8)

$C + O_2 \rightarrow CO_2$ ΔH_r = - 394 kJ/mol (1.9)

Gas-phase reaction: $CO + \frac{1}{2}O_2 \rightarrow CO_2$ ΔH_r = - 283 kJ/mol (1.10)

Model III: Oxygen cannot reach the carbon surface. It reacts with the CO in a gas-phase reaction away from the carbon surface. One part of the CO_2 formed diffused back to the carbon surface to be reduced to CO. However some literatures against the hypothesis of reduction of CO_2 on the carbon surface because of the slow rate of CO oxidation and the low concentration of carbon in a fluidized bed (Basu et al., 1975; Ross et al., 1981 cited in Basu, 1999).

Surface reactions, from eq. (1.8):

$C + \frac{1}{2}O_2 \rightarrow CO$ ΔH_r = - 111 kJ/mol

$C + CO_2 \rightarrow 2CO$ ΔH_r = + 172 kJ/mol (1.11)

Gas-phase reaction, from eq. (1.10)

$CO + \frac{1}{2}O_2 \rightarrow CO_2$ ΔH_r = - 283 kJ/mol

The oxidation reaction of char can be represented for all three models as

$$C + \left(\frac{1}{\phi}\right)O_2 \rightarrow \left(2 - \frac{2}{\phi}\right)CO + \left(\frac{2}{\phi} - 1\right)CO_2 \quad (1.12)$$

The mechanism factor, ϕ is equal to 1 for CO_2 transport from surface (Model I), and is equal 2 for CO transport (Model II or III) (Rajan and Wen, 1980 cited in Basu, 1999). The emissions of CO and CO_2 were simulated by Sotudeh-Gharebaagh et al. (1998) in the 0.8 MW_{th} CFBC and Huilin et al. (2000) in 35 t/h CFB boiler.

For nitrogen and nitrous oxides emissions, Nordin et al. (1993) studied the reduction of NO emissions from 20 MW CFB boiler. The results showed that most important factors for NO reduction were air: fuel ratio, and the amount of NH_3 added. Bonn et al. (1995) studied the formation and decomposition of N_2O from coal combustion. They founded that N_2O emitted low level at the operating conditions of fluidized bed boiler (<30 mg m^{-3}) but increased when the temperature in the system increased. However these results disagreed with Kilpinen et al. (2002). Finally, limestone addition and the variation of secondary/primary air ratio did not affect N_2O emissions significantly. In 2001, Shimizu et al., investigated that NO_x emission decreased with limestone feed in the bubbling fluidized bed combustor. Winter et al. (1999) summarized 85 kinetic model reactions of the combustion chemistry of the nitrogen containing species from the single particle to the pilot-scale.

In the part of co-combustion or biomass combustion, the advantage of fluidized bed systems over other systems is that they form less thermal NO_x, which will often mean that further NO_x removal is superfluous (Broek et al., 1996). Liu and Gibbs (2002) presented the model applied to a 12 MW_{th} CFB boiler using a typical wood biomass-pinewood chips as the fuel to predicted the NO and N_2O emissions. The predicted of N_2O emissions were always less than 5 ppmv. Leckner et al. (2004) experimented on co-combustion of sewage sludge and coal/wood. Although sewage sludge contained large quantities of nitrogen and sulfur, the beneficial properties of CFB lead to considerable reduction of nitrogen oxides, and only a few percent of the nitrogen was effectively converted to NO or N_2O. However, sewage sludge had the highest overall trace element inventory of the fuels tested and that sewage sludge may cause problems related to emissions of Cd and Hg from fluidized bed combustion due to its high volatilization observed (Miller et al., 2002 cited in Åmand and Lecker 2004). Li et al. (2004) investigated the emissions of NO and N_2O from co-firing municipal solid waste

(MSW). The results showed that increasing the co-firing rates leaded to reduction of N_2O emission, but an increase of NO emission. The disadvantage of biomass combustion is the fouling of combustor surfaces (Sami et al., 2001). The main contributions to fouling come from inorganic material in the fuel such as Na, Mg, Ca. Slagging and fouling reduce heat transfer and cause corrosion and erosion problems, which reduce the lifetime of the equipment.

For SO_2 emission, during the coal combustion, the sulfur in it is oxidized to the pollutant. Limestone ($CaCO_3$) of the bed materials calcine to CaO which reacts with SO_2 producing $CaSO_4$ (Basu, 1999) following the reaction:

$$CaCO_3 \rightarrow CaO + CO_2 \quad (1.13)$$

$$CaO + SO_2 + \frac{1}{2}O_2 \rightarrow CaSO_4 \quad (1.14)$$

Thus instead of leaving the boiler as a gaseous pollutant, sulfur is discharged as a solid residue. The molar volume of $CaSO_4$ is greater than that of CaO. As a result the reaction product $CaSO_4$ blocks passages to the internal pores of CaO. For this reason 30-50 % of the CaO remain unutilized. The level of sorbent utilization depends on the reactivity of the sorbent, its size, temperature and cyclone efficiency. The kinetics of the SO_2 reaction with calcined limestone were studied by Borgwardt (1970). Mattisson and Lyngfelt (1998) developed a sulfur capture model for CFB boiler.

In the cases of co-combustion, the alkaline ash from biomass also captures some of the SO_2 produced during combustion and therefore the net SO_2 emissions can also be reduced by co-firing (Sami et al., 2001 and Gayan et al., 2004). Nordin (1995) studied the co-combusion of high sulfur fuels and biomass fuels in a small pilot scale fluidized bed. The optimization of sulfur retention in ash was studied in this experiment. The results showed that by optimizing the process when co-combusting a biomass fuel with high sulfur retentions, a sulfur capture corresponding to, or even better than, conventional techniques (utilizing $CaCO_3$) was obtained.

1.6 Studies in CFBC modeling and simulations

Douglas and Young (1991) simulated the Atmospheric Fluidized Bed Combustion (AFBC) steam heating plant using ASPEN/SP (advanced system for process engineering). A sensitivity analysis showed that the combustion air flowrate has the greatest effect on the predicted carbon burnout. An economic sensitivity analysis showed that the plant's economic viability versus electric heating is extremely sensitivity to the price of the electricity. Sotudeh-Gharebaagh et al. (1998) simulated the CFBC for coal combustion using ASPEN PLUS based on the isothermal assumption. The kinetic and hydrodynamic subroutines were used for calculated the rate of reaction and predicted the mean axial voidage profile at the upper region. The results were expressed in terms of combustion efficiency and emission level. Huilin et al. (2000) computed a Circulating Fluidized Bed Boiler with wide particle size distributions by considering the hydrodynamics, heat transfer and combustion of coal. The models predicted the flue gas temperature, the chemical gas species such as O_2, CO, CO_2 and the char concentration distributions in both the axial and radial location along the furnace. Mukadi et al. (2000) developed the mathematical model of kinetic reactions to predict the gas emissions in an internally circulating fluidized bed (ICFB) combustor for treatment of industrial solid wastes. The trends of model predictions were in qualitative agreement with experimental observations from thermal treatment of spent foundry sand in 20 kW ICFB pilot unit. According to the kinetics and experimental data, bed materials were strongly responsible for low-level emissions of nitrogen oxides and sulfur dioxide. In 2003, Adánez et al. developed a mathematical model for the combustion of wood chips in a 12 MW_{th} CFB boiler. The model considered the process of wood chip drying and devolatilization, population balances of devolatilizing particles, volatiles combustion, population balances of char burning particles, and heat generation in the different regions of the combustion chamber. Chen et al. (2001) developed the model of fluidized bed combustion and studied the emissions of NO_x and N_2O for char combustion and Chaiklangmuang (2001) developed the mathematical modeling of emissions from solid fuel combustion. Gayan et al. (2004) developed model to predict gas concentration along the riser (O_2, CO, CH_4, etc.) and the carbon efficiency of co-combustion between coal and biomass.

CHAPTER II

EXPERIMENTS

In this research, the laboratory scale of circulating fluidized bed combustor was focused on the fuels comminution. The fuels that were used in the experiments were coal and biomass. Bagasse is the most available biomass in Thailand (Department of Alternative Energy Development and Efficiency, 2003). Thus bagasse was selected as the fuel in this study. The comminution study was divided into three parts: attrition, primary fragmentation, and secondary fragmentation. The details in each part will be described in the following sections.

2.1 Material preparation

The fuels in these experiments are coal from Electricity Generating Authority of Thailand (EGAT, Mae Moh) and bagasse. The size of them was between 2.0-3.0 mm diameter prepared by sieve analysis. The bed material in the CFBC is sand with the size between 425-600 μm. For the fluidizing gas, in this research, two types of gas were used. Nitrogen gas was used for the primary fragmentation study, and air was used for attrition and secondary fragmentation studies, respectively.

2.2 Instrument and apparatus

The dimensions of laboratory-scale CFBC in this research was shown in Figure 2.1 to 2.3. The CFBC was constructed with stainless steel. The main reactor was composed of a riser with 2.5 cm inside diameter and 160 cm height. It was electrically heated up to the desired temperature by five external heater furnaces surrounding the main reactor. Five thermocouples were used to measure the temperatures in the middle of each heater. At the top of the riser, the cyclone was installed and the dimension was illustrated in Figure 2.2. At the bottom of the cyclone, connected with 1.2 cm inside diameter tube were the downcomer and the valve for adjusting solid recirculation rate.

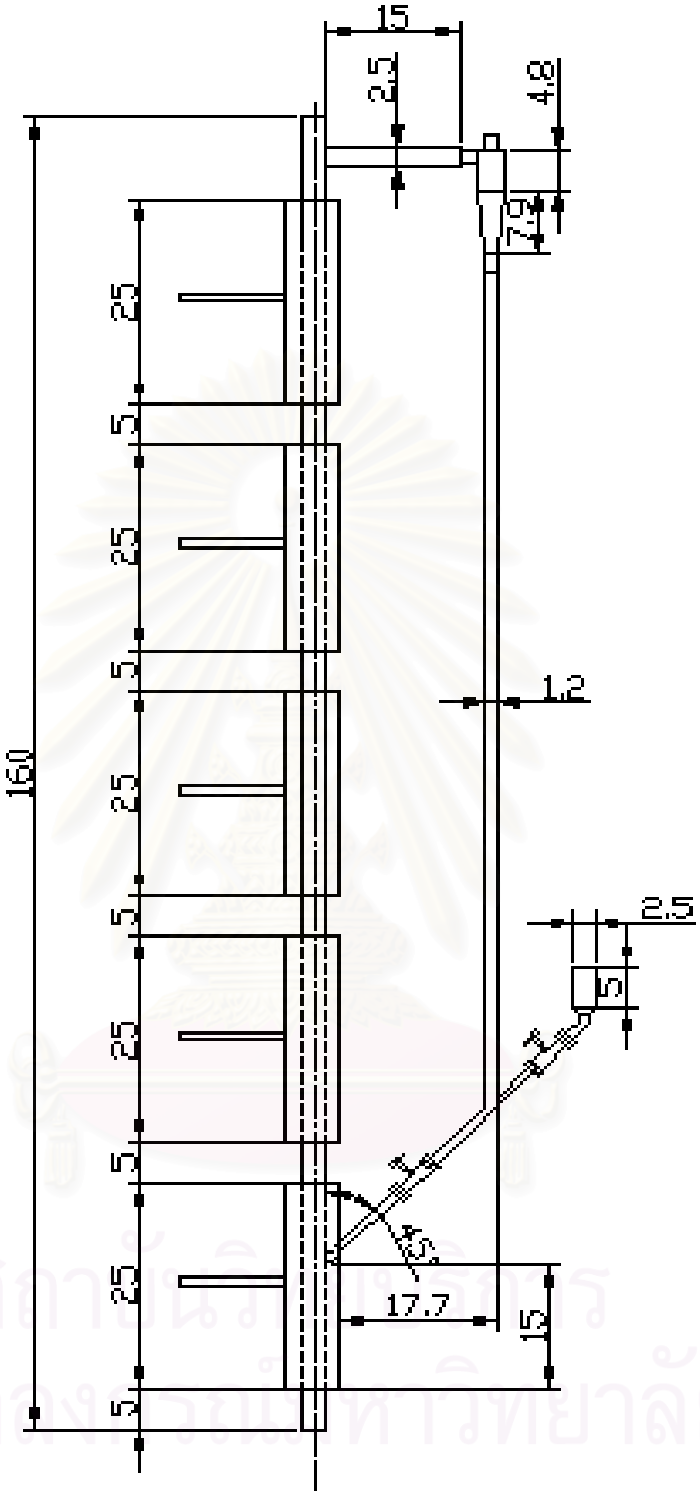


Figure 2.1 The dimensions of CFBC in the experiments (unit in centimeter).

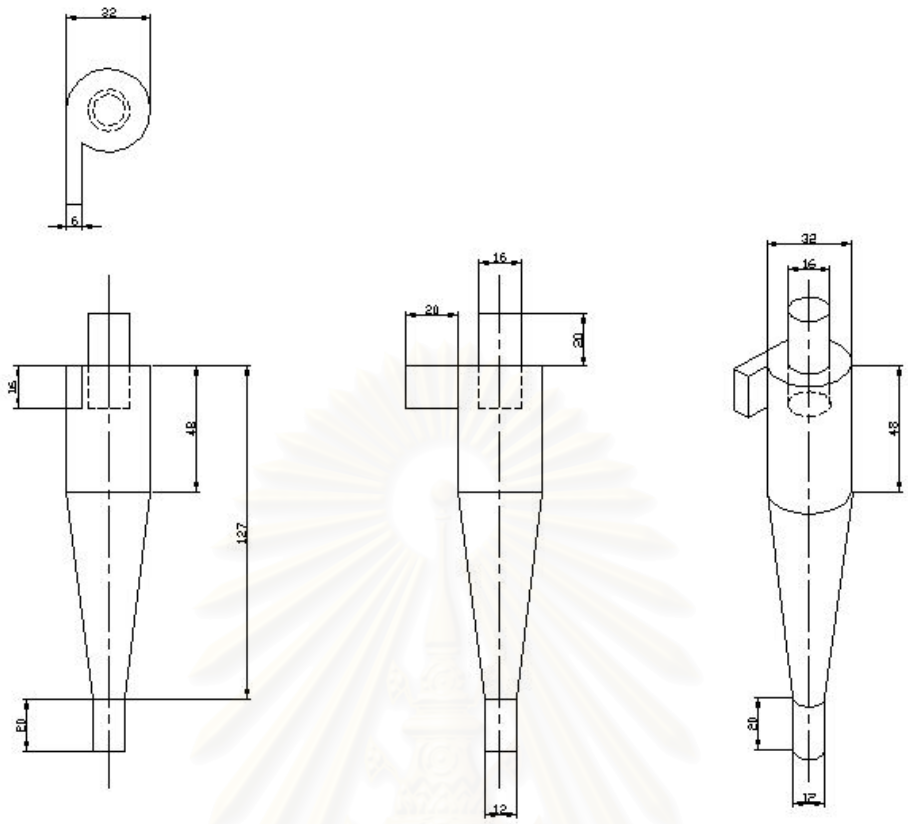


Figure 2.2 Dimensions of the cyclone.

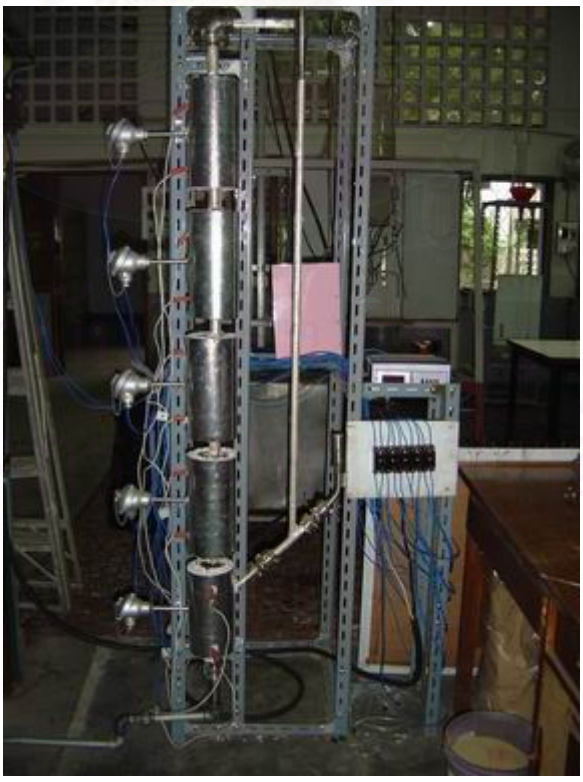


Figure 2.3 CFBC in the experiments.

2.3 Experiments

The experiment in this research was composed of a batch experiment with 4 g of fuel and 250 g of bed material. The experiments were divided into four parts to study the coal comminution that described in the following section. The method to measure the particle size was the problem in this research because of the brittle of particles after the devolatilization and combustion processes. Thus two methods of particle size distribution measurements were considered. The first method, CCD camera was used to measure the size of particles larger than 1 mm. The second one, particle size laser analyzer was used to measure the size of particles that was smaller than 1 mm.

2.3.1 Blank study

It was difficult to separate unburnt fuels or ashes from bed material. To analyze the particles size after fuels combustion in the CFBC by the particle size laser analyzer, blank study was used for the comparison of the particle size distribution between mixed particles and bed material particles after combustion.

In the blank study, only the bed material was used during the combustion in the CFBC. The operating conditions were 850 ^{o}C and 1 atm with air as the fluidizing gas. The residence time was equal to that used in the secondary fragmentation study as described later. After combustion, the sizes of particles were measured by particle size laser analyzer. The result of particle size distribution was shown in Figure 2.4.

2.3.2 Attrition study

This experiment was studied the attrition of fuels due to the collisions between particles and those between wall and particles. The operating conditions were room temperature and 1 atm with the same resident time as secondary fragmentation study section. The mixed particles between coal and sand were shown in Figure 2.5.

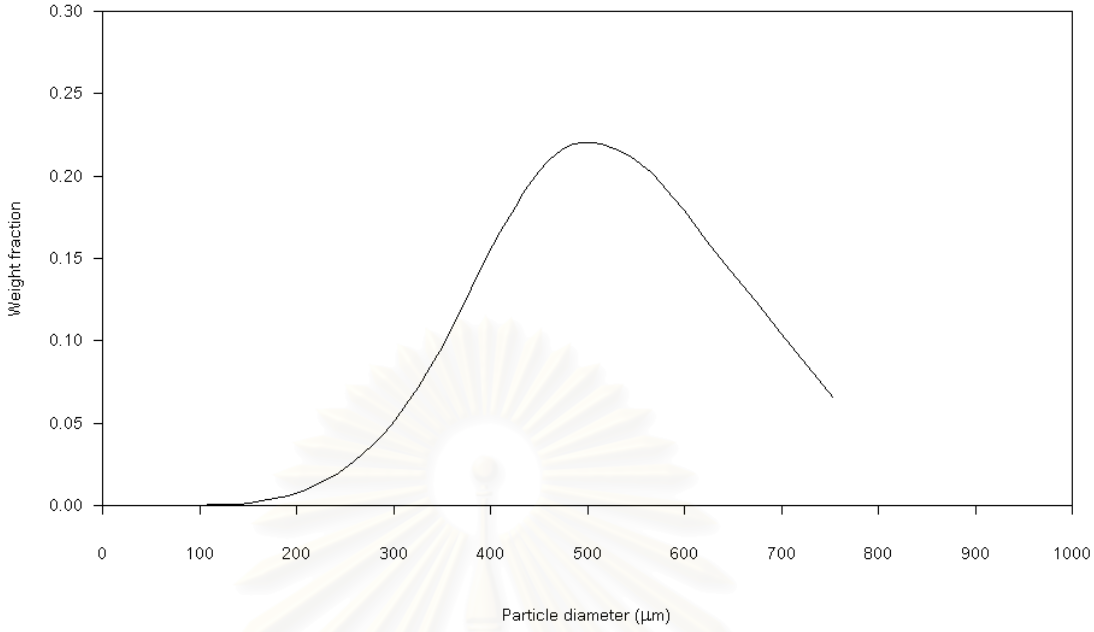


Figure 2.4 The PSD of sand from blank study at 850 °C, 1 atm that analyzed by particle size laser analyzer.

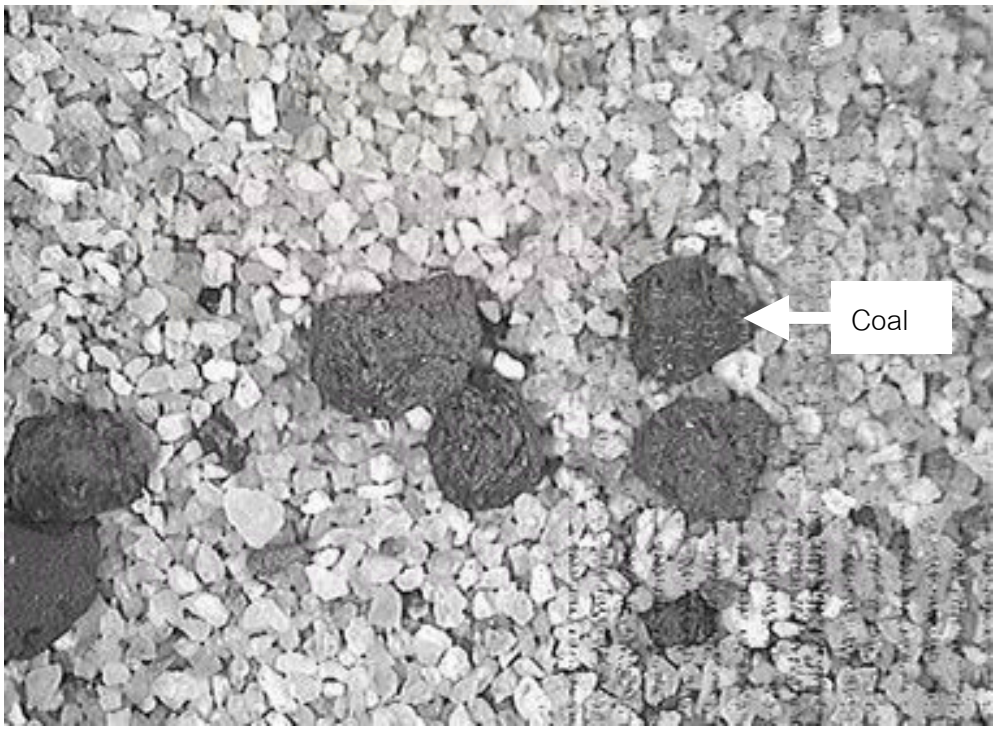


Figure 2.5 Mixed particles between coal and sand after attrition study at the ambient environment by CCD camera.

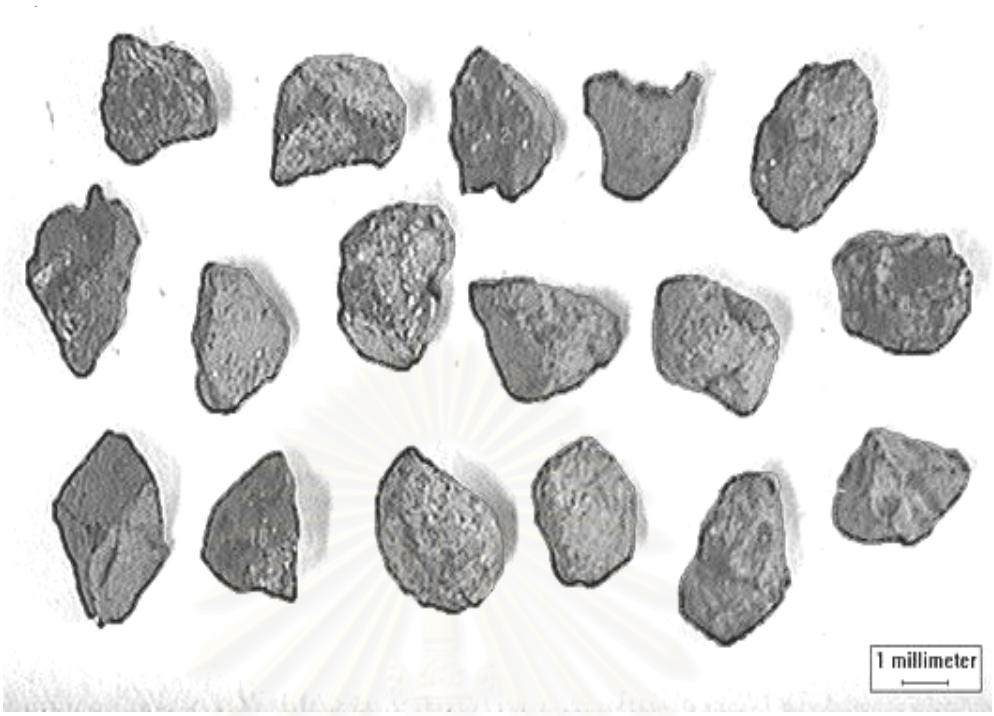


Figure 2.6 Coal particles after attrition at ambient environment that captured by CCD camera and analyzed by Image Pro Plus.

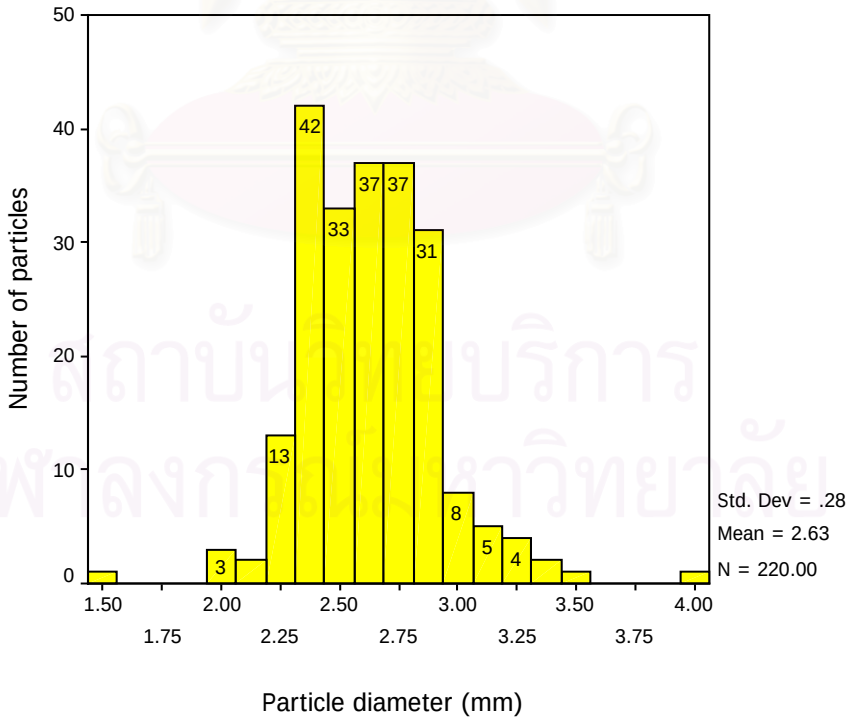


Figure 2.7 PSD from Image Pro Plus of attrition particles.

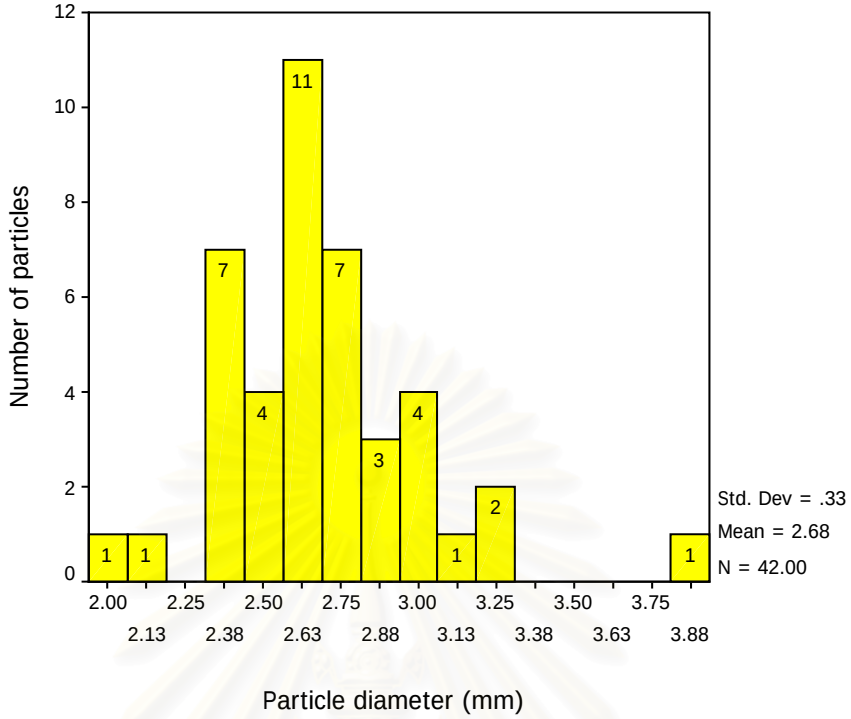


Figure 2.8 PSD from Image Pro Plus of raw material particle.

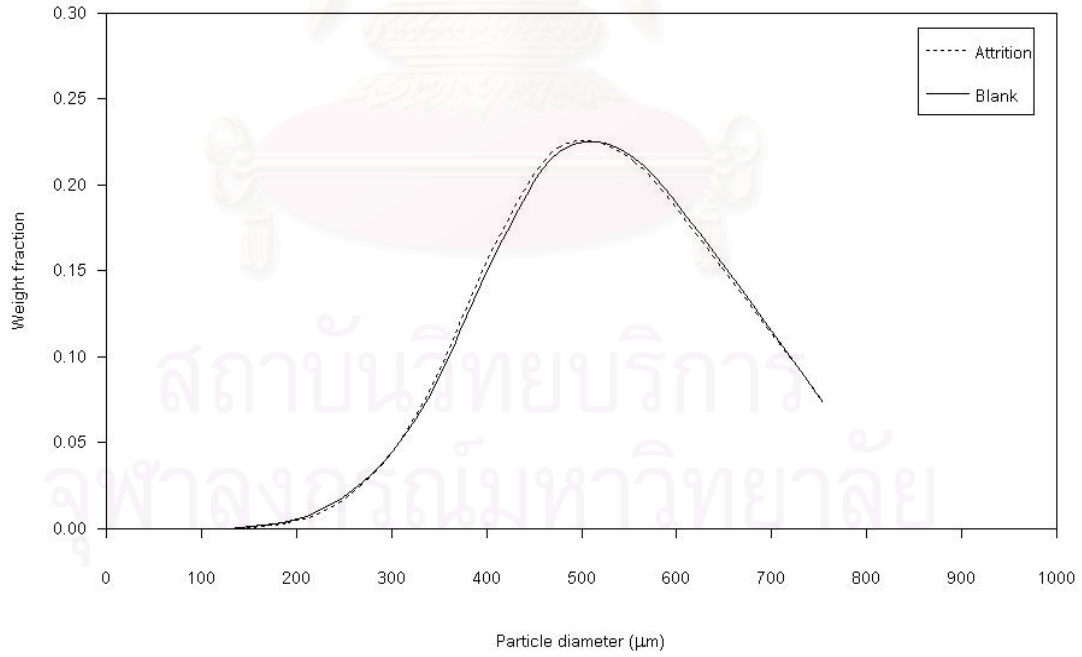


Figure 2.9 The PSD of mixed particles from attrition study at ambient environment that analyzed by particle size laser analyzer compare with blank study at 850 °C, 1 atm.

From Figure 2.5, after these experiments, the particles were measured by CCD camera and particle size laser analyzer in the following steps.

Steps to measure the size of particles.

- Drop off the particles through 1 mm sieve after complete the attrition study to separate coarse and fine particles.
- For the particles that were larger than 1 mm, sample 1 g of particles to capture their pictures with CCD camera. Then measure the size of particles with Image Pro Plus version 4.5.1. The result was shown in Figure 2.6 and 2.7.
- For the particles that were smaller than 1 mm, measure the size of particles with particle size laser analyzer. The result was shown in Figure 2.9.

For the large particles, Figure 2.7, the mean diameter of coal particles after attrition test was equal to 2.63 mm. Compare with Figure 2.8, the mean diameter of raw materials was equal to 2.68 mm. The particle size was slightly decreased by attrition. However, the standard deviations of both cases were relatively high. It could be summarized that the attrition has insignificant effect on the changing size of coal particles.

For the small particles, Figure 2.9, the particle size distribution of the coal after the attrition study was the same as that of the blank test. From this result, it could be mentioned that the coal particles were not changed their sizes after the collisions among particles in the CFBC reactor at the ambient condition. This result was the same as the attrition study for shale particles in a cold fast fluidized bed (Donsi et al., 1981 cited in Tardin, et al., 2001), but disagreed for the friable material particle (Tardin, et al., 2001). This was due to the attrition rate constant for coal particle was small (Soutdeh-Gharebaagh et al., 1998, and Halder and Basu, 1992).

2.3.3 Primary fragmentation study

To study the primary fragmentation process, nitrogen was used as fluidizing gas in the devolatilization process at 850 ^{o}C and 1 atm. The resident time and the methods to measure the size of particles were the same as in the previous section. The results were shown in Figure 2.10 and 2.13.

At high temperature, the volatile pressure was built up in the pore network of the combustible particles. Then the coal particles were bursted out into the smaller ones. From Figure 2.12, the mean particle diameter was reduced to 2.08 mm compared with the raw material in Figure 2.8. This was due to the effect of devolatilization process in the CFBC reactor. For the small particles, Figure 2.13 showed the increasing of particle size between 500-750 μm. The reason is that the mother particles were bursted out into small particles due to the weaken structure of particles and the build up of volatile pressure.

To model the prediction of PSD of the primary fragmentation, two models were used for the prediction. The first model was used for large particles that were larger than 1 mm. The second model was used for predicting smaller ones. Weibull distribution was used for predicting the cumulative mass of fragmented particles (Brown, 1989; Chirone and Massimilla, 1991, and Zobeck et al., 1995).

The cumulative particle size distribution for the fragmented particles was fitted to a two-parameter Weibull of the form;

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{\sigma}\right)^k\right] \qquad (2.1)$$

where $M(<l)$ is cumulative mass of fragments of size less than l, l is the diameter of particle, M_T is total mass of fragments in the distribution, σ is size related to the average size, and k is free parameter.

Figure 2.10 Mixed particles between coal and sand after primary fragmentation study at 850 ^{o}C, 1 atm with N_2 as the fluidizing gas by CCD camera.

Figure 2.11 Coal particles after primary fragmentation at 850 ^{o}C, 1 atm with N_2 as the fluidizing gas that captured by CCD camera and analyzed by Image Pro Plus.

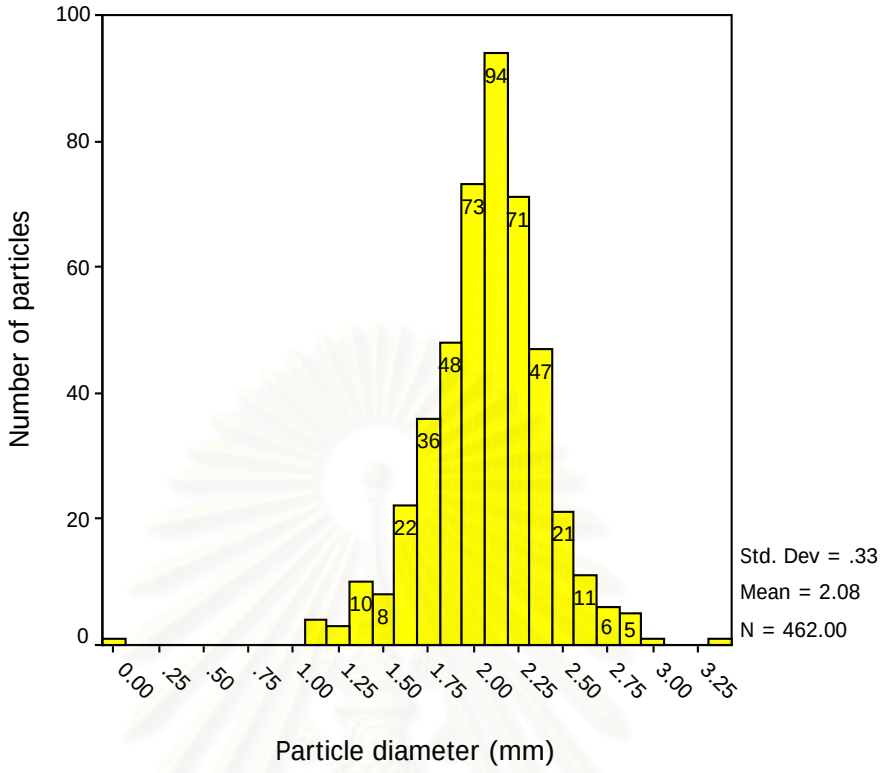


Figure 2.12 PSD from Image Pro Plus of primary fragmentation particles.

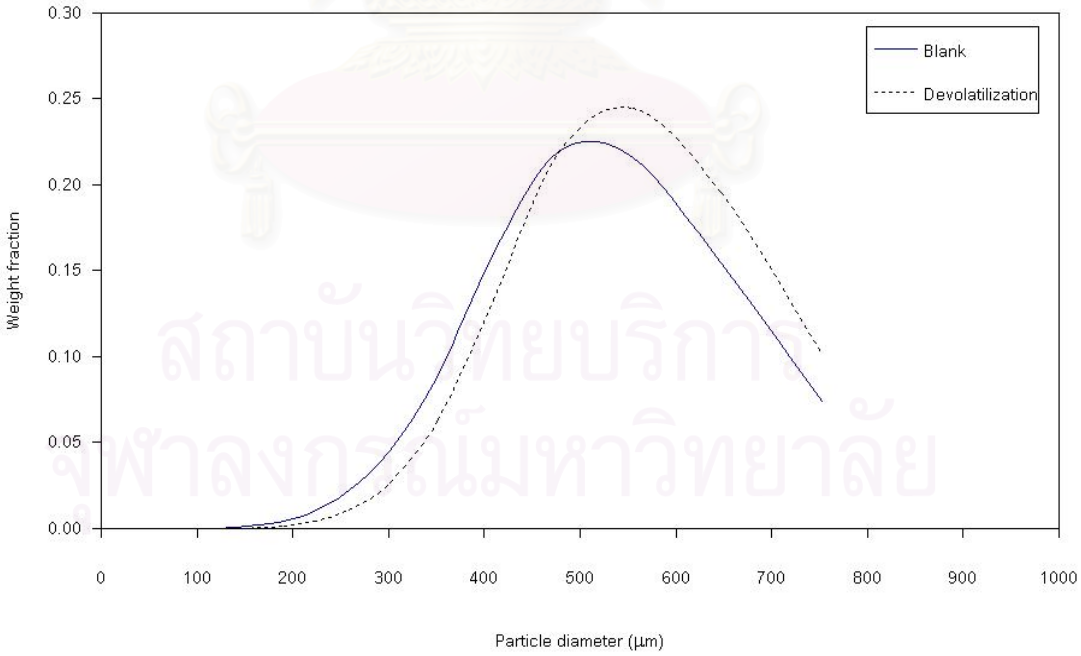


Figure 2.13 The PSD of mixed particles from primary fragmentation study at 850 °C, 1 atm with N_2 as the fluidizing gas that analyzed by particle size laser analyzer compare with blank study at 850 °C, 1 atm.

For the large particles, from Figure 2.12, the weight fractions of fragmented particles to construct a prediction model were calculated by multiplying the average weight of single fragmented particle that shown in Table A-1.

From the Weibull distribution, the prediction of cumulative fragmented particle model was shown in eq (2.2) and Figure 2.14.

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{2.13\times10^{-3}}\right)^{7.5}\right] \quad (2.2)$$

For the small particles, the difference of weight fractions over the blank study, in Figure 2.13, were modeled to predict the cumulative fraction as shown in eq (2.3) and Figure 2.15.

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{627}\right)^{7.5}\right] \quad (2.3)$$

2.3.4 Secondary fragmentation study

The secondary fragmentation was occurred in the combustion process. In the CFBC, fuels were combusted with air at 850 ^{o}C and 1 atm until complete combustion. In this study, the time for complete combustion of the fuels based on the emission analyses of volatiles, CO and CO_2, were about 1000 s as shown in Table A-2.

After complete combustion, only fine particles were observed. The mixed particles were difficult to separate between ash and sand. Therefore, the size of mixed particles was measured by the particle size laser analyzer. The result was shown in Figure 2.16.

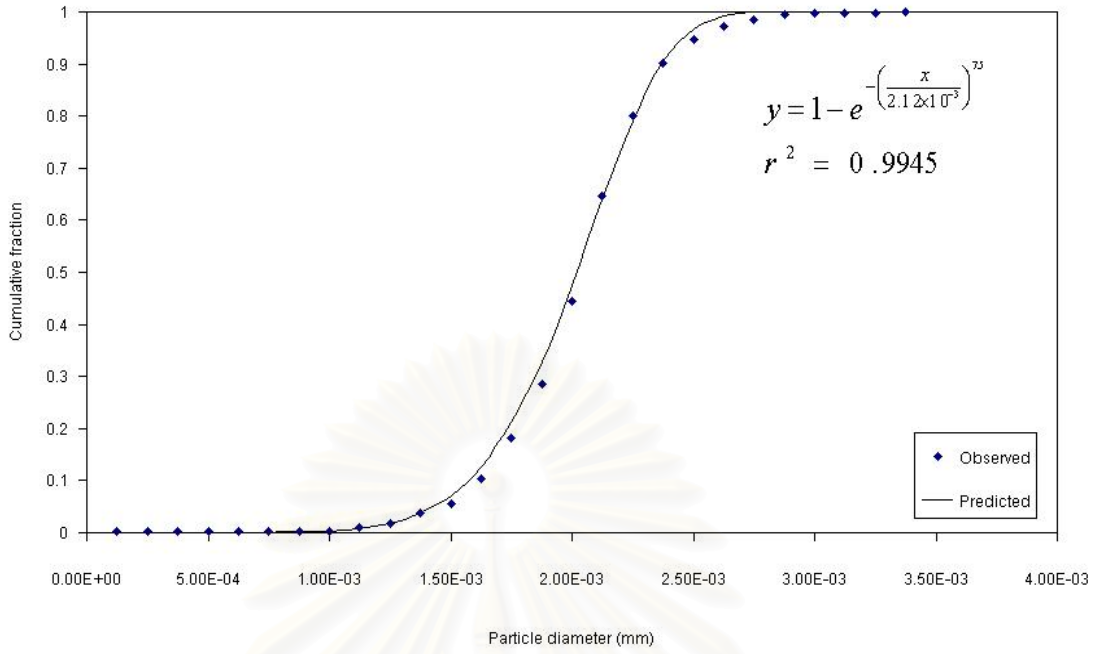


Figure 2.14 Comparison of the cumulative fraction between the experiment of primary fragmentation at 850 °C, 1 atm with N_2 as the fluidizing gas and the model prediction for large particles.

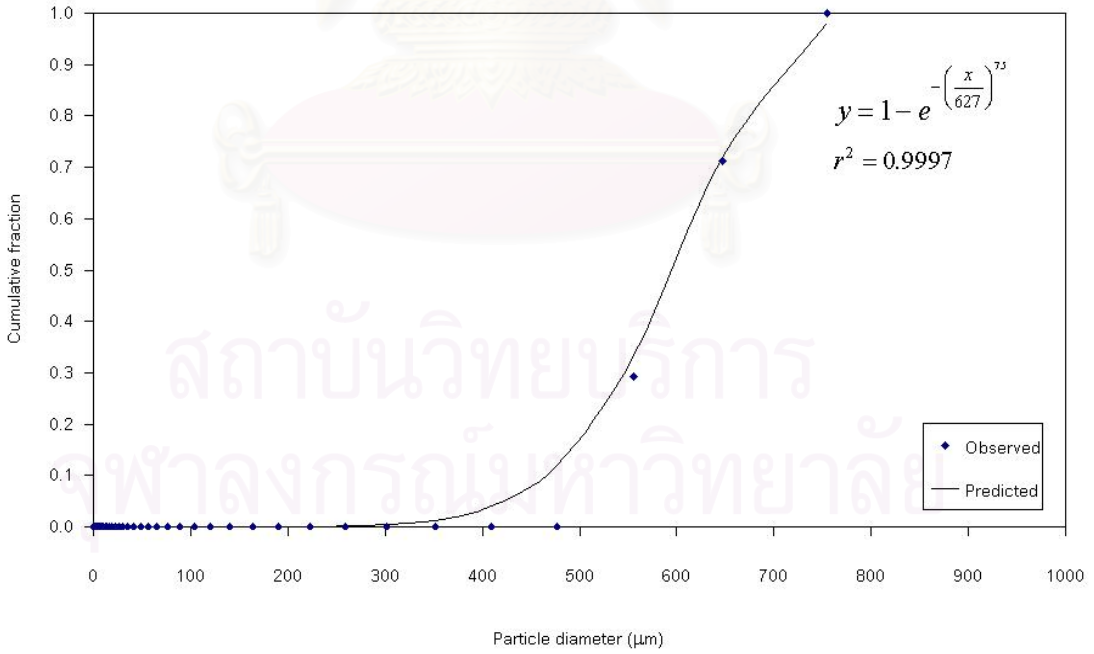


Figure 2.15 Comparison of the cumulative fraction between the experiment of primary fragmentation at 850 °C, 1 atm with N_2 as the fluidizing gas and the model prediction for small particles.

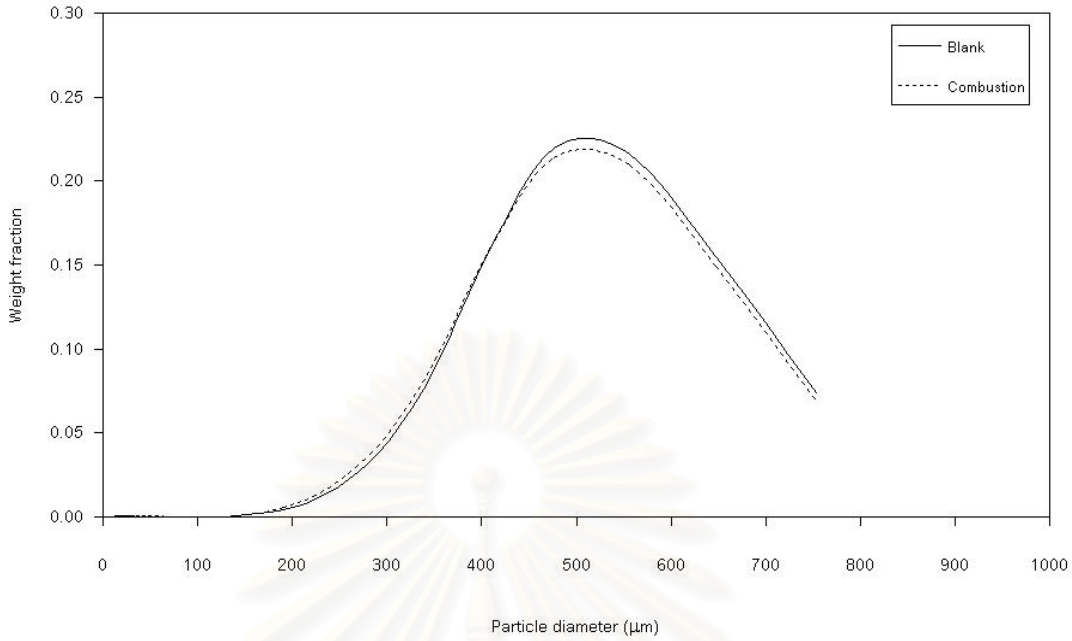


Figure 2.16 The PSD of mixed particles from secondary fragmentation study at 850 °C, 1 atm with air as the fluidizing gas that analyzed by particle size laser analyzer compare with blank study at 850 °C, 1 atm.

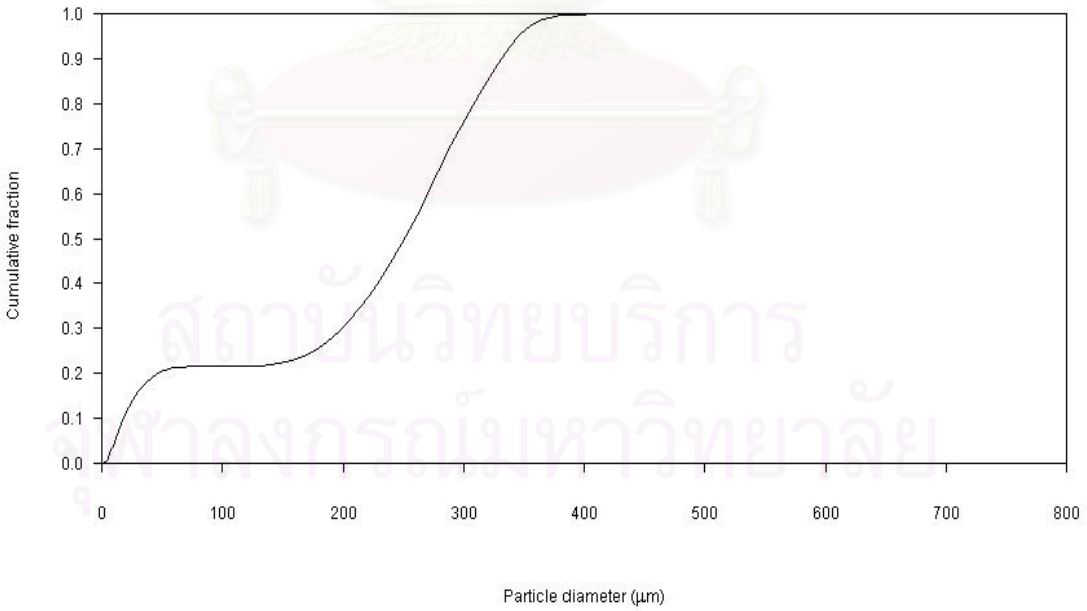


Figure 2.17 Cumulative fraction of secondary fragmentation at 850 °C, 1 atm with air as the fluidizing gas.

From Figure 2.16, the particle size distribution shifted to the left hand side. This was due to the small particles were increased from the combustion. The small particles in this experiment were divided into two parts, but it was not observed here due to the improper scale of the plot for these particles. Then this evidence was plotted in the form of cumulative fraction by the different weight fraction of secondary study over the blank study. The result was shown in Figure 2.17.

From Figure 2.17, the curve was divided into two intervals. The average sizes of particles were approximately 20 μm and 300 μm for the first and second intervals, respectively. The reasons were that the coal after combustion was divided into ash and unburnt carbon. The particles that were cumulated in the first interval were ash because the size of particle was closed to the size of Mae Moh ash, which equals 14 μm reported by Jaturapitakkul et al. (1999). For the second interval, the unburnt carbon was accumulated (Marban et al., 1996; and Lee et al, 2003).

The model to predict the size distribution of ash and unburnt carbon was also used the Weibull distribution. The prediction models were divided into two models. The first model predicted the particles that was smaller than 120 μm as shown in eq. (2.4). The second one was predicted the larger particles as shown in eq. (2.5).

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{25}\right)^{1.6}\right] \tag{2.4}$$

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{295}\right)^{6}\right] \tag{2.5}$$

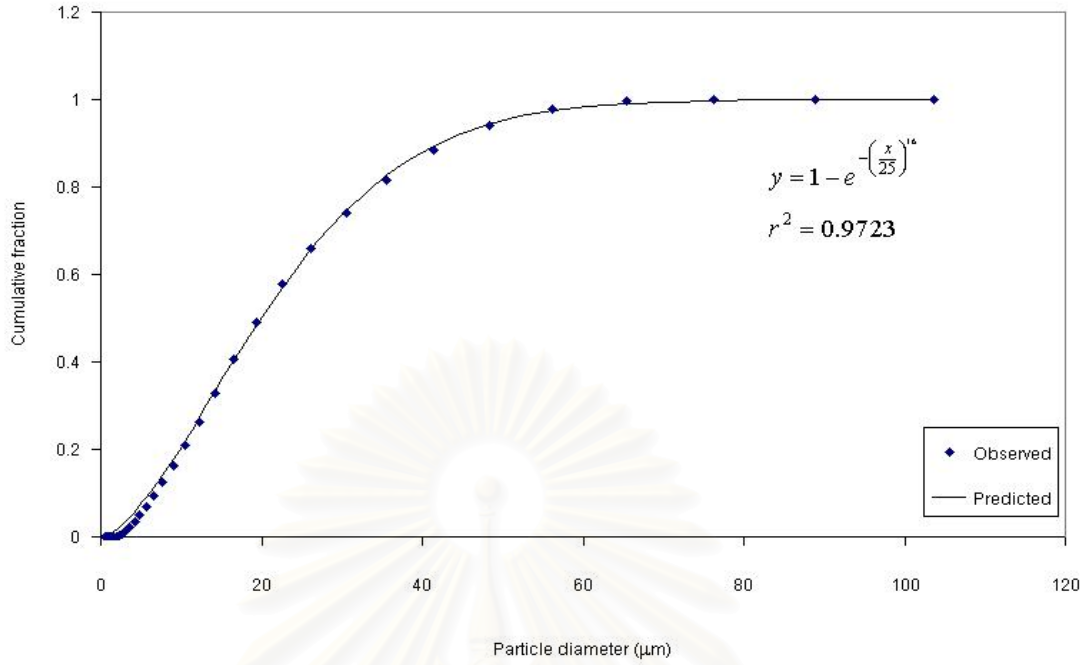


Figure 2.18 Comparison of the cumulative fraction between the experiment of secondary fragmentation at 850 °C, 1 atm with air as the fluidizing gas and the model prediction for ash particles.

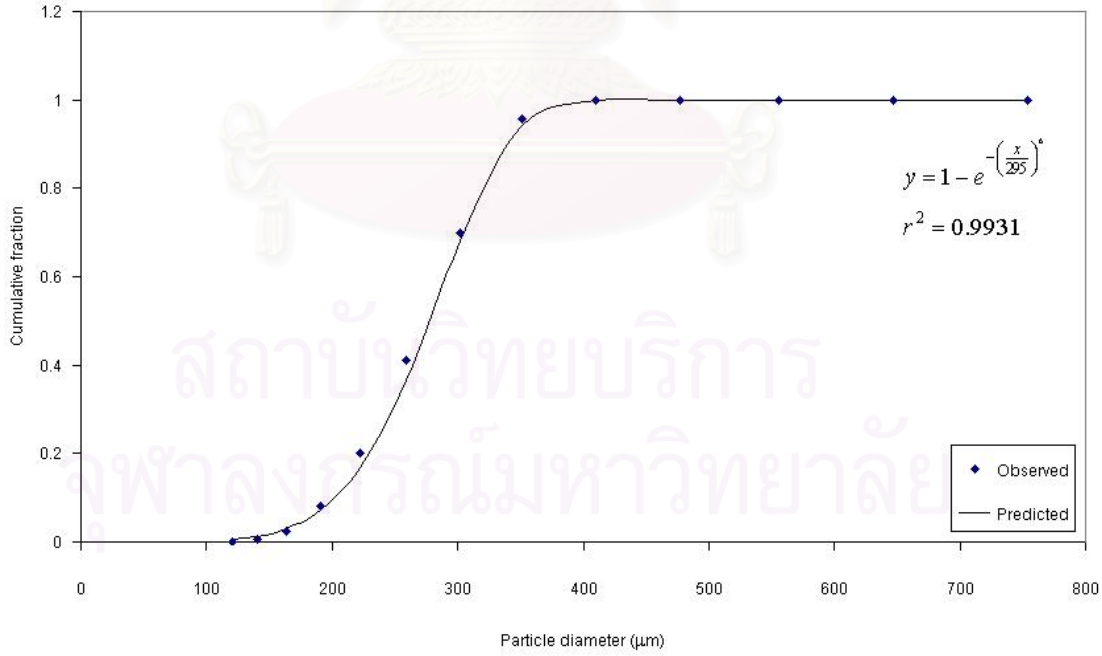


Figure 2.19 Comparison of the cumulative fraction between the experiment of secondary fragmentation at 850 °C, 1 atm with air as the fluidizing gas and the model prediction for unburnt particles.

2.3.5 Biomass study

The biomass in this research is bagasse. Bagasse was prepared by crushing and sieving to 2-3 mm. For the comminution study of bagasse, it was difficult to predict the size distribution of bagasse combustion. Only the primary and secondary fragmentation were studied. For the primary fragmentation study, the size distribution of fragmented bagasse could not be predicted, because the bagasse is very brittle after the devolatilization process. The bagasse fibers were changed to the very fine particles with the same size of the particles after the secondary fragmentation study. The result was shown in Figure 2.20 and 2.21.

From both figures, it was difficult to differentiate between sand particles from blank study and bagasse-sand particles from both primary and secondary fragmentation studies. This was due to the small amount of ash in bagasse. The peak that represents the ash in bagasse would not be observed as was observed for the case of coal combustion.

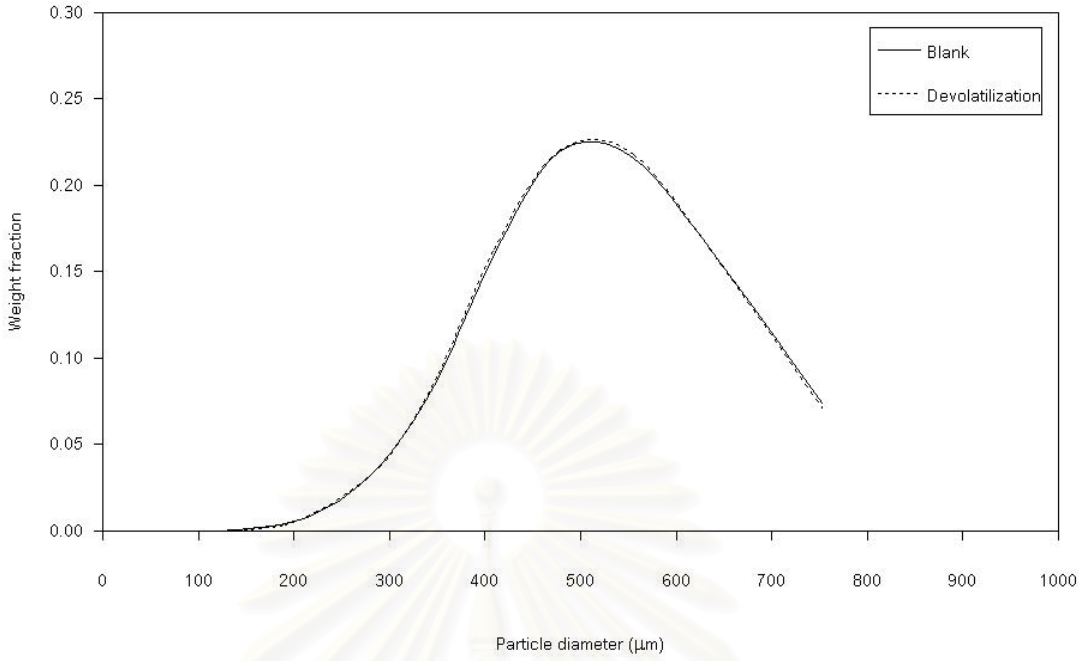


Figure 2.20 The PSD of bagasse-sand particles from primary fragmentation study at 850 °C, 1 atm with N_2 as the fluidizing gas that analyzed by particle size laser analyzer compared with blank study at 850 °C, 1 atm.

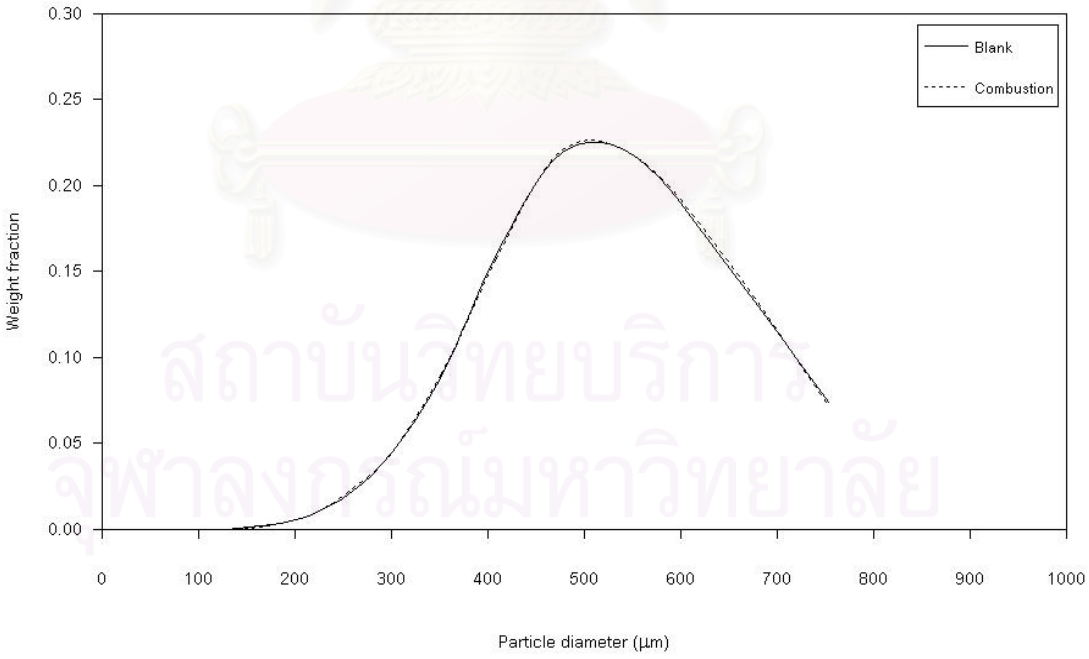


Figure 2.21 The PSD of bagasse-sand particles from secondary fragmentation study at 850 °C, 1 atm with air as the fluidizing gas that analyzed by particle size laser analyzer compared with blank study at 850 °C, 1 atm.

CHAPTER III

MODELING

The models of CFBC in this research were divided into three parts: combustion reactions and particle size distribution, hydrodynamics, and gas emissions.

3.1 Combustion reactions and particle size distribution

The combustion model allows for the determination of chemical change and heat released during the combustion. Since coal combustion in the CFBC is quite complex, only the three major steps of coal combustion were considered in the model (Soutdeh-Gharebaagh et al., 1998, and Huilin et al., 2000).

From eq. (1.8), (1.10), and (1.11):

$$C + \frac{1}{2}O_2 \rightarrow CO$$

$$CO + \frac{1}{2}O_2 \rightarrow CO_2$$

$$C + CO_2 \rightarrow 2CO$$

The first and third reactions are heterogeneous and the second is homogeneous. The third reaction was neglected in the model because the temperature of the burning particles in the CFBC was not sufficiently high. The effect of this reaction on the combustion was minimal (LaNauze, 1985 cited in Soutdeh-Gharebaagh et al., 1998) due to the low concentration of carbon in a fluidized bed (Ross et al., 1981 cited in Basu, 1999; Basu et al., 1975 cited in Basu, 1999).

The second reaction, emission level of CO from CFBC is strongly dependent on the temperature and reactive concentration. The rate of reaction can be calculated from the following equation (Soutdeh-Gharebaagh et al., 1998).

$$Rt_{CO} = 1.18 \times 10^{13} \cdot f_{CO} \cdot f_{O_2}^{0.5} \cdot f_{H_2O}^{0.5} \cdot \left(\frac{P}{R_{g1}T}\right) \cdot \exp\left(-\frac{25000}{R_g T}\right) \cdot C \cdot \varepsilon \qquad (3.1)$$

where Rt is the rate of reaction, C is combustion gas concentration, f is the mole fraction of each component, P is bed pressure, R_g and R_{g1} are universal gas constant, T is bed temperature, and ε is void fraction.

The reaction rate and particle size distribution from the combustion of the first reaction were calculated by shrinking particle model.

The shrinking particle model for an isothermal spherical particle is divided into three steps as shown in Figure 3.1 (Levenspile 1972):

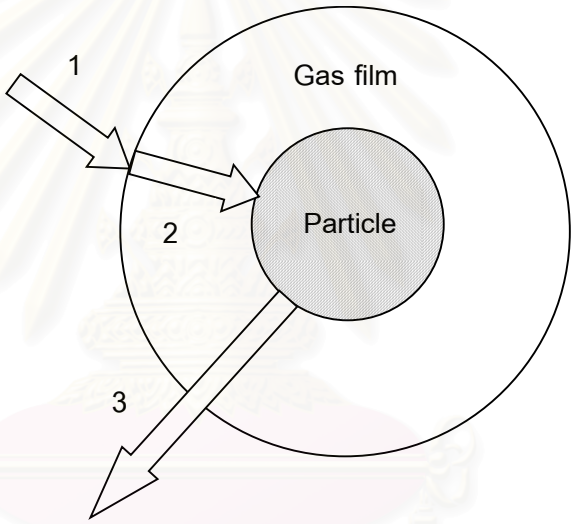


Figure 3.1 Three steps of shrinking particle model.

1. Diffusion of reactant A from the main body of gas through the gas film to the surface of the solid.
2. Reaction on the surface between reactant A and solid.
3. Diffusion of reaction products from the surface of the solid through the gas film back into the main body of the gas.

In this model the ash layer was absent and did not contribute any resistance. Then the complete conversion time was calculated from above step.

Consider the correlation for estimating k_{Ag} for spherical particles given by Ranz and Marshall (Ranz and Marshall 1952, cited in Missen et al., 1999). For a free-falling spherical particle of radius (R), moving with velocity (U) relative to a fluid of density (ρ), and viscosity (μ), and in which the molecular diffusion coefficient for species A (D_A), the Ranz and Marshall correlation relates the Sherwood number which incorporates k_{Ag}, to the Schmidt number and the Reynolds number, according to the following equation:

$$Sh = 2 + 0.6Sc^{1/3}\,\mathrm{Re}^{1/2} \tag{3.2}$$

where Sc is Schmidt number, Re is Reynolds number

That is,

$$\frac{2Rk_{Ag}}{D_A} = 2 + 0.6\left(\frac{\mu}{\rho D_A}\right)^{1/3}\left(\frac{2RU\rho}{\mu}\right)^{1/2} \tag{3.3}$$

where D_A is diffusion coefficient of A, k_{Ag} is mass transfer coefficient of A, R is radius of particle, U is gas velocity, μ is gas viscosity, and ρ is gas density.

This correlation may be used to estimate k_{Ag} given sufficient information about the other quantities.

rearrange eq. (3.3)

$$k_{Ag} = \frac{D_A}{R} + 0.3D_A\frac{\left(\frac{\mu}{\rho D_A}\right)^{1/3}\left(\frac{2U\rho}{\mu}\right)^{1/2}}{R^{1/2}} \tag{3.4}$$

or $$k_{Ag} = \frac{K_1}{R} + \frac{K_2}{R^{1/2}} \tag{3.5}$$

where $$K_1 = D_A \tag{3.6}$$

$$K_2 = 0.3D_A\left(\frac{\mu}{\rho D_A}\right)^{1/3}\left(\frac{2U\rho}{\mu}\right)^{1/2} \tag{3.7}$$

With the gas-film mass transfer control, this condition occurs when the mass transfer rate is very slow compared to the kinetic rate. The kinetic rate is so fast

that the amount of oxygen reaching the external surface of the char through the relatively slow mass transfer process is entirely consumed before it has a chance to enter the pores. This type of combustion occurs in large particles, and where the mass transfer is small compared to the reaction rate (Basu and Fraser, 1991). The complete conversion time can be calculated using the following equations (Missen et al., 1999):

Small particles $$\tau = \frac{\rho_B R^2 f_B}{3bc_{Ag} K_1} \quad (3.8)$$

Where b is stoichiometric coefficient of gas in the combustion reaction, c_{Ag} is concentration of A, f_B is size parameters, and ρ_B is solid molar density.

Large particles $$\tau = \frac{\rho_B R^{3/2} f_B}{3bc_{Ag} K_2} \quad (3.9)$$

$$f_B = 1 - \left(\frac{r_c}{R}\right)^3 \quad (3.10)$$

where r_c is residual radius.

With chemical reaction control, the chemical kinetic rate is much slower than the diffusion rate. This regime would occur on the exterior surface of coarse non porous particles at temperatures around 900 °C. In porous coarse particles, it would not occur until the temperature is lower than 600 °C. For fine porous particles if the mass transfer rate is correspondingly high, this regime may occurs even at 800 °C. In porous chars, oxygen diffuses into the char and combustion occurs uniformly throughout the char. As a result, the density of particle, rather than its diameter, decreases with combustion. Oxygen concentration is uniform throughout the char. Typical situations when this regime is prevalent are (Basu and Fraser, 1991):

1. During light-up in a CFB when the temperature is low and consequently the kinetic rate is very slow.
2. Fine particle where the diffusion resistance is very small.

The complete conversion time in this regime can be calculated using the following equations:

$$\tau = \frac{\rho_B R}{b k_s c_{Ag}} \tag{3.11}$$

$$k_{s1} = k_0 \exp\left(-\frac{Ea_1}{R_{g2} T}\right) \tag{3.12}$$

where k_0 is frequency factor, Ea_1 is activation energy, k_{s1} is first order reaction rate constant base on unit surface, and R_{g2} is universal gas constant.

The mean residence time for mixed flow in the reactor is:

$$\hat{t} = \frac{V(1-\varepsilon)}{F_t} \tag{3.13}$$

where F_t is volumetric flow rate of solid, and V is reactor volume.

The residual radius from the combustion can be calculated using the following equations:

for the gas-film mass transfer control

small particle

$$\hat{t} = \frac{\rho_B R^2 \left(1-\left(\frac{r_c}{R}\right)^3\right)}{3 b c_{Ag} D_A} \tag{3.14}$$

rearrange eq. (3.14)

$$r_c = \sqrt[3]{R^3 - \frac{3 b c_{Ag} D_A R \hat{t}}{\rho_B}} \tag{3.15}$$

large particle

$$\hat{t} = \frac{\rho_B R^{3/2}}{3 b c_{Ag} K_2}\left(1-\left(\frac{r_c}{R}\right)^3\right) \tag{3.16}$$

substitute K_2 from eq. (3.7) to eq. (3.16)

$$\hat{t} = \frac{\rho_B R^{3/2}\left(1-\left(\frac{r_c}{R}\right)^3\right)}{0.9 b c_{Ag} D_A \left(\frac{\mu}{\rho D_A}\right)^{1/3}\left(\frac{2U\rho}{\mu}\right)^{1/2}} \tag{3.17}$$

rearrange eq. (3.17)

$$r_c = \sqrt[3]{R^3 - \frac{0.9\hat{t}bc_{Ag}D_A R^{3/2}\left(\frac{\mu}{\rho D_A}\right)^{1/3}\left(\frac{2U\rho}{\mu}\right)^{1/2}}{\rho_B}} \tag{3.18}$$

for the chemical reaction control

$$\hat{t} = \frac{\rho_B}{bk_s c_{Ag}}\left(R - r_c\right) \tag{3.19}$$

rearrange eq. (3.19)
$$r_c = R - \frac{\hat{t}bk_s c_{Ag}}{\rho_B} \tag{3.20}$$

The unconverted fraction of the reactant was given by the following equations (Levenspiel, 1972):

$$\begin{pmatrix}\text{mean value}\\ \text{for fraction of}\\ \text{B unconverted}\end{pmatrix} = \sum_{\text{all sizes}} \begin{pmatrix}\text{fraction}\\ \text{unconverted}\\ \text{in particles}\\ \text{of size } R_i\end{pmatrix}\begin{pmatrix}\text{fraction of}\\ \text{exit or entering}\\ \text{stream consisting}\\ \text{of particles}\\ \text{of size } R_i\end{pmatrix} \tag{3.21}$$

or in symbols:

$$1 - \overline{X}_B = \sum_{R=0}^{R_m}\left[1 - \overline{X}_B(R_i)\right]\frac{F_c(R_i)}{F_c} \tag{3.22}$$

for gas-film mass transfer control,

$$1 - \overline{X}_B = \sum_{R=0}^{R_m}\left\{\frac{1}{2!}\frac{\tau(R_i)}{t} - \frac{1}{3!}\left[\frac{\tau(R_i)}{t}\right]^2 + \ldots\right\}\frac{F_c(R_i)}{F_c} \tag{3.23}$$

for reaction control,

$$1 - \overline{X}_B = \sum_{R=0}^{R_m}\left\{\frac{1}{4}\frac{\tau(R_i)}{t} - \frac{1}{20}\left[\frac{\tau(R_i)}{t}\right]^2 + \ldots\right\}\frac{F_c(R_i)}{F_c} \tag{3.24}$$

3.2 Hydrodynamics

For steady-state condition, the model considers that the CFBC is divided into two regions: a dense zone in the bottom, which is located right above the distributor, and a dilute region in the upper portion of the furnace, which is located between the upper surface of the dense bed and the riser exit, with a suspension density decaying with height. The height of each region depends on the superficial gas velocity, solids mass flux and properties of solids and fluid (Huilin et al., 2000 and Sabbaghan et al., 2004).

In the dense bed, the phenomena can be explained by the gas-solid flow. According to the two-phase theory of fluidization, the dense bed is divided into two regions: a solids-free bubble phase and a solids-laden emulsion phase (Jin et al., 2001). The emulsion phase remains at incipient fluidization conditions and with the gas in the so-called excess gas flow (U- U_{mf}), in excess of what is required to maintain incipient fluidization in the emulsion phase, assumed to pass through the bed as solid-free bubbles (Hayhurst and Tucker, 1990 cited in Jin et al., 2001).

The upper region is assumed to be axially composed of three zones (Sabbaghan et al., 2004):

1. The acceleration zone is at the bottom part of the upper region where the solids are accelerated to a constant upward velocity.
2. The fully developed zone is located above the acceleration zone, where the flow characteristics are invariant with height.
3. The deceleration zone is located above the fully developed zone, where the solids are decelerated depending on the exit geometry of the riser.

The variation of solid fraction with length is illustrated in Figure 3.2.

3.2.1 Lower region calculation

In this region, the perfect mixing between the solid and the gas phase was assumed. The mean void can be considered constant and may be obtained using the correlation of Kunni and Levenspiel (1991) as shown in Figure 3.3.

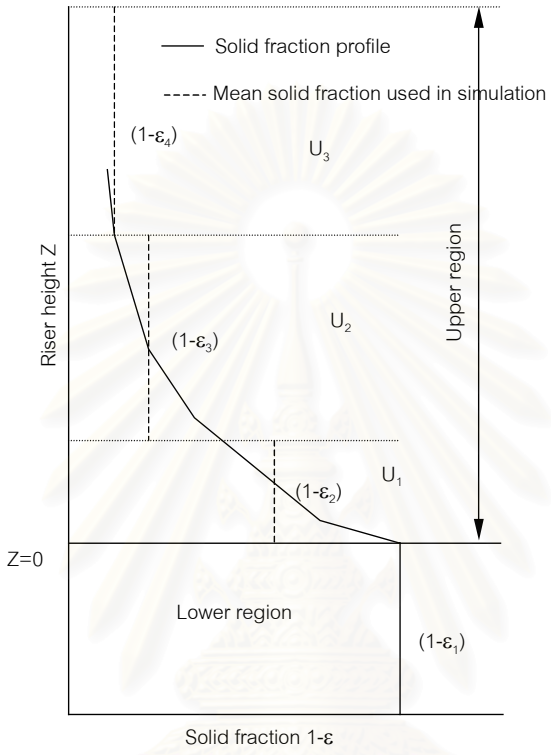


Figure 3.2 Variation of void fraction with height in the riser (Soutdeh-Gharebaagh et al., 1998).

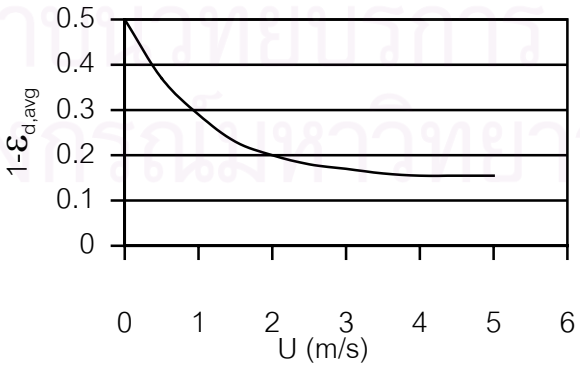


Figure 3.3 Mean void of the dense bed of the CFBC as a function of superficial gas velocities (Kunni and Levenspiel, 1991).

3.2.2 Upper region calculation

In order to predict the mean void in this region, the proposed model assumes that the upper region consists of two zones: an acceleration zone, and a fully developed zone.

The decay constant was obtained using the correlation of Kunni and Levenspiel as shown in Figure 3.4 (Basu and Fraser, 1991).

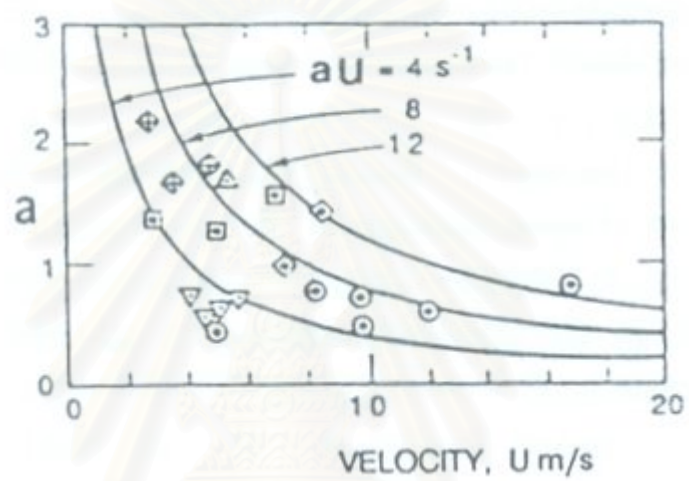


Figure 3.4 Decay constant in a axial bed density profile (Basu and Fraser, 1991).

The asymptotic voidage in the dilute phase (ε^*) was assumed to be equal to the choking voidage (ε_c) (Basu and Fraser 1991) that can be calculated by using following equations:

$$\frac{U_{ch}}{\varepsilon_c} = U_t + \left[\frac{2gd\left(\varepsilon_c^{-4.7}-1\right)\rho_p^{2.2}}{6.81\times10^5\,\rho^{2.2}}\right]^{0.5} \tag{3.26}$$

$$G_s = \left(U_{ch}-U_t\right)\left(1-\varepsilon_c\right)\rho_p \tag{3.27}$$

where U_{ch} is choking velocity, U_t is terminal velocity, g is acceleration due to gravity, ρ_p is particle density, ρ is gas density, and G_s is solid circulation rate.

$$Ar = \frac{\rho\left(\rho_p-\rho\right)gd^3}{\mu^2} \tag{3.28}$$

$$U_t = \frac{\mu}{d\rho}\left[\frac{Ar}{7.5}\right]^{0.666} \tag{3.29}$$

where Ar is Archimedes number.

$$\mathrm{Re}_{mf} = \left[27.2^2 + 0.0408\,Ar\right]^{0.5} - 27.2 \tag{3.30}$$

where Re_{mf} is Reynolds number at minimum fluidized condition.

$$U_{mf} = \frac{\mathrm{Re}_{mf}\,\mu}{d\rho} \tag{3.31}$$

The axial voidage in the dilute phase (ε_u) was calculated from:

$$\varepsilon_u = \frac{1}{1+\dfrac{\Phi G_s}{U_2\rho_p}} \tag{3.32}$$

where Φ is slip factor, and U_2 is superficial gas velocity in dilute bed.

$$\Phi = 1 + \frac{5.6}{F_r} + 0.47F_{rt}^{0.41} \tag{3.33}$$

where F_r is Froude number, and F_{rt} is particle Froude number.

$$F_r = \frac{U_2}{\sqrt{gD_r}} \tag{3.34}$$

$$F_{rt} = \frac{U_t}{\sqrt{gD_r}} \tag{3.35}$$

where D_r is riser diameter.

The mean voidage in each section of the upper region was calculated from the following equation.

$$\varepsilon_{u,ni,avg} = \varepsilon^* - \frac{1}{a\cdot\Delta L}\left(\varepsilon_{d,avg} - \varepsilon^*\right)\left(\exp\left(-aZ_{ni}\right) - \exp\left(-aZ_{ni-1}\right)\right) \tag{3.36}$$

where ΔL is height of the nith interval, Z_{ni} and Z_{ni-1} are the corresponding distances for the nith and (ni – 1)th interval above the lower region.

3.3 Gas emissions

3.3.1 CO and CO_2 emissions

The reaction rate emissions of CO and CO_2 were calculated from the reaction (1.8) and (1.10):

$$C + \frac{1}{2}O_2 \rightarrow CO$$

$$CO + \frac{1}{2}O_2 \rightarrow CO_2$$

The methods of calculation were described in the section 3.1.

3.3.2 NO_x and N_2O emissions

NO_x and N_2O formation in combustion processes result from an oxidation nitrogen in the combustion air and in the fuel. The formation of NO_x is highly dependent upon temperature and excess air. The nitrogen oxides include several nitrogen-based air pollutants. The heterogeneous reactions of char with O_2, CO_2, NO, and N_2O within porous particles, and the homogeneous reactions involving CO, O_2, NO, and N_2O in the boundary layer were described in the following sections (Chen et al., 2001).

3.3.2.1 Heterogeneous reactions

3.3.2.1.1 *Formation of NO*

Char bound nitrogen is first oxidized to NO by a reaction which is first order with respect to oxygen concentration (De Soete et al., 1999 cited in Chen et al., 2001).

$$C_{Char} - N_{\gamma} + \frac{\gamma + 1}{2}O_2 \rightarrow \gamma NO + C_{Char} - O \qquad (3.37)$$

The rate of this reaction was assumed to be proportional to the rate of char combustion with the constant of proportionally defined as γ. On an average, every char-N atom is expected to be linked to one carbon atom suggesting that $\gamma = 1$. Thus the rate of NO formation is:

$$Rt_A = K_A C_{O_2} \tag{3.38}$$

$$K_A = \frac{1000}{3} F_P T \exp(-19000/T) \tag{3.39}$$

where F_p is specific surface area.

3.3.2.1.2 *Formation of N_2O*

NO further reacts with bound nitrogen to produce N_2O according to the following reaction:

$$C_{Char} - N + NO \rightarrow N_2O + C_{Char} \tag{3.40}$$

The rate of N_2O formation is also proportional to γ. The modified first order rate expression is:

$$Rt_B = K_B C_{NO} \tag{3.41}$$

$$K_B = \gamma k_0 F_P \exp(-9000/T) \tag{3.42}$$

where k_0 is adjustable parameter; k_0 = 3 was suggested by Chen et al. (2001).

3.3.2.1.3 *Reduction of NO by char*

A number of mechanisms were proposed for the reduction of NO on the surface of char. The mechanism proposed by Chan et al. (Chan et al., 1983 cited in Chen et al., 2001) assumed reaction between NO and a single carbon site to form chemisorbed oxygen and the release of nitrogen as shown in the following reaction.

$$NO + C_{Char} \rightarrow \frac{1}{2} N_2 + CO \tag{3.43}$$

$$Rt_C = K_C C_{NO} \tag{3.44}$$

$$K_C = 555.6 F_P \exp(-14193/T) \tag{3.45}$$

The presence of CO in the gas phase is known to enhance the rate of NO reduction. This may occur through reaction of CO with surface bound oxygen atoms, leading to regeneration of surface sites for reaction with NO. Alternatively, this reaction has also been considered as a part of the heterogeneous reaction between NO and carbon in the presence of CO—thus, CO acts as an oxygen scavenger from the surface of carbon leaving behind a free active carbon site. This reaction can be written as:

$$NO + CO \rightarrow \frac{1}{2}N_2 + CO_2 \tag{3.46}$$

$$Rt_D = K_D C_{NO} \tag{3.47}$$

$$K_D = 5.67 \times 10^3 \exp(-13952/T) \tag{3.48}$$

3.3.2.1.4 *Reduction of N_2O by char*

This reaction, observed to be faster than that between char and NO, involves several steps. N_2O reacts with carbon to form N_2 and carbon-oxygen surface complex. This surface complex can, subsequently, react with N_2O to form nitrogen and carbon dioxide (Amand et al., 1989 cited in Chen et al., 2001). Alternatively, the chemisorbed oxygen may be released as CO. In principle, then, CO, CO_2, and N_2 are the products of reaction with production of CO being favored at high temperatures (Li YH et al., 1998 cited in Chen et al., 2001). The following reaction has been adopted.

$$N_2O + C_{Char} \rightarrow N_2 + CO \tag{3.49}$$

$$Rt_E = K_E C_{N_2O} \tag{3.50}$$

$$K_E = 13.36 F_P \exp(-16677/T) \tag{3.51}$$

3.3.2.2 Homogeneous reactions

3.3.2.2.1 *Homogeneous destruction of N_2O*

Homogeneous of N_2O in conditions of interest in fluidized bed combustor can be expressed by the following reaction:

$$N_2O + CO \rightarrow N_2 + CO_2 \tag{3.52}$$

$$Rt_F = K_F C_{N_2O} \tag{3.53}$$

$$K_F = 2.51 \times 10^{11} \exp(-23180/T) C_{CO} \tag{3.54}$$

The concentration of CO is expected to be comparatively high, and N_2O is likely to be the rate limiting species.

3.3.2.2.2 *Thermal decomposition of N_2O*

$$N_2O \rightarrow N_2 + \frac{1}{2}O_2 \tag{3.55}$$

$$Rt_G = K_G C_{N_2O} \tag{3.56}$$

$$K_G = 1.75 \times 10^8 \exp(-23800/T) \tag{3.57}$$

3.3.3 SO_2 emission

In the fluidized bed combustor, sulfur was captured by a sorbent, e.g. limestone or dolomite, to form $CaSO_4$. In this research, the SO_2 captured by limestone can be represented by the following reactions:

From reaction (1.13) and (1.14)

$$CaCO_3 \rightarrow CaO + CO_2$$

$$CaO + SO_2 + \frac{1}{2}O_2 \rightarrow CaSO_4$$

The fractional conversion of CaO to $CaSO_4$ is strongly affected by the physical and chemical properties of limestone, hydrodynamic parameters, mass transfer resistance, temperature, reactive concentration, particle size distribution, and operating conditions, and can be calculated from the following expression (Soutdeh-Gharebaagh et al., 1998):

$$X_{CaO,i} = \frac{V_{CaO}}{1-\varepsilon_i}\left[\frac{t_i - \frac{1}{a_1}\ln\left(1+\frac{3\alpha C Y_{SO_{2,i}}}{R_s K_V}\left(e^{a_1 t_i}-1\right)\right)}{\frac{R_s}{3\alpha C Y_{SO_{2,i}}} - \frac{1}{K_V}}\right] \tag{3.58}$$

$$a_1 = 3.33\times 10^{-4}\exp\left(\gamma R_s\right) \tag{3.59}$$

$$\alpha = 35 D_P^{0.3} \tag{3.60}$$

where $X_{CaO,i}$ is fractional conversion of CaO in the i[th] interval, V_{CaO} is molar volume of CaO, ε_i is porosity of particle after calcinations, t_i is mean residence time of sorbent particles in i[th] interval of the bed(s), $Y_{SO_{2,i}}$ is mole fraction of SO_2 in the i[th] interval, R_s is mean sorbent particle radius, K_v is volumetric rate constant, a_1 is parameter in eq. (3.58), α is external mass transfer coefficient, and D_p is average sorbent surface particle diameter.

Using eq. (3.58), the moles of SO_2 removed per unit volume become:

$$r_{SO_{2,i}} = \frac{V_{CaO} F_l}{1-\varepsilon_i A_c \Delta L \times 100}\left[\frac{t_i - \frac{1}{a_1}\ln\left(1+\frac{3\alpha C Y_{SO_{2,i}}}{R_s K_V}\left(e^{a_1 t_i}-1\right)\right)}{\frac{R_s}{3\alpha C Y_{SO_{2,i}}} - \frac{1}{K_V}}\right] \tag{3.61}$$

where A_c is cross-sectional area of combustor, and F_l is mass flow rate of limestone in the feed.

The mean residence time of sorbent particles can be calculated by the following equation:

$$t_1 = \rho_l \sigma_{sp} \frac{A_c L_1}{F_l} \tag{3.62}$$

and

$$t_i = \rho_l \sigma_{sp} \frac{A_c \Delta L}{\xi F_l} \qquad (i \neq 1) \tag{3.63}$$

where t_1 is mean residence of sorbent particles in dense bed, ρ_l is density of limestone, L_1 is height of dense bed, σ_{sp} is volume fraction occupied by sorbent particles, and ξ is parameter in eq. (3.63).

$$\xi = \left(1 - \sum_{2}^{4} X_{CaO,i-1}\right) \tag{3.64}$$

Since SO_2 is well mixed in each interval of the bed, an overall SO_2 balance gives:

$$Y_{SO_2,1} = \frac{L_1 \left(R_{SO_2,1} - r_{SO_2,1}\right)}{CU_1} \tag{3.65}$$

$$Y_{SO_2,i} = \frac{\Delta L \left(R_{SO_2,i} - r_{SO_2,i}\right)}{CU_2} \qquad (i \neq 1) \tag{3.66}$$

where

$$R_{SO_2,1} = \frac{F_c W_s}{32 A_c L_1} \tag{3.67}$$

and

$$R_{SO_2,1} = \frac{\left(1 - X_{SO_2,i-1}\right) F_c W_s}{32 A_c \Delta L} \qquad (i \neq 1) \tag{3.68}$$

where $R_{SO_2,1}$ is rate SO_2 generate per unit volume of dense bed, U_1 is superficial gas velocity of dense bed, $r_{SO_2,1}$ is rate of removal of SO_2 per unit volume of dense bed, and W_s is sulfur weight fraction in dry-based coal.

The fraction sulfur capture for each interval $\left(X_{SO_2,i}\right)$ can be calculated from:

$$X_{SO_2,1} = 1 - \left[\frac{Y_{SO_2,i} CU_1 A_c}{F_C \frac{W_s}{32}} \right] \tag{3.69}$$

$$X_{SO_2,i} = 1 - \left[\frac{Y_{SO_2,i} CU_2 A_c}{F_C \frac{W_s}{32}\left(1 - X_{SO_2,i-1}\right)} \right] \qquad (i \neq 1) \tag{3.70}$$

CHAPTER IV

DEVELOPMENT OF THE CFBC SIMULATION

4.1 Introduction

The circulating fluidized bed combustor simulations in this work were divided in two parts. In the first part, the dimension of the CFBC was developed from the CFBC industrial scale of Siam Kraft Industry Co., Ltd. that described in the next chapter. The simulation in this part was focused on mixed fuels between coal and biomass. The model included the shrinking particle models for estimating the size change of the solid along the riser. Moreover, the simulation models were extended by including detail reactions of emissions. The emission models such as the rates of N_2O and NO_x formation and the fractional conversion of limestone to absorb SO_2 were added. In the second part, the simulation emphasized on the particle size distributions that change by the attrition, fragmentation, and combustion in the laboratory scale. The simulation in this part was described in the chapter 6. In this chapter, the development of the CFBC using ASPEN PLUS was described for each unit operation that used in the simulation.

4.2 CFBC simulation

4.2.1 Steps to develop the CFBC simulation with ASPEN PLUS (Yamskulna, 2000)

1. Define the process flowsheet.
2. Determine the components in the process.
3. Describe the NC (Non Conventional) components such as lignite by its attributes (proximate, ultimate, and sulfur analysis).
4. Choose a density and an enthalpy model for NC.
5. Choose the methods for calculating the thermodynamic properties of conventional components.
6. Determine the particle size distribution for the fuels.
7. Represent the CFBC flowsheet with the unit operation blocks.

8. Define the stream structure.
9. Specify the feed streams and block specifications.
10. Insert the user Fortran codes and subroutines into the simulation.
11. Calculate and analyze the process.

4.2.2 The combustion unit operation developments

To simulate the CFBC using ASPEN PLUS, three type reactors, RYIELD, RSTOIC, and RCSTR were selected for the combustion process. In each region, the combustion of coal particles was modeled using the following reactions (Soutdeh-Gharebaagh et al., 1998):

1. Devolatilization and volatilite combustion
2. Char combustion
3. NO_x formation
4. SO_2 absorption

4.2.2.1 Devolatilization and volatile combustion

The RYIELD (yield reactor) was used to simulate the decomposition of char or biomass to the constituting components (Figure 4.1) such as carbon, oxygen, hydrogen, nitrogen, sulfur and ash at the lower region under the following assumption (Aspen Technology Inc., 2001):

- Reaction stiochiometry is unknown or unimportant.
- Reaction kinetics are unknown or unimportant.
- Yield distribution is known

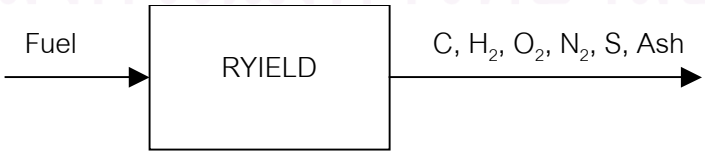


Figure 4.1 The decomposition in yield reactor.

The RSTOIC (stoichiometric reactor) was used to simulate the volatile combustion process under the following assumption (Aspen Technology Inc., 2001):

- Reaction kinetics are unknown or unimportant.
- Stoichiometry and the molar extent or conversion is known for each reaction.

Three reactions were considered in this model as shown in Table 4.1. The combustion of the volatile matter is based on the following hypotheses (Soutdeh-Gharebaagh, 1998):

Table 4.1 Conversion for each reaction in volatile combustion process

Reaction	Key component	Fractional conversion	Reference
$C + \frac{1}{2}O_2 \rightarrow CO$	C	0.3	Yamskulna, 2000
$S + O_2 \rightarrow SO_2$	S	1	Soutdeh-Gharebaagh, 1998
$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$	H_2	1	Soutdeh-Gharebaagh, 1998

- Considering the volatile matter in the coal, (obtained from a proximate analysis) consists exclusively of carbon, hydrogen, and sulfur. This supposed that the entire hydrogen content of the coal is found in the volatile matter. The volatile carbon fraction reacts to form CO only during the volatile combustion process because of the oxygen depletion in the lower region of the riser.
- The coal hydrogen content is entirely consumed during the volatile combustion process.
- The coal sulfur content is assumed to be converted completely to SO_2 during the volatile combustion process.

In this unit, limestone was added to capture SO_2 then the products from this unit were shown in Figure 4.2.

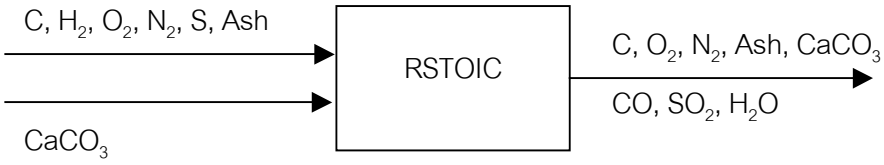


Figure 4.2 The volatile process in stoichiometric reactor.

4.2.2.2 Char combustion

RCSTR (continuous stirred tank reactor) was used to model a well-mixed reaction with known kinetics. The products from this reactor were shown in Figure 4.3. Two reactions considered in this reaction are:

from eq. (1.8), and (1.10)

$$C + \frac{1}{2}O_2 \rightarrow CO$$

$$CO + \frac{1}{2}O_2 \rightarrow CO_2$$

Figure 4.3 The combustion process in continuous stirred tank reactor.

The rate of the first reaction was calculated by shrinking particle model and hydrodynamics subroutine that described in section 3.1 and 3.2. The basic flowchart for calculating reaction rate was shown in Figure 4.4.

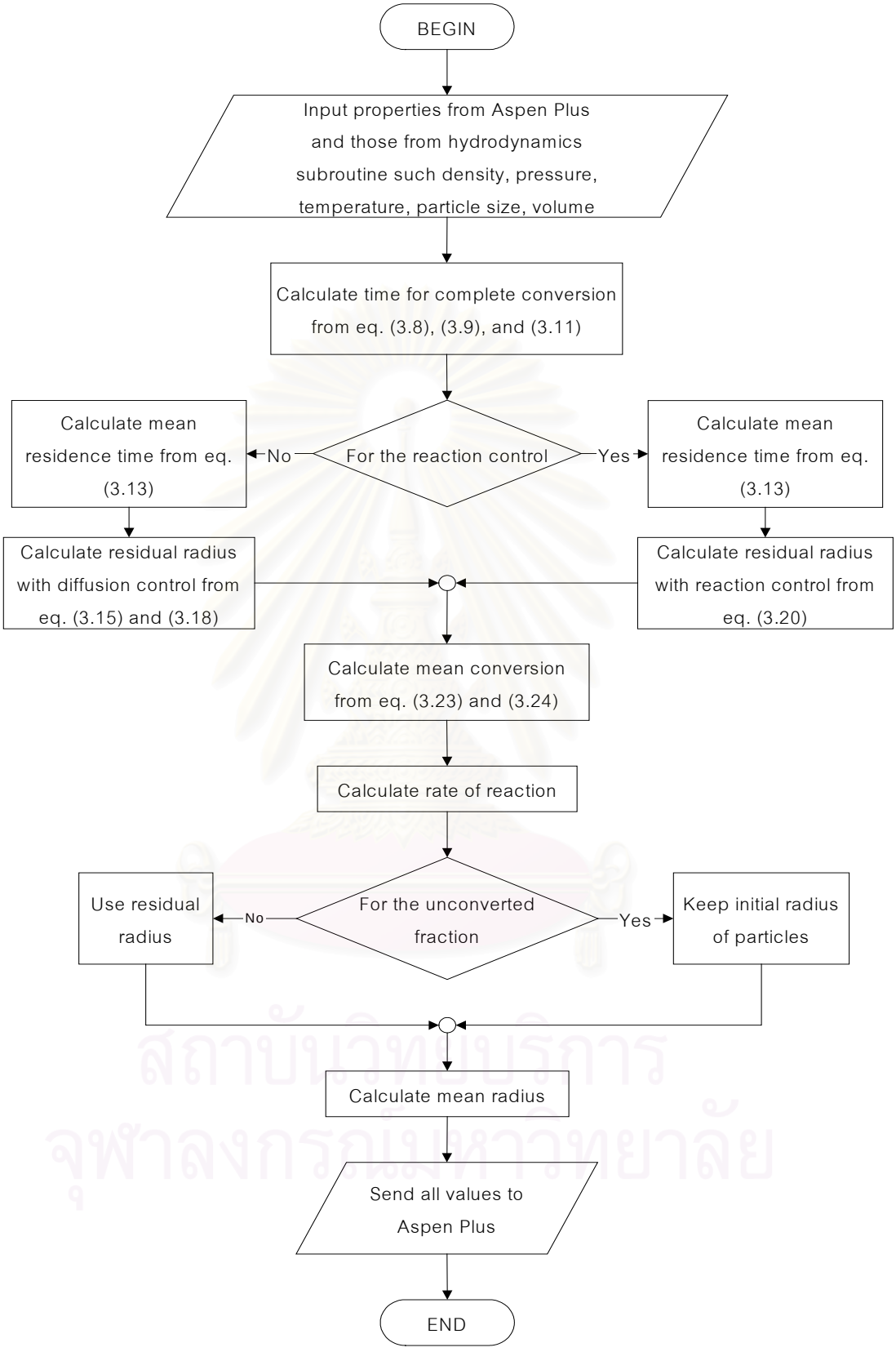


Figure 4.4 The basic flowchart for calculating reaction rate and particle sizes for a solid fuel by apply shrinking particle model.

4.2.2.3 No_x formation

RCSTR was also used to simulate the emission of NO_x and N_2O. This process calculated the rate of reaction for NO_x and N_2O formation. Finally the products from every reaction were shown in Figure 4.5

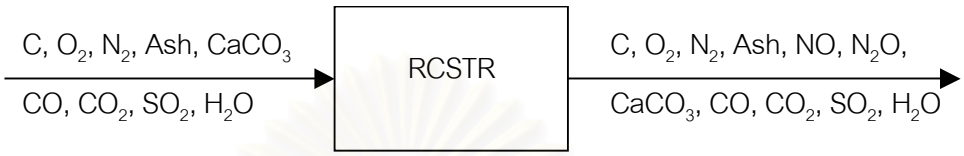


Figure 4.5 The NO_x and N_2O emission from the combustion process.

4.2.2.4 SO_2 absorption

The RSTOIC was used to model the capture of sulfur in the CFBC. The products from this reactor were shown in Figure 4.6. The SO_2 captured by limestone can be represented by the following reactions:

from eq. (3.58) and (3.59)

$$CaCO_3 \rightarrow CaO + CO_2$$

$$CaO + SO_2 + \frac{1}{2}O_2 \rightarrow CaSO_4$$

Figure 4.6 The SO_2 absorption from the combustion process.

4.2.2.5 Heat exchanger

The duty of this unit is to exchange the heat from the wall of the CFBC to the water tubes for steam producing. The inlet and outlet streams were shown in Figure 4.7.

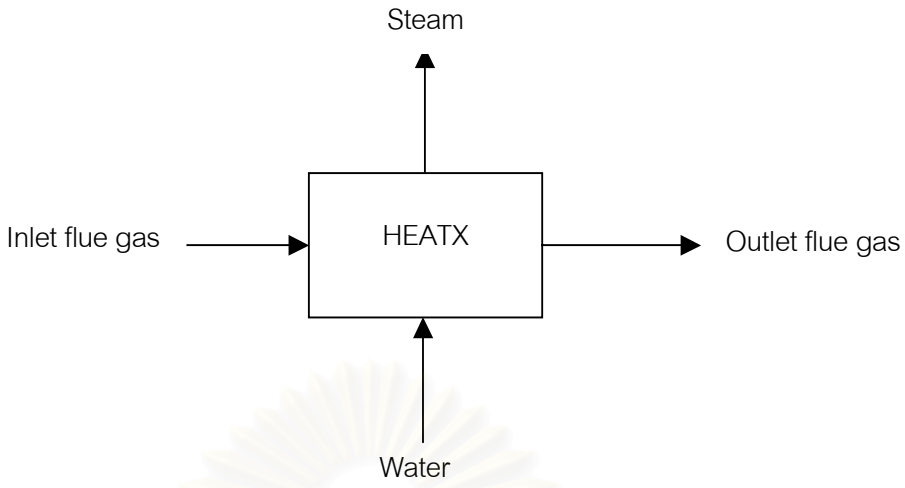


Figure 4.7 Heat exchanger.

4.2.2.6 Cyclone

Cyclone is the unit operation for solid-gas separation. The flue gas outlet from heat exchanger was fed into the cyclone to recover unburnt coal to the riser as shown in Figure 4.8.

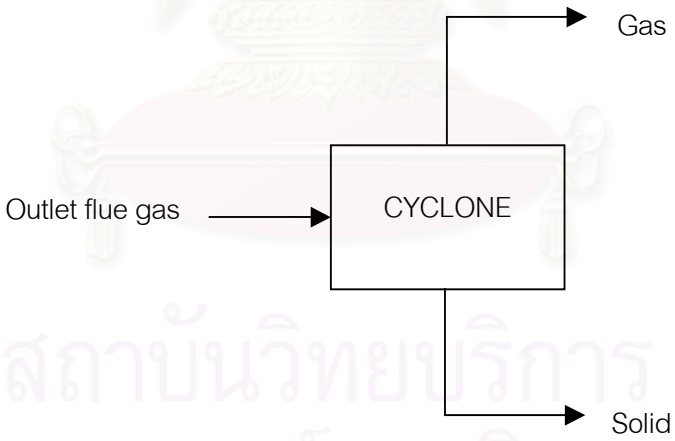


Figure 4.8 Cyclone.

CHAPTER V

INDUSTRIAL SCALE CFBC SIMULATION

5.1 Dimension of the CFBC

The dimension of the CFBC in this simulation was developed from the CFBC industrial scale of Siam Kraft Industry Co., Ltd. The CFBC was divided into two regions: the lower and upper regions. The lower region represented the dense bed and the upper region represented the dilute bed fluidization. Each region was composed of kinetic reactions, hydrodynamics and emission sections. In lower region or dense bed, the primary air was fed at the bottom of the combustor. The secondary and the tertiary airs were fed at the height of 1.703 m. and 3.203 m., respectively.

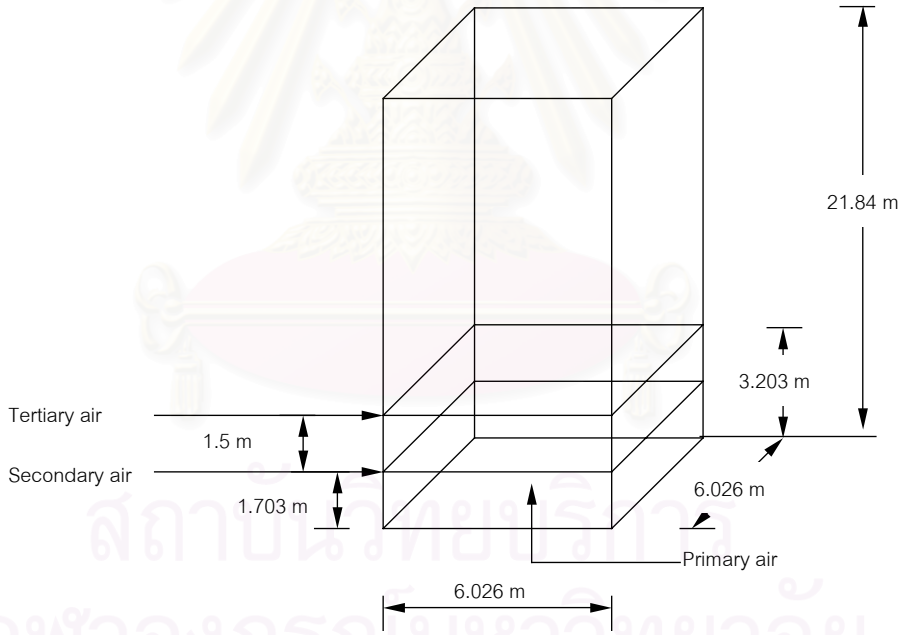


Figure 5.1 Dimension of the industrial scale CFBC simulation.

5.2 Assumptions of the reaction model

1. The fuels, limestone, and primary air were fed at the bottom of the CFBC with uniform temperature.

2. The simulated combustor was a rectangular column with the surface area of 36.31 m^2 and the height of 21.84 m. as illustrated in Figure 5.1. In the proposed model, the secondary and tertiary airs were fed into the combustor at the specified heights.
3. The combustion of volatile matters occurred instantaneously at the bottom of the combustor.
4. Char combustion occurred slowly after volatile matters were combusted.
5. Gas and fuel particle temperatures were equal to the bed temperature varying with respect to the height of the riser.
6. The attrition of the char particles was neglected.
7. All steps of the reactions were calculated with an isothermal at 850 ^{O}C.

5.3 Simulation procedures

For the combustion in each region, the combustion of coal particles can be modeled using the following reactions:

1. Devolatilization and volatilite combustion
2. Char combustion
3. NO_x formation
4. SO_2 absorption

The algorithms of simulations were divided in three parts: reaction, hydrodynamic, and gas emission part. The reaction and gas emission part were used in the char combustion step. The gas emission part was used for calculate the NO_x formation and SO_2 absorption.

Each reaction was simulated by using reaction modules of ASPEN depended on the type of the reactions. All blocks were simulated as shown in Figure 5.2.

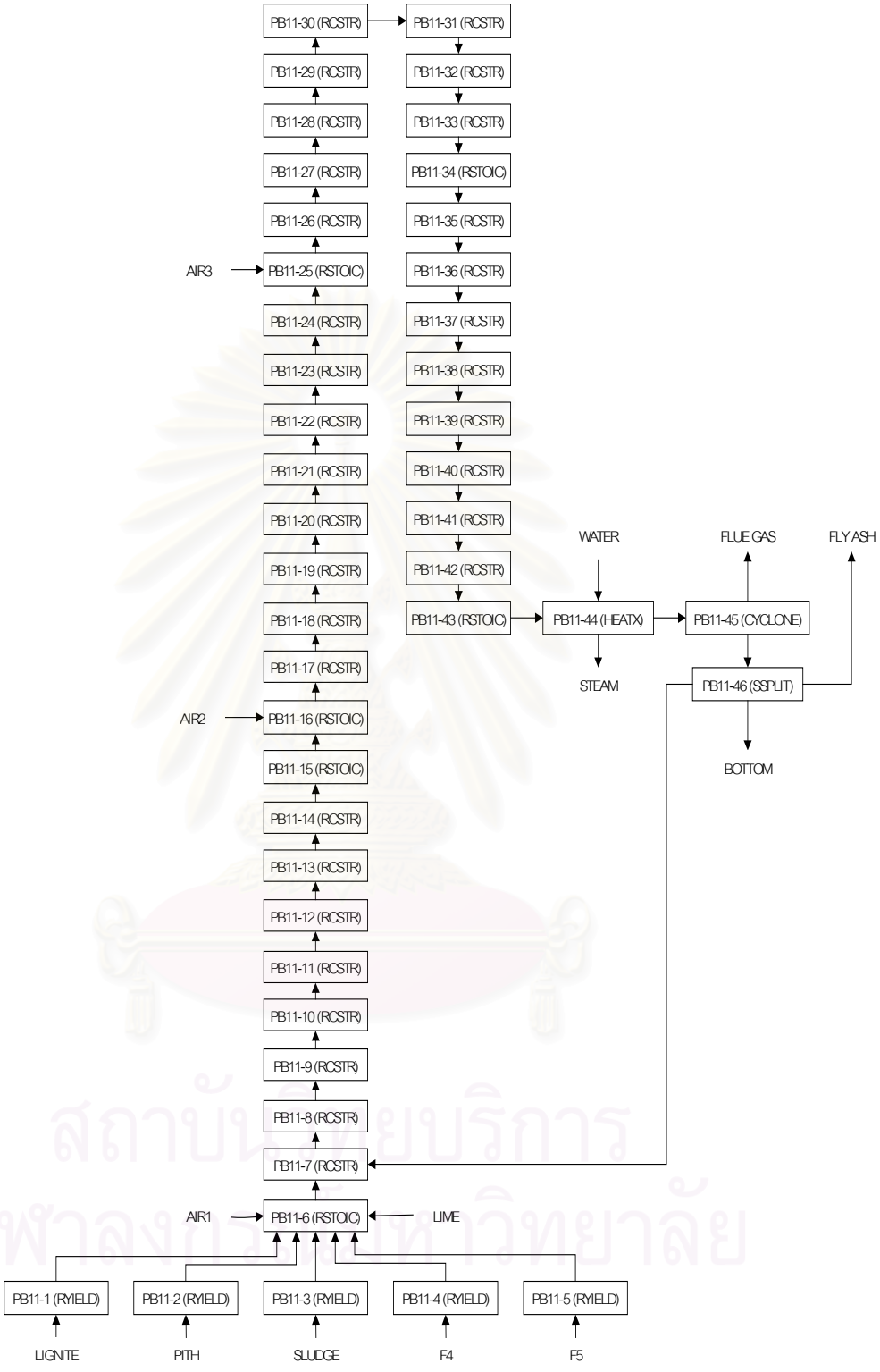


Figure 5.2 Simulation diagram for the CFBC.

5.3.1 Lower region

5.3.1.1. Decomposition of lignite or biomass

From Figure 5.2, RYIELDs were used to decompose lignite or biomass in block PB11-1 to PB 11-5. The fuels in this simulation are lignite, bagasse, bark, and sludge. The yield distribution for each fuel was specified by the proximate and ultimate analyses as shown in the following tables.

Table 5.1 Proximate analysis for each type of fuel (Siam Kraft Industry Co., Ltd., 1992)

Proximate analysis (wt.%)	Lignite	Bagasse	Bark	Sludge
Moisture	19.86	35.49	39.66	63.20
Fixed carbon	34.85	7.71	9.09	3.44
Volatile matter	34.84	55.23	48.85	13.15
Ash	10.45	1.57	2.40	20.21

Table 5.2 Ultimate analysis for each type of fuel (Siam Kraft Industry Co., Ltd., 1992)

Ultimate analysis (wt.%)	Lignite	Bagasse	Bark	Sludge
Ash	13.04	2.44	2.82	23.00
Carbon	68.15	48.64	48.40	39.77
Hydrogen	5.09	5.87	6.72	4.71
Nitrogen	1.24	0.16	0.19	1.50
Sulfur	0.59	0.07	0.00	0.82
Oxygen	11.89	42.82	41.87	30.20

5.3.1.2. Volatile combustion process

In block PB11-6, RSTOIC was used to simulate the volatile combustion process in the lower region. In this block, primary air and limestone were added for combustion and sulfur capture, respectively. The volatile reactions were shown in Table 4.1.

5.3.1.3. Char combustion

RCSTR was used to simulate the char combustion process in block PB11-7. The combustion occurred as the following reactions:

From eq. (1.8), and (1.10)

$$C + \frac{1}{2}O_2 \rightarrow CO$$

$$CO + \frac{1}{2}O_2 \rightarrow CO_2$$

The rates of reactions were calculated by using subroutine showed in Appendix B. The kinetic expressions and basic flowchart of the subroutine were described in section 3.1 and Figure 4.4, respectively. The physical and chemical properties used in the simulation were shown in Table 5.3.

Table 5.3 Physical and chemical properties used in the shrinking particle model subroutine

Parameter		Value	Unit	Reference
Activation energy	Lignite	1.492×10^{8}	$J\cdot kmol^{-1}$	Yamskulna, 2000
	Bagasse	1.246×10^{7}	$J\cdot kmol^{-1}$	Gaur and Reed, 1998
	Bark	4.207×10^{7}	$J\cdot kmol^{-1}$	Gaur and Reed, 1998
	Sludge	4.476×10^{7}	$J\cdot kmol^{-1}$	Gaur and Reed, 1998
Frequency factor	Lignite	59,600	$m\cdot s^{-1}\cdot K^{-1}$	Yamskulna, 2000
	Bagasse	210,870	$m\cdot s^{-1}$	Gaur and Reed, 1998
	Bark	86,560	$m\cdot s^{-1}$	Gaur and Reed, 1998
	Sludge	22,140	$m\cdot s^{-1}$	Gaur and Reed, 1998
Diffusivity		1.525×10^{-4}	$m^2\cdot s^{-1}$	Soutdeh-Gharebaagh, 1998

5.3.1.4. NO_x formation

Blocks PB11-8 to PB11-14 were used to calculate the rate of reactions for NO_x and N_2O emissions using the following reactions.

From eq. (3.37), (3.40), (3.43), (3.46), (3.49), (3.52), and (3.53)

$$C_{Char} - N_\gamma + \frac{\gamma + 1}{2} O_2 \rightarrow \gamma NO + C_{Char} - O \quad (3.37)$$

$$C_{Char} - N + NO \rightarrow N_2O + C_{Char} \quad (3.40)$$

$$NO + C_{Char} \rightarrow \frac{1}{2} N_2 + CO \quad (3.43)$$

$$NO + CO \rightarrow \frac{1}{2} N_2 + CO_2 \quad (3.46)$$

$$N_2O + C_{Char} \rightarrow N_2 + CO \quad (3.49)$$

$$N_2O + CO \rightarrow N_2 + CO_2 \quad (3.52)$$

$$N_2O \rightarrow N_2 + \frac{1}{2} O_2 \quad (3.53)$$

The kinetic expressions for the above equations were described in section 3.3.2. The subroutines for NO_x and N_2O formation were shown in Appendix C.

5.3.1.5. SO_2 absorption

The RSTOIC reactor was used to calculate the fraction of sulfur capture in block PB11-15. SO_2 absorption was written by internal subroutine in the ASPEN PLUS. The model of fractional sulfur capture for this process was described in section 3.3.3. Figure 5.3 showed the flowchart of sulfur capture subroutine for the lower region.

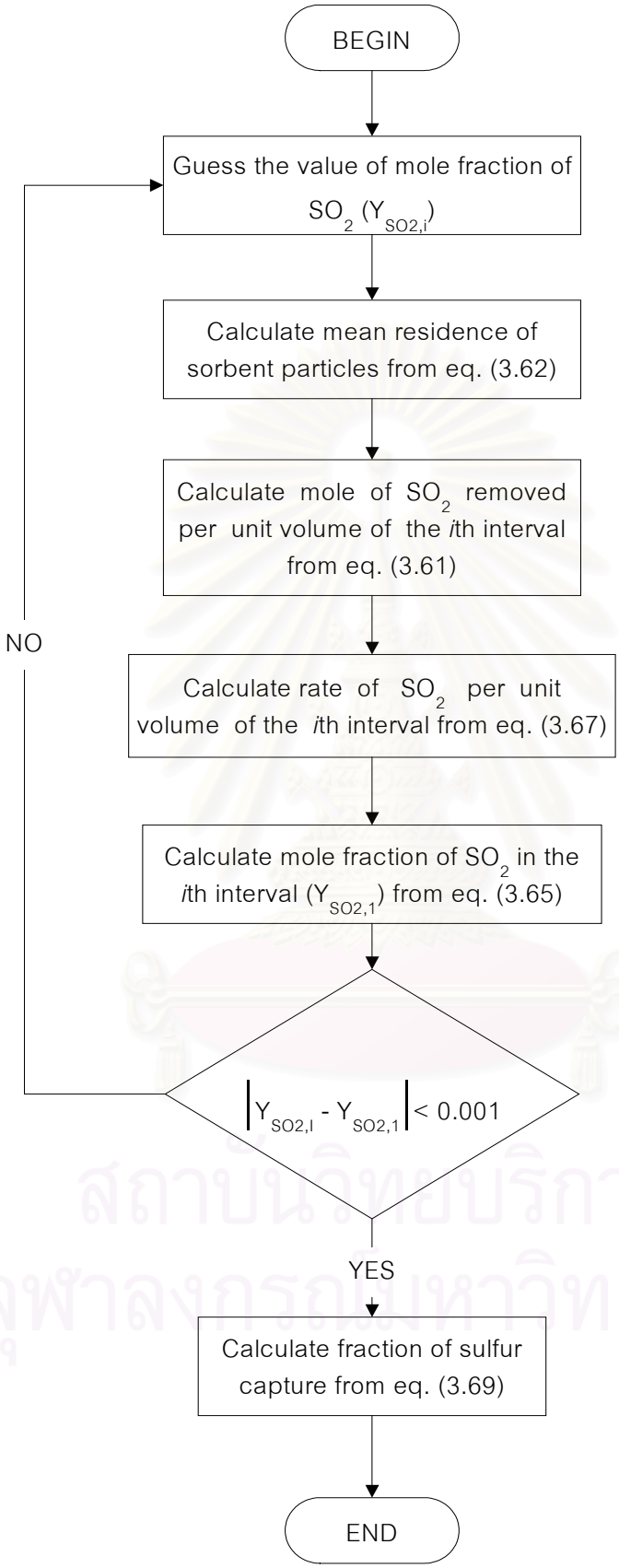


Figure 5.3 The flowchart to calculate the fraction of sulfur capture.

5.3.2 Upper region

To model this region, the dilute bed was divided into three intervals. Each interval the char combustion, NO_x formation, and SO_2 absorption were calculated like in the lower region. In the first interval, the calculation started from block PB11-16 to PB11-25. The secondary and tertiary airs were fed into the CFBC in block PB11-16 and PB11-25, respectively, to increase the rate of char combustion. Consequently, in the second and third interval, the calculation started from block PB11-26 to PB11-34 and PB11-35 to 11-43. At the top of the riser, the heat exchanger and cyclone were simulated for the completion of CFBC simulation. The details of these units were expressed in the next section.

5.3.2.1. Heat exchanger

The shell and tube heat exchanger was used to simulate the heat exchange between hot gas from combustion and water to produce steam in block PB11-44. The details of this unit were shown in Table 5.4.

Table 5.4 The details of heat exchanger (Siam Kraft Industry Co., Ltd., 1994)

Details	Value	Unit
Inside shell diameter	6.8	m
Inner tube diameter	52.32	mm
Outer tube diameter	63.5	mm
Tube length	15	m
Number of tubes	272	-
Pitch	88	mm
Fin height	5	mm

5.3.2.2 Cyclone

In block PB11-45, cyclone model was used to simulate the separation between the recalculating solid and flue gas. The efficiency of cyclone was calculated by Leith-Licht model. The dimensions of cyclone were shown in Table 5.5.

Table 5.5 Dimensions of cyclone (Siam Kraft Industry Co., Ltd., 1994)

Dimensions	Value (m)
Length of cylinder	6.25
Length of cone section	7.25
Length of overflow	2.25
Diameter of overflow	2.54
Diameter of underflow	1
Height of inlet	4.52
Width of inlet	1.81
Cyclone diameter	5

The input data to simulate the CFBC was shown in Appendix D.

5.4 Results and discussion

The fuels included in the simulator were lignite, bagasse, bark, and sludge. The simulation results for both single fuel and mixed fuels between lignite and biomass were investigated. In case of mixed fuels, since there are a number of combinations among fuels, the mixtures of bagasse, bark and sludge were selected to demonstrate the model prediction.

The model was used to simulate the operation of a CFBC that produced 110 tons·hr^{-1} of steam at 510 ^{o}C and 110 barg. The fuels to be considered were both a single fuel and mixed fuels. In case of a single fuel, 4 kg·s^{-1} of lignite was fed into the combustor. The other case, the mixed fuels between lignite and biomass were considered. In each simulation the lignite flow rate was decreased by 10 %. The flow rate of biomass was increased by keeping the amount of carbon inlet constant. The results of the simulation were shown in Figure 5.4 to 5.6.

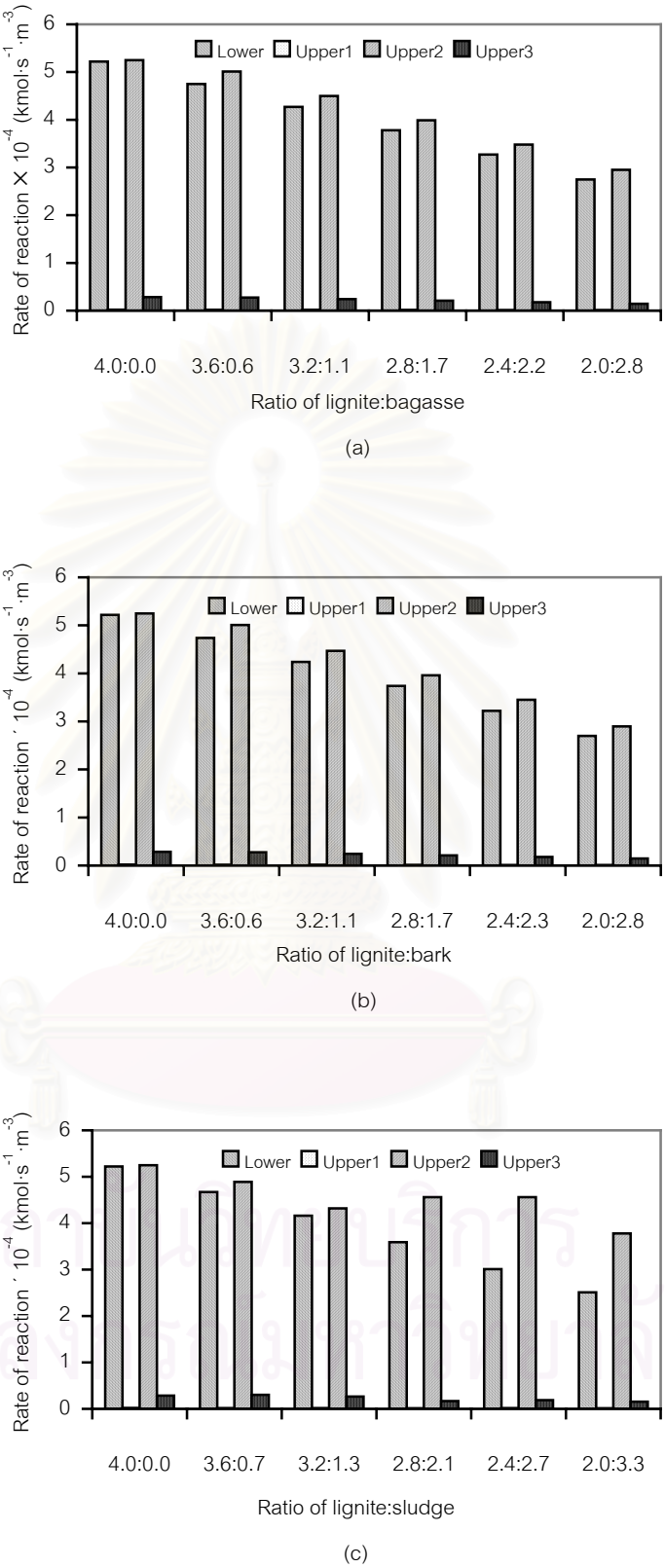
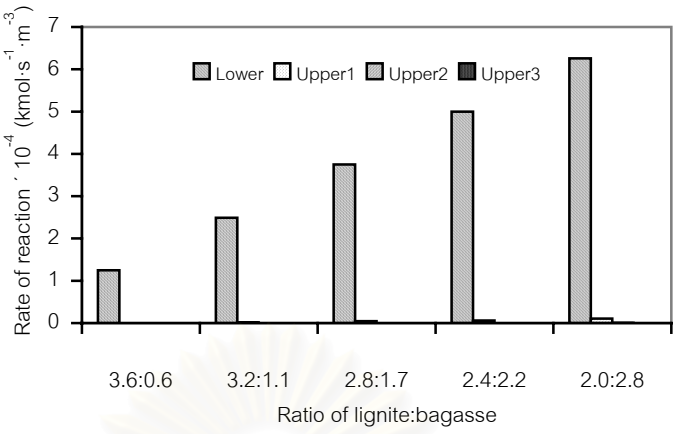
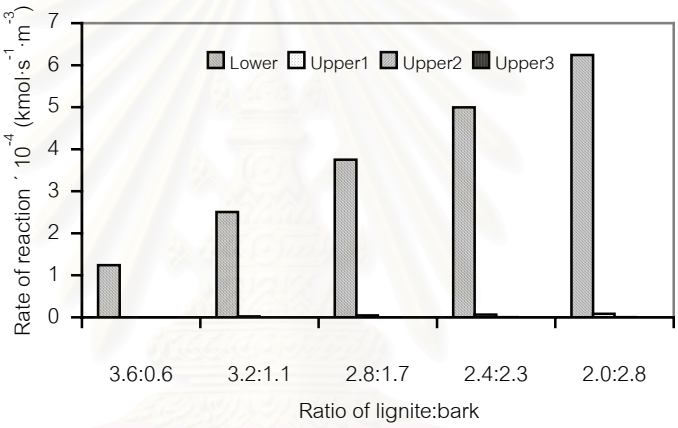


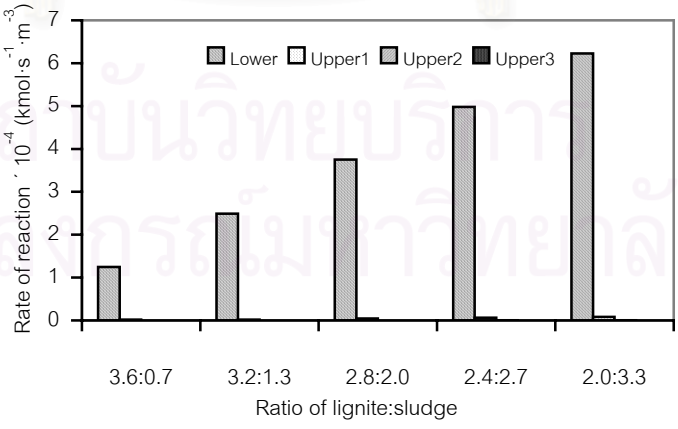
Figure 5.4 Reaction rates of carbon in lignite in mixed fuels for each region in the CFBC: (a) lignite&bagasse (b) lignite&bark (c) lignite&sludge



(a)

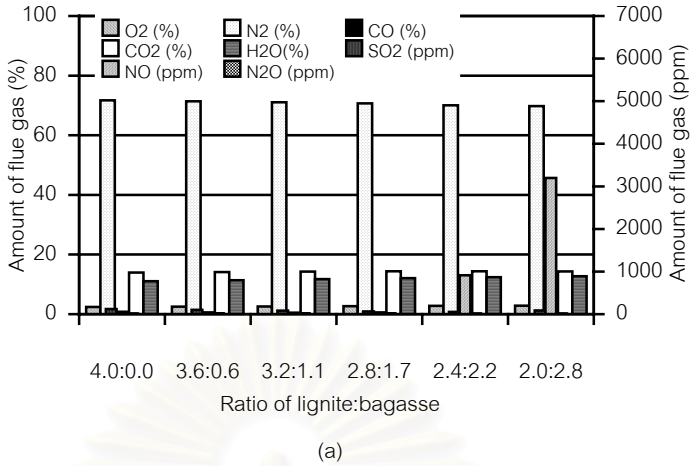


(b)

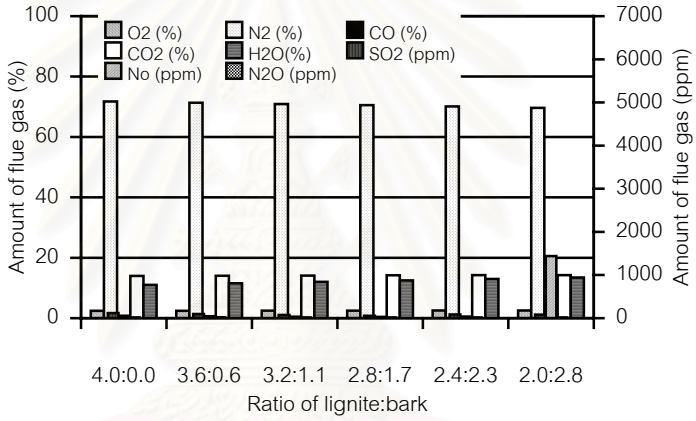


(c)

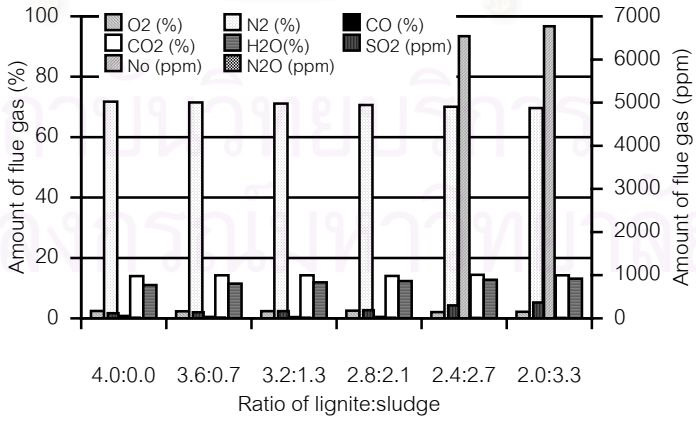
Figure 5.5 Reaction rates of carbon in biomass in mixed fuels for each region in the CFBC: (a) lignite&bagasse (b) lignite&bark (c) lignite&sludge



(a)



(b)



(c)

Figure 5.6 The composition of flue gas for different kind of mixed fuels: (a) lignite&bagasse (b) lignite&bark (c) lignite&sludge

Table 5.6 The results of reactor data for 4.0 $kg \cdot s^{-1}$ of lignite

Region	Volume (m^3)	Height (m)	Residence time (min)
Lower	61.84	1.70	316.82
Upper1	16.70	0.46	26.68
Upper2	33.34	0.92	183.33
Upper3	681.14	18.76	1425.73

Table 5.7 Reaction rates of carbon in bagasse at ratio 3.6:0.6

Region	Rate of reaction ($kmol \cdot s^{-1} \cdot m^{-3}$)
Lower	1.24×10^{-4}
Upper1	1.59×10^{-8}
Upper2	4.98×10^{-12}
Upper3	3.83×10^{-16}

Table 5.8 The emissions of lignite and bagasse combustion

Ratio of lignite and bagasse	Amount of gas emission					
	(%)			(ppm)		
	O_2	CO	CO_2	SO_2	NO	N_2O
4.0:0.0	2.42	0.81	13.97	120	1	16
3.6:0.6	2.51	0.59	14.10	101	22	18
3.2:1.1	2.59	0.34	14.26	83	33	18
2.8:1.7	2.69	0.12	14.38	65	41	17
2.4:2.2	2.78	0.01	14.41	51	915	17
2.0:2.8	2.85	0.01	14.31	87	3197	17

Figure 5.4 shows the reaction rates of carbon in lignite in mixed fuels for each region in the CFBC when there were three kinds of mixed fuels and three compositions. All simulation cases showed the same trend. In lower region, the rate of reaction was high because of the high carbon concentration due to the feed. In upper region zone 1, the rate of reaction was closed to zero because of the lower oxygen concentration left over from the lower region. However in the upper region zone 2, the rate of reaction was high due to more oxygen injected as secondary and the tertiary airs. In upper region zone 3, the rate of reaction was low because there was only residual carbon left over from the previous zone. Compared with various ratios of lignite and biomass, when increased the flow rate of biomass, the reaction rates of lignite were slightly decreased. This is due to the decrease of the concentration of lignite in mixed fuels.

Figure 5.5 shows the combustion rates of biomass for different types of materials in mixed fuels. The reaction rates were increased with the increase of its fraction in the fuels. For example, at the 2.0:2.8 of lignite and bagasse ratio, the reaction rate was increased to 6.25×10^{-4} $kmol\cdot s^{-1}\cdot m^{-3}$ or about 5 times when compared with the lignite and bagasse ratio at 3.6:0.6. This is due to the higher concentration of carbon from biomass. The rates were decreased rapidly at high position of the riser since most of the biomass was burnt in lower region. The reaction rates in upper region were close to zero. The example for reaction rates of carbon in bagasse at 3.6:0.6 was shown in Table 5.7.

Figure 5.6 shows the compositions of gas emission when different mixed fuels were used. All the simulation cases show the same patterns of responses. For example, Table 5.8 shows the emissions gas from lignite and bagasse combustion. The results show that the amount of N_2O was small, which is in agreement with those reported in literatures (Chen et al., 2001; Liu and Gibbs, 2002). The amount of NO was high when increased the amount of biomass. However, this result does not agree with Liu et al. experiment (Liu et al., 2002). This reason is that rate of NO formation in this simulation, eq. (3.38), was dependent only on oxygen concentration. Then, the amount

of nitrogen does not affect the NO conversion. The amount of CO was decreased because of complete combustion with higher oxygen concentration when increasing the biomass. Finally, the results also showed that the amount of SO_2 was small.

In the part of size distribution prediction, this example demonstrated the size distribution predictions in each region of the riser. The particle sizes of biomass and lignite were divided into 2 and 3 subintervals, respectively. The case showed here was the combustion of single fuel, lignite. The initial radius and weight fraction of lignite were shown in Table 5.9. The predictions of the size distribution and the weight fraction in each region were shown in Table 5.10.

In the lower region, when the combustion occurred, most of the smallest particles were burnt. Therefore, its weight fraction almost disappeared. However the combustion was not occurred completely, some particle might be unburnt. Then the algorithm of calculation was divided into two parts. In the first part, the burnt carbon was combusted completely. The radii of particles were equal zero because the mean residence time was higher than the time to complete conversion. In the second part, the unburnt particle was not combusted in this region. Then the result showed the initial radius because algorithm program kept the initial radius for the unconverted. For the second interval, weight fraction was reduced from 0.52 to 0.16, while that for the third interval was increased. This was due to the lower region having small volume that implied the short residence time. That is, only the small particles would be burnt completely. Thus, the mass of the larger particles was reduced slower, causing its weight fraction in this interval high. Nevertheless, the combustion in this region caused the mean particle size in the third-interval to reduce to 0.0552 m.

The upper region was divided into three regions. The weight fraction of the second-interval particles was increased in the first upper regions. The reason is that the large particles had time to reduce their sizes into the second-interval particles.

Since the second and third upper regions had large volume, their residence times would be long. Therefore, most of the small and medium particles were burnt in the regions. Thus, the particles left in these regions were the particles falling in

the third-interval size. This observation was noticed with high weight fraction in this interval and the mean particle size was reduced to 0.0524 m. as shown in Table 5.10.

Table 5.9 Initial radius and weight fraction of lignite

No.	Interval size (m)	Mean initial radius (m)	Weight fraction
1	0-0.001	0.0005	0.08
2	0.001-0.04	0.0205	0.52
3	0.04-0.075	0.0575	0.40

Table 5.10 The predictions of size distribution and weight fraction in each region

Region	Volume (m^3)	Mean radius (m)			Weight fraction		
		Interval 1	Interval 2	Interval 3	Interval 1	Interval 2	Interval 3
Lower	61.84	0.0005	0.0205	0.0552	0.0007	0.16	0.84
Upper 1	16.70	0.0005	0.0201	0.0551	0.0116	0.61	0.38
Upper 2	33.34	0.0005	0.0201	0.0524	0.0018	0.15	0.85
Upper 3	681.14	0.0005	0.0201	0.0524	0.0022	0.22	0.78

CHAPTER VI

LABORATORY SCALE CFBC SIMULATION

In the previous chapter, the CFBC was only investigated the changing sizes of particles by applying the shrinking particle model. In this chapter, the simulation for laboratory-scale apparatus was conducted and focused on the particle size distribution. The particle comminution models developed from the experiments were added. The calculations of PSD were divided into two steps. First, the model of primary fragmentation due to the devolatilization process was added to the simulation. Second, the model of secondary fragmentation due to the combustion including shrinking particle model was added. The dimension of the laboratory scale CFBC to simulate in this section was shown in Figure 2.1.

6.1 Assumptions of the reaction model

1. The fuels, and air were fed at the bottom of the CFBC with uniform temperature.
2. The combustion of volatile matters occurred instantaneously at the bottom of the combustor.
3. Char combustion occurred slowly after volatile matters were combusted.
4. Gas and fuel particle temperatures were equal to the bed temperature varying with respect to the height of the riser.
5. All steps of the reactions were calculated with an isothermal at 850 ^{o}C.

6.2 Simulation procedures

Simulation procedures or the algorithms of computation in this part are the same as in the previous chapter, but in this part, the simulation only emphasizes on the particle size distribution along the riser. From the previous chapter, the CFBC

simulation was divided into lower and upper regions. Each region was calculated the hydrodynamics and the rates of reactions. The shrinking particle model was added in every interval to predict the PSD along the riser. The RCSCR was added to calculate the changing sizes of particles due to the devolatilization in block B9 as shown in Figure 6.1.

6.2.1 Lower region

RYIELD was used to decompose lignite in block B1. The proximate and ultimate analyses were specified for yield distribution as shown in the following tables.

Table 6.1 Proximate analysis

Element	Value (wt.%)
Moisture	26.5
Fixed carbon	21.0
Volatile matter	38.4
Ash	14.1

Table 6.2 Ultimate analysis

Element	Value (wt.%)
Ash	20.0
Carbon	54.3
Hydrogen	9.8
Nitrogen	2.3
Sulfur	3.7
Oxygen	9.9

RSTOIC was used to represent the volatile combustion process only for the lower region, block B2, because only primary air was fed into the main reactor, in case of the experiments. The volatile reactions were shown in Table 4.1.

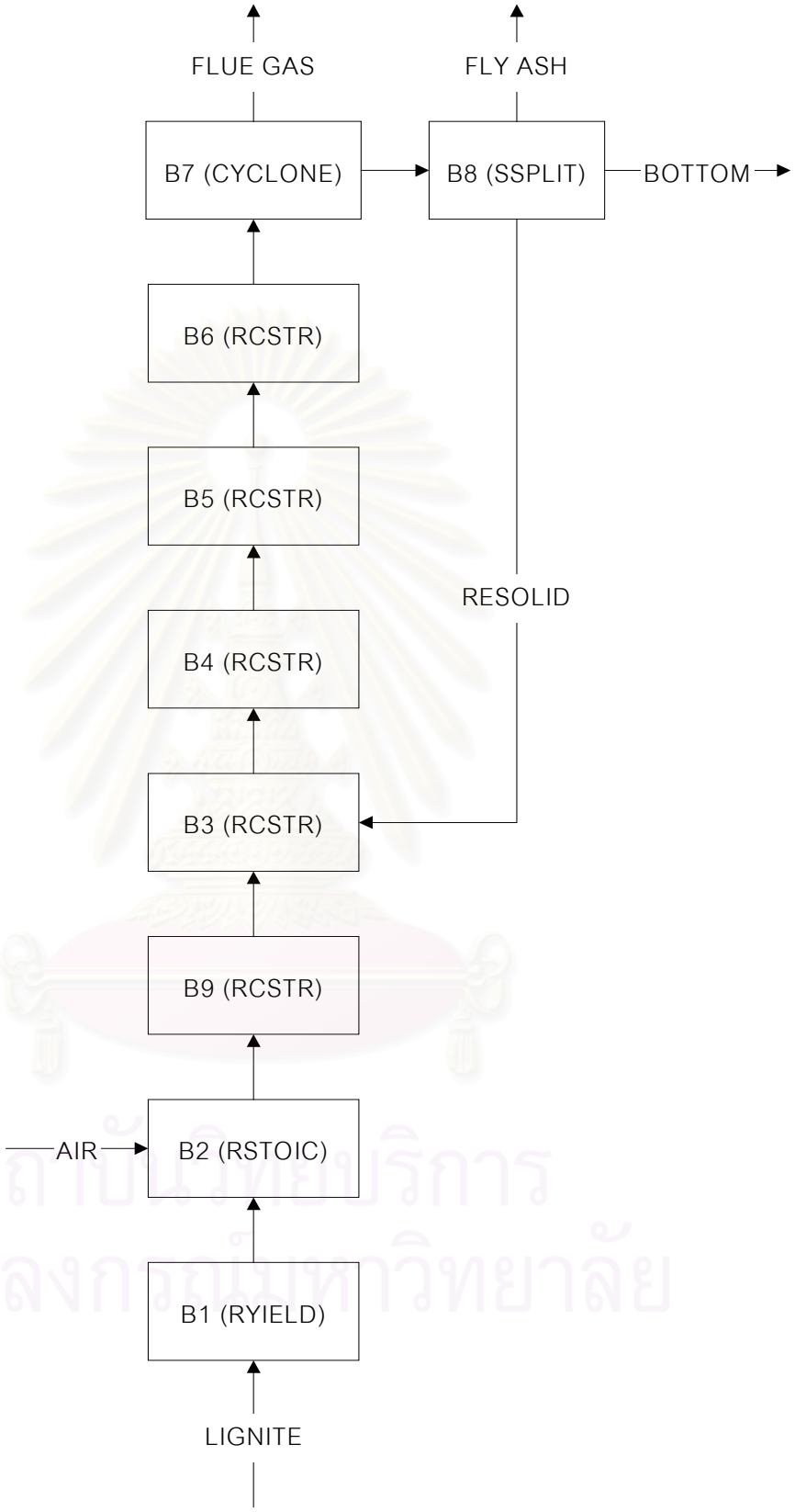


Figure 6.1 Simulation diagram for the laboratory scale CFBC.

The RCSTR was used to calculate the PSD by adding the subroutine that showed in Appendix E. In this block (B9), it was assumed that no reaction occurred because all volatile reactions were calculated from the previous block (B2). Then this block only calculated the PSD. The primary fragmentation of particles due to the devolatilization was predicted by the Weibull distribution that was obtained from the experiments as shown by the following equations.

From eq. (2.2)

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{2.13\times10^{-3}}\right)^{7.5}\right]$$

For small particle, from eq. (2.3)

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{627}\right)^{7.5}\right]$$

For the changing sizes of particles due to the combustion process, in block B3, the RCSTR was used to calculate the rates of reactions and to predict the PSD as shown in Appendix F. The reactions and algorithms were shown in section 5.3.1.3.

6.2.2 Upper region

In this region, the dilute bed was divided into three intervals as same as in the previous chapter. The predictions of size distributions were only considered for the combustion process since the assumption was that the combustion of volatile matters occurred instantaneously at the bottom of the combustor. Then the changing of particle size was neglected.

At the top of the riser, cyclone model (B7) was used to simulate the recirculation solid. The dimensions of cyclone were shown in Table 6.3. The input data to simulate the CFBC using the ASPEN PLUS was shown in Appendix G.

Table 6.3 Dimensions of cyclone

Dimensions	Value (m)
Length of cylinder	0.048
Length of cone section	0.079
Length of overflow	0.008
Diameter of overflow	0.016
Diameter of underflow	0.012
Height of inlet	0.016
Width of inlet	0.006
Cyclone diameter	0.032

6.3 Results and discussion

In the simulation, coal and air was fed at 0.015 $g \cdot s^{-1}$ and 7 $l \cdot min^{-1}$. The simulations were divided in two cases. The first case, the PSD was calculated only by the shrinking particle model subroutine. The second one, the primary fragmentation model that fitted by Weibull distribution was added in the lower region to predict the coal comminution from the devolatilization process. The results were shown in Figure 6.2 to 6.7.

The algorithm to predict the PSD in this simulation was divided into 61 discrete intervals that was arranged from small to large particles. This program supported the size of particles between 0-4 mm. Normally, the PSD is the continuous function, but in the simulation, the discrete function was used to represent the function by dividing to small intervals. Thus, the shape of PSD resulted from the simulation was depended upon to the width of range in each interval.

Figure 6.2 showed the particle size distribution of raw material that was obtained from the experiment mentioned in chapter 2. This PSD of coal was the input data for both cases of simulations as the initial size distribution of the feed stream.

Figure 6.3 showed the size prediction of particles after devolatilization process. From Figure 6.3 (a), the simulation only reported the yield from the volatile reactions. Thus the particle sizes were not changed by this process. From Figure 6.3 (b), the primary fragmentation model was added to the simulation. The sizes of particles were smaller because of the burst of particles due to the volatile pressure in the pore of particles.

Figure 6.4 showed the PSD of coal in the lower region of the CFBC. The simulation showed the difference of PSD between the first and the second cases. In the first case, the prediction of PSD showed that the weight fractions of the particles between 2.5 and 3 mm was reduced from 0.45 to 0.25 due to the combustion process. The weight fractions of the particles that was smaller than 2 mm were increased because the reducing size from the larger particles. In the last node, the weight fraction of 3.5 mm particle size was occurred from the reducing size of 4 mm particles.

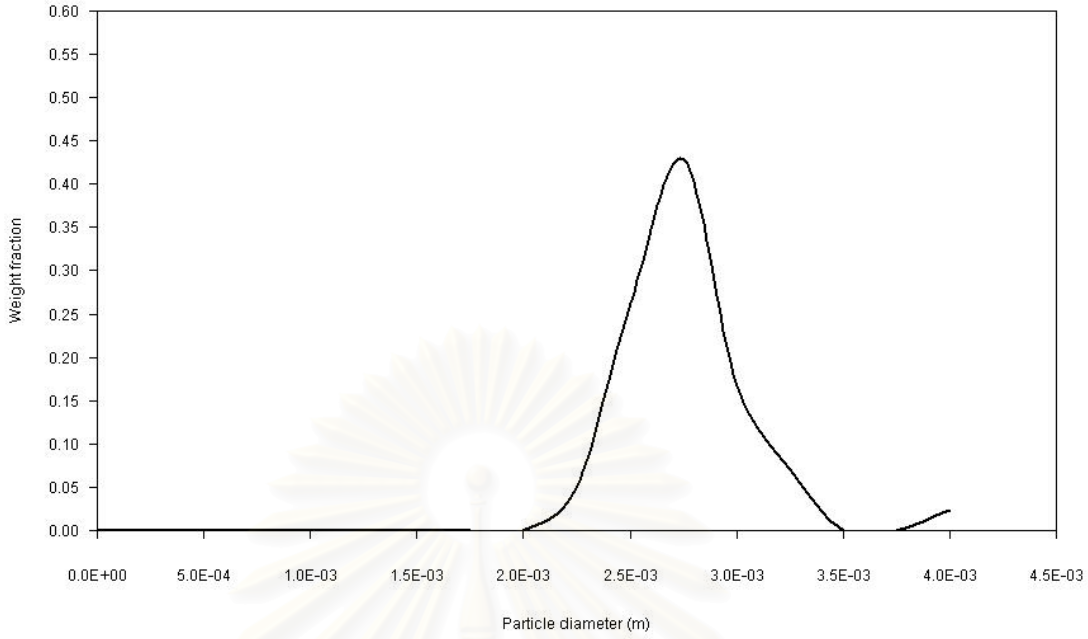
In the second case, only the particles smaller than 3.25 mm was observed. This is due to the effect of the devolatilization process as shown in Figure 6.3 (b). For the smaller particles, the prediction of PSD was the same as the first case.

Figure 6.5 showed the PSD of coal in the first interval of the upper region. With longer residence time, the smallest particles were combusted, then the weight fractions was decreased in the first node as shown in Figure 6.5 (a) and (b). Most of the particles were reduced their sizes as observed from the shift of the curve to the left hand side. For example, the 1.5 mm particles reduced their size to 1.25 mm diameter. For the large particles, the weight fractions seem to be increased because of the normalized curve from the program.

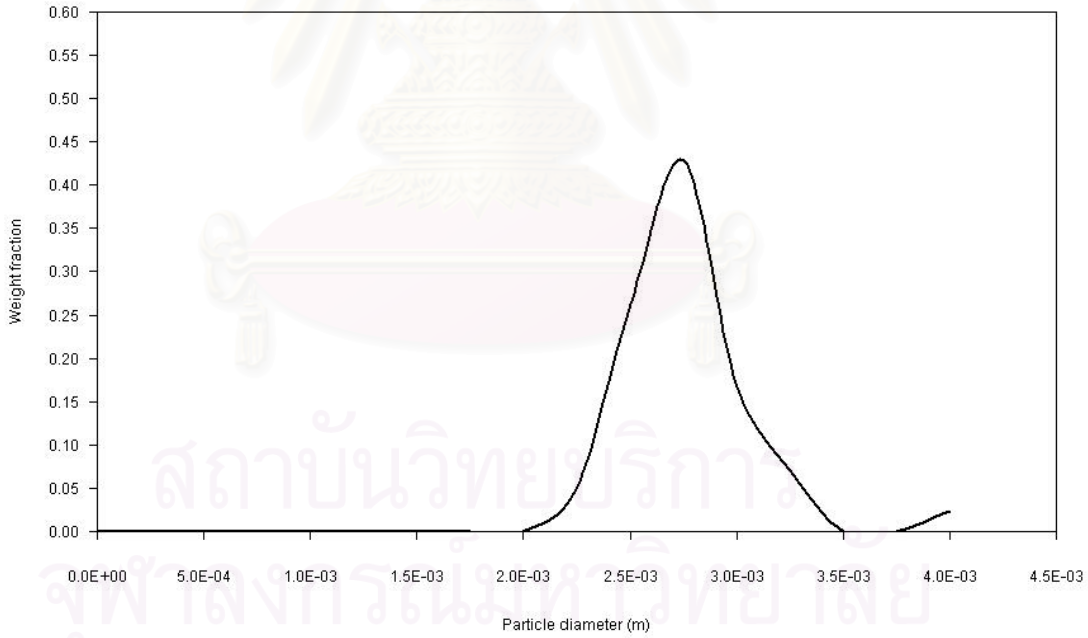
Figure 6.6 showed the PSD of coal in the second interval of the upper region. From Figure 6.6 (a), the results of PSD were considered in three intervals. The first interval, the weight fraction of smaller than 1mm particles was still closed to zero. The second interval, the particles with the size between 1.6-2.5 mm were reduced their size into 1.25- 1.5 mm by observing the increase of weight fraction that increased in this interval. The last interval, the 2.75 mm particles were reduced their size to 2.0 mm. The

weight fraction of 3.5 mm particles was increased due to the effect of curve normalization. From Figure 6.6 (b), the weight fraction of the small particles was also closed to zero. For the particles between 1.75-2.3 mm, the weight fraction was also decreased.

Figure 6.7 showed the PSD of coal in the third interval of the upper region. It was compared with that of the experiment after complete combustion. From both cases, the particles larger than 1.75 mm were reduced their size to 1.5 mm. For the small particles with the range of 0.4-0.75 mm, their weight fractions were increased. However, only the case of considering the primary fragmentation, the weight fractions of the particles smaller than 0.4 mm were observed but there were small amount when compared with those observed from the experiment. The reason was that the experiment was operated in batch operation, while the simulation was conducted in continuous operation. Thus, the large particles still can be observed in the simulation results.

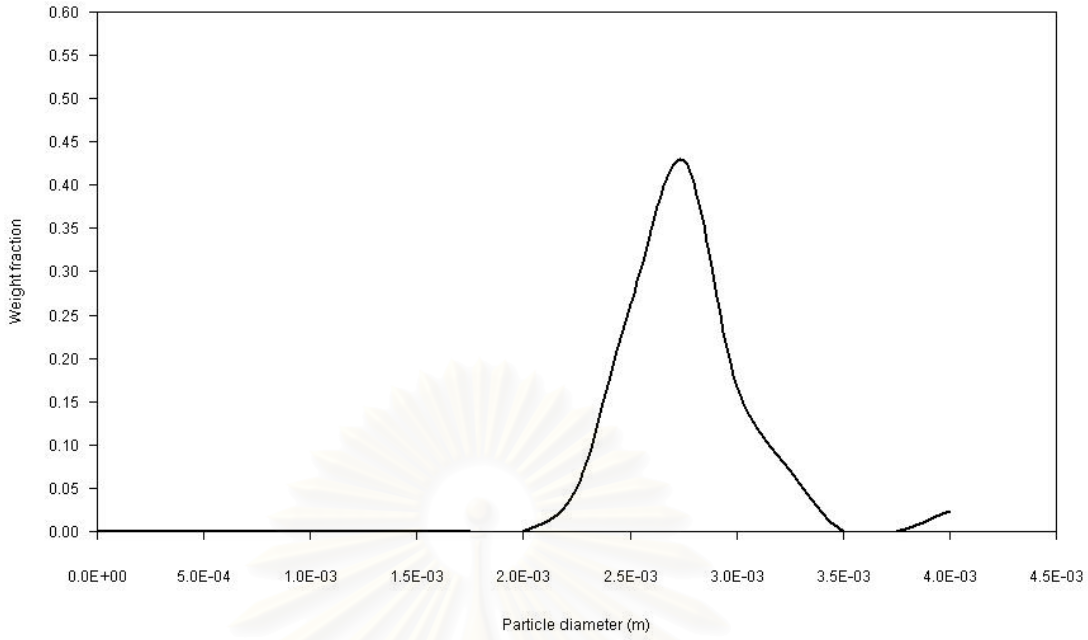


(a)

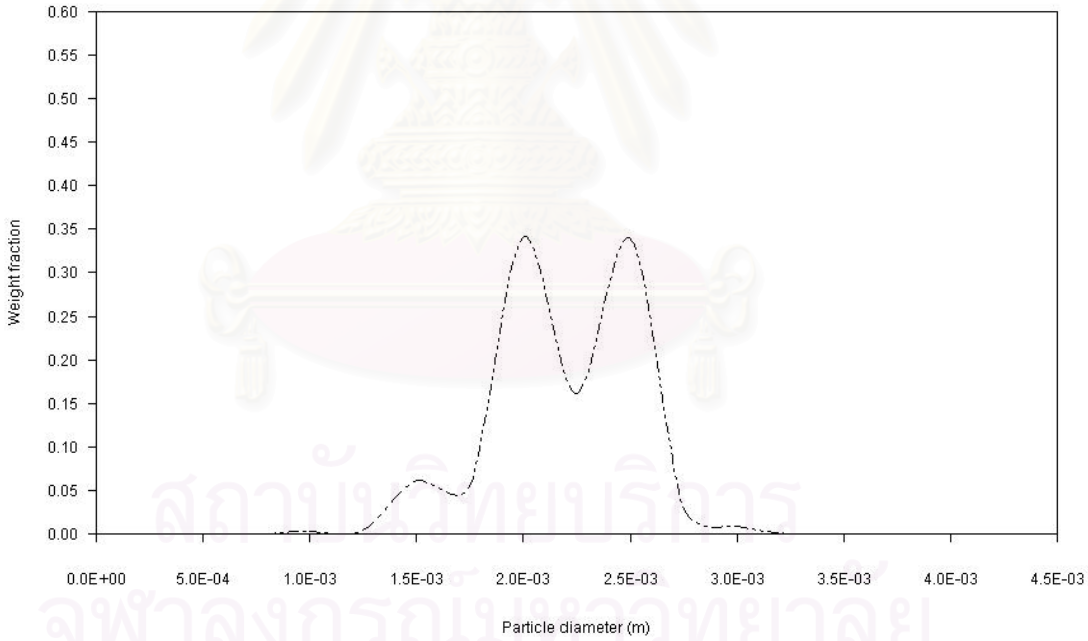


(b)

Figure 6.2 Particle size distribution of initial particle: (a) input to shrinking particle model simulation, (b) input to shrinking particle model with primary fragmentation model.

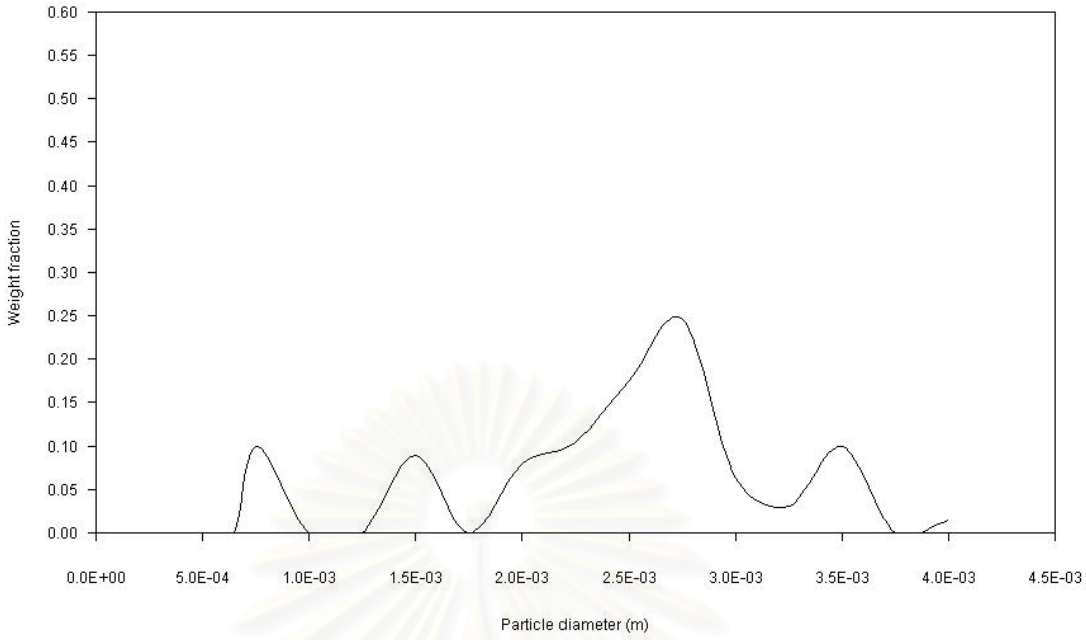


(a)

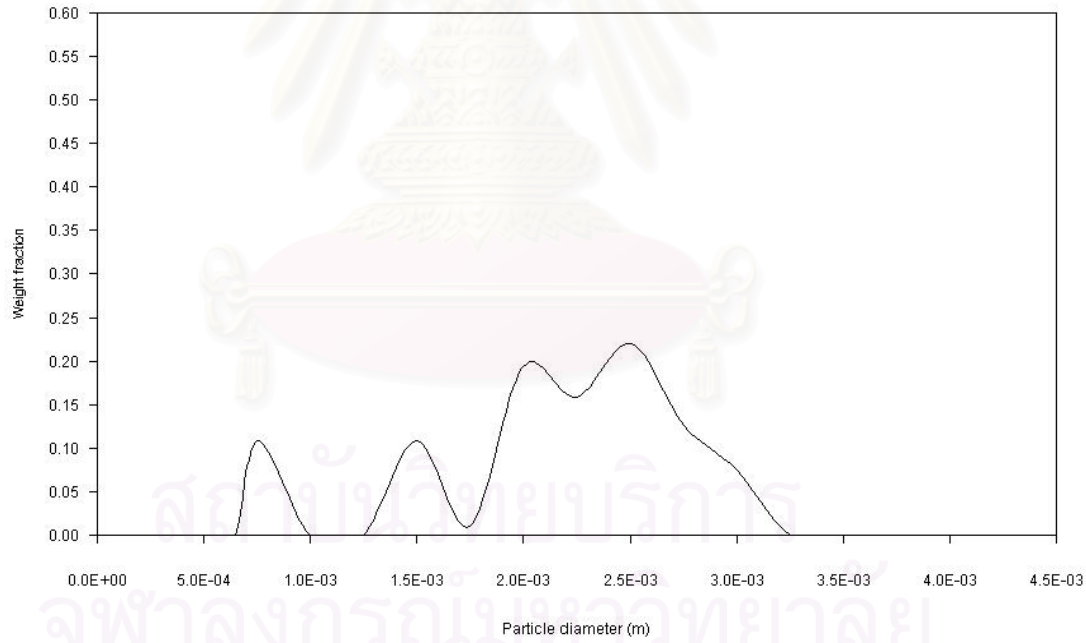


(b)

Figure 6.3 Particle size distribution after devolatilization process at 850 ^{o}C, 1 atm: (a) no adding primary fragmentation model, (b) adding primary fragmentation model.

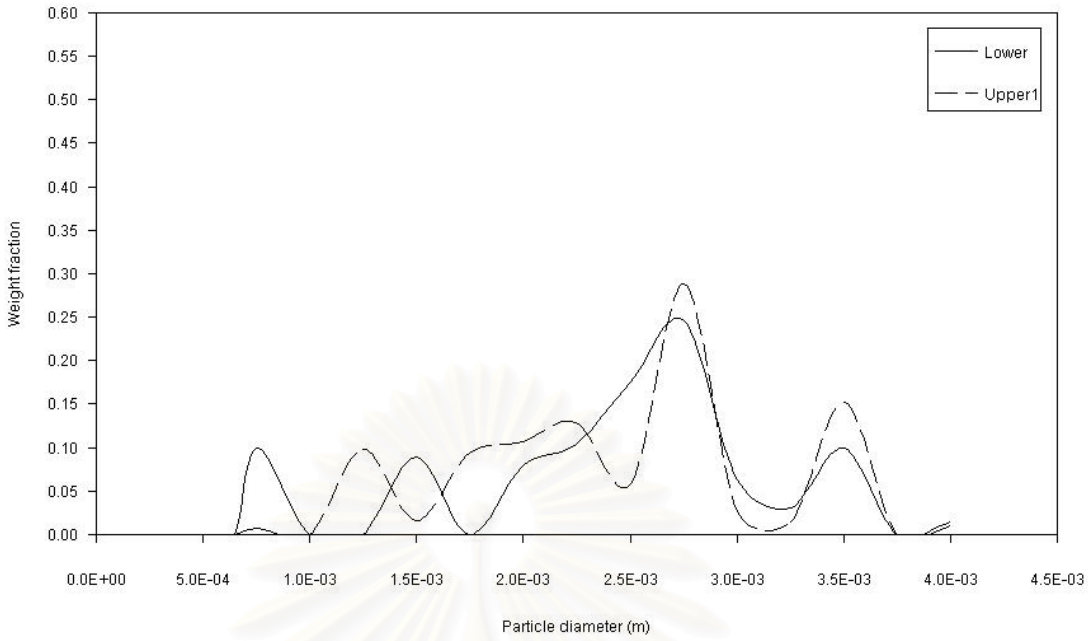


(a)

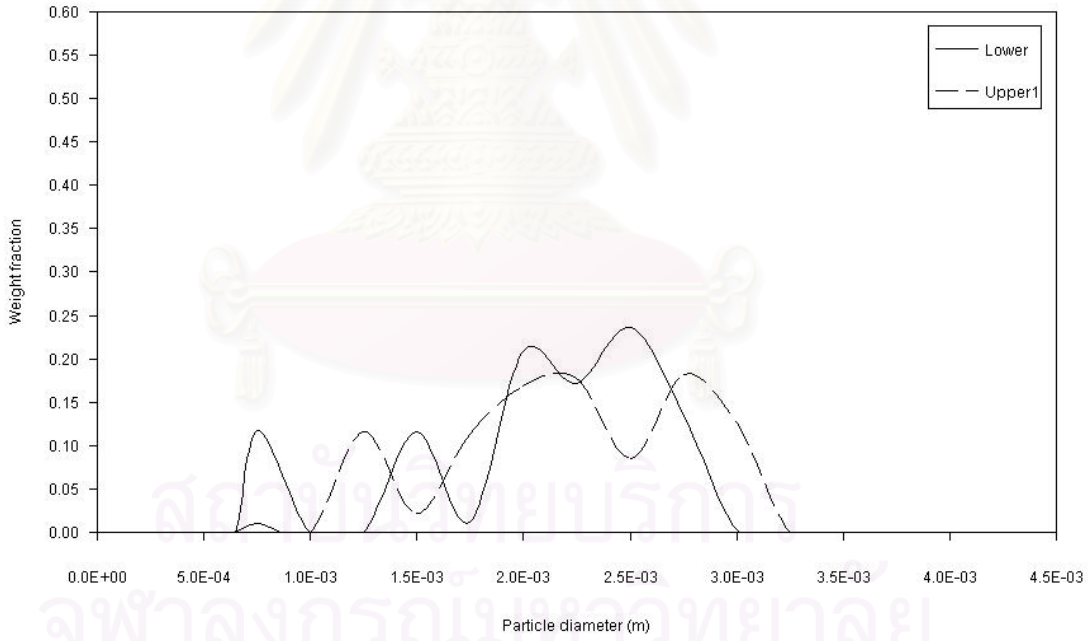


(b)

Figure 6.4 Particle size distribution after combustion in lower region at 850 ^{o}C, 1 atm: (a) no adding primary fragmentation model, (b) adding primary fragmentation model.

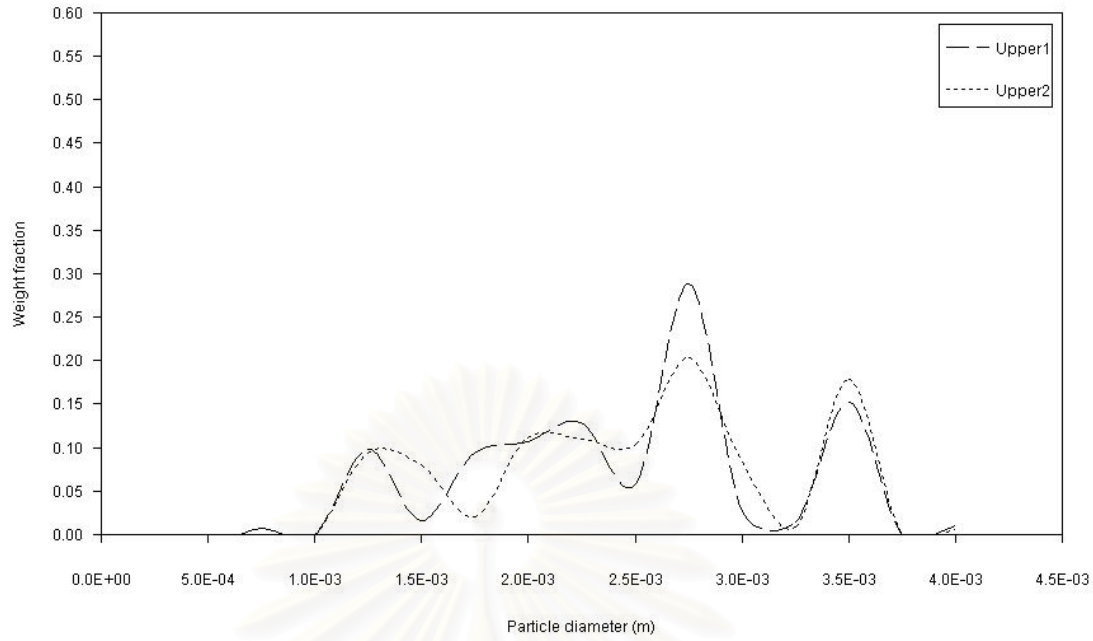


(a)

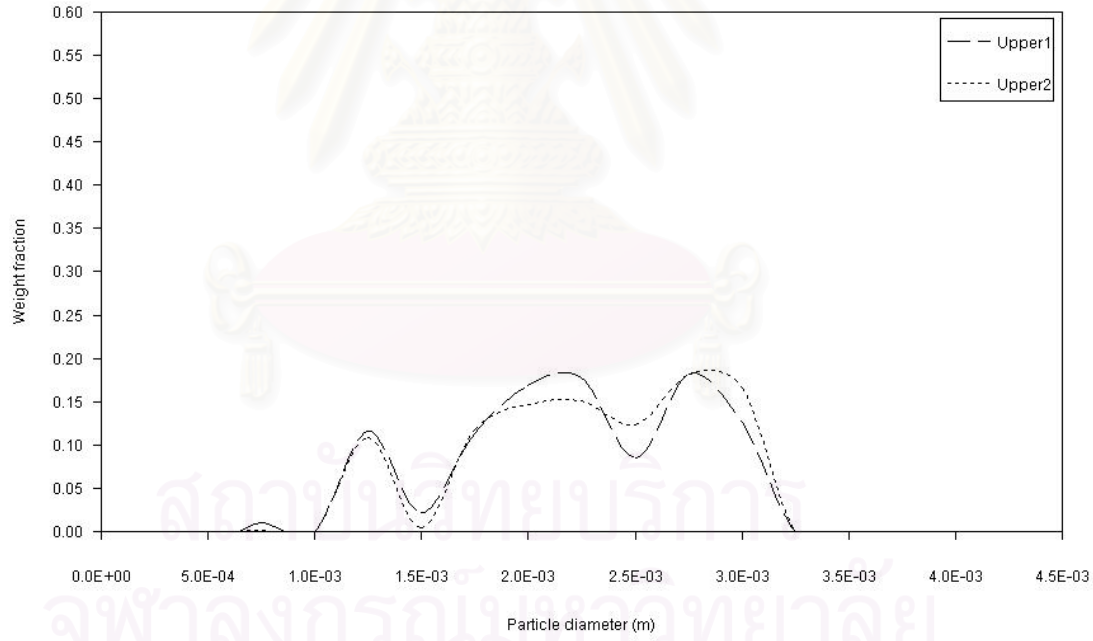


(b)

Figure 6.5 Compare the particle size distribution after combustion between lower and the first interval upper region at 850 ^{o}C, 1 atm: (a) no adding primary fragmentation model, (b) adding primary fragmentation model.

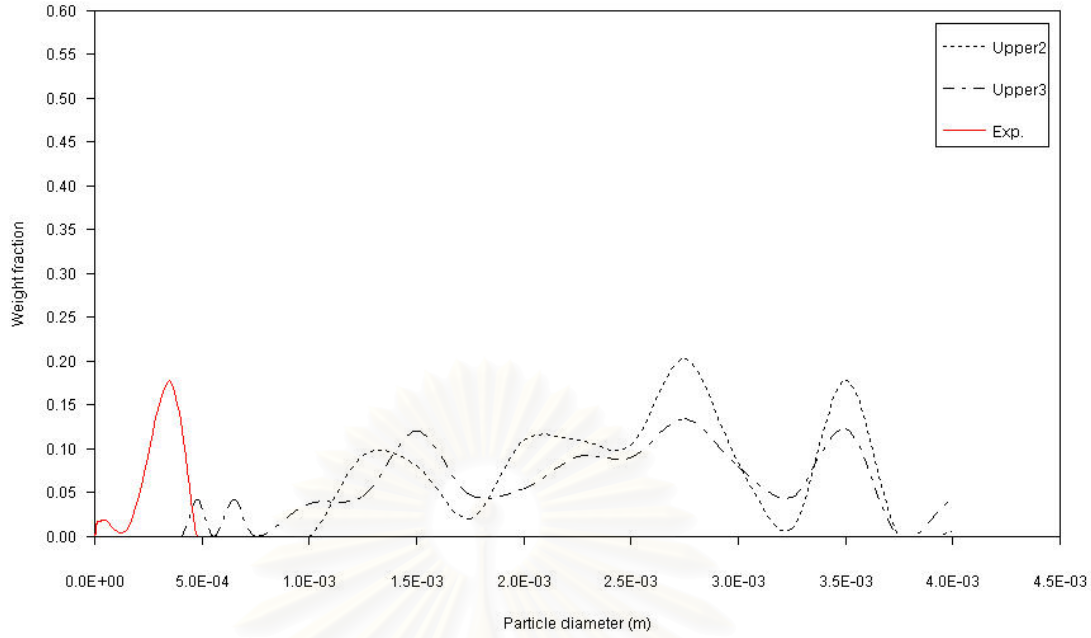


(a)

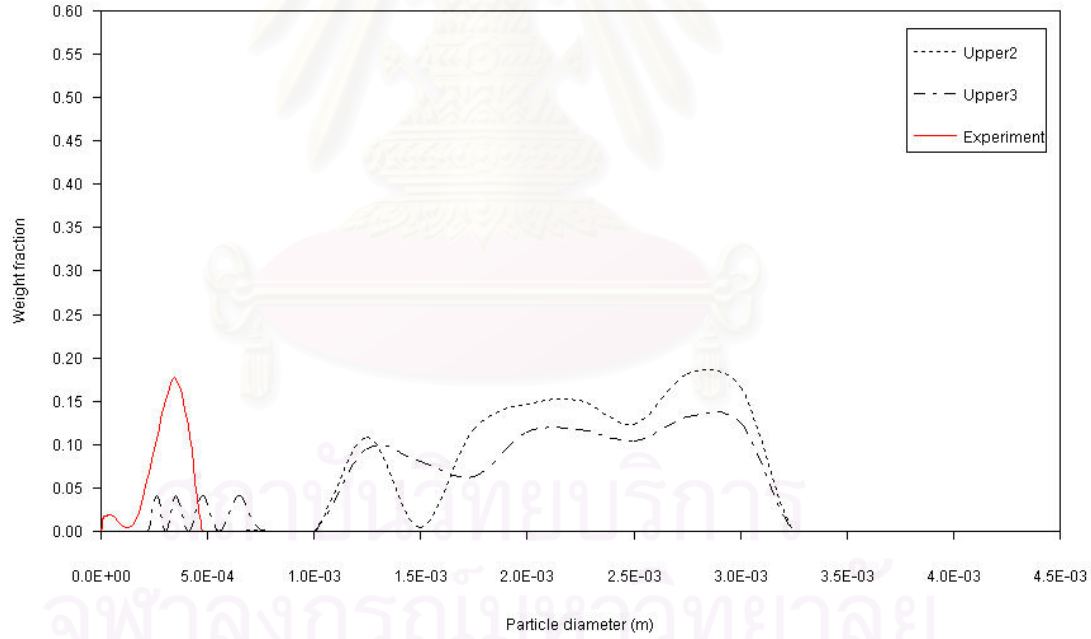


(b)

Figure 6.6 Compare the particle size distribution after combustion between the first and the second interval upper region at 850 ^{o}C, 1 atm: (a) no adding primary fragmentation model, (b) adding primary fragmentation model.



(a)



(b)

Figure 6.7 Compare the particle size distribution after combustion between the second and the third interval upper region at 850 ^{o}C, 1 atm compare with experiment: (a) no adding primary fragmentation model, (b) adding primary fragmentation model.

CHAPTER VII

CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

7.1.1 The experiments on the fuels comminution

In this research, the experiments on the fuels comminution in the laboratory-scale circulating fluidized bed combustor were divided into three parts: attrition, primary fragmentation, and secondary fragmentation parts. The fuels in the research were coal and bagasse.

The study of coal comminution was found that the attrition has insignificant effect on the changing size of coal particles. In the primary fragmentation study, the coal particles were fragmented due to the volatile pressure in the pores. The models to predict the particle size distribution were divided into two models as shown in the following equations.

For the small particles with size between 500-750 μm

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{627}\right)^{7.5}\right]$$

For the large particles with size between 1-3 mm

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{2.13\times10^{-3}}\right)^{7.5}\right]$$

where $M(<l)$ is cumulative mass of fragments of size less than l, l is the diameter of particle, M_T is total mass of fragments in the distribution.

For the secondary fragmentation study, it was found that the coal particles were divided into fine and coarse particles after the combustion process. The fine particles were the ash from the coal combustion. The coarse particles were the

unburnt particles in the system. Thus the models to predict the particle size distribution for the coal particles after combustion were divided into two models as shown in the following equations:

For the fine particles

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{25}\right)^{1.6}\right]$$

For the coarse particles

$$\frac{M(<l)}{M_T} = 1 - \exp\left[-\left(\frac{l}{295}\right)^{6}\right]$$

For the study on bagasse communition, it could not predict the size distribution of fragmented bagasse both the cases of primary and secondary fragmentation studies. Because the bagasse is very brittle after the devolatilization process. In the case of combustion, all bagasses were burnt in the combustor and remained small amount of the ash which was difficult to separate from the bed material.

7.1.2 Industrial scale CFBC simulation

This section was proposed a model for simulating a CFBC using single or mixed fuels. The shrinking particle model was included in the simulation to calculate the size distribution and weight fractions in each region of the riser. The modification will reflect the phenomena in the riser better. Moreover, the detail of emission models were added in the simulation to predict the formation of NO, N_2O, and SO_2. For different biomass fractions in the fuel, the simulation output will demonstrate the trend of gas emission, which can be used for environment protection consideration.

7.1.3 Laboratory-scale CFBC simulation

The simulation in this section emphasized on the particle size distribution in the riser of the CFBC. Two case studies were simulated. The first case, only shrinking particle model was added to predict the PSD along the riser. The second case, the Weibull distribution was added at the bottom of riser to predict the PSD after

the devolatilization process. It was found that the sizes of particles were reduced along the riser. The second case could be predicted the fine particles better than the first case. This was due to only the shrinking particle model could not eliminate the large particle in the system. The original size of particles still remains at the top of riser. However, the result of the second case simulation was not coincided with the experiment result because of the difference in operating modes.

7.2 Recommendations

A future study in the circulating fluidized bed combustor simulation should be performed in the following areas:

1. The apparatus should be improved for validating the simulation result by:
   - Modifying feed system from batch to continuous operation.
   - Scaling up the apparatus to increase the amount of feed and sampling points along the riser.
2. The emissions from the CFBC are taking place in the network reactions, but the simulations were calculated in the series reactions. Thus the complex algorithms should be developed.
3. For the emission from biomass combustion, the component of alkaline earth in biomass such as Ca should be included so that the better prediction of the amount of SO_2 and Ca/S ratio can be obtained.

REFERENCES

Adanez, J.; Gayan, P.; De Diego, L.F.; Garcia-Labiano, F.; and Abad, A. Combustion of wood chips in a CFBC. modeling and validation. Ind, Eng, Chem, Res. 42 (2003): 987-999.

Åmand, L.-E.; and Leckner, B. Metal emissions from co-combustion of sewage sludge and coal/wood in fluidized bed. Fuel 83 (2004): 1803-1821.

Arena, U; D'amore, M.; and Massimilla, L. Carbon attrition during the fluidized combustion of a coal. AIChE J. 29 (January 1983): 40-49.

Arena, U; D'amore, M.; Massimilla, L.; Meo, S.; and Miccio, M. Evaluation of attrition rate constants of char burning in fluidized beds by means of laboratory-scale combustors. AIChE J. 32 (May 1986): 869-871.

Aspen Technology Inc., Aspen Plus 11.1 Unit Operation Models. U.S.A.: Cambridge, September 2001.

Barrett, P. Selecting in Process Particle Size Analyzers [Online]. August 2003. Available from: http://www.cepmagazine.org [2003, September 17]

Basu, P. Combustion of coal in circulating fluidized bed boilers: a Review. Chemical Engineering Science 54 (1999): 5547-5557.

Basu, P.; and Fraser, S.A. Circulating Fluidized Bed Boilers. Stoneham: Butterworth-Heinemann, 1991.

Bemrose, C.R.; and Bridgwater, J. A review of attrition and attrition test methods. Powder Technology 49 (1987): 97-126.

Black, D.L.; Mcquay, M.Q.; and Bonin, M.P. Laser-based techniques for particle-size measurement: a review of sizing methods and their industrial applications. Prog. Energy Combust. Sci. 22 (1996): 267-306.

Boëlle, A., et al. Coal Comminution Characterization for Industrial Scale Circulating Fluidized Bed. Final Joint report corrected version: Electricité de France, 2002. (a Research Program in the frame of the International Energy Agency implementing agreement for co-operation in the field of fluidized bed conversion of fuels applied to clean energy production.)

Bonn, B.; Pelz, G.; and Baumann, H. Formation and decomposition of N_2O in fluidized bed boilers. Fuel 74 (1995): 165-171.

Borgwardt, R.H. Kinetics of the reaction of SO_2 with calcined limestone. Environmental Science & Technology 4 (1970): 59-63.

Broek, R.V.D.; Faaij, André; and Wijk, A.V. Biomass combustion for power generation. Biomass and Bioenergy 11 (1996): 271-281.

Brown, R.C.; Ahrens, J.; and Christofides, N. The Contributions of attrition and fragmentation to char elutriation from fluidized beds. Combustion and Flame 89 (1992): 95-102.

Brown, W.K. A theory of sequential fragmentation and its astronomical applications. J. Astrophys. Astr. 10 (1989): 89-112.

Bruni, G., et al. Self-segregation of High-volatile fuel particles during devolatilization in a fluidized bed reactor. Powder Technology 128 (2002): 11-21.

Chaiklangmuang, S. Mathematical Modelling of Emissions from Solid Fuel Combustion. Doctor of Dissertation, Department of Fuel and Energy, School of Process and Materials Engineering, United Kingdom, 2001.

Chen, Z., et al. Mathematical modeling of fluidized bed combustion. 4: N_2O and NO_x emissions from the combustion of char. Fuel 80 (2001): 1259-1272.

Chirone, R.; and Massimilla, L. Primary fragmentation in fluidized bed combustion of antracites. Powder Technology 64 (1991): 249-258.

Chirone, R.; Massimilla, L.; and Salatino, P. Comminution of carbons in fluidized bed combustion. Prog. Energy Combust. Sci. 17 (1991): 297-326.

Chirone, R.; Salatino, P.; and Massimilla, L. Secondary fragmentation of char particles during combustion in a fluidized bed. Combustion and Flame 77 (1989): 79-90.

Douglas, P.L.; and Young, B.E. Modelling and simulation of an AFBC steam heating plant using ASPEN/SP. Fuel 70 (1991): 145-154.

Gaur, S.; and Reed, T.B. Thermal Data for Natural and Synthetic Fuels. New York: Marcel Dekker, 1998.

Gayan, P., et al. Circulating fluidised bed co-combustion of coal and biomass. Fuel 83 (2004): 277-286.

Grace, J.R.; Avidan, A.A.; and Knowlton, T.M. Circulating Fluidized Beds. London: Blackie Academic & Professional, 1997.

Halder, P.K.; and Basu, P. Attrition of spherical electrode carbon particles during combustion in a turbulent fluidized bed. Chemical Engineering Science 47 (1992): 527-532.

Huilin, L.; Rushan, B.; Wenti, L.; Binxi, L.; and Lidan, Y. Computations of a circulating fluidized-bed boiler with wide particle size distributions. Ind, Eng. Chem. Res. 39 (2000): 3212-3220.

Jaturapitakkul, C., et al. Strength activity index of single size fly ash mixed with Portland cement typy I and type III. The 7th East Asia-Pacific Conference on Structural Engineering & Construction, pp. 1396-1401. Kochi, Japan, 1999.

Jin, X., et al. Comprehensive mathematical model for coal combustion in the circulating fluidized bed combustor. Tsinghua Science and Technology 6 (2001): 319-325.

Kadambi, J.R.; Martin, W.T.; Amirthaganesh, S.; and Wernet, M.P. Particle sizing using particle image velocimetry for Two-phase Flows. Powder Technology 100 (1998): 251-259.

Kamall, R. Cleaner Coal Technologies. [online]. (n.d.). Available from:http:// www.iea.org [2002, October 7]

Kilpinen, P.; Kallio, S.; Konttinen, J.; and Barisic, V. Char-nitrogen oxidation under fluidised bed combustion condition: single particle studies. Fuel 81 (2002): 2349-2362.

Kunii, D.; and Levenspiel, O. Fluidization Engineering. 2nd ed. Boston: Butterworth-Heinemann, 1991.

Laux, S.; Grusha, J.; and Mccarthy, K. Real Time Coal Flow and Particle Size Measurement for Improved Boiler Operation [Online]. (n.d.). Available from: http://www.fwc.com [2003, August 27]

Leckner, B.; Åmand, L.-E.; Lücke, K.; and Werther, J. Gaseous emissions from co-combustion of sewage sludge and coal/wood in a fludized bed. Fuel 83 (2004): 477-486.

Lee, J.M.; Kim, J.S.; and Kim, J.J. Comminution characteristics of Korean antracite in a CFB reactor. Fuel 82 (2003): 1349-1357.

Levenspiel, O. Chemical Reaction Engineering. 2nd ed. Singapore: John Wiley & Sons, 1972.

Li, Z; Lu, Q.; and Na, Y. N2O and NO emissions from co-firing MSW with coals in pilot scale CFBC. Fuel Processing Technology 85 (2004): 1539-1549.

Liu, D.C.; Mi, T.; Shen B.X.; and Feng, B. Reducing N_2O Emission by Co-Combustion of Coal and Biomass. Energy & Fuels 16 (2002): 525-526.

Liu, H.; and Gibbs, B.M. Modelling of NO and N_2O emissions from biomass-fired circulating fluidized bed combustors. Fuel 81 (2002): 271-280.

Ministry of Energy, Thailand Alternative Energy Situation. Bangkok: Department of Alternative Energy Development and Efficiency, 2003. (Mimeographed)

Missen, R.W.; Mims, C.A.; and Saville, B.A. Introduction to Chemical Reaction Engineering and Kinetics. New York: John Wiley & Sons, 1999.

Mukadi, L.; Guy, C.; and Legros, R. Prediction of gas emissions in an internally circulating fluidized bed combustor for treatment of industrial solid wastes. Fuel 79 (2000): 1125-1136.

Nordin, A. Optimization of sulfur retention in ash when cocombusting high sulfur fuels and biomass fuels in a small pilot scale fluidized bed. Fuel 74 (1995): 615-622.

Nordin, A.; Eriksson, L.; and Ohman, M. NO Reduction in a fluidized bed combustor with primary measures and selective non-catalytic reduction: a screening study using statistical experimental designs. Fuel 74 (1993): 128-135.

Paul, J.; Peeler, K.; and Howard, J.P. Devolatilization of large coal particles under fluidized bed conditions. Fuel 71 (1992): 425-430.

Sabbaghan, H.; Sotudeh-Gharebaagh, R.; and Mostoufi, N. Modeling the acceleration zone in the riser of circulating fluidized beds. Powder Technology 142 (2004): 129-135.

Sami, M.; Annamalia, K.; and Wooldridge, M. Co-firing of coal and biomass fuel blends. Prog. Energy Combust. Sci. 27 (2001): 171-214.

Scala, F.; and Salatino, P. Fluidized bed combustion of a biomass char (*Robinia pseudoacacia*). Energy & Fuels 14 (2000): 781-790.

Shimizu, T.; Fujikawa, T.; Tonsho, M.; and Inagaki, M. Effect of batch feeding of limestone on NO_x and SO_2 emissions during petroleum coke combustion in a bubbling fluidized bed combustor. Energy & Fuels 15 (2001): 1220-1224.

Siam Kraft Industry, Boiler Plant Design Basis. Ratchaburi: Energy division, June 1992. (Mimeographed)

Siam Kraft Industry, Summary of Technical Data of Pyroflow 30.6 $kg \cdot s^{-1}$. Ratchaburi: Energy division, January 1994. (Mimeographed)

Sotudeh-Gharebaagh, R.; Legros, R.; Chaouki, J.; and Paris, J. Simulation of circulating fluidized bed reactors using ASPEN PLUS. Fuel 77 (1998): 327-337.

Tardin, P.R., Jr.; Goldstein, L., Jr.; Lombardi, G.; and Pagliuso, J.D. On the mechanical attrition and fragmentation of particles in a fast fluidized bed. Ind, Eng. Chem. Res. 40 (2001): 4141-4150.

Walsh, P.M.; and Li, T. Fragmentation and attrition of coal char particles undergoing collisions at temperatures from 900 to 1100 K. Combustion and Flame 99 (1994): 749-757.

Winter, Z., et al. The NO and N_2O formation mechanism under circulating fluidized bed combustor conditions: from the single particle to the pilot-scale. The Canadian Journal of Chemical Engineering 77 (April 1999): 275-283.

Yamskulna, S. Energy management system design for steam power plant. Master's thesis, Department of Chemical Technology, Graduate School, Chulalongkorn University, 2000.

Yan, Y.; and Stewart, D. Guide to the Flow Measurement of Particulate Solids in Pipelines. London: The Institute of Measurement and Control, 2001.

Zhang, M.; Qian, Z.; Yu, Ha.; and Wei, F. The solid flow structure in a circulating fluidized bed riser/downer of 0.42 m diameter. Powder Technology 129 (2003): 46-52.

Zobeck, T.M.; Gill, T.E.; and Popham, T.W. A two-parameter Weibull function to describe airborne dust particle size distribution. Earth Surf. Process. Landforms 24 (1999): 943-955.

APPENDICES

Appendix A

Weight of particles and data of flue gas

Weight of single fragmented particle determined by sampling 30 particles and weighting for each particle. Then calculated for the average of the single particle as showed in the following table.

Table A-1 Weight of single fragmented particle

Particle number	Weight (g)	Particle number	Weight (g)
1	0.0034	16	0.0020
2	0.0055	17	0.0044
3	0.0069	18	0.0032
4	0.0041	19	0.0049
5	0.0033	20	0.0069
6	0.0042	21	0.0038
7	0.0027	22	0.0034
8	0.0036	23	0.0039
9	0.0045	24	0.0026
10	0.0059	25	0.0042
11	0.0025	26	0.0029
12	0.0040	27	0.0048
13	0.0044	28	0.0037
14	0.0036	29	0.0016
15	0.0044	30	0.0040
		Average	0.0040

Table A-2 Time to complete combustion of coal by flue gas detecting.

Amount of flue gas						
Time (s)	O_2 (%)	CO2 (%)	NO (ppm)	NO_x (ppm)	CO (ppm)	SO_2 (ppm)
30	20.8	-	0	0	24	0
60	20.4	-	5	5	289	5
90	19	1.8	7	7	1893	37
120	16.4	4	29	30	6065	313
150	11.7	8.1	192	201	7773	970
180	4.9	14.1	244	256	4841	638
210	4.7	14.3	194	203	364	365
240	6.9	12.3	360	379	61	368
270	9	10.5	398	418	42	414
300	14	6.2	227	238	24	477
330	20.2	-	24	25	17	281
360	20.5	-	12	12	15	226
390	20.6	-	4	5	12	191
420	20.7	-	2	2	9	139
450	20.7	-	0	0	7	104
480	20.7	-	0	0	6	86
510	20.7	-	0	0	5	71
540	20.8	-	0	0	5	48
570	20.9	-	0	0	5	38
600	21	-	0	0	5	40
630	21	-	0	0	4	33
660	21	-	0	0	4	29
690	21	-	0	0	5	26
720	21	-	0	0	3	24
750	21	-	0	0	3	21
780	21	-	0	0	3	17

Table A-2 (Continued)

Amount of flue gas						
Time (s)	O_2 (%)	CO2 (%)	NO (ppm)	NO_x (ppm)	CO (ppm)	SO_2 (ppm)
810	21	-	0	0	2	28
840	21	-	0	0	1	18
870	21	-	0	0	1	13
900	20.9	-	0	0	1	10
930	20.9	-	0	0	1	8
960	20.9	-	0	0	1	8
990	20.9	-	0	0	1	7
1020	20.9	-	0	0	1	5

Appendix B

Shrinking particle model subroutine for RCSTR

```
*==========================================================================*
C     User Subroutine for 5 component by apply Shrinking Particle Model
*==========================================================================*

      Subroutine USRKI1  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*--------------------------------------------------------------------------*

      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

      DATA EPSIC/0.30/, PIE/3.141592654/

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)


C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

C     DECLARE LOCAL VARIABLES
      COMMON /USER1/ FCBSD, FCBRS,   DCIPN, FMOLE, FRAC
      COMMON /USER2/ WPSD,  RWPSD
      COMMON /USER3/ FIRC,  Ea,      RD,    K0
      COMMON /USER5/ AREA,  VFAIR1,  VAIR1, VVOID, BEDW, BEDVV
      COMMON /USER7/ FRFN,  FIPSDN2, RLOW,  UPPER

      INTEGER IMISS, DMS_KCCIDC
      REAL*8  RMISS

      DIMENSION SUMTAU(5,5),      RLOW(26),     UPPER(25),
     .          K0(5),            Ea(5),        ID(5,5),
     .          RKCR(5),          WPSD(5,5),    RWPSD(5,5),
     .          FCBSD(5),         FCINV(5,5),   FCBRS(5),
     .          FCRINV(5,5),      FTOLINV(5,5), FTOTAL(5),
```

```
     .          WPSDNEW(5,5),     PPSD(5,5),    R1PSD(5,5),
     .          R2PSD(5,5),       RMEAN(5,5),   R1PS(25),
     .          R2PS(25),         RM1(25),      RM2(25),
     .          SRM(25),          DCIPN(5),     TAUD(5,5),
     .          TAUR(5,5),        RC(5,5),      UXB(5,5),

     .          FUXB(5,5),        FXB(5,5),     TOTAL(5),
     .          XB(5),            FMOLE(5),     R1(5),
     .          FRAC(3),          RCD(5,5),     RRC(5,5),
     .          RC1(5,5),         RC2(5,5),     RC3(5,5),
     .          RC4(5,5),         RC5(5,5),     XB1N(5,5),

     .          XB2N(5,5),        XB3N(5,5),    XB4N(5,5),
     .          XB5N(5,5),        XBN(5,5),     SUM1(5),
     .          SUM2(5),          SUM3(5),      SUM4(5),
     .          SUM5(5),          XB1N2(5,5),   XB2N2(5,5),
     .          XB3N2(5,5),       XB4N2(5,5),   XB5N2(5,5),

     .          SIGMA(5,5),       RCN2(5,5),    SUMM(5),
     .          FIPSD(5,5),       UXBNR(5,5),   XBNNR(5,5),
     .          WBYR1(5,5),       WBYR2(5,5),   SWBYR(5,5),
     .          FIRC(5,5),        SUMFI(5),     FIPSDN(5,5),
     .          F(NCOMP_NCC),     FIPSDN2(5,5), VVOID(4),

     .          UXB01(5,5),       RF1(5,5),     RF2(5,5),
     .          RF3(5,5),         RF4(5,5),     RF5(5,5),
     .          FIPSD1(5,5),      FIPSD2(5,5),  FIPSD3(5,5),
     .          FIPSD4(5,5),      FIPSD5(5,5),  SM1(5),
     .          SM2(5),           SM3(5),       SM4(5),

     .          SM5(5),           FXB1(5,5),    FXB2(5,5),
     .          FXB3(5,5),        FXB4(5,5),    FXB5(5,5),
     .          FSIGMA(5,5),      FRFN(5,5),    SUMF(5),
     .          BEDVV(4),         RD(5)

      OPEN (7,FILE='KINETIC1.txt')

*---------------------------------------------------------------------*
C     ORDER OF SUBSTREAM MIXED, CISOLID, CIPSD1, NCPSD1, CIPSD2, NCPSD2,
C     CIPSD3, NCPSD3, CIPSD4, NCPSD4, CIPSD5 AND NCPSD5
*---------------------------------------------------------------------*


C     MEAN RESIDENT TIME
      VFSUM = REAL(1)
      RTIME = RCSTRR_VOLRC*(1-VVOID(1)) / VFSUM
      WRITE (7,*) 'RESIDENT TIME (s)',RTIME
C     WRITE (7,*) 'VOLUMETRIC FLOW RATE OF TOTAL FLOW (m^3/s)', VFSUM
C     WRITE (7,*) 'VOID AT DENSE BED', VVOID(1)
C     WRITE (7,*) 'VOLUME (m^3)                = ',RCSTRR_VOLRC

C     DO 5 I = 1,5
C5    WRITE (7,*) 'MOLAR DENSITY IN CIPSD (Kgmole/m^3)', I, DCIPN(I)
C5    WRITE (7,*) 'MOLE FLOW IN CIPSD (Kgmole/s)', I,FMOLE(I)

C     DECLARE LOCAL OF CARBON
      IDXC   = DMS_KCCIDC('C')
C     WRITE (7,*) 'LOCAL ID. OF C    =',IDXC

C     DECLARE LOCAL OF OXYGEN
      IDXO2   = DMS_KCCIDC('O2')
C     WRITE (7,*) 'LOCAL ID. OF O2   =',IDXO2

C     DECLARE LOCAL OF CARBON MONOXIDE
      IDXCO   = DMS_KCCIDC('CO')
C     WRITE (7,*) 'LOCAL ID. OF CO   =',IDXCO

C     DECLARE LOCAL OF CARBON DIOXIDE
      IDXCO2  = DMS_KCCIDC('CO2')
```

```
C     WRITE (7,*) 'LOCAL ID. OF CO2  =',IDXCO2

C     DECLARE LOCAL OF WATER
      IDXH2O  = DMS_KCCIDC('H2O')
C     WRITE (7,*) 'LOCAL ID. OF H2O  =',IDXH2O

C     SET MISSING VALUE FOR RADIUS OF PARTICLES TO ZERO
      DO 10 I = 2,26
      IF (REAL(I).GT.1E34) THEN
      REAL(I) = 0.0
10    END IF

      DO 15 I = 30,104
      IF (REAL(I).GT.1E34) THEN
      REAL(I) = 0.0
15    END IF

*=====================================================================*
C          LOWER AND UPPER BOUNDARY FOR EACH INTERVEL OF PSD          C
*=====================================================================*
      DO 16 I = 1,26
16    RLOW(I) = 0.0

      DO 17 I = 1,25
17    UPPER(I) = 0.0

C     FOR PSD 1
      RLOW(1)  = 0.0
          DO 20 I = 1,5

          UPPER(I) = ( 2.*REAL(I+1) - RLOW(I) )
              IF(UPPER(I).LT.0.) THEN
                  UPPER(I) = RLOW(I) + 1.
              END IF
20        RLOW(I+1)  = UPPER(I)
C20       WRITE (7,*) 'BOUNDARY FOR PSD1',RLOW(I),UPPER(I)

C     FOR PSD2
      RLOW(6) = 0.0
          DO 25 I = 6,10
          UPPER(I) = ( 2.*REAL(I+1) - RLOW(I) )
              IF(UPPER(I).LT.0.) THEN
                  UPPER(I) = RLOW(I) + 1.
              END IF
25        RLOW(I+1)  = UPPER(I)
C25       WRITE (7,*) 'BOUNDARY FOR PSD2',RLOW(I),UPPER(I)

C     FOR PSD3
      RLOW(11) = 0.0
          DO 30 I = 11,15
          UPPER(I) = ( 2.*REAL(I+1) - RLOW(I) )
              IF(UPPER(I).LT.0.) THEN
                  UPPER(I) = RLOW(I) + 1.
              END IF
30        RLOW(I+1)  = UPPER(I)
C30       WRITE (7,*) 'BOUNDARY FOR PSD3',RLOW(I),UPPER(I)

C     FOR PSD4
      RLOW(16) = 0.0
          DO 35 I = 16,20
          UPPER(I) = ( 2.*REAL(I+1) - RLOW(I) )
              IF(UPPER(I).LT.0.) THEN
                  UPPER(I) = RLOW(I) + 1.
              END IF
35        RLOW(I+1)  = UPPER(I)
C35       WRITE (7,*) 'BOUNDARY FOR PSD4',RLOW(I),UPPER(I)

C     FOR PSD5
      RLOW(21) = 0.0
          DO 40 I = 21,25
```

```
          UPPER(I) = ( 2.*REAL(I+1) - RLOW(I) )
              IF(UPPER(I).LT.0.) THEN
                  UPPER(I) = RLOW(I) + 1.
              END IF
40        RLOW(I+1)  = UPPER(I)
C40       WRITE (7,*) 'BOUNDARY FOR PSD5',RLOW(I),UPPER(I)

*=======================================================================*
C             CONCENTRATION OF OXYGEN IN SUBSTREAM MIXED               C
*=======================================================================*
C     CONCENTRATION (Kgmole/m^3)
      CONO2 = REAL(29)
C     WRITE (7,*)'CONCENTRATION (Kgmole/m^3)        = ',CONO2

*-----------------------------------------------------------------------*

*=======================================================================*
C     PROPETIES OF EACH COMPONENT FOR CALCULATION
*=======================================================================*

C     FREQUENCY FACTOR
C     LANNA (m/(K s))
      K0(1) = 59600.

C     SIRAMANI (m/s)
      K0(2) = 59600.

C     BAGASSE (m/s)
      K0(3) = 210870.

C     F4 (m/s)
      K0(4) = 86560.

C     F5 (m/s)
      K0(5) = 22140.
*-----------------------------------------------------------------------*

C     ACTIVATED ENERGY (J/Kgmole)
C     LANNA
      Ea(1) = 1.492E8

C     SIRAMANI
      Ea(2) = 1.492E8

C     BAGASSE
      Ea(3) = 1.246E7

C     F4
      Ea(4) = 4.207E7

C     F5
      Ea(5) = 4.476E7
*-----------------------------------------------------------------------*

C     DIFFUSIVITY (m^2/s)
C     LANNA
      RD(1) = 1.525E-4

C     SIRAMANI
      RD(2) = 1.525E-4

C     SLUDGE
      RD(3) = 1.525E-4

C     F4
      RD(4) = 1.525E-4

C     F5
      RD(5) = 1.525E-4
*-----------------------------------------------------------------------*
```

```
*========================================================================*
C                          PROPERTIES IN RCSTR                           C
*========================================================================*
      TOTF = SOUT(NCOMP_NCC + 1)
      Tp   = SOUT(NCOMP_NCC + 2)
      PPAS = SOUT(NCOMP_NCC + 3)
      DEN  = SOUT(NCOMP_NCC + 8)
      WM   = SOUT(NCOMP_NCC + 9)
C     WRITE (7,*) 'TOTAL MOLE FLOW (Kgmole/s)       = ', TOTF
C     WRITE (7,*) 'TEMPERATURE (K)                  = ', Tp
C     WRITE (7,*) 'PRESSURE (Pa)                    = ', PPAS
C     WRITE (7,*) 'TOTAL MASS DENSITY (Kg/m^3)      = ', DEN
C     WRITE (7,*) 'MOLECULAR WEIGHT (Kg/Kgmole)     = ', WM

C     CONVERTED UNIT TO atm
      PATM = PPAS/1.01325E5
*------------------------------------------------------------------------*

C     RATE CONSTANT

C     LANNA
      DO 900 I = 1,2
      RKCR(I) = K0(I) * Tp * DEXP( -Ea(I) / (PPGLOB_RGAS*Tp) )
C     WRITE (7,*) 'GAS CONSTANT',PPGLOB_RGAS
900   WRITE (7,*) 'RATE CONSTANT FOR LIGNITE',RKCR(I)

C     PITH, SLUDGE, F4 AND F5
      DO 45 I = 3,5
      RKCR(I) = K0(I) * DEXP( -Ea(I) / (PPGLOB_RGAS*Tp) )
45    WRITE (7,*) 'RATE CONSTANT FOR PITH,SLUDGE, F4 AND F5',RKCR(I)


*========================================================================*
C                  NEW FRACTION FOR EACH INTERVAL                        C
*========================================================================*
C     INTERVAL = ROW, COMPONENT = COLUMN

C     WEIGHT PARTICLE SIZE DISTRIBUTION FOR RECYCLE STREAM
      DO 49 J = 1,5
      DO 49 I = 1,5
      IF(RWPSD(I,J).GT.1E34) THEN
      RWPSD(I,J) = 0.0
      END IF

      FCINV(I,J)   = 0.0
      FCRINV(I,J)  = 0.0
      FTOLINV(I,J) = 0.0
49    WPSDNEW(I,J) = 0.0

C     FLOW IN EACH INTERVAL OF EACH COMPONENT BOTH INPUT AND RECYCLE
C     FCINV = INPUT, FCRINV = RECYCLE
      DO 50 J = 1,5
      DO 50 I = 1,5
      FCINV(I,J)   = WPSD(I,J) * FCBSD(J)
      FCRINV(I,J)  = RWPSD(I,J) * FCBRS(J)
50    FTOLINV(I,J) = FCINV(I,J) + FCRINV(I,J)

!     WRITE (7,51) ((FCINV(I,J),J=1,5),I=1,5)
!51   FORMAT(2X, 'INPUT FLOW IN EACH INTERVAL',/5(1X,E10.3))
!     WRITE (7,52) ((FCRINV(I,J),J=1,5),I=1,5)
!52   FORMAT(2X, 'RECYCLE FLOW IN EACH INTERVAL',/5(1X,E10.3))
!     WRITE (7,53) ((FTOLINV(I,J),J=1,5),I=1,5)
!53   FORMAT(2X, 'TOTAL FLOW IN EACH INTERVAL',/5(1X,E10.3))

C     NEW TOTAL FLOW IN EACH COMPONENT
      DO 55 I = 1,5
55    FTOTAL(I) = 0.0

      DO 60 J = 1,5
```

```
      DO 60 I = 1,5
60    FTOTAL(I) = FTOTAL(I) + FTOLINV(J,I)

C     DO 61 I = 1,5
C61   WRITE (7,*) 'TOTAL IN EACH COMPONENT',FTOTAL(I)

C     NEW FRACTION FOR EACH INTERVAL AND EACH COMPONENT
      DO 65 J = 1,5
      DO 65 I = 1,5
65    WPSDNEW(I,J) =  FTOLINV(I,J)/FTOTAL(J)

!     WRITE (7,66) ((WPSDNEW(I,J),J=1,5),I=1,5)
!66   FORMAT(2X, 'NEW FRACTION IN EACH INTERVAL',/5(1X,E10.3))
*---------------------------------------------------------------------*

*=====================================================================*
C             NEW RADIUS OF PARTICLE FOR EACH INTERVAL                C
*=====================================================================*

C     NEW WEIGHT FRACTION FOR FIND MEAN RADIUS
      DO 70 J = 1,5
      DO 70 I = 1,5
      R1PSD(I,J) = 0.0
      R2PSD(I,J) = 0.0
70    PPSD(I,J)  = 0.0

      DO 75 J = 1,5
      DO 75 I = 1,5
      PPSD(I,J)  = WPSD(I,J) + RWPSD(I,J)

C     NORMALIZED NEW WEIGHT FRACTION BETWEEN INPUT AND RECYCLE
          IF (PPSD(I,J).NE.0.) THEN
          R1PSD(I,J) = WPSD(I,J)/PPSD(I,J)
          R2PSD(I,J) = RWPSD(I,J)/PPSD(I,J)
75        END IF

!     WRITE (7,76) ((R1PSD(I,J),J=1,5),I=1,5)
!76   FORMAT(2X, 'R1PSD',/5(1X,E10.3))

!     WRITE (7,77) ((R2PSD(I,J),J=1,5),I=1,5)
!77   FORMAT(2X, 'R2PSD',/5(1X,E10.3))

!     WRITE (7,78) ((PPSD(I,J),J=1,5),I=1,5)
!78   FORMAT(2X, 'PPSD',/5(1X,E10.3))

C     ARRANGE R1PSD AND R2PSD MATRIX TO VECTOR

      DO 79 I = 1,5
      R1PS(I) = 0.0
79    R2PS(I) = 0.0

      DO 80 I = 1,5
      R1PS(I) = R1PSD(I,1)
80    R2PS(I) = R2PSD(I,1)

      DO 85 I = 6,10
      R1PS(I) = R1PSD(I-5,2)
85    R2PS(I) = R2PSD(I-5,2)

      DO 90 I = 11,15
      R1PS(I) = R1PSD(I-10,3)
90    R2PS(I) = R2PSD(I-10,3)

      DO 95 I = 16,20
      R1PS(I) = R1PSD(I-15,4)
95    R2PS(I) = R2PSD(I-15,4)

      DO 100 I = 21,25
      R1PS(I) = R1PSD(I-20,5)
100   R2PS(I) = R2PSD(I-20,5)
```

```
C     WRITE (7,101) (R1PS(I),I=1,25)
C101  FORMAT(2X,'R1PS',/1(E10.3))

C     WRITE (7,102) (R2PS(I),I=1,25)
C102  FORMAT(2X,'R2PS',/1(E10.3))

C     MEAN RADIUS
      DO 105 I = 1,25
      RM1(I) = 0.0
      RM2(I) = 0.0
105   SRM(I) = 0.0

!     DO 104 I = 1,25
!104  WRITE (7,*) 'INPUT RADIUS', REAL(I+1)

!     DO 106 I = 1,25
!106  WRITE (7,*) 'RECYCLE RADIUS', REAL(I+29)


      DO 110 I = 1,25
      IF (REAL(I+1).EQ.0.0) THEN
      RM1(I) = 0.0
      ELSE
      RM1(I) = R1PSD(I,1)/REAL(I+1)
110   END IF
C     WRITE (7,*) 'RM1', I,RM1(I)

      DO 115 I = 1,25
      IF (REAL(I+29).EQ.0.0) THEN
      RM2(I) = 0.0
      ELSE
      RM2(I) = R2PSD(I,1)/REAL(I+29)
115   END IF
C     WRITE (7,*) 'RM2', I,RM2(I)

      DO 120 I = 1,25
      SRM(I) = RM1(I) + RM2(I)
      IF (SRM(I).NE.0.0) THEN
      REAL(I+54) = 1/SRM(I)
120   END IF
C     WRITE (7,*) 'SRM', I,SRM(I)
C     WRITE (7,*) 'MEAN RADIUS', I,REAL(I+54)
*-----------------------------------------------------------------------*
C     ARRANGE MEAN RADIUS VECTOR TO MATRIX
C     ROW = RADIUS, COLUMN = COMPONENT

      DO 124 J = 1,5
      DO 124 I = 1,5
124   RMEAN(I,J) = 0.0

      DO 125 I = 1,5
      RMEAN(I,1) = REAL(I+54)
      RMEAN(I,2) = REAL(I+59)
      RMEAN(I,3) = REAL(I+64)
      RMEAN(I,4) = REAL(I+69)
125   RMEAN(I,5) = REAL(I+74)

      WRITE (7,126) ((RMEAN(I,J),J=1,5),I=1,5)
126   FORMAT(2X, 'MEAN RADIUS',/5(1X,E10.3))

*=======================================================================*
C      TIME REQUIRED FOR COMPLETE CONVERSION (TAU) IN INPUT STREAM      C
*=======================================================================*
      DO 127 J = 1,5
      DO 127 I = 1,5
      TAUD(I,J)   = 0.0
      TAUR(I,J)   = 0.0
      SUMTAU(I,J) = 0.0
      RC(I,J)     = 0.0
```

```
      UXB(I,J)    = 0.0
      FUXB(I,J)   = 0.0
      FXB(I,J)    = 0.0
127   RRC(I,J)    = 0.0

      DO 130 J = 1,5
      DO 130 I = 1,5

C     FOR SMALL PARTICLE

          IF (RMEAN(I,J).LE.5E-3) THEN

C     TAUD IS TIME IN FILM DIFFUSION CONTROLS
C     TAUR IS TIME IN REACTION CONTROLS FOR SMALL PARTICLE

              TAUD(I,J) = DCIPN(J) * RMEAN(I,J)**2./ (4.*RD(J)*CONO2)
              TAUR(I,J) = DCIPN(J) * RMEAN(I,J) /(2.*RKCR(J)*CONO2)

          ELSE

C     FOR LARGE PARTICLE

C     TAUD IN FILM DIFFUSION CONTROLS
C     TAUR IN REACTION CONTROLS

              TAUD(I,J) = DCIPN(J)*RMEAN(I,J)**(3./2.)/( 1.8*CONO2*RD(J)
     .                    * ( REAL(108)/(DEN*RD(J)) )**(1./3.)
     .                    * ( 2.*VAIR1*DEN/REAL(108) )**(1./2.)  )
              TAUR(I,J) = DCIPN(J) * RMEAN(I,J) /(2.*RKCR(J)*CONO2)

          END IF

130           SUMTAU(I,J) = TAUD(I,J) + TAUR(I,J)

      WRITE (7,131) ((TAUD(I,J),J=1,5),I=1,5)
131   FORMAT(2X, 'TAUD',/5(1X,E10.3))

      WRITE (7,132) ((TAUR(I,J),J=1,5),I=1,5)
132   FORMAT(2X, 'TAUR',/5(1X,E10.3))

      WRITE (7,133) ((SUMTAU(I,J),J=1,5),I=1,5)
133   FORMAT(2X, 'SUMMATION TAU',/5(1X,E10.3))

*---------------------------------------------------------------------*

*=====================================================================*
C                    RESIDUAL RADIUS AFTER BURNING                    C
*=====================================================================*
      DO 135 J = 1,5
      DO 135 I = 1,5

              IF (TAUD(I,J).LE.TAUR(I,J)) THEN
C     FOR REACTION CONTROLLING
                  RC(I,J) =  RMEAN(I,J) - 2.*RTIME*RKCR(J)*CONO2
     .                     / DCIPN(J)
              ELSE

C     FOR DIFFUSION CONTROLLING
                  IF (RMEAN(I,J).LE.5E-3) THEN

C     CALCULATED FOR SMALL PARTICLES
                  RRC(I,J) = RMEAN(I,J)**3 - 6.*CONO2*RD(J)*RTIME
     .                                     *RMEAN(I,J) / DCIPN(J)

                      IF (RRC(I,J).GT.0.) THEN
                          RC(I,J) = RRC(I,J)**(1./3.)
                      END IF

                  ELSE
```

```
                RRC(I,J) = RMEAN(I,J)**3 - ( 1.8*RTIME*CONO2*RD(J)
     .                     *RMEAN(I,J)**(3./2.)
     .                     *( REAL(108)/(DEN*RD(J)) )**(1./3.)
     .                     *( 2.*VAIR1*DEN/REAL(108) )**(1./2.) )
     .                     / DCIPN(J)

                    IF (RRC(I,J).GT.0.) THEN
                        RC(I,J) = RRC(I,J)**(1./3.)
                    END IF

                END IF
            END IF

      IF (RC(I,J).LT.0.) THEN
      RC(I,J) = 0.0
135   END IF

      WRITE (7,136) ((RC(I,J),J=1,5),I=1,5)
136   FORMAT(2X, 'RESIDUAL RADIUS AFTER BURNING',/5(1X,E10.3))

*---------------------------------------------------------------------*

*=====================================================================*
C               CONVERSION FOR CHEMICAL CONTROLLING                   C
*=====================================================================*
C     FRACTION UNCONVERTED IN PARTICLES OF EACH SIZE

      DO 140 J = 1,5
      DO 140 I = 1,5

          IF (TAUD(I,J).LE.TAUR(I,J)) THEN
                  UXB(I,J) =   (1./4.)   * (SUMTAU(I,J)/RTIME)
     .                       - (1./20.)  * (SUMTAU(I,J)/RTIME)**2
     .                       + (1./120.) * (SUMTAU(I,J)/RTIME)**3
              ELSE
                  UXB(I,J) =   (1./2.)   * (SUMTAU(I,J)/RTIME)
     .                       - (1./6.)   * (SUMTAU(I,J)/RTIME)**2
     .                       + (1./24.)  * (SUMTAU(I,J)/RTIME)**3
          END IF

          IF (UXB(I,J).GT.1.) THEN
              UXB(I,J) = 1.
          END IF

C     CONVERTED AND UNCONVERTED FOR EACH STREAM

      FUXB(I,J) = UXB(I,J) * FTOLINV(I,J)/FTOTAL(J)
          IF (FUXB(I,J).NE.0.0) THEN
          FXB(I,J)  = 1-FUXB(I,J)
140       END IF

!     WRITE (7,141) ((UXB(I,J),J=1,5),I=1,5)
!141  FORMAT(2X, 'FRACTION UNCONVERTED SOLID',/5(1X,E10.3))
C     WRITE (7,142) ((FUXB(I,J),J=1,5),I=1,5)
C142  FORMAT(2X, 'UNCONVERTED FOR EACH INTEVAL',/5(1X,E10.3))
C     WRITE (7,143) ((FXB(I,J),J=1,5),I=1,5)
C143  FORMAT(2X, 'CONVERSION FOR EACH INTERVAL',/5(1X,E10.3))

      DO 150 I = 1,5
      TOTAL(I) = 0.0
      XB(I)    = 0.0
150   R1(I)    = 0.0

      DO 155 J = 1,5
      DO 155 I = 1,5
      TOTAL(J) = TOTAL(J) + FUXB(I,J)
155   XB(J) = 1 - TOTAL(J)

      DO 160 I = 1,5
C     WRITE (7,*) 'TOTAL', TOTAL(I)
```

```
160   WRITE (7,*) 'MEAN CONVERSION', XB(I)
*-------------------------------------------------------------------*

*===================================================================*
C                     FIRST RATE OF COMBUSTION
*===================================================================*
      DO 165 I = 1,5
      R1(I) = FMOLE(I)*XB(I)/2.
!     WRITE (7,*) 'MOLAR FLOW',FMOLE(I)
165   WRITE (7,*) 'FIRST RATE OF COMBUSTION FOR MATERIAL',I,R1(I)

*-------------------------------------------------------------------*

*===================================================================*
C                     SECOND RATE OF COMBUSTION
*===================================================================*
C     CONVERT UNIT OF GAS LAW CONSTANT TO Kcal/(Kgmole K)
      RGASN  = PPGLOB_RGAS*0.239/1E3

C     CONVERT UNIT OF GAS LAW CONSTANT TO (atm cm^3)/(gmole K)
      RGASN1 = PPGLOB_RGAS*1E3/1.01325E5

C     MOLE FRACTION
      DO 175 I = 1,NCOMP_NCC
175   F(I) = SOUT(I)/TOTF

C     MOLAR DENSITY
      DENMOL = DEN/WM

      R2 = 1.18E13 * F(IDXCO) * F(IDXO2)**0.5 * F(IDXH2O)**0.5
     .     * (PATM/(RGASN1*Tp)) * DEXP(-25000./(RGASN*Tp)) * DENMOL
     .     * VVOID(1) * RCSTRR_VOLRC

      WRITE (7,*) 'SECOND RATE OF COMBUSTION', R2
*-------------------------------------------------------------------*

*===================================================================*
C                     REACTION RATES IN MIXED
*===================================================================*
      DO 180 I = 1,NCOMP_NCC
180   RATES(I) = 0.0

C     FOR OXYGEN
      RATES(IDXO2) = - ( R1(1) + R1(2) + R1(3) + R1(4) + R1(5) + R2 )
C     WRITE (7,*) 'RATES O2 IN MIXED  = ', RATES(IDXO2)

C     FOR CARBON MONOXIDE
      RATES(IDXCO) = 2. * ( R1(1) + R1(2) + R1(3) + R1(4) + R1(5) - R2 )
C     WRITE (7,*) 'RATES CO IN MIXED  = ', RATES(IDXCO)

C     FOR CARBON DIOXIDE
      RATES(IDXCO2) = 2. * R2
C     WRITE (7,*) 'RATES CO2 IN MIXED = ', RATES(IDXCO2)

*===================================================================*
C                     REACTION RATES IN CISOLID
*===================================================================*
      L1 = NCOMP_NCC + 1
      L2 = L1 + NCOMP_NCC - 1

      DO 185 I = L1, L2
185   RATES(I) = 0.0

*===================================================================*
C                     REACTION RATES IN CIPSD1
*===================================================================*
      L3 = L2 + 1
      L4 = L3 + NCOMP_NCC - 1

      DO 190 I = L3, L4
```

```
190   RATES(I) = 0.0

C     FOR CARBON
      CCPSD1 = IDXC + L3 - 1
      RATES(CCPSD1) = -2.*R1(1)
C     WRITE (7,*) 'RATES C IN CIPSD1  = ', RATES(CCPSD1)

*=====================================================================*
C                     REACTION RATES IN CIPSD2
*=====================================================================*
      L5 = L4 + NCOMP_NNCC + 1
      L6 = L5 + NCOMP_NCC - 1

      DO 195 I = L5, L6
195   RATES(I) = 0.0

C     FOR CARBON
      CCPSD2 = IDXC + L5 - 1
      RATES(CCPSD2) = -2. * R1(2)
C     WRITE (7,*) 'RATES C IN CIPSD2  = ', RATES(CCPSD2)

*=====================================================================*
C                     REACTION RATES IN CIPSD3
*=====================================================================*

      L7 = L6 + NCOMP_NNCC + 1
      L8 = L7 + NCOMP_NCC - 1

      DO 200 I = L7, L8
200   RATES(I) = 0.0

C     FOR CARBON
      CCPSD3 = IDXC + L7 - 1
      RATES(CCPSD3) = -2. * R1(3)
C     WRITE (7,*) 'RATES C IN CIPSD3  = ', RATES(CCPSD3)

*=====================================================================*
C                     REACTION RATES IN CIPSD4
*=====================================================================*
      L9  = L8 + NCOMP_NNCC + 1
      L10 = L9 + NCOMP_NCC - 1

      DO 205 I = L9, L10
205   RATES(I) = 0.0

C     FOR CARBON
      CCPSD4 = IDXC + L9 - 1
      RATES(CCPSD4) = -2. * R1(4)
C     WRITE (7,*) 'RATES C IN CIPSD4  = ', RATES(CCPSD4)

*=====================================================================*
C                     REACTION RATES IN CIPSD5
*=====================================================================*
      L11 = L10 + NCOMP_NNCC + 1
      L12 = L11 + NCOMP_NCC - 1

      DO 210 I = L11, L12
210   RATES(I) = 0.0

C     FOR CARBON
      CCPSD5 = IDXC + L11 - 1
      RATES(CCPSD5) = -2. * R1(5)
C     WRITE (7,*) 'RATES C IN CIPSD5  = ', RATES(CCPSD5)
*---------------------------------------------------------------------*

*=====================================================================*
C                  NEW MEAN RADIUS AND NEW FRACTION
*=====================================================================*

C     FOR UNCONVERTED PARTICLES THE SIZE ARE UNCHANGING
```

```
C     REAL(55-79) = RMEAN(I,J)

C     WEIGHT FRACTION OF PSD FOR CONVERTED SOLID

C     PREPARE MATRIX FOR NEW RADIUS
      DO 230 J = 1,5
      DO 230 I = 1,5
      RC1(I,J)  = 0.0
      RC2(I,J)  = 0.0
      RC3(I,J)  = 0.0
      RC4(I,J)  = 0.0
      RC5(I,J)  = 0.0
      XB1N(I,J) = 0.0
      XB2N(I,J) = 0.0
      XB3N(I,J) = 0.0
      XB4N(I,J) = 0.0
230   XB5N(I,J) = 0.0


C     WRITE (7,231) ((FXB(I,J),J=1,5),I=1,5)
C231  FORMAT(2X, 'WEIGHT FRACTION FOR SOLID CONVERTED',/5(1X,E10.3))
*=====================================================================*
C         ARRANGE NEW RADIUS AND FRACTION MATRIX FOR COMPONENT 1
C                        FOR CONVERT PARTICLES
*=====================================================================*

      DO 240 J = 1,5
      DO 240 I = 1,5

      IF (RC(I,1).GE.RLOW(J).AND.RC(I,1).LT.UPPER(J)) THEN
          RC1(I,J)  = RC(I,1)
          XB1N(I,J) = FXB(I,1)

              IF (RC1(I,J).EQ.0.) THEN
                  XB1N(I,J) = 0.0
              END IF

      END IF

*=====================================================================*
C         ARRANGE NEW RADIUS AND FRACTION MATRIX FOR COMPONENT 2
C                        FOR CONVERT PARTICLES
*=====================================================================*
      IF (RC(I,2).GE.RLOW(J+5).AND.RC(I,2).LT.UPPER(J+5)) THEN
          RC2(I,J)  = RC(I,2)
          XB2N(I,J) = FXB(I,2)

              IF (RC2(I,J).EQ.0.) THEN
                  XB2N(I,J) = 0.0
              END IF
      END IF

*=====================================================================*
C         ARRANGE NEW RADIUS AND FRACTION MATRIX FOR COMPONENT 3
C                        FOR CONVERT PARTICLES
*=====================================================================*
      IF (RC(I,3).GE.RLOW(J+10).AND.RC(I,3).LT.UPPER(J+10)) THEN
          RC3(I,J)  = RC(I,3)
          XB3N(I,J) = FXB(I,3)

              IF (RC3(I,J).EQ.0.) THEN
                  XB3N(I,J) = 0.0
              END IF
      END IF

*=====================================================================*
C         ARRANGE NEW RADIUS AND FRACTION MATRIX FOR COMPONENT 4
C                        FOR CONVERT PARTICLES
*=====================================================================*
      IF (RC(I,4).GE.RLOW(J+15).AND.RC(I,4).LT.UPPER(J+15)) THEN
```

```
          RC4(I,J)  = RC(I,4)
          XB4N(I,J) = FXB(I,4)

              IF (RC4(I,J).EQ.0.) THEN
                  XB4N(I,J) = 0.0
              END IF
      END IF

*=====================================================================*
C         ARRANGE NEW RADIUS AND FRACTION MATRIX FOR COMPONENT 5
C                         FOR CONVERT PARTICLES
*=====================================================================*
      IF (RC(I,5).GE.RLOW(J+20).AND.RC(I,5).LT.UPPER(J+20)) THEN
              RC5(I,J)  = RC(I,5)
              XB5N(I,J) = FXB(I,5)

              IF (RC5(I,J).EQ.0.) THEN
                  XB5N(I,J) = 0.0
              END IF
240   END IF
*---------------------------------------------------------------------*

!     WRITE (7,241) ((RC1(I,J),J=1,5),I=1,5)
!241   FORMAT(2X, 'ARRANGE NEW RADIUS FOR COMPONENT 1',/5(1X,E10.3))

!     WRITE (7,242) ((XB1N(I,J),J=1,5),I=1,5)
!242   FORMAT(2X, 'ARRANGE NEW FRACTION FOR COMPONENT 1',/5(1X,E10.3))

C     WRITE (7,243) ((RC2(I,J),J=1,5),I=1,5)
C243  FORMAT(2X, 'ARRANGE NEW RADIUS FOR COMPONENT 2',/5(1X,E10.3))

C     WRITE (7,244) ((XB2N(I,J),J=1,5),I=1,5)
C244  FORMAT(2X, 'ARRANGE NEW FRACTION FOR COMPONENT 2',/5(1X,E10.3))

C     WRITE (7,246) ((RC3(I,J),J=1,5),I=1,5)
C246  FORMAT(2X, 'ARRANGE NEW RADIUS FOR COMPONENT 3',/5(1X,E10.3))

C     WRITE (7,247) ((XB3N(I,J),J=1,5),I=1,5)
C247  FORMAT(2X, 'ARRANGE NEW FRACTION FOR COMPONENT 3',/5(1X,E10.3))

C     WRITE (7,248) ((RC4(I,J),J=1,5),I=1,5)
C248  FORMAT(2X, 'ARRANGE NEW RADIUS FOR COMPONENT 4',/5(1X,E10.3))

C     WRITE (7,249) ((XB4N(I,J),J=1,5),I=1,5)
C249  FORMAT(2X, 'ARRANGE NEW FRACTION FOR COMPONENT 4',/5(1X,E10.3))

C     WRITE (7,251) ((RC5(I,J),J=1,5),I=1,5)
C251  FORMAT(2X, 'ARRANGE NEW RADIUS FOR COMPONENT 5',/5(1X,E10.3))

C     WRITE (7,252) ((XB5N(I,J),J=1,5),I=1,5)
C252  FORMAT(2X, 'ARRANGE NEW FRACTION FOR COMPONENT 5',/5(1X,E10.3))
*---------------------------------------------------------------------*

*=====================================================================*
C     NORMALIZE WEIGHT FRACTION FOR EACH INTERVAL AND EACH COMPONENT
C                         FOR CONVERT PARTICLES
*=====================================================================*
      DO 265 I = 1,5
      SUM1(I) = 0.0
      SUM2(I) = 0.0
      SUM3(I) = 0.0
      SUM4(I) = 0.0
265   SUM5(I) = 0.0

      DO 270 J = 1,5
      DO 270 I = 1,5
      SUM1(J) = SUM1(J) + XB1N(I,J)
      SUM2(J) = SUM2(J) + XB2N(I,J)
      SUM3(J) = SUM3(J) + XB3N(I,J)
      SUM4(J) = SUM4(J) + XB4N(I,J)
```

```
      SUM5(J) = SUM5(J) + XB5N(I,J)

C     PREPARE MATRIX FOR NORMALIZED WEIGHT FRACTION
      XB1N2(I,J) = 0.0
      XB2N2(I,J) = 0.0
      XB3N2(I,J) = 0.0
      XB4N2(I,J) = 0.0
270   XB5N2(I,J) = 0.0

      DO 280 J = 1,5
      DO 280 I = 1,5

      IF (SUM1(J).NE.0.) THEN
      XB1N2(I,J) = XB1N(I,J)/SUM1(J)
      END IF

              IF (SUM2(J).NE.0.) THEN
              XB2N2(I,J) = XB2N(I,J)/SUM2(J)
              END IF

                  IF (SUM3(J).NE.0.) THEN
                  XB3N2(I,J) = XB3N(I,J)/SUM3(J)
                  END IF

              IF (SUM4(J).NE.0.) THEN
              XB4N2(I,J) = XB4N(I,J)/SUM4(J)
              END IF

      IF (SUM5(J).NE.0.) THEN
      XB5N2(I,J) = XB5N(I,J)/SUM5(J)
280   END IF

!     WRITE (7,281) ((XB1N2(I,J),J=1,5),I=1,5)
!281   FORMAT(2X, 'NORMALIZED FRACTION FOR COMPONENT 1',/5(1X,E10.3))

C     WRITE (7,282) ((XB2N2(I,J),J=1,5),I=1,5)
C282  FORMAT(2X, 'NORMALIZED FRACTION FOR COMPONENT 2',/5(1X,E10.3))

C     WRITE (7,283) ((XB3N2(I,J),J=1,5),I=1,5)
C283  FORMAT(2X, 'NORMALIZED FRACTION FOR COMPONENT 3',/5(1X,E10.3))

C     WRITE (7,284) ((XB4N2(I,J),J=1,5),I=1,5)
C284  FORMAT(2X, 'NORMALIZED FRACTION FOR COMPONENT 4',/5(1X,E10.3))

C     WRITE (7,286) ((XB5N2(I,J),J=1,5),I=1,5)
C286  FORMAT(2X, 'NORMALIZED FRACTION FOR COMPONENT 5',/5(1X,E10.3))
*--------------------------------------------------------------------*

*====================================================================*
C     MEAN RADIUS FOR EACH INTERVAL AND EACH COMPONENT
C                    FOR CONVERTED PARTICLES
*====================================================================*
      DO 285 J = 1,5
      DO 285 I = 1,5
      SIGMA(I,J) = 0.0
285   RCN2(I,J)  = 0.0

      DO 290 J = 1,5
      DO 290 I = 1,5

      IF (RC1(I,J).NE.0.) THEN
      SIGMA(J,1) = SIGMA(J,1) + XB1N2(I,J)/RC1(I,J)
      END IF

          IF (RC2(I,J).NE.0.) THEN
          SIGMA(J,2) = SIGMA(J,2) + XB2N2(I,J)/RC2(I,J)
          END IF

              IF (RC3(I,J).NE.0.) THEN
              SIGMA(J,3) = SIGMA(J,3) + XB3N2(I,J)/RC3(I,J)
```

```
              END IF

          IF (RC4(I,J).NE.0.) THEN
          SIGMA(J,4) = SIGMA(J,4) + XB4N2(I,J)/RC4(I,J)
          END IF

      IF (RC5(I,J).NE.0.) THEN
      SIGMA(J,5) = SIGMA(J,5) + XB5N2(I,J)/RC5(I,J)
290   END IF

C     WRITE (7,291) ((SIGMA(I,J),J=1,5),I=1,5)
C291  FORMAT(2X, 'SIGMA',/5(1X,E10.3))

C     ROW = RADIUS, COLUMN = COMPONENT

      DO 300 J = 1,5
      DO 300 I = 1,5
      IF (SIGMA(I,J).NE.0.) THEN
      RCN2(I,J) = 1./SIGMA(I,J)
300   END IF

C     WRITE (7,301) ((RCN2(I,J),J=1,5),I=1,5)
C301   FORMAT(2X, 'NEW RADIUS FOR EACH INTERVAL',/5(1X,E10.3))
*-----------------------------------------------------------------------*

*=======================================================================*
C         NEW FRACTION FOR NEXT STEP OF CONVERT PARTICLES
*=======================================================================*
C     ROW = WEIGHT FRACTION, COLUMN = COMPONENT
      DO 305 I = 1,5
305   SUMM(I) = 0.0

      DO 310 I = 1,5
      SUMM(1) = SUMM(1) + SUM1(I)
      SUMM(2) = SUMM(2) + SUM2(I)
      SUMM(3) = SUMM(3) + SUM3(I)
      SUMM(4) = SUMM(4) + SUM4(I)
310   SUMM(5) = SUMM(5) + SUM5(I)

      DO 315 J = 1,5
      DO 315 I = 1,5
315   XBN(I,J) = 0.0

      DO 320 I = 1,5
      IF (SUMM(1).NE.0.) THEN
      XBN(I,1) = SUM1(I)/SUMM(1)
      END IF

          IF (SUMM(2).NE.0.) THEN
          XBN(I,2) = SUM2(I)/SUMM(2)
          END IF

              IF (SUMM(3).NE.0.) THEN
              XBN(I,3) = SUM3(I)/SUMM(3)
              END IF

          IF (SUMM(4).NE.0.) THEN
          XBN(I,4) = SUM4(I)/SUMM(4)
          END IF

      IF (SUMM(5).NE.0.) THEN
      XBN(I,5) = SUM5(I)/SUMM(5)
320   END IF

!     WRITE (7,321) ((XBN(I,J),J=1,5),I=1,5)
!321   FORMAT(2X, 'NEW FRACTION FOR NEXT STEP OF CONVERTED',/5(1X,E10.3))
*-----------------------------------------------------------------------*

*=======================================================================*
C            MEAN RADIUS AND WEIGHT FRACTION FOR NEXT STEP
```

```
C              BOTH CONVERTED AND UNCONVERTED PARTICLES
*=====================================================================*

C     UNCONVERTED PARTICLES SIZE DISTRIBUTION
      DO 325 J = 1,5
      DO 325 I = 1,5
      UXB01(I,J) = 0.0
      FIPSD(I,J) = 0.0
      UXBNR(I,J) = 0.0
      XBNNR(I,J) = 0.0
      WBYR1(I,J) = 0.0
      WBYR2(I,J) = 0.0
      SWBYR(I,J) = 0.0
325   FIRC(I,J)  = 0.0

      DO 330 J = 1,5
      DO 330 I = 1,5
      UXB01(I,J) = WPSDNEW(I,J) - FXB(I,J)

C     NORMALIZE WEIGHT FRACTION FOR FIND MEAN RADIUS

C     SUMMATION OF FRACTION
      FIPSD(I,J) = UXB(I,J) + XBN(I,J)

C     NORMALIZE UXB(I,J) AND XBN(I,J)
          IF (FIPSD(I,J).NE.0.0) THEN
              UXBNR(I,J) = UXB(I,J)/FIPSD(I,J)
              XBNNR(I,J) = XBN(I,J)/FIPSD(I,J)
330       END IF

!     WRITE (7,331) ((UXB01(I,J),J=1,5),I=1,5)
!331   FORMAT(2X, 'UXB01',/5(1X,E10.3))

!     WRITE (7,336) ((FIPSD(I,J),J=1,5),I=1,5)
!336  FORMAT(2X, 'SUMMATION OF FRACTION',/5(1X,E10.3))

!     WRITE (7,341) ((UXBNR(I,J),J=1,5),I=1,5)
!341  FORMAT(2X, 'NORMALIZED UXB',/5(1X,E10.3))

!     WRITE (7,342) ((XBNNR(I,J),J=1,5),I=1,5)
!342  FORMAT(2X, 'NORMALIZED XBN',/5(1X,E10.3))

C     FINAL RADIUS FOR NEXT STEP
      DO 345 J = 1,5
      DO 345 I = 1,5

      IF (RMEAN(I,J).NE.0.) THEN
      WBYR1(I,J) = UXBNR(I,J)/RMEAN(I,J)
      END IF

      IF (RCN2(I,J).NE.0.) THEN
      WBYR2(I,J) = XBNNR(I,J)/RCN2(I,J)
      END IF

      SWBYR(I,J) = WBYR1(I,J) + WBYR2(I,J)

      IF (SWBYR(I,J).NE.0.) THEN
      FIRC(I,J) = 1./SWBYR(I,J)
345   END IF



C     WRITE (7,346) ((WBYR1(I,J),J=1,5),I=1,5)
C346  FORMAT(2X, '',/5(1X,E10.3))

C     WRITE (7,347) ((WBYR2(I,J),J=1,5),I=1,5)
C347  FORMAT(2X, '',/5(1X,E10.3))

!     WRITE (7,348) ((FIRC(I,J),J=1,5),I=1,5)
!348  FORMAT(2X, 'FINAL RADIUS FOR NEXT STEP',/5(1X,E10.3))
```

```
*-------------------------------------------------------------------*
C     NEW FRACTION FOR NEXT STEP
C     NORMALIZE SUMMATION OF FRACTION
C     PREPARE MATRIX OF NEW FRACTION FOR NEXT STEP

      DO 450 I = 1,5
450   SUMFI(I) = 0.0

      DO 355 J = 1,5
      DO 355 I = 1,5
355   SUMFI(J) = SUMFI(J) + FIPSD(I,J)

      DO 360 J = 1,5
      DO 360 I = 1,5
360   FIPSDN(I,J) = FIPSD(I,J)/SUMFI(J)

!     WRITE (7,361) ((FIPSDN(I,J),J=1,5),I=1,5)
!361  FORMAT(2X, 'FINAL WEIGHT FRACTION FOR NEXT STEP',/5(1X,E10.3))
*-------------------------------------------------------------------*

*===================================================================*
C         ARRANGE FINAL RADIUS AND FRACTION MATRIX FOR COMPONENT 1
*===================================================================*
      DO 350 I = 1,5
      DO 350 J = 1,5
      RF1(I,J) = 0.0
      RF2(I,J) = 0.0
      RF3(I,J) = 0.0
      RF4(I,J) = 0.0
      RF5(I,J) = 0.0
      FIPSD1(I,J) = 0.0
      FIPSD2(I,J) = 0.0
      FIPSD3(I,J) = 0.0
      FIPSD4(I,J) = 0.0
350   FIPSD5(I,J) = 0.0

      DO 365 J = 1,5
      DO 365 I = 1,5

      IF (FIRC(I,1).GE.RLOW(J).AND.FIRC(I,1).LT.UPPER(J)) THEN
          RF1(I,J)    = FIRC(I,1)
          FIPSD1(I,J) = FIPSDN(I,1)

              IF (RF1(I,J).EQ.0.) THEN
                  FIPSD1(I,J) = 0.0
              END IF

      END IF

*===================================================================*
C         ARRANGE FINAL RADIUS AND FRACTION MATRIX FOR COMPONENT 2
*===================================================================*
      IF (FIRC(I,2).GE.RLOW(J+5).AND.FIRC(I,2).LT.UPPER(J+5)) THEN
          RF2(I,J)    = FIRC(I,2)
          FIPSD2(I,J) = FIPSDN(I,2)

              IF (RF2(I,J).EQ.0.) THEN
                  FIPSD2(I,J) = 0.0
              END IF
      END IF

*===================================================================*
C         ARRANGE FINAL RADIUS AND FRACTION MATRIX FOR COMPONENT 3
*===================================================================*
      IF (FIRC(I,3).GE.RLOW(J+10).AND.FIRC(I,3).LT.UPPER(J+10)) THEN
          RF3(I,J)    = FIRC(I,3)
          FIPSD3(I,J) = FIPSDN(I,3)

              IF (RF3(I,J).EQ.0.) THEN
                  FIPSD3(I,J) = 0.0
```

```
              END IF
      END IF

*=====================================================================*
C         ARRANGE FINAL RADIUS AND FRACTION MATRIX FOR COMPONENT 4
*=====================================================================*
      IF (FIRC(I,4).GE.RLOW(J+15).AND.FIRC(I,4).LT.UPPER(J+15)) THEN
          RF4(I,J)    = FIRC(I,4)
          FIPSD4(I,J) = FIPSDN(I,4)

              IF (RF4(I,J).EQ.0.) THEN
                  FIPSD4(I,J) = 0.0
              END IF
      END IF

*=====================================================================*
C         ARRANGE FINAL RADIUS AND FRACTION MATRIX FOR COMPONENT 5
*=====================================================================*
      IF (FIRC(I,5).GE.RLOW(J+20).AND.FIRC(I,5).LT.UPPER(J+20)) THEN
              RF5(I,J)    = FIRC(I,5)
              FIPSD5(I,J) = FIPSDN(I,5)

              IF (RF5(I,J).EQ.0.) THEN
                  FIPSD5(I,J) = 0.0
              END IF
365   END IF

*---------------------------------------------------------------------*
!     WRITE (7,366) ((RF1(I,J),J=1,5),I=1,5)
!366   FORMAT(2X, 'ARRANGE FINAL RADIUS FOR COMPONENT 1',/5(1X,E10.3))

!     WRITE (7,367) ((FIPSD1(I,J),J=1,5),I=1,5)
!367   FORMAT(2X, 'ARRANGE FINAL FRACTION FOR COMPONENT 1',/5(1X,E10.3))

C     WRITE (7,368) ((RF2(I,J),J=1,5),I=1,5)
C368   FORMAT(2X, 'ARRANGE FINAL RADIUS FOR COMPONENT 2',/5(1X,E10.3))

C     WRITE (7,369) ((FIPSD2(I,J),J=1,5),I=1,5)
C369   FORMAT(2X, 'ARRANGE FINAL FRACTION FOR COMPONENT 2',/5(1X,E10.3))

C     WRITE (7,371) ((RF3(I,J),J=1,5),I=1,5)
C371   FORMAT(2X, 'ARRANGE FINAL RADIUS FOR COMPONENT 3',/5(1X,E10.3))

C     WRITE (7,372) ((FIPSD3(I,J),J=1,5),I=1,5)
C372   FORMAT(2X, 'ARRANGE FINAL FRACTION FOR COMPONENT 3',/5(1X,E10.3))

C     WRITE (7,373) ((RF4(I,J),J=1,5),I=1,5)
C373   FORMAT(2X, 'ARRANGE FINAL RADIUS FOR COMPONENT 4',/5(1X,E10.3))

C     WRITE (7,374) ((FIPSD4(I,J),J=1,5),I=1,5)
C374   FORMAT(2X, 'ARRANGE FINAL FRACTION FOR COMPONENT 4',/5(1X,E10.3))

C     WRITE (7,376) ((RF5(I,J),J=1,5),I=1,5)
C376   FORMAT(2X, 'ARRANGE FINAL RADIUS FOR COMPONENT 5',/5(1X,E10.3))

C     WRITE (7,377) ((FIPSD5(I,J),J=1,5),I=1,5)
C377   FORMAT(2X, 'ARRANGE FINAL FRACTION FOR COMPONENT 5',/5(1X,E10.3))
*---------------------------------------------------------------------*


*=====================================================================*
C     NORMALIZE WEIGHT FRACTION FOR EACH INTERVAL AND EACH COMPONENT
*=====================================================================*
      DO 380 I = 1,5
      SM1(I) = 0.0
      SM2(I) = 0.0
      SM3(I) = 0.0
      SM4(I) = 0.0
380   SM5(I) = 0.0
```

```
      DO 385 J = 1,5
      DO 385 I = 1,5
      SM1(J) = SM1(J) + FIPSD1(I,J)
      SM2(J) = SM2(J) + FIPSD2(I,J)
      SM3(J) = SM3(J) + FIPSD3(I,J)
      SM4(J) = SM4(J) + FIPSD4(I,J)
      SM5(J) = SM5(J) + FIPSD5(I,J)

C     PREPARE MATRIX FOR NORMALIZED WEIGHT FRACTION
      FXB1(I,J) = 0.0
      FXB2(I,J) = 0.0
      FXB3(I,J) = 0.0
      FXB4(I,J) = 0.0
385   FXB5(I,J) = 0.0

      DO 390 J = 1,5
      DO 390 I = 1,5

      IF (SM1(J).NE.0.) THEN
      FXB1(I,J) = FIPSD1(I,J)/SM1(J)
      END IF

              IF (SM2(J).NE.0.) THEN
              FXB2(I,J) = FIPSD2(I,J)/SM2(J)
              END IF

                  IF (SM3(J).NE.0.) THEN
                  FXB3(I,J) = FIPSD3(I,J)/SM3(J)
                  END IF

              IF (SM4(J).NE.0.) THEN
              FXB4(I,J) = FIPSD4(I,J)/SM4(J)
              END IF

      IF (SM5(J).NE.0.) THEN
      FXB5(I,J) = FIPSD5(I,J)/SM5(J)
390   END IF

!     WRITE (7,391) ((FXB1(I,J),J=1,5),I=1,5)
!391   FORMAT(2X, 'NORMALIZED FINAL FRACTION COMPONENT 1',/5(1X,E10.3))

C     WRITE (7,392) ((FXB2(I,J),J=1,5),I=1,5)
C392   FORMAT(2X, 'NORMALIZED FINAL FRACTION COMPONENT 2',/5(1X,E10.3))

C     WRITE (7,393) ((FXB3(I,J),J=1,5),I=1,5)
C393   FORMAT(2X, 'NORMALIZED FINAL FRACTION COMPONENT 3',/5(1X,E10.3))

C     WRITE (7,394) ((FXB4(I,J),J=1,5),I=1,5)
C394   FORMAT(2X, 'NORMALIZED FINAL FRACTION COMPONENT 4',/5(1X,E10.3))

C     WRITE (7,396) ((FXB5(I,J),J=1,5),I=1,5)
C396   FORMAT(2X, 'NORMALIZED FINAL FRACTION COMPONENT 5',/5(1X,E10.3))
*--------------------------------------------------------------------*

*====================================================================*
C     MEAN RADIUS FOR EACH INTERVAL AND EACH COMPONENT
C                        FOR FINAL PARTICLES
*====================================================================*
      DO 400 J = 1,5
      DO 400 I = 1,5
      FSIGMA(I,J) = 0.0
400   FRFN(I,J) = 0.0

      DO 405 J = 1,5
      DO 405 I = 1,5

      IF (RF1(I,J).NE.0.) THEN
      FSIGMA(J,1) = FSIGMA(J,1) + FXB1(I,J)/RF1(I,J)
      END IF
```

```
          IF (RF2(I,J).NE.0.) THEN
          FSIGMA(J,2) = FSIGMA(J,2) + FXB2(I,J)/RF2(I,J)
          END IF

              IF (RF3(I,J).NE.0.) THEN
              FSIGMA(J,3) = FSIGMA(J,3) + FXB3(I,J)/RF3(I,J)
              END IF

          IF (RF4(I,J).NE.0.) THEN
          FSIGMA(J,4) = FSIGMA(J,4) + FXB4(I,J)/RF4(I,J)
          END IF

      IF (RF5(I,J).NE.0.) THEN
      FSIGMA(J,5) = FSIGMA(J,5) + FXB5(I,J)/RF5(I,J)
405   END IF

!     WRITE (7,406) ((FSIGMA(I,J),J=1,5),I=1,5)
!406  FORMAT(2X, 'FSIGMA',/5(1X,E10.3))

C     ROW = RADIUS, COLUMN = COMPONENT

      DO 410 J = 1,5
      DO 410 I = 1,5
      IF (FSIGMA(I,J).NE.0.) THEN
      FRFN(I,J) = 1./FSIGMA(I,J)
410   END IF

      WRITE (7,411) ((FRFN(I,J),J=1,5),I=1,5)
411   FORMAT(2X, 'NEW FINAL RADIUS FOR EACH INTERVAL',/5(1X,E10.3))
*-----------------------------------------------------------------------*

*=======================================================================*
C         NEW FRACTION FOR NEXT STEP OF FINAL PARTICLES
*=======================================================================*
C     ROW = WEIGHT FRACTION, COLUMN = COMPONENT
      DO 415 I = 1,5
415   SUMF(I) = 0.0

      DO 420 I = 1,5
      SUMF(1) = SUMF(1) + SM1(I)
      SUMF(2) = SUMF(2) + SM2(I)
      SUMF(3) = SUMF(3) + SM3(I)
      SUMF(4) = SUMF(4) + SM4(I)
420   SUMF(5) = SUMF(5) + SM5(I)

      DO 425 J = 1,5
      DO 425 I = 1,5
425   FIPSDN2(I,J) = 0.0

      DO 430 I = 1,5

      IF (SUMF(1).NE.0.) THEN
      FIPSDN2(I,1) = SM1(I)/SUMF(1)
      END IF

          IF (SUMF(2).NE.0.) THEN
          FIPSDN2(I,2) = SM2(I)/SUMF(2)
          END IF

              IF (SUMF(3).NE.0.) THEN
              FIPSDN2(I,3) = SM3(I)/SUMF(3)
              END IF

          IF (SUMF(4).NE.0.) THEN
          FIPSDN2(I,4) = SM4(I)/SUMF(4)
          END IF

      IF (SUMF(5).NE.0.) THEN
      FIPSDN2(I,5) = SM5(I)/SUMF(5)
430   END IF
```

```
      WRITE (7,431) ((FIPSDN2(I,J),J=1,5),I=1,5)
431   FORMAT(2X, 'NEW FRACTION FOR FINAL STEP ',/5(1X,E10.3))
*-----------------------------------------------------------------------*


C     INPUT WEIGHT FRACTION FOR NEXT STEP
      DO 435 I = 1,5
      ID(I,1) = IDXSUB(3) -1 + NCOMP_NCC + (I+9)
      ID(I,2) = IDXSUB(5) -1 + NCOMP_NCC + (I+9)
      ID(I,3) = IDXSUB(7) -1 + NCOMP_NCC + (I+9)
      ID(I,4) = IDXSUB(9) -1 + NCOMP_NCC + (I+9)
435   ID(I,5) = IDXSUB(11) -1 + NCOMP_NCC + (I+9)

C     WRITE (7,366) ((ID(I,J),J=1,5),I=1,5)
C366  FORMAT(2X, 'ID',/5(1X,I3))


      DO 440 J = 1,5
      DO 440 I = 1,5
440   SOUT(ID(I,J)) = FIPSDN2(I,J)

      RETURN
      END
```

Appendix C

Subroutine for NOx emissions

C-1 Subroutine of NO formation

```
*==========================================================================*
C     User Subroutine for NOx formation.
*==========================================================================*
      Subroutine USRKI5  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*--------------------------------------------------------------------------*
      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)

C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

C     DECLARE LOCAL VARIABLES
      COMMON /USER7/ FRFN,  FIPSDN2, RLOW,  UPPER
      COMMON /USER18/ SPAREA, Tp

      DIMENSION FRFN(5,5),     FIPSDN2(5,5),     RLOW(26),
     .          UPPER(25),     FDR(5,5),         SFDR(5),
     .          SFDRM(5),      SFIPSDN2(5),      WTN(5),
     .          WTND(5),       RK(7)

      INTEGER IMISS, DMS_KCCIDC
      REAL*8  RMISS

      OPEN(7,FILE='NOX1.txt')

*--------------------------------------------------------------------------*
C     ORDER OF SUBSTREAM MIXED, CISOLID, CIPSD1, NCPSD1, CIPSD2, NCPSD2,
C     CIPSD3, NCPSD3, CIPSD4, NCPSD4, CIPSD5 AND NCPSD5
*--------------------------------------------------------------------------*

C     DECLARE LOCAL OF OXYGEN
```

```
      IDXO2   = DMS_KCCIDC('O2')
C     WRITE (7,*) 'LOCAL ID. OF O2   =',IDXO2

C     DECLARE LOCAL OF NITROGEN
      IDXN2   = DMS_KCCIDC('N2')
C     WRITE (7,*) 'LOCAL ID. OF N2   =',IDXN2

C     DECLARE LOCAL OF NITRIC OXIDE
      IDXNO  = DMS_KCCIDC('NO')
C     WRITE (7,*) 'LOCAL ID. OF NO  =',IDXNO

*---------------------------------------------------------------------*
C                    MEAN RADIUS OF ALL PARTICLES
*---------------------------------------------------------------------*

C     INPUT THE RADIUS AND WEIGHT FRACTION FROM THE CSRT BLOCK (USRKI1)

C     WRITE (7,411) ((FRFN(I,J),J=1,5),I=1,5)
C411  FORMAT(2X, 'NEW FINAL RADIUS FOR EACH INTERVAL',/5(1X,E10.3))
C     WRITE (7,431) ((FIPSDN2(I,J),J=1,5),I=1,5)
C431   FORMAT(2X, 'NEW FRACTION FOR FINAL STEP ',/5(1X,E10.3))

C     CALCULATE MEAN RADIUS OF EACH FUEL
C     FRACTION DIVIDED BY RADIUS
      DO 5 J = 1,5
      DO 5 I = 1,5
5     FDR(I,J) = 0.0

      DO 10 J = 1,5
      DO 10 I = 1,5
      IF (FRFN(I,J).NE.0.) THEN
      FDR(I,J) = FIPSDN2(I,J)/FRFN(I,J)
10    END IF

C     WRITE (7,11) ((FDR(I,J),J=1,5),I=1,5)
C11   FORMAT(2X, 'FRACTION DIVIDED BY RADIUS',/5(1X,E10.3))

C     SUMMATION OF FRACTION DIVIDED BY RADIUS OF EACH FUEL
      DO 15 I = 1,5
      SFDR(I) = 0.0
      SFDRM(I) = 0.0
      SFIPSDN2(I) = 0.0
15    WTN(I) = 0.0

      DO 20 J = 1,5
      DO 20 I = 1,5
20    SFDR(I) = SFDR(I) + FDR(J,I)

C     WRITE (7,21) (SFDR(I),I=1,5)
C21   FORMAT(2X, 'SFDR',/5(1X,E10.3))

C     MEAN RADIUS FOR EACH PARTICLE
      DO 25 I = 1,5
      IF (SFDR(I).NE.0.) THEN
      SFDRM(I) = 1/SFDR(I)
25    END IF

C     WRITE (7,22) (SFDRM(I),I=1,5)
C22   FORMAT(2X, 'SFDRM',/5(1X,E10.3))

C     NORMALIZE WEIGHT FRACTION OF EACH FUEL
C     SUMMATION OF WEIGHT FRACTION OF EACH FUEL

      DO 30 J = 1,5
      DO 30 I = 1,5
30    SFIPSDN2(I) = SFIPSDN2(I) + FIPSDN2(J,I)

C     WRITE (7,31) (SFIPSDN2(I),I=1,5)
C31   FORMAT(2X, 'SFIPSDN2',/5(1X,E10.3))
```

```
C     NEW WEIGHT FRACTION FOR EACH FUEL
      SUMM = 0.0
      DO 35 I = 1,5
35    SUMM = SUMM + SFIPSDN2(I)

      DO 40 I = 1,5
40    WTN(I) = SFIPSDN2(I)/SUMM

C     WRITE (7,41) (WTN(I),I=1,5)
C41   FORMAT(2X, 'WTN',/5(1X,E10.3))

C     MEAN RADIUS OF ALL PARTICLES
      DO 45 I = 1,5
45    WTND(I) = WTN(I)/SFDRM(I)

C     WRITE (7,46) (WTND(I),I=1,5)
C46   FORMAT(2X, 'WTND',/5(1X,E10.3))

      SUMM = 0.0
      DO 50 I = 1,5
50    SUMM = SUMM + WTND(I)

      RADIUS = 1/SUMM
      WRITE (7,*) 'MEAN RADIUS OF ALL PATICLE', RADIUS

C     NO FORMATION    N2 + O2 --> 2NO
C     CALCULATE THE SPECIFIC AREA OF PARTICLE (1/m)
      SPAREA = 3./RADIUS
      Tp   = SOUT(NCOMP_NCC + 2)
      RKA = 250.*Tp*DEXP(-19000/Tp)*SPAREA
      RK(1) = 4.*RKA*REAL(1)*RCSTRR_VOLRC / 3.
      WRITE (7,*) 'RKA, RK(1)', RKA, RK(1)

*=====================================================================*
C                     REACTION RATES IN MIXED
*=====================================================================*
      DO 55 I = 1,NCOMP_NCC
55    RATES(I) = 0.0

C     CHECK KINETIC RATE

      RKN = RK(1)
      IF (RKN.GT.REAL(2).OR.RKN.GT.REAL(3)) THEN

          IF (REAL(2).GT.REAL(3)) THEN
              RKN = REAL(3)*0.99
                  RK(1) = RKN
                      ELSE IF (REAL(3).GT.REAL(2)) THEN
                  RKN = REAL(2)*0.99
              RK(1) = RKN
          END IF
      ELSE
          GOTO 60
      END IF

C     FOR NITROGEN
60    RATES(IDXN2) = -RK(1)
      WRITE (7,*) 'RATES N2 IN MIXED  = ', RATES(IDXN2)

C     FOR OXYGEN
      RATES(IDXO2) = -RK(1)
      WRITE (7,*) 'RATES O2 IN MIXED  = ', RATES(IDXO2)

C     FOR NITRIC-OXIDE
      RATES(IDXNO) = 2.*RK(1)
      WRITE (7,*) 'RATES NO IN MIXED  = ', RATES(IDXNO)
*---------------------------------------------------------------------*
      RETURN
      END
```

C-2 Subroutine of N2O Formation

```
*=====================================================================*
C     User Subroutine for NOx formation.
*=====================================================================*

      Subroutine USRKI6  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*---------------------------------------------------------------------*

      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)

C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

C     DECLARE LOCAL VARIABLES
      COMMON /USER18/ SPAREA, Tp

      DIMENSION RK(7)

      INTEGER IMISS, DMS_KCCIDC
      REAL*8  RMISS

      OPEN(7,FILE='NOX2.txt')

*---------------------------------------------------------------------*
C     ORDER OF SUBSTREAM MIXED, CISOLID, CIPSD1, NCPSD1, CIPSD2, NCPSD2,
C     CIPSD3, NCPSD3, CIPSD4, NCPSD4, CIPSD5 AND NCPSD5
*---------------------------------------------------------------------*

C     DECLARE LOCAL OF NITROGEN
      IDXN2   = DMS_KCCIDC('N2')
C     WRITE (7,*) 'LOCAL ID. OF N2   =',IDXN2

C     DECLARE LOCAL OF NITRIC OXIDE
      IDXNO  = DMS_KCCIDC('NO')
C     WRITE (7,*) 'LOCAL ID. OF NO  =',IDXNO

C     DECLARE LOCAL OF NITROUS OXIDE
```

```
      IDXN2O  = DMS_KCCIDC('N2O')
C     WRITE (7,*) 'LOCAL ID. OF N2O  =',IDXN2O

*---------------------------------------------------------------------*
C                       NOx FORMATION AND REDUCTION                   C
*---------------------------------------------------------------------*

C     N2O FORMATION   N2 + 2NO --> 2N2O
      RKD = 3.*SPAREA*DEXP(-9000/Tp)
      RK(2) = RKD*REAL(1)*RCSTRR_VOLRC

*---------------------------------------------------------------------*

*=====================================================================*
C                     REACTION RATES IN MIXED
*=====================================================================*
      DO 55 I = 1,NCOMP_NCC
55    RATES(I) = 0.0

      RKN = 2.*RK(2)
      IF (RKN.GT.REAL(2).OR.RKN.GT.REAL(3)) THEN

          IF (REAL(2).GT.REAL(3)) THEN
              RKN = REAL(3)*0.99
                  RK(2) = RKN/2.
                      ELSE IF (REAL(3).GT.REAL(2)) THEN
                  RKN = REAL(2)*0.99
              RK(2) = RKN/2.
          END IF
      ELSE
          GOTO 60
      END IF

C     FOR NITROGEN
60    RATES(IDXN2) = -RK(2)
      WRITE (7,*) 'RATES N2 IN MIXED  = ', RATES(IDXN2)

C     FOR NITRIC-OXIDE
      RATES(IDXNO) = -2.*RK(2)
      WRITE (7,*) 'RATES NO IN MIXED  = ', RATES(IDXNO)

C     FOR NITROUS-OXIDE
      RATES(IDXN2O) = 2.*RK(2)
      WRITE (7,*) 'RATES N2O IN MIXED  = ', RATES(IDXN2O)

      RETURN
      END
```

C-3 Subroutine of Reduction of NO by Char

```
*=====================================================================*
C     User Subroutine for NOx formation.
*=====================================================================*

      Subroutine USRKI7  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*---------------------------------------------------------------------*

      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP),         SORT1(6),      SORT2(6),
     .          SORT3(6)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)

C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

C     DECLARE LOCAL VARIABLES
      COMMON /USER18/ SPAREA, Tp

      DIMENSION RK(7)

      INTEGER IMISS, DMS_KCCIDC
      REAL*8  RMISS

      OPEN(7,FILE='NOX3.txt')

*---------------------------------------------------------------------*
C     ORDER OF SUBSTREAM MIXED, CISOLID, CIPSD1, NCPSD1, CIPSD2, NCPSD2,
C     CIPSD3, NCPSD3, CIPSD4, NCPSD4, CIPSD5 AND NCPSD5
*---------------------------------------------------------------------*

C     DECLARE LOCAL OF CARBON
      IDXC   = DMS_KCCIDC('C')
C     WRITE (7,*) 'LOCAL ID. OF C    =',IDXC

C     DECLARE LOCAL OF CARBON-MONOXIDE
      IDXCO   = DMS_KCCIDC('CO')
C     WRITE (7,*) 'LOCAL ID. OF CO   =',IDXCO
```

```
C     DECLARE LOCAL OF NITROGEN
      IDXN2   = DMS_KCCIDC('N2')
C     WRITE (7,*) 'LOCAL ID. OF N2   =',IDXN2

C     DECLARE LOCAL OF NITRIC OXIDE
      IDXNO  = DMS_KCCIDC('NO')
C     WRITE (7,*) 'LOCAL ID. OF NO  =',IDXNO

C     NO REDUCTION    2NO + 2C --> N2 + CO
      IF (Tp.LE.973.) THEN
              RKE = 0.159*SPAREA*DEXP(-6255/Tp)
          ELSE
              RKE = 555.6*SPAREA*DEXP(-14193/Tp)
      END IF
      RK(3) = RKE*REAL(1)*RCSTRR_VOLRC

*=======================================================================*
C                     REACTION RATES IN MIXED
*=======================================================================*
      DO 55 I = 1,NCOMP_NCC
55    RATES(I) = 0.0

      DO 90 I = 1,6
      SORT1(I) = REAL(I+1)
90    WRITE (7,*) 'BEFORE SORT REAL(I)', I,SORT1(I)

      N = 6
      LAST = N-1
      DO 95 I = 1,LAST
          M = I
          NEXT = M + 1

              DO 100 IN = NEXT,N
                      IF (SORT1(IN).GT.SORT1(M)) M = IN
100           CONTINUE

                  IF (M.NE.I) THEN
                      TEMP = SORT1(M)
                      SORT1(M) = SORT1(I)
                      SORT1(I) = TEMP
                      TEMP = SORT2(M)
                      SORT2(M) = SORT2(I)
                      SORT2(I) = TEMP
                  END IF
95    CONTINUE

C     DO 105 I = 1,N
C105  WRITE (7,*) 'AFTER SORT REAL(I)', I,SORT1(I)

      K = 0
      DO 110 I = 1,N
110       IF (SORT1(I).GT.1E-11) K = K+1

      DO 115 I = 1,K
          IF (SORT1(I).GT.1E-11) THEN
              SORT3(I) = SORT1(I)
115       END IF

      DO 120 I=1,K
120   WRITE (7,*) 'SORT3', SORT3(I)

      RKN = 2.*RK(3)

      IF (RKN.GT.SORT3(K)) THEN
          RKN = SORT3(K)*0.99
          RK(3) = RKN/2.
      ELSE
          GOTO 600
      END IF
```

```
C     FOR NITRIC-OXIDE
600   RATES(IDXNO) = -2.*RK(3)
      WRITE (7,*) 'RATES NO IN MIXED  = ', RATES(IDXNO)

C     FOR NITROGEN
      RATES(IDXN2) = 1.*RK(3)
      WRITE (7,*) 'RATES N2 IN MIXED  = ', RATES(IDXN2)

C     FOR CARBON MONOXIDE
      RATES(IDXCO) = 2.*RK(3)
      WRITE (7,*) 'RATES CO IN MIXED  = ', RATES(IDXCO)
*---------------------------------------------------------------------*

*=====================================================================*
C                     REACTION RATES IN CISOLID
*=====================================================================*
      L1 = NCOMP_NCC + 1
      L2 = L1 + NCOMP_NCC - 1

      DO 60 I = L1, L2
60    RATES(I) = 0.0

*=====================================================================*
C                     REACTION RATES IN CIPSD1
*=====================================================================*
      L3 = L2 + 1
      L4 = L3 + NCOMP_NCC - 1

      DO 65 I = L3, L4
65    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(3).GT.1E-11) THEN
          CCPSD1 = IDXC + L3 - 1
          RATES(CCPSD1) = -2.*RK(3)
          WRITE (7,*) 'RATES C IN CIPSD1  = ', RATES(CCPSD1)
      END IF
*=====================================================================*
C                     REACTION RATES IN CIPSD2
*=====================================================================*
      L5 = L4 + NCOMP_NNCC + 1
      L6 = L5 + NCOMP_NCC - 1

      DO 70 I = L5, L6
70    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(4).GT.1E-11) THEN
          CCPSD2 = IDXC + L5 - 1
          RATES(CCPSD2) = -2.*RK(3)
          WRITE (7,*) 'RATES C IN CIPSD2  = ', RATES(CCPSD2)
      END IF
*=====================================================================*
C                     REACTION RATES IN CIPSD3
*=====================================================================*

      L7 = L6 + NCOMP_NNCC + 1
      L8 = L7 + NCOMP_NCC - 1

      DO 75 I = L7, L8
75    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(5).GT.1E-11) THEN
          CCPSD3 = IDXC + L7 - 1
          RATES(CCPSD3) = -2.*RK(3)
          WRITE (7,*) 'RATES C IN CIPSD3  = ', RATES(CCPSD3)
      END IF
*=====================================================================*
C                     REACTION RATES IN CIPSD4
```

```
*=====================================================================*
      L9  = L8 + NCOMP_NNCC + 1
      L10 = L9 + NCOMP_NCC - 1

      DO 80 I = L9, L10
80    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(6).GT.1E-11) THEN
          CCPSD4 = IDXC + L9 - 1
          RATES(CCPSD4) = -2.*RK(3)
          WRITE (7,*) 'RATES C IN CIPSD4  = ', RATES(CCPSD4)
      END IF
*=====================================================================*
C                    REACTION RATES IN CIPSD5
*=====================================================================*
      L11 = L10 + NCOMP_NNCC + 1
      L12 = L11 + NCOMP_NCC - 1

      DO 85 I = L11, L12
85    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(7).GT.1E-11) THEN
          CCPSD5 = IDXC + L11 - 1
          RATES(CCPSD5) = -2.*RK(3)
          WRITE (7,*) 'RATES C IN CIPSD5  = ', RATES(CCPSD5)
      END IF
*---------------------------------------------------------------------*

      RETURN
      END
```

C-4 Subroutine of Reduction of NO by Char (2)

```
*======================================================================*
C     User Subroutine for NOx formation.
*======================================================================*

      Subroutine USRKI8  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*----------------------------------------------------------------------*

      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)

C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

C     DECLARE LOCAL VARIABLES
      COMMON /USER18/ SPAREA, Tp

      DIMENSION RK(7)

      INTEGER IMISS, DMS_KCCIDC
      REAL*8  RMISS

      OPEN(7,FILE='NOX4.txt')
*----------------------------------------------------------------------*
C     ORDER OF SUBSTREAM MIXED, CISOLID, CIPSD1, NCPSD1, CIPSD2, NCPSD2,
C     CIPSD3, NCPSD3, CIPSD4, NCPSD4, CIPSD5 AND NCPSD5
*----------------------------------------------------------------------*

C     DECLARE LOCAL OF CARBON-MONOXIDE
      IDXCO   = DMS_KCCIDC('CO')
C     WRITE (7,*) 'LOCAL ID. OF CO   =',IDXCO

C     DECLARE LOCAL OF CARBON-DIOXIDE
      IDXCO2   = DMS_KCCIDC('CO2')
C     WRITE (7,*) 'LOCAL ID. OF CO2   =',IDXCO2

C     DECLARE LOCAL OF NITROGEN
```

```
      IDXN2   = DMS_KCCIDC('N2')
C     WRITE (7,*) 'LOCAL ID. OF N2   =',IDXN2

C     DECLARE LOCAL OF NITRIC OXIDE
      IDXNO  = DMS_KCCIDC('NO')
C     WRITE (7,*) 'LOCAL ID. OF NO  =',IDXNO

C     NO REDUCTION    2NO + 2CO --> N2 + 2CO2
      RKF = 5.67E3*Tp*DEXP(-13952/Tp)
      RK(4) = RKF*REAL(1)*RCSTRR_VOLRC

*=====================================================================*
C                     REACTION RATES IN MIXED
*=====================================================================*
      DO 55 I = 1,NCOMP_NCC
55    RATES(I) = 0.0

      RKN = 2.*RK(4)

      IF (RKN.GT.REAL(2).OR.RKN.GT.REAL(3)) THEN

          IF (REAL(2).GT.REAL(3)) THEN
              RKN = REAL(3)*0.99
                  RK(4) = RKN/2.
                      ELSE IF (REAL(3).GT.REAL(2)) THEN
                  RKN = REAL(2)*0.99
              RK(4) = RKN/2.
          END IF
      ELSE
          GOTO 600
      END IF

C     FOR NITRIC-OXIDE
600   RATES(IDXNO) = -2.*RK(4)
      WRITE (7,*) 'RATES NO IN MIXED  = ', RATES(IDXNO)

C     FOR CARBON MONOXIDE
      RATES(IDXCO) = -2.*RK(4)
      WRITE (7,*) 'RATES CO IN MIXED  = ', RATES(IDXCO)

C     FOR NITROGEN
      RATES(IDXN2) = RK(4)
      WRITE (7,*) 'RATES N2 IN MIXED  = ', RATES(IDXN2)

C     FOR CARBON DIOXIDE
      RATES(IDXCO2) = 2.*RK(4)
      WRITE (7,*) 'RATES CO2 IN MIXED = ', RATES(IDXCO2)
*---------------------------------------------------------------------*

      RETURN
      END
```

C-5 Subroutine of Reduction of N2O by Char

```
*=====================================================================*
C     User Subroutine for NOx formation.
*=====================================================================*

      Subroutine USRKI9  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*---------------------------------------------------------------------*

      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP),         SORT1(6),      SORT2(6),
     .          SORT3(6)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)

C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

C     DECLARE LOCAL VARIABLES
      COMMON /USER18/ SPAREA, Tp

      DIMENSION RK(7)

      INTEGER IMISS, DMS_KCCIDC
      REAL*8  RMISS

      OPEN(7,FILE='NOX5.txt')

*---------------------------------------------------------------------*
C     ORDER OF SUBSTREAM MIXED, CISOLID, CIPSD1, NCPSD1, CIPSD2, NCPSD2,
C     CIPSD3, NCPSD3, CIPSD4, NCPSD4, CIPSD5 AND NCPSD5
*---------------------------------------------------------------------*

C     DECLARE LOCAL OF CARBON
      IDXC   = DMS_KCCIDC('C')
C     WRITE (7,*) 'LOCAL ID. OF C    =',IDXC

C     DECLARE LOCAL OF CARBON-MONOXIDE
      IDXCO   = DMS_KCCIDC('CO')
C     WRITE (7,*) 'LOCAL ID. OF CO   =',IDXCO
```

```
C     DECLARE LOCAL OF NITROGEN
      IDXN2   = DMS_KCCIDC('N2')
C     WRITE (7,*) 'LOCAL ID. OF N2   =',IDXN2

C     DECLARE LOCAL OF NITROUS OXIDE
      IDXN2O  = DMS_KCCIDC('N2O')
C     WRITE (7,*) 'LOCAL ID. OF N2O  =',IDXN2O

C     N2O REDUCTION   N2O + C --> N2 + CO
      RKG = 13.36*SPAREA*DEXP(-16677/Tp)
      RK(5) = RKG*REAL(1)*RCSTRR_VOLRC
*--------------------------------------------------------------------*

*====================================================================*
C                     REACTION RATES IN MIXED
*====================================================================*
      DO 55 I = 1,NCOMP_NCC
55    RATES(I) = 0.0

      DO 90 I = 1,6
90    SORT1(I) = REAL(I+1)
C90   WRITE (7,*) 'BEFORE SORT REAL(I)', I,SORT1(I)

      N = 6
      LAST = N-1
      DO 95 I = 1,LAST
          M = I
          NEXT = M + 1

              DO 100 IN = NEXT,N
                      IF (SORT1(IN).GT.SORT1(M)) M = IN
100           CONTINUE

                  IF (M.NE.I) THEN
                      TEMP = SORT1(M)
                      SORT1(M) = SORT1(I)
                      SORT1(I) = TEMP
                      TEMP = SORT2(M)
                      SORT2(M) = SORT2(I)
                      SORT2(I) = TEMP
                  END IF
95    CONTINUE

C     DO 105 I = 1,N
C105  WRITE (7,*) 'AFTER SORT REAL(I)', I,SORT1(I)

      K = 0
      DO 110 I = 1,N
110       IF (SORT1(I).GT.1E-11) K = K+1

      DO 115 I = 1,K
          IF (SORT1(I).GT.1E-11) THEN
              SORT3(I) = SORT1(I)
115       END IF

C     DO 120 I=1,K
C120  WRITE (7,*) 'SORT3', SORT3(I)

      RKN = 1.*RK(5)

      IF (RKN.GT.SORT3(K)) THEN
          RKN = SORT3(K)*0.99
          RK(5) = RKN/1.
      ELSE
          GOTO 600
      END IF

C     FOR NITROUS-OXIDE
600   RATES(IDXN2O) = -1.*RK(5)
      WRITE (7,*) 'RATES N2O IN MIXED  = ', RATES(IDXN2O)
```

```
C     FOR NITROGEN
      RATES(IDXN2) = 1.*RK(5)
      WRITE (7,*) 'RATES N2 IN MIXED  = ', RATES(IDXN2)

C     FOR CARBON MONOXIDE
      RATES(IDXCO) = 1.*RK(5)
      WRITE (7,*) 'RATES CO IN MIXED  = ', RATES(IDXCO)
*-----------------------------------------------------------------------*

*=======================================================================*
C                     REACTION RATES IN CISOLID
*=======================================================================*
      L1 = NCOMP_NCC + 1
      L2 = L1 + NCOMP_NCC - 1

      DO 60 I = L1, L2
60    RATES(I) = 0.0

*=======================================================================*
C                     REACTION RATES IN CIPSD1
*=======================================================================*
      L3 = L2 + 1
      L4 = L3 + NCOMP_NCC - 1

      DO 65 I = L3, L4
65    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(3).GT.1E-11) THEN
          CCPSD1 = IDXC + L3 - 1
          RATES(CCPSD1) = -RK(5)
          WRITE (7,*) 'RATES C IN CIPSD1  = ', RATES(CCPSD1)
      END IF
*=======================================================================*
C                     REACTION RATES IN CIPSD2
*=======================================================================*
      L5 = L4 + NCOMP_NNCC + 1
      L6 = L5 + NCOMP_NCC - 1

      DO 70 I = L5, L6
70    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(4).GT.1E-11) THEN
          CCPSD2 = IDXC + L5 - 1
          RATES(CCPSD2) = -RK(5)
          WRITE (7,*) 'RATES C IN CIPSD2  = ', RATES(CCPSD2)
      END IF
*=======================================================================*
C                     REACTION RATES IN CIPSD3
*=======================================================================*

      L7 = L6 + NCOMP_NNCC + 1
      L8 = L7 + NCOMP_NCC - 1

      DO 75 I = L7, L8
75    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(5).GT.1E-11) THEN
          CCPSD3 = IDXC + L7 - 1
          RATES(CCPSD3) = -RK(5)
          WRITE (7,*) 'RATES C IN CIPSD3  = ', RATES(CCPSD3)
      END IF
*=======================================================================*
C                     REACTION RATES IN CIPSD4
*=======================================================================*
      L9  = L8 + NCOMP_NNCC + 1
      L10 = L9 + NCOMP_NCC - 1
```

```
      DO 80 I = L9, L10
80    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(6).GT.1E-11) THEN
          CCPSD4 = IDXC + L9 - 1
          RATES(CCPSD4) = -RK(5)
          WRITE (7,*) 'RATES C IN CIPSD4  = ', RATES(CCPSD4)
      END IF
*=====================================================================*
C                     REACTION RATES IN CIPSD5
*=====================================================================*
      L11 = L10 + NCOMP_NNCC + 1
      L12 = L11 + NCOMP_NCC - 1

      DO 85 I = L11, L12
85    RATES(I) = 0.0

C     FOR CARBON
      IF (REAL(7).GT.1E-11) THEN
          CCPSD5 = IDXC + L11 - 1
          RATES(CCPSD5) = -RK(5)
          WRITE (7,*) 'RATES C IN CIPSD5  = ', RATES(CCPSD5)
      END IF
*---------------------------------------------------------------------*

      RETURN
      END
```

C-6 Subroutine of Homogeneous Destruction of N2O

```
*=====================================================================*
C     User Subroutine for NOx formation.
*=====================================================================*

      Subroutine USRK10  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*---------------------------------------------------------------------*

      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)

C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

C     DECLARE LOCAL VARIABLES
      COMMON /USER18/ SPAREA, Tp

      DIMENSION RK(7)

      INTEGER IMISS, DMS_KCCIDC
      REAL*8  RMISS

      OPEN(7,FILE='NOX6.txt')

*---------------------------------------------------------------------*
C     ORDER OF SUBSTREAM MIXED, CISOLID, CIPSD1, NCPSD1, CIPSD2, NCPSD2,
C     CIPSD3, NCPSD3, CIPSD4, NCPSD4, CIPSD5 AND NCPSD5
*---------------------------------------------------------------------*

C     DECLARE LOCAL OF CARBON-MONOXIDE
      IDXCO   = DMS_KCCIDC('CO')
C     WRITE (7,*) 'LOCAL ID. OF CO   =',IDXCO

C     DECLARE LOCAL OF CARBON-DIOXIDE
      IDXCO2   = DMS_KCCIDC('CO2')
C     WRITE (7,*) 'LOCAL ID. OF CO2   =',IDXCO2

C     DECLARE LOCAL OF NITROGEN
```

```
      IDXN2   = DMS_KCCIDC('N2')
C     WRITE (7,*) 'LOCAL ID. OF N2   =',IDXN2

C     DECLARE LOCAL OF NITROUS OXIDE
      IDXN2O  = DMS_KCCIDC('N2O')
C     WRITE (7,*) 'LOCAL ID. OF N2O  =',IDXN2O

C     N2O REDUCTION   N2O + CO --> N2 + CO2
      RKI = 2.51E11*DEXP(-23180/Tp)*REAL(1)
      RK(6) = RKI*REAL(2)*RCSTRR_VOLRC

*=====================================================================*
C                    REACTION RATES IN MIXED
*=====================================================================*
      DO 55 I = 1,NCOMP_NCC
55    RATES(I) = 0.0

      RKN = RK(6)

      IF (RKN.GT.REAL(3).OR.RKN.GT.REAL(4)) THEN

          IF (REAL(3).GT.REAL(4)) THEN
              RKN = REAL(4)*0.99
                  RK(6) = RKN
                      ELSE IF (REAL(4).GT.REAL(3)) THEN
                  RKN = REAL(3)*0.99
              RK(6) = RKN
          END IF
      ELSE
          GOTO 600
      END IF

C     FOR NITROUS-OXIDE
600   RATES(IDXN2O) = -RK(6)
      WRITE (7,*) 'RATES N2O IN MIXED  = ', RATES(IDXN2O)

C     FOR CARBON MONOXIDE
      RATES(IDXCO) = -RK(6)
      WRITE (7,*) 'RATES CO IN MIXED  = ', RATES(IDXCO)

C     FOR NITROGEN
      RATES(IDXN2) = RK(6)
      WRITE (7,*) 'RATES N2 IN MIXED  = ', RATES(IDXN2)

C     FOR CARBON DIOXIDE
      RATES(IDXCO2) = RK(6)
      WRITE (7,*) 'RATES CO2 IN MIXED = ', RATES(IDXCO2)
*---------------------------------------------------------------------*

      RETURN
      END
```

C-7 Subroutine of Thermal Decomposition of N2O

```
*===================================================================*
C     User Subroutine for NOx formation.
*===================================================================*

      Subroutine USRK11  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*-------------------------------------------------------------------*

      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)


C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

C     DECLARE LOCAL VARIABLES
      COMMON /USER18/ SPAREA, Tp

      DIMENSION RK(7)

      INTEGER IMISS, DMS_KCCIDC
      REAL*8  RMISS

      OPEN(7,FILE='NOX7.txt')

*-------------------------------------------------------------------*
C     ORDER OF SUBSTREAM MIXED, CISOLID, CIPSD1, NCPSD1, CIPSD2, NCPSD2,
C     CIPSD3, NCPSD3, CIPSD4, NCPSD4, CIPSD5 AND NCPSD5
*-------------------------------------------------------------------*

C     DECLARE LOCAL OF OXYGEN
      IDXO2   = DMS_KCCIDC('O2')
C     WRITE (7,*) 'LOCAL ID. OF O2   =',IDXO2

C     DECLARE LOCAL OF NITROGEN
      IDXN2   = DMS_KCCIDC('N2')
C     WRITE (7,*) 'LOCAL ID. OF N2   =',IDXN2
```

```
C     DECLARE LOCAL OF NITROUS OXIDE
      IDXN2O  = DMS_KCCIDC('N2O')
C     WRITE (7,*) 'LOCAL ID. OF N2O  =',IDXN2O

C     N2O REDUCTION   2N2O --> 2N2 + O2
      RKJ = 1.75E8*DEXP(-23800/Tp)
      RK(7) = RKJ*REAL(1)*RCSTRR_VOLRC
*---------------------------------------------------------------------*

*=====================================================================*
C                     REACTION RATES IN MIXED
*=====================================================================*
      DO 55 I = 1,NCOMP_NCC
55    RATES(I) = 0.0

      RKN = 2.* RK(7)

      IF (RKN.GT.REAL(2)) THEN
          RKN = REAL(2)*0.99
              RK(7) = RKN/2.
          ELSE
      GOTO 600
      END IF

C     FOR NITROUS-OXIDE
600   RATES(IDXN2O) = -2.*RK(7)
      WRITE (7,*) 'RATES N2O IN MIXED  = ', RATES(IDXN2O)

C     FOR NITROGEN
      RATES(IDXN2) = 2.*RK(7)
      WRITE (7,*) 'RATES N2 IN MIXED  = ', RATES(IDXN2)

C     FOR OXYGEN
      RATES(IDXO2) = RK(7)
      WRITE (7,*) 'RATES O2 IN MIXED  = ', RATES(IDXO2)
*---------------------------------------------------------------------*

      RETURN
      END
```

Appendix D

ASPEN PLUS input file for industrial scale

```
     7    DYNAMICS
     8        DYNAMICS RESULTS=ON
     9
    10    TITLE 'PLEASE SEE DESCRIPTION'
    11
    12    IN-UNITS SI
    13
    14    DEF-STREAMS CONVEN ALL
    15
    16    SIM-OPTIONS
    17                IN-UNITS  MET  VOLUME-FLOW='cum/hr'  ENTHALPY-
FLO='MMkcal/hr'  &
    18                      HEAT-TRANS-C='kcal/hr-sqm-K'  PRESSURE=bar
TEMPERATURE=C  &
    19                       VOLUME=cum  DELTA-T=C  HEAD=meter  MOLE-
DENSITY='kmol/cum'  &
    20            MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol'  &
    21                      MASS-ENTHALP='kcal/kg'  HEAT=MMkcal  MOLE-
CONC='mol/l'  &
    22            PDROP=bar
    23        SIM-OPTIONS FLASH-MAXIT=500
    24
    25    RUN-CONTROL MAX-FORT-ERR=200
    26
    27    DESCRIPTION "
    28           Subroutine for calculate RCSTR is reserved for 5
component.
    29           Each component can specific 5 interval of PSD.
    30             At lower boundary of the first interval you must
input zero value.
    31
    32           In block RCSTR (PB11-7)
    33                 REAL(1)      = Total volumetric flow rate to
RCSTR
    34                REAL(2-6)   = Radius of particle in first input
stream (m)
    35               REAL(7-11)  = Radius of particle in second input
stream (m)
    36                REAL(12-16) = Radius of particle in third input
stream (m)
    37               REAL(17-21) = Radius of particle in fourth input
stream (m)
    38                REAL(22-26) = Radius of particle in fifth input
stream (m)
    39
    40               REAL(29)    = Oxygen concentration
    41
```

```
    42
    43                REAL(30-34) = Radius of particle in recycle for
component 1 (m)
    44                REAL(35-39) = Radius of particle in recycle for
component 2 (m)
    45                REAL(40-44) = Radius of particle in recycle for
component 3 (m)
    46                REAL(45-49) = Radius of particle in recycle for
component 4 (m)
    47
    48                REAL(50-54) = Radius of particle in recycle for
component 5 (m)
    49
    50                REAL(55-59) = Mean radius of mixed particle for
component 1 (m)
    51                REAL(60-64) = Mean radius of mixed particle for
component 2 (m)
    52                REAL(65-69) = Mean radius of mixed particle for
component 3 (m)
    53                REAL(70-74) = Mean radius of mixed particle for
component 4 (m)
    54                REAL(75-79) = Mean radius of mixed particle for
component 5 (m)
    55
    56                REAL(80-84)   = Radius from output of RCSTR for
component 1 (m)
    57                REAL(85-89)   = Radius from output of RCSTR for
component 2 (m)
    58                REAL(90-94)   = Radius from output of RCSTR for
component 3 (m)
    59                REAL(95-99)   = Radius from output of RCSTR for
component 4 (m)
    60                REAL(100-104) = Radius from output of RCSTR for
component 5 (m)
    61
    62              REAL(105)     = Maximum error tolerance for mass
balance
    63              REAL(106)     = Tolerance for mass balance
    64              REAL(107)     = Molar density in mixed stream
    65              REAL(108)     = Viscosity of mixed stream
    66         "
    67
    68    DATABANKS PURE12  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
    69              NOASPENPCD
    70
    71    PROP-SOURCES PURE12  / AQUEOUS  / SOLIDS  / INORGANIC
    72
    73    COMPONENTS
    74        C C /
    75        O2 O2 /
    76        N2 N2 /
    77        CO CO /
    78        CO2 CO2 /
    79        H2 H2 /
    80        H2O H2O /
```

```
 81        S S /
 82        SO2 O2S /
 83        NO NO /
 84        N2O N2O /
 85        NO2 NO2 /
 86        CACO3 CACO3 /
 87        CAO CAO /
 88        CASO4 CASO4 /
 89        ASH /
 90        LANNA /
 91        SIRA /
 92        SLUDGE /
 93        BAGASSE /
 94        BARK
 95
 96    FLOWSHEET
 97        BLOCK P11-1 IN=LANNA OUT=S1
 98        BLOCK P11-2 IN=SIRA OUT=S2
 99        BLOCK P11-3 IN=SLUDGE OUT=S3
100        BLOCK P11-4 IN=BAGASSE OUT=S4
101        BLOCK P11-5 IN=BARK OUT=S5
102        BLOCK P11-6 IN=S1 S2 S3 S4 S5 AIR1 LIME OUT=S6
103        BLOCK P11-7 IN=S6 RESOLID OUT=S7
104        BLOCK P11-15 IN=S8-7 OUT=S10
105        BLOCK P11-16 IN=S10 AIR2 OUT=S11
106        BLOCK P11-17 IN=S11 OUT=S12
107        BLOCK P11-25 IN=AIR3 S13-7 OUT=S15
108        BLOCK P11-26 IN=S15 OUT=S16
109        BLOCK P11-34 IN=S17-7 OUT=S19
110        BLOCK P11-35 IN=S19 OUT=S20
111        BLOCK P11-43 IN=S21-7 OUT=S23
112        BLOCK P11-45 IN=S24 OUT=FLUEGAS S25
113        BLOCK P11-46 IN=S25 OUT=RESOLID FLUEGAS2 BOTTOM
114        BLOCK P11-44 IN=S23 WATER OUT=S24 STEAM
115        BLOCK P11-8 IN=S7 OUT=S8-1
116        BLOCK P11-9 IN=S8-1 OUT=S8-2
117        BLOCK P11-14 IN=S8-6 OUT=S8-7
118        BLOCK P11-10 IN=S8-2 OUT=S8-3
119        BLOCK P11-11 IN=S8-3 OUT=S8-4
120        BLOCK P11-12 IN=S8-4 OUT=S8-5
121        BLOCK P11-13 IN=S8-5 OUT=S8-6
122        BLOCK P11-18 IN=S12 OUT=S13-1
123        BLOCK P11-19 IN=S13-1 OUT=S13-2
124        BLOCK P11-20 IN=S13-2 OUT=S13-3
125        BLOCK P11-21 IN=S13-3 OUT=S13-4
126        BLOCK P11-22 IN=S13-4 OUT=S13-5
127        BLOCK P11-23 IN=S13-5 OUT=S13-6
128        BLOCK P11-24 IN=S13-6 OUT=S13-7
129        BLOCK P11-27 IN=S16 OUT=S17-1
130        BLOCK P11-28 IN=S17-1 OUT=S17-2
131        BLOCK P11-29 IN=S17-2 OUT=S17-3
132        BLOCK P11-30 IN=S17-3 OUT=S17-4
133        BLOCK P11-31 IN=S17-4 OUT=S17-5
134        BLOCK P11-32 IN=S17-5 OUT=S17-6
135        BLOCK P11-33 IN=S17-6 OUT=S17-7
```

```
   136        BLOCK P11-36 IN=S20 OUT=S21-1
   137        BLOCK P11-37 IN=S21-1 OUT=S21-2
   138        BLOCK P11-39 IN=S21-3 OUT=S21-4
   139        BLOCK P11-40 IN=S21-4 OUT=S21-5
   140        BLOCK P11-38 IN=S21-2 OUT=S21-3
   141        BLOCK P11-41 IN=S21-5 OUT=S21-6
   142        BLOCK P11-42 IN=S21-6 OUT=S21-7
   143
   144    PROPERTIES SYSOP0
   145
   146    NC-COMPS ASH PROXANAL ULTANAL SULFANAL
   147
   148    NC-PROPS ASH ENTHALPY HCOALGEN / DENSITY DCOALIGT
   149
   150    NC-COMPS LANNA PROXANAL ULTANAL SULFANAL
   151
   152    NC-PROPS LANNA ENTHALPY HCOALGEN / DENSITY DCOALIGT
   153
   154    NC-COMPS SIRA PROXANAL ULTANAL SULFANAL
   155
   156    NC-PROPS SIRA ENTHALPY HCOALGEN / DENSITY DCOALIGT
   157
   158    NC-COMPS SLUDGE PROXANAL ULTANAL SULFANAL
   159
   160    NC-PROPS SLUDGE ENTHALPY HCOALGEN / DENSITY DCOALIGT
   161
   162    NC-COMPS BAGASSE PROXANAL ULTANAL SULFANAL
   163
   164    NC-PROPS BAGASSE ENTHALPY HCOALGEN / DENSITY DCOALIGT
   165
   166    NC-COMPS BARK PROXANAL ULTANAL SULFANAL
   167
   168    NC-PROPS BARK ENTHALPY HCOALGEN / DENSITY DCOALIGT
   169
   170    DEF-SUBS-ATTR PSD PSD
   171        IN-UNITS ENG
   172        INTERVALS 5
   173           SIZE-LIMITS 0.0 <meter> / 5E-005 <meter> / 0.0001
<meter> /  &
   174            0.0002 <meter> / 0.0005 <meter> / 0.001 <meter>
   175
   176    DEF-SUBS-ATTR PSD1 PSD
   177        INTERVALS 5
   178         SIZE-LIMITS 0. <mm> / 1. <mm> / 40. <mm> / 75. <mm> /
&
   179            76. <mm> / 77. <mm>
   180
   181    DEF-SUBS-ATTR PSD2 PSD
   182        INTERVALS 5
   183         SIZE-LIMITS 0. <mm> / 1. <mm> / 40. <mm> / 75. <mm> /
&
   184            76. <mm> / 77. <mm>
   185
   186    DEF-SUBS-ATTR PSD3 PSD
   187        INTERVALS 5
```

```
   188         SIZE-LIMITS 0. <mm> / 3.175 <mm> / 4. <mm> / 5. <mm> /
&
   189             6. <mm> / 7. <mm>
   190
   191     DEF-SUBS-ATTR PSD4 PSD
   192         INTERVALS 5
   193         SIZE-LIMITS 0. <mm> / 3.175 <mm> / 4. <mm> / 5. <mm> /
&
   194             6. <mm> / 7. <mm>
   195
   196     DEF-SUBS-ATTR PSD5 PSD
   197         INTERVALS 5
   198         SIZE-LIMITS 0. <mm> / 3.175 <mm> / 4. <mm> / 5. <mm> /
&
   199             6. <mm> / 7. <mm>
   200
   201     DEF-SUBS CISOLID CISOLID
   202
   203     DEF-SUBS-CLA CISOLID
   204         DEF TYPE=CISOLID ATTR=PSD
   205
   206     DEF-SUBS CIPSD1 CIPSD1
   207
   208     DEF-SUBS-CLA CIPSD1
   209         DEF TYPE=CISOLID ATTR=PSD1
   210
   211     DEF-SUBS NCPSD1 NCPSD1
   212
   213     DEF-SUBS-CLA NCPSD1
   214         DEF TYPE=NC ATTR=PSD1
   215
   216     DEF-SUBS CIPSD2 CIPSD2
   217
   218     DEF-SUBS-CLA CIPSD2
   219         DEF TYPE=CISOLID ATTR=PSD2
   220
   221     DEF-SUBS NCPSD2 NCPSD2
   222
   223     DEF-SUBS-CLA NCPSD2
   224         DEF TYPE=NC ATTR=PSD2
   225
   226     DEF-SUBS CIPSD3 CIPSD3
   227
   228     DEF-SUBS-CLA CIPSD3
   229         DEF TYPE=CISOLID ATTR=PSD3
   230
   231     DEF-SUBS NCPSD3 NCPSD3
   232
   233     DEF-SUBS-CLA NCPSD3
   234         DEF TYPE=NC ATTR=PSD3
   235
   236     DEF-SUBS CIPSD4 CIPSD4
   237
   238     DEF-SUBS-CLA CIPSD4
   239         DEF TYPE=CISOLID ATTR=PSD4
```

```
   240
   241    DEF-SUBS NCPSD4 NCPSD4
   242
   243    DEF-SUBS-CLA NCPSD4
   244        DEF TYPE=NC ATTR=PSD4
   245
   246    DEF-SUBS CIPSD5 CIPSD5
   247
   248    DEF-SUBS-CLA CIPSD5
   249        DEF TYPE=CISOLID ATTR=PSD5
   250
   251    DEF-SUBS NCPSD5 NCPSD5
   252
   253    DEF-SUBS-CLA NCPSD5
   254        DEF TYPE=NC ATTR=PSD5
   255
   256      DEF-STREAM-C  CONVEN  MIXED  CISOLID  CIPSD1  NCPSD1  CIPSD2
NCPSD2  &
   257           CIPSD3 NCPSD3 CIPSD4 NCPSD4 CIPSD5 NCPSD5
   258
   259    PROP-SET PS-1 MUMX SUBSTREAM=MIXED PHASE=V
   260
   261    STREAM AIR1
   262        SUBSTREAM MIXED TEMP=306. PRES=1. <atm> VOLUME-FLOW=22.
   263        MOLE-FRAC O2 0.2 / N2 0.7525 / H2O 0.0475
   264
   265    STREAM AIR2
   266        SUBSTREAM MIXED TEMP=306. PRES=1. <atm> VOLUME-FLOW=10.
   267        MOLE-FRAC O2 0.2 / N2 0.7525 / H2O 0.0475
   268
   269    STREAM AIR3
   270        SUBSTREAM MIXED TEMP=306. PRES=1. <atm> VOLUME-FLOW=5.
   271        MOLE-FRAC O2 0.2 / N2 0.7525 / H2O 0.0475
   272
   273    STREAM BAGASSE
   274        SUBSTREAM NCPSD4 TEMP=306. PRES=1. <atm>
   275        MASS-FLOW BAGASSE 1E-012
   276        COMP-ATTR BAGASSE PROXANAL ( 35.49 7.71 55.23 1.57 )
   277        COMP-ATTR BAGASSE ULTANAL ( 2.44 48.64 5.87 0.16 0.  &
   278            0.07 42.82 )
   279        COMP-ATTR BAGASSE SULFANAL ( 0. 0. 0. )
   280        SUBS-ATTR PSD4 ( 0.8 0.2 0. 0. 0. )
   281
   282    STREAM BARK
   283        SUBSTREAM NCPSD5 TEMP=306. PRES=1. <atm>
   284        MASS-FLOW BARK 1E-012
   285        COMP-ATTR BARK PROXANAL ( 39.66 9.09 48.85 2.4 )
   286        COMP-ATTR BARK ULTANAL ( 2.82 48.4 6.72 0.19 0. 0.  &
   287            41.87 )
   288        COMP-ATTR BARK SULFANAL ( 0. 0. 0. )
   289        SUBS-ATTR PSD5 ( 0.8 0.2 0. 0. 0. )
   290
   291    STREAM LANNA
   292        SUBSTREAM NCPSD1 TEMP=306. PRES=1. <atm>
   293        MASS-FLOW LANNA 4.
```

```
   294        COMP-ATTR LANNA PROXANAL ( 19.86 34.85 34.84 10.45 )
   295        COMP-ATTR LANNA ULTANAL ( 13.04 68.15 5.09 1.24 0. 0.59
&
   296            11.89 )
   297        COMP-ATTR LANNA SULFANAL ( 0. 0. 0. )
   298        SUBS-ATTR PSD1 ( 0.08 0.52 0.4 0. 0. )
   299
   300    STREAM LIME
   301        SUBSTREAM CISOLID TEMP=306. PRES=1. <atm>
   302        MASS-FLOW CACO3 0.2
   303        SUBS-ATTR PSD ( 0.02 0.07 0.45 0.405 0.055 )
   304
   305    STREAM S6
   306
   307    STREAM SIRA
   308        SUBSTREAM NCPSD2 TEMP=306. PRES=1. <atm>
   309        MASS-FLOW SIRA 1E-012
   310        COMP-ATTR SIRA PROXANAL ( 25.04 32.47 37.86 4.63 )
   311         COMP-ATTR SIRA ULTANAL ( 6.18 68.16 4.51 0.36 0. 1.75
&
   312            19.04 )
   313        COMP-ATTR SIRA SULFANAL ( 0. 0. 0. )
   314        SUBS-ATTR PSD2 ( 0.08 0.52 0.4 0. 0. )
   315
   316    STREAM SLUDGE
   317        SUBSTREAM NCPSD3 TEMP=306. PRES=1. <atm>
   318        MASS-FLOW SLUDGE 1E-012
   319        COMP-ATTR SLUDGE PROXANAL ( 65.42 2.9 13.19 18.5 )
   320         COMP-ATTR SLUDGE ULTANAL ( 18.5 41.19 5.4 1.7 0. 0.72
&
   321            32.49 )
   322        COMP-ATTR SLUDGE SULFANAL ( 0. 0. 0. )
   323        SUBS-ATTR PSD3 ( 0.8 0.2 0. 0. 0. )
   324
   325    STREAM WATER
   326        SUBSTREAM MIXED TEMP=406. PRES=106.6 <barg>
   327        MASS-FLOW H2O 30.6
   328
   329    BLOCK P11-44 HEATX
   330        PARAM T-COLD=510. CALC-TYPE=RATING TYPE=COCURRENT  &
   331                    PRES-HOT=1.  <atm>  PRES-COLD=100.  <barg>  U-
OPTION=FILM-COEF  &
   332            F-OPTION=GEOMETRY CALC-METHOD=DETAILED
   333        FEEDS HOT=S23 COLD=WATER
   334        PRODUCTS HOT=S24 COLD=STEAM
   335                          EQUIP-SPECS   TUBE-NPASS=1   TEMA-TYPE=E
ORIENTATION=VERTICAL  &
   336            TUBE-FLOW=UP SHELL-DIAM=6.8
   337        TUBES TOTAL-NUMBER=272 TUBE-TYPE=FINNED LENGTH=15.  &
   338            INSIDE-DIAM=52.32 <mm> OUTSIDE-DIAM=63.5 <mm>  &
   339            PITCH=88. <mm>
   340        FINS HEIGHT=5. <mm> THICKNESS=5.
   341        SEGB-SHELL NBAFFLE=268 BAFFLE-CUT=0.005
   342        HOT-SIDE H-OPTION=GEOMETRY SHELL-TUBE=SHELL  &
   343            DP-OPTION=CONSTANT
```

```
344         COLD-SIDE H-OPTION=GEOMETRY DP-OPTION=CONSTANT
345
346     BLOCK P11-6 RSTOIC
347         PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
348         STOIC 1 CIPSD1 C -2. / MIXED O2 -1. / CO 2.
349         STOIC 2 CIPSD1 S -1. / MIXED O2 -1. / SO2 1.
350         STOIC 3 CIPSD2 C -2. / MIXED O2 -1. / CO 2.
351         STOIC 4 CIPSD2 S -1. / MIXED O2 -1. / SO2 1.
352         STOIC 5 CIPSD3 C -2. / MIXED O2 -1. / CO 2.
353         STOIC 6 CIPSD3 S -1. / MIXED O2 -1. / SO2 1.
354         STOIC 7 CIPSD4 C -2. / MIXED O2 -1. / CO 2.
355         STOIC 8 CIPSD4 S -1. / MIXED O2 -1. / SO2 1.
356         STOIC 9 CIPSD5 C -2. / MIXED O2 -1. / CO 2.
357         STOIC 10 CIPSD5 S -1. / MIXED O2 -1. / SO2 1.
358         STOIC 11 MIXED H2 -2. / O2 -1. / H2O 2.
359         CONV 1 CIPSD1 C 0.3
360         CONV 2 CIPSD1 S 1.
361         CONV 3 CIPSD2 C 0.3
362         CONV 4 CIPSD2 S 1.
363         CONV 5 CIPSD3 C 0.3
364         CONV 6 CIPSD3 S 1.
365         CONV 7 CIPSD4 C 0.3
366         CONV 8 CIPSD4 S 1.
367         CONV 9 CIPSD5 C 0.3
368         CONV 10 CIPSD5 S 1.
369         CONV 11 MIXED H2 1.
370         BLOCK-OPTION FREE-WATER=NO
371
372     BLOCK P11-15 RSTOIC
373         PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
374         STOIC 1 CISOLID CACO3 -1. / CAO 1. / MIXED CO2 1.
375         STOIC 2 CISOLID CAO -2. / MIXED SO2 -2. / O2 -1. /  &
376            CISOLID CASO4 2.
377         CONV 1 CISOLID CACO3 1.
378         CONV 2 MIXED SO2 0.4
379         BLOCK-OPTION FREE-WATER=NO
380
381     BLOCK P11-16 RSTOIC
382         PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
383         STOIC 1 CIPSD1 S -1. / MIXED O2 -1. / SO2 1.
384         STOIC 2 CIPSD2 S -1. / MIXED O2 -1. / SO2 1.
385         STOIC 3 CIPSD3 S -1. / MIXED O2 -1. / SO2 1.
386         STOIC 4 CIPSD4 S -1. / MIXED O2 -1. / SO2 1.
387         STOIC 5 CIPSD5 S -1. / MIXED O2 -1. / SO2 1.
388         STOIC 6 MIXED H2 -2. / O2 -1. / H2O 2.
389         CONV 1 CIPSD1 S 1.
390         CONV 2 CIPSD2 S 1.
391         CONV 3 CIPSD3 S 1.
392         CONV 4 CIPSD4 S 1.
393         CONV 5 CIPSD5 S 1.
394         CONV 6 MIXED H2 1.
395         BLOCK-OPTION FREE-WATER=NO
396
397     BLOCK P11-25 RSTOIC
398         PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
```

```
399         STOIC 1 CISOLID CAO -1. / MIXED SO2 -1. / O2 -0.5 /  &
400             CISOLID CASO4 1.
401         CONV 1 MIXED SO2 0.4
402         BLOCK-OPTION FREE-WATER=NO
403
404     BLOCK P11-34 RSTOIC
405         PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
406         STOIC 1 CISOLID CAO -1. / MIXED SO2 -1. / O2 -0.5 /  &
407             CISOLID CASO4 1.
408         CONV 1 MIXED SO2 0.4
409         BLOCK-OPTION FREE-WATER=NO
410
411     BLOCK P11-43 RSTOIC
412         PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
413         STOIC 1 CISOLID CAO -1. / MIXED SO2 -1. / O2 -0.5 /  &
414             CISOLID CASO4 1.
415         CONV 1 MIXED SO2 0.4
416         BLOCK-OPTION FREE-WATER=NO
417
418     BLOCK P11-1 RYIELD
419         PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
420         MASS-YIELD CIPSD1 C 0.6815 / MIXED H2 0.0509 / N2  &
421             0.0124 / CIPSD1 S 0.0059 / MIXED O2 0.1189 / NCPSD1
&
422             ASH 0.1304
423         BLOCK-OPTION FREE-WATER=NO
424         COMP-ATTR NCPSD1 ASH PROXANAL ( 0. 0. 0. 100. )
425          COMP-ATTR NCPSD1 ASH ULTANAL ( 100. 0. 0. 0. 0. 0. 0.
&
426             )
427         COMP-ATTR NCPSD1 ASH SULFANAL ( 0. 0. 0. )
428         SUBS-ATTR 1 CIPSD1 PSD1 ( 0.08 0.52 0.4 0. 0. )
429
430     BLOCK P11-2 RYIELD
431         PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
432         MASS-YIELD CIPSD2 C 0.6816 / MIXED H2 0.0451 / N2  &
433             0.0036 / CIPSD2 S 0.0175 / MIXED O2 0.1904 / NCPSD2
&
434             ASH 0.0618
435         BLOCK-OPTION FREE-WATER=NO
436         COMP-ATTR NCPSD2 ASH PROXANAL ( 0. 0. 0. 100. )
437          COMP-ATTR NCPSD2 ASH ULTANAL ( 100. 0. 0. 0. 0. 0. 0.
&
438             )
439         COMP-ATTR NCPSD2 ASH SULFANAL ( 0. 0. 0. )
440         SUBS-ATTR 1 CIPSD2 PSD2 ( 0.08 0.52 0.4 0. 0. )
441
442     BLOCK P11-3 RYIELD
443         PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
444          MASS-YIELD CIPSD3 C 0.4119 / MIXED H2 0.054 / N2 0.017
/ &
445             CIPSD3 S 0.0072 / MIXED O2 0.3249 / NCPSD3 ASH  &
446             0.185
447         BLOCK-OPTION FREE-WATER=NO
448         COMP-ATTR NCPSD3 ASH PROXANAL ( 0. 0. 0. 100. )
```

```
   449         COMP-ATTR NCPSD3 ASH ULTANAL ( 100. 0. 0. 0. 0. 0. 0.
&
   450           )
   451        COMP-ATTR NCPSD3 ASH SULFANAL ( 0. 0. 0. )
   452        SUBS-ATTR 1 CIPSD3 PSD3 ( 0.8 0.2 0. 0. 0. )
   453
   454    BLOCK P11-4 RYIELD
   455        PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
   456        MASS-YIELD CIPSD4 C 0.4864 / MIXED H2 0.0587 / N2  &
   457           0.0016 / CIPSD4 S 0.0007 / MIXED O2 0.4282 / NCPSD4
&
   458           ASH 0.0244
   459        BLOCK-OPTION FREE-WATER=NO
   460        COMP-ATTR NCPSD4 ASH PROXANAL ( 0. 0. 0. 100. )
   461        COMP-ATTR NCPSD4 ASH SULFANAL ( 0. 0. 0. )
   462         COMP-ATTR NCPSD4 ASH ULTANAL ( 100. 0. 0. 0. 0. 0. 0.
&
   463           )
   464        SUBS-ATTR 1 CIPSD4 PSD4 ( 0.8 0.2 0. 0. 0. )
   465
   466    BLOCK P11-5 RYIELD
   467        PARAM TEMP=1173. PRES=1. <atm> NPHASE=1 PHASE=V
   468        MASS-YIELD CIPSD5 C 0.484 / MIXED H2 0.0672 / N2  &
   469           0.0019 / CIPSD5 S 0. / MIXED O2 0.4187 / NCPSD5  &
   470           ASH 0.0282
   471        BLOCK-OPTION FREE-WATER=NO
   472        COMP-ATTR NCPSD5 ASH PROXANAL ( 0. 0. 0. 100. )
   473         COMP-ATTR NCPSD5 ASH ULTANAL ( 100. 0. 0. 0. 0. 0. 0.
&
   474           )
   475        COMP-ATTR NCPSD5 ASH SULFANAL ( 0. 0. 0. )
   476        SUBS-ATTR 1 CIPSD5 PSD5 ( 0.8 0.2 0. 0. 0. )
   477
   478    BLOCK P11-7 RCSTR
   479        USER-VECS NREAL=110
   480           REAL  VALUE-LIST=*  0.0005  0.0205  0.0575  *  *  0.0005
0.0205  &
   481           0.0575 * * 0.0015875 0.0035875 * * * 0.0015875  &
   482           0.0035875 * * * 0.0015875 0.0035875
   483        PARAM VOL=61.84 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
   484        CONVERGENCE SOLVER=NEWTON
   485        REACTIONS RXN-IDS=R-1
   486
   487    BLOCK P11-8 RCSTR
   488        USER-VECS NREAL=3
   489        PARAM VOL=61.84 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
   490        CONVERGENCE SOLVER=NEWTON
   491        REACTIONS RXN-IDS=R-5
   492
   493    BLOCK P11-9 RCSTR
   494        USER-VECS NREAL=3
   495        PARAM VOL=61.84 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
   496        CONVERGENCE SOLVER=NEWTON
   497        REACTIONS RXN-IDS=R-6
   498
```

```
 499    BLOCK P11-10 RCSTR
 500        USER-VECS NREAL=7
 501          PARAM VOL=61.84 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
&
 502             MB-TOL=0.0001
 503        CONVERGENCE SOLVER=NEWTON
 504        REACTIONS RXN-IDS=R-7
 505
 506    BLOCK P11-11 RCSTR
 507        USER-VECS NREAL=3
 508          PARAM VOL=61.84 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
&
 509             MB-TOL=0.001
 510        CONVERGENCE SOLVER=NEWTON
 511        REACTIONS RXN-IDS=R-8
 512
 513    BLOCK P11-12 RCSTR
 514        USER-VECS NREAL=7
 515          PARAM VOL=61.84 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
&
 516             MB-TOL=0.0001
 517        CONVERGENCE SOLVER=NEWTON
 518        REACTIONS RXN-IDS=R-9
 519
 520    BLOCK P11-13 RCSTR
 521        USER-VECS NREAL=4
 522        PARAM VOL=61.84 TEMP=1173. PRES=1. <atm>
 523        REACTIONS RXN-IDS=R-10
 524
 525    BLOCK P11-14 RCSTR
 526        USER-VECS NREAL=2
 527          PARAM VOL=61.84 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
&
 528             MB-TOL=0.001
 529        CONVERGENCE SOLVER=NEWTON
 530        REACTIONS RXN-IDS=R-11
 531
 532    BLOCK P11-17 RCSTR
 533        USER-VECS NREAL=108
 534        PARAM VOL=54.75 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
 535        CONVERGENCE SOLVER=NEWTON
 536        REACTIONS RXN-IDS=R-2
 537
 538    BLOCK P11-18 RCSTR
 539        USER-VECS NREAL=3
 540        PARAM VOL=54.75 TEMP=1173. PRES=1. <atm>
 541        REACTIONS RXN-IDS=R-12
 542
 543    BLOCK P11-19 RCSTR
 544        USER-VECS NREAL=3
 545        PARAM VOL=54.75 TEMP=1173. PRES=1. <atm>
 546        REACTIONS RXN-IDS=R-13
 547
 548    BLOCK P11-20 RCSTR
 549        USER-VECS NREAL=7
```

```
550          PARAM VOL=54.75 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
&
551             MB-TOL=0.0001
552         CONVERGENCE SOLVER=NEWTON
553         REACTIONS RXN-IDS=R-14
554
555     BLOCK P11-21 RCSTR
556         USER-VECS NREAL=3
557         PARAM VOL=54.75 TEMP=1173. PRES=1. <atm>
558         REACTIONS RXN-IDS=R-15
559
560     BLOCK P11-22 RCSTR
561         USER-VECS NREAL=7
562         PARAM VOL=54.75 TEMP=1173. PRES=1. <atm>
563         REACTIONS RXN-IDS=R-16
564
565     BLOCK P11-23 RCSTR
566         USER-VECS NREAL=4
567         PARAM VOL=54.75 TEMP=1173. PRES=1. <atm>
568         REACTIONS RXN-IDS=R-17
569
570     BLOCK P11-24 RCSTR
571         USER-VECS NREAL=2
572         PARAM VOL=54.75 TEMP=1173. PRES=1. <atm>
573         REACTIONS RXN-IDS=R-18
574
575     BLOCK P11-26 RCSTR
576         USER-VECS NREAL=108
577         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
578         CONVERGENCE SOLVER=NEWTON
579         REACTIONS RXN-IDS=R-3
580
581     BLOCK P11-27 RCSTR
582         USER-VECS NREAL=3
583         PARAM VOL=388.4 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
584         CONVERGENCE SOLVER=NEWTON
585         REACTIONS RXN-IDS=R-19
586
587     BLOCK P11-28 RCSTR
588         USER-VECS NREAL=3
589         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
590         REACTIONS RXN-IDS=R-20
591
592     BLOCK P11-29 RCSTR
593         USER-VECS NREAL=7
594         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
595         REACTIONS RXN-IDS=R-21
596
597     BLOCK P11-30 RCSTR
598         USER-VECS NREAL=3
599         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
600         REACTIONS RXN-IDS=R-22
601
602     BLOCK P11-31 RCSTR
603         USER-VECS NREAL=7
```

```
604          PARAM VOL=338.4 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
&
605             ALGORITHM=INTEGRATOR
606         CONVERGENCE SOLVER=NEWTON
607         REACTIONS RXN-IDS=R-23
608
609     BLOCK P11-32 RCSTR
610         USER-VECS NREAL=4
611         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
612         REACTIONS RXN-IDS=R-24
613
614     BLOCK P11-33 RCSTR
615         USER-VECS NREAL=2
616         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
617         REACTIONS RXN-IDS=R-25
618
619     BLOCK P11-35 RCSTR
620         USER-VECS NREAL=108
621         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
622         CONVERGENCE SOLVER=NEWTON
623         REACTIONS RXN-IDS=R-4
624
625     BLOCK P11-36 RCSTR
626         USER-VECS NREAL=3
627         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
628         REACTIONS RXN-IDS=R-26
629
630     BLOCK P11-37 RCSTR
631         USER-VECS NREAL=3
632         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
633         CONVERGENCE SOLVER=NEWTON
634         REACTIONS RXN-IDS=R-27
635
636     BLOCK P11-38 RCSTR
637         USER-VECS NREAL=7
638         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm> MB-MAXIT=500
639         CONVERGENCE SOLVER=NEWTON
640         REACTIONS RXN-IDS=R-28
641
642     BLOCK P11-39 RCSTR
643         USER-VECS NREAL=3
644         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
645         REACTIONS RXN-IDS=R-29
646
647     BLOCK P11-40 RCSTR
648         USER-VECS NREAL=7
649         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
650         REACTIONS RXN-IDS=R-30
651
652     BLOCK P11-41 RCSTR
653         USER-VECS NREAL=4
654         PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
655         REACTIONS RXN-IDS=R-31
656
657     BLOCK P11-42 RCSTR
```

```
      USER-VECS NREAL=2
      PARAM VOL=338.4 TEMP=1173. PRES=1. <atm>
      REACTIONS RXN-IDS=R-32

  BLOCK P11-46 SSPLIT
      FRAC MIXED FLUEGAS2 1. / BOTTOM 0.
      FRAC CISOLID FLUEGAS2 0.8 / BOTTOM 0.1
      FRAC CIPSD1 FLUEGAS2 0. / BOTTOM 0.
      FRAC NCPSD1 FLUEGAS2 0.8 / BOTTOM 0.2
      FRAC CIPSD2 FLUEGAS2 0. / BOTTOM 0.
      FRAC NCPSD2 FLUEGAS2 0.8 / BOTTOM 0.2
      FRAC CIPSD3 FLUEGAS2 0. / BOTTOM 0.
      FRAC NCPSD3 FLUEGAS2 0.8 / BOTTOM 0.2
      FRAC CIPSD4 FLUEGAS2 0. / BOTTOM 0.
      FRAC NCPSD4 FLUEGAS2 0.8 / BOTTOM 0.2
      FRAC CIPSD5 FLUEGAS2 0. / BOTTOM 0.
      FRAC NCPSD5 FLUEGAS2 0.8 / BOTTOM 0.2

  BLOCK P11-45 CYCLONE
      PARAM TYPE=USER
      SIMULATION DIAM=5.
           DIMENSIONS  LEN-CYLINDER=6.25  LEN-CONE=7.25  DIAM-
OVER=2.54  &
         LEN-OVER=2.25 WIDTH-INLET=1.805 HT-INLET=4.515  &
         DIAM-UNDER=1.

  EO-CONV-OPTI

  CALCULATOR C-1
  F     COMMON /USER1/ FCBSD, FCBRS, DCIPN, FMOLE,
  F    .               FRAC
  F
  F     COMMON /USER2/ WPSD, RWPSD
  F     COMMON /USER5/ AREA, VFAIR1, VAIR1, VVOID,
  F    .               BEDW
  F
  F     REAL*8 VVOID(4),  WPSD(5,5), RWPSD(5,5),
  F    .       FCBSD(5),  FCBRS(5),  DCIPN(5),
  F    .       FMOLE(5),  FRAC(3)
  F
  F     DATA BEDW/6.026/
      DEFINE FCPSD1 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD1  &
         VARIABLE=MASS-FLOW
      DEFINE FCPSD2 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD2  &
         VARIABLE=MASS-FLOW
      DEFINE FCPSD3 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD3  &
         VARIABLE=MASS-FLOW
      DEFINE FCPSD4 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD4  &
         VARIABLE=MASS-FLOW
      DEFINE FCPSD5 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD5  &
         VARIABLE=MASS-FLOW
      DEFINE DPSD1 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD1  &
         VARIABLE=MASS-DENSITY
      DEFINE DPSD2 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD2  &
         VARIABLE=MASS-DENSITY
```

```
DEFINE DPSD3 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD3  &
    VARIABLE=MASS-DENSITY
DEFINE DPSD4 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD4  &
    VARIABLE=MASS-DENSITY
DEFINE DPSD5 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD5  &
    VARIABLE=MASS-DENSITY
 DEFINE VFSUM BLOCK-VAR BLOCK=P11-7 VARIABLE=VALUE-LIST
&
    SENTENCE=REAL ELEMENT=1
DEFINE DAIR1 STREAM-VAR STREAM=AIR1 SUBSTREAM=MIXED  &
    VARIABLE=MASS-DENSITY
DEFINE FAIR1 STREAM-VAR STREAM=AIR1 SUBSTREAM=MIXED  &
    VARIABLE=MASS-FLOW
 DEFINE FLIME STREAM-VAR STREAM=LIME SUBSTREAM=CISOLID
&
    VARIABLE=MASS-FLOW
 DEFINE DLIME STREAM-VAR STREAM=LIME SUBSTREAM=CISOLID
&
    VARIABLE=MASS-DENSITY
DEFINE FNPSD1 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD1  &
    VARIABLE=MASS-FLOW
DEFINE FNPSD2 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD2  &
    VARIABLE=MASS-FLOW
DEFINE FNPSD3 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD3  &
    VARIABLE=MASS-FLOW
DEFINE FNPSD4 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD4  &
    VARIABLE=MASS-FLOW
DEFINE FNPSD5 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD5  &
    VARIABLE=MASS-FLOW
DEFINE DNPSD1 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD1  &
    VARIABLE=MASS-DENSITY
DEFINE DNPSD2 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD2  &
    VARIABLE=MASS-DENSITY
DEFINE DNPSD3 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD3  &
    VARIABLE=MASS-DENSITY
DEFINE DNPSD4 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD4  &
    VARIABLE=MASS-DENSITY
DEFINE DNPSD5 STREAM-VAR STREAM=S6 SUBSTREAM=NCPSD5  &
    VARIABLE=MASS-DENSITY
DEFINE FCBSD1 MASS-FLOW STREAM=S6 SUBSTREAM=CIPSD1  &
    COMPONENT=C
DEFINE FCBSD2 MASS-FLOW STREAM=S6 SUBSTREAM=CIPSD2  &
    COMPONENT=C
DEFINE FCBSD3 MASS-FLOW STREAM=S6 SUBSTREAM=CIPSD3  &
    COMPONENT=C
DEFINE FCBSD4 MASS-FLOW STREAM=S6 SUBSTREAM=CIPSD4  &
    COMPONENT=C
DEFINE FCBSD5 MASS-FLOW STREAM=S6 SUBSTREAM=CIPSD5  &
    COMPONENT=C
VECTOR-DEF PSD1 SUBS-ATTR STREAM=S6 SUBSTREAM=CIPSD1  &
    ATTRIBUTE=PSD1
VECTOR-DEF PSD2 SUBS-ATTR STREAM=S6 SUBSTREAM=CIPSD2  &
    ATTRIBUTE=PSD2
VECTOR-DEF PSD3 SUBS-ATTR STREAM=S6 SUBSTREAM=CIPSD3  &
    ATTRIBUTE=PSD3
```

```
   764        VECTOR-DEF PSD4 SUBS-ATTR STREAM=S6 SUBSTREAM=CIPSD4  &
   765            ATTRIBUTE=PSD4
   766        VECTOR-DEF PSD5 SUBS-ATTR STREAM=S6 SUBSTREAM=CIPSD5  &
   767            ATTRIBUTE=PSD5
   768        DEFINE MOFRAC MOLE-FRAC STREAM=S6 SUBSTREAM=MIXED  &
   769            COMPONENT=O2
   770        DEFINE MDMIX STREAM-VAR STREAM=S6 SUBSTREAM=MIXED  &
   771            VARIABLE=MOLE-DENSITY
   772         DEFINE CONO2 BLOCK-VAR BLOCK=P11-7 VARIABLE=VALUE-LIST
&
   773            SENTENCE=REAL ELEMENT=29
   774                   DEFINE   FCRSD1   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD1  &
   775            VARIABLE=MASS-FLOW
   776                   DEFINE   FCRSD2   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD2  &
   777            VARIABLE=MASS-FLOW
   778                   DEFINE   FCRSD3   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD3  &
   779            VARIABLE=MASS-FLOW
   780                   DEFINE   FCRSD4   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD4  &
   781            VARIABLE=MASS-FLOW
   782                   DEFINE   FCRSD5   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD5  &
   783            VARIABLE=MASS-FLOW
   784                   DEFINE   FNRSD1   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=NCPSD1  &
   785            VARIABLE=MASS-FLOW
   786                   DEFINE   FNRSD2   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=NCPSD2  &
   787            VARIABLE=MASS-FLOW
   788                   DEFINE   FNRSD3   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=NCPSD3  &
   789            VARIABLE=MASS-FLOW
   790                   DEFINE   FNRSD4   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=NCPSD4  &
   791            VARIABLE=MASS-FLOW
   792                   DEFINE   FNRSD5   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=NCPSD5  &
   793            VARIABLE=MASS-FLOW
   794                   DEFINE   DRPSD1   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD1  &
   795            VARIABLE=MASS-DENSITY
   796                   DEFINE   DRPSD2   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD2  &
   797            VARIABLE=MASS-DENSITY
   798                   DEFINE   DRPSD3   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD3  &
   799            VARIABLE=MASS-DENSITY
   800                   DEFINE   DRPSD4   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD4  &
   801            VARIABLE=MASS-DENSITY
   802                   DEFINE   DRPSD5   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CIPSD5  &
```

```
   803            VARIABLE=MASS-DENSITY
   804                    DEFINE   FRLIME   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CISOLID  &
   805            VARIABLE=MASS-FLOW
   806                    DEFINE   DRLIME   STREAM-VAR   STREAM=RESOLID
SUBSTREAM=CISOLID  &
   807            VARIABLE=MASS-DENSITY
   808         DEFINE DMPSD1 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD1  &
   809            VARIABLE=MOLE-DENSITY
   810         DEFINE DMPSD2 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD2  &
   811            VARIABLE=MOLE-DENSITY
   812         DEFINE DMPSD3 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD3  &
   813            VARIABLE=MOLE-DENSITY
   814         DEFINE DMPSD4 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD4  &
   815            VARIABLE=MOLE-DENSITY
   816         DEFINE DMPSD5 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD5  &
   817            VARIABLE=MOLE-DENSITY
   818         DEFINE FMPSD1 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD1  &
   819            VARIABLE=MOLE-FLOW
   820         DEFINE FMPSD2 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD2  &
   821            VARIABLE=MOLE-FLOW
   822         DEFINE FMPSD3 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD3  &
   823            VARIABLE=MOLE-FLOW
   824         DEFINE FMPSD4 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD4  &
   825            VARIABLE=MOLE-FLOW
   826         DEFINE FMPSD5 STREAM-VAR STREAM=S6 SUBSTREAM=CIPSD5  &
   827            VARIABLE=MOLE-FLOW
   828         DEFINE FRACO MOLE-FRAC STREAM=S6 SUBSTREAM=MIXED  &
   829            COMPONENT=CO
   830         DEFINE FRAH2O MOLE-FRAC STREAM=S6 SUBSTREAM=MIXED  &
   831            COMPONENT=H2O
   832         DEFINE DENMOL BLOCK-VAR BLOCK=P11-7 VARIABLE=VALUE-LIST
&
   833            SENTENCE=REAL ELEMENT=107
   834         DEFINE VISCO STREAM-PROP STREAM=S6 PROPERTY=PS-1
   835         DEFINE VIS BLOCK-VAR BLOCK=P11-7 VARIABLE=VALUE-LIST  &
   836            SENTENCE=REAL ELEMENT=108
   837     F     OPEN (7,FILE='C-1.txt')
   838     F
   839     F
   840     C     TOTAL MASS FLOW RATE OF SUBSTREAM CIPSD
   841     F     FTOTAL =   FCPSD1 + FCPSD2 + FCPSD3 + FCPSD4 + FCPSD5
   842     F     .        + FNPSD1 + FNPSD2 + FNPSD3 + FNPSD4 + FNPSD5
   843     F     .        + FCRSD1 + FCRSD2 + FCRSD3 + FCRSD4 + FCRSD5
   844     F     .        + FNRSD1 + FNRSD2 + FNRSD3 + FNRSD4 + FNRSD5
   845     F     .        + FLIME  + FRLIME
   846      F      WRITE (7,*) 'TOTAL MASS FLOW RATE OF CIPSD (kg/s)',
FTOTAL
   847     F
   848     C     MEAN MASS DENSITY OF TOTAL FLOW TO RCSTR
   849      F      DENS = 1/FTOTAL * (FCPSD1*DPSD1  + FCPSD2*DPSD2  +
FCPSD3*DPSD3
   850     F     .               +  FCPSD4*DPSD4  + FCPSD5*DPSD5
   851      F     .                  +  FNPSD1*DNPSD1 + FNPSD2*DNPSD2 +
FNPSD3*DNPSD3
```

```
   852    F    .                +  FNPSD4*DNPSD4 + FNPSD5*DNPSD5
   853     F    .                  +  FCRSD1*DRPSD1 + FCRSD2*DRPSD2 +
FCRSD3*DRPSD3
   854    F    .                +  FCRSD4*DRPSD4 + FCRSD5*DRPSD5
   855     F    .                  +  FNRSD1*DRNSD1 + FNRSD2*DRNSD2 +
FNRSD3*DRNSD3
   856    F    .                +  FNRSD4*DRNSD4 + FNRSD5*DRNSD5
   857    F    .                +  FLIME*DLIME   + FRLIME*DRLIME)
   858    F     WRITE (7,*) 'MEAN MASS DENSITY (Kg/m^3)',DENS
   859    F
   860    C     VOLUMETRIC FLOW RATE OF TOTAL FLOW TO RCSTR
   861    F     VFSUM = FTOTAL/DENS
   862     F       WRITE (7,*) 'VOLUMETRIC FLOW RATE OF TOTAL FLOW
(m^3/s)', VFSUM
   863    F
   864    C     CONCENTRATION OF OXYGEN
   865    F     DENMOL = MDMIX
   866    F     CONO2 = MOFRAC*MDMIX
   867    C      WRITE (7,*) 'CONCENTRATION ',CONO2
   868    F
   869    C     CONCENTRATION OF MIXED STREAM
   870    F     CONM = CONMIX
   871    F
   872                                                                C
*===============================================================*
   873    C                              LOWER REGION
   874                                                                C
*===============================================================*
   875    C     SECTION AREA OF REACTOR
   876    F     PIE  = 3.141592654
   877    F     AREA = BEDW**2.
   878    F     WRITE (7,*)'AREA',AREA
   879    F
   880    C     AIR VOLUMETRIC FLOW RATE (m^3/s)
   881    F     VFAIR1 = FAIR1/DAIR1
   882        F         WRITE  (7,*)  'VOLUMETRIC  FLOW  RATE  OF  AIR
(m^3/s)',VFAIR1
   883    F
   884    C     AIR VELOCITY (m/s)
   885    F     VAIR1 = VFAIR1/AREA
   886    F     WRITE (7,*) 'AIR VELOCITY (m/s)',VAIR1
   887    F
   888    C     MEAN VOIDAGE OF DENSE BED
   889    C     FUNCTION BETWEEN VELOCITY AND 1-VOIDAGE
   890    F     VOI = -0.0884*DLOG(VAIR1)+0.279
   891    F     VVOID(1) = 1.-VOI
   892    F     WRITE (7,*)'MEAN VOIDAGE OF DENSE BED',VVOID(1)
   893    C      VOID1 = VOID(1)
   894    C     *-------------------------------------------------
------------*
   895    F
   896    C     DEFINED MOLAR DENSITY TO EXTERNAL SUBROUTINE
   897    F     DCIPN(1) = DMPSD1
   898    F     DCIPN(2) = DMPSD2
   899    F     DCIPN(3) = DMPSD3
```

```
   900    F     DCIPN(4) = DMPSD4
   901    F     DCIPN(5) = DMPSD5
   902    F
   903    C     DEFINED MOLAR FLOW RATE TO EXTERNAL SUBROUTINE
   904    F     FMOLE(1) = FMPSD1
   905    F     FMOLE(2) = FMPSD2
   906    F     FMOLE(3) = FMPSD3
   907    F     FMOLE(4) = FMPSD4
   908    F     FMOLE(5) = FMPSD5
   909    F
   910    C     MOLE FRACTION FOR CALCULATED
   911    F     FRAC(1) = MOFRAC
   912    F     FRAC(2) = FRACO
   913    F     FRAC(3) = FRAH2O
   914    F
   915                                                                C
*================================================================*
   916    C                     PREPARE WEIGHT FRACTION OF PSD
   917                                                                C
*================================================================*
   918    F     DO 5 I=1,5
   919    F     WPSD(I,1) = PSD1(I)
   920    F     WPSD(I,2) = PSD2(I)
   921    F     WPSD(I,3) = PSD3(I)
   922    F     WPSD(I,4) = PSD4(I)
   923    F   5 WPSD(I,5) = PSD5(I)
   924    F     WRITE (7,6) ((WPSD(I,J),J=1,5),I=1,5)
   925    F   6 FORMAT(2X, 'WPSD',/5(1X,E10.3))
   926    F
   927    F
   928                                                                C
*================================================================*
   929     C         MASS FLOW RATE OF CARBON FOR EACH COMPONENT IN
INPUT STREAM
   930                                                                C
*================================================================*
   931    F     FCBSD(1) = FCBSD1
   932    F     FCBSD(2) = FCBSD2
   933    F     FCBSD(3) = FCBSD3
   934    F     FCBSD(4) = FCBSD4
   935    F     FCBSD(5) = FCBSD5
   936    F
   937    C     VISCOSITY OF MIXED STREAM
   938    F     VIS = VISCO
   939    F
   940     C     5 WRITE (7,*)'MASS FLOW RATE FOR EACH PSD, Kg/s',
FPSD(I)
   941        EXECUTE BEFORE BLOCK P11-7
   942
   943    CALCULATOR C-2
   944    F     COMMON /USER4/ DCIPNU, FMOLU1, W2PSD, FBSD2, DP
   945    F     COMMON /USER5/ AREA, VFAIR1, VAIR1, VVOID,
   946    F    .               BEDW, BEDVV
   947    F     COMMON /USER6/ VAIRU1
   948    F     COMMON /USER15/ BEDT2
```

```
 949    F
 950    F     REAL*8 DCIPNU(5), FMOLU1(5), W2PSD(5,5),
 951    F    .       FBSD2(5),  VVOID(4),  BEDL(4),
 952    F    .       UGAS(4),   BDL(4),    BEDVV(4)
 953    F
 954    F     DATA PHIS/0.806/, BEDLT/21.84/, VOIDS/0.999/
 955    F
 956         DEFINE FCPSD1 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD1  &
 957             VARIABLE=MASS-FLOW
 958         DEFINE FCPSD2 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD2  &
 959             VARIABLE=MASS-FLOW
 960         DEFINE FCPSD3 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD3  &
 961             VARIABLE=MASS-FLOW
 962         DEFINE FCPSD4 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD4  &
 963             VARIABLE=MASS-FLOW
 964         DEFINE FCPSD5 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD5  &
 965             VARIABLE=MASS-FLOW
 966         DEFINE FNPSD1 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD1  &
 967             VARIABLE=MASS-FLOW
 968         DEFINE FNPSD2 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD2  &
 969             VARIABLE=MASS-FLOW
 970         DEFINE FNPSD3 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD3  &
 971             VARIABLE=MASS-FLOW
 972         DEFINE FNPSD4 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD4  &
 973             VARIABLE=MASS-FLOW
 974         DEFINE FNPSD5 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD5  &
 975             VARIABLE=MASS-FLOW
 976         DEFINE FLIME STREAM-VAR STREAM=S11 SUBSTREAM=CISOLID  &
 977             VARIABLE=MASS-FLOW
 978         DEFINE DPSD1 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD1  &
 979             VARIABLE=MASS-DENSITY
 980         DEFINE DPSD2 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD2  &
 981             VARIABLE=MASS-DENSITY
 982         DEFINE DPSD3 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD3  &
 983             VARIABLE=MASS-DENSITY
 984         DEFINE DPSD4 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD4  &
 985             VARIABLE=MASS-DENSITY
 986         DEFINE DPSD5 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD5  &
 987             VARIABLE=MASS-DENSITY
 988         DEFINE DNPSD1 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD1  &
 989             VARIABLE=MASS-DENSITY
 990         DEFINE DNPSD2 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD2  &
 991             VARIABLE=MASS-DENSITY
 992         DEFINE DNPSD3 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD3  &
 993             VARIABLE=MASS-DENSITY
 994         DEFINE DNPSD4 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD4  &
 995             VARIABLE=MASS-DENSITY
 996         DEFINE DNPSD5 STREAM-VAR STREAM=S11 SUBSTREAM=NCPSD5  &
 997             VARIABLE=MASS-DENSITY
 998         DEFINE DLIME STREAM-VAR STREAM=S11 SUBSTREAM=CISOLID  &
 999             VARIABLE=MASS-DENSITY
1000         DEFINE VFSUM BLOCK-VAR BLOCK=P11-17 VARIABLE=VALUE-LIST
&
1001             SENTENCE=REAL ELEMENT=1
1002         DEFINE DMPSD1 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD1  &
```

```
1003            VARIABLE=MOLE-DENSITY
1004          DEFINE DMPSD2 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD2  &
1005            VARIABLE=MOLE-DENSITY
1006          DEFINE DMPSD3 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD3  &
1007            VARIABLE=MOLE-DENSITY
1008          DEFINE DMPSD4 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD4  &
1009            VARIABLE=MOLE-DENSITY
1010          DEFINE DMPSD5 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD5  &
1011            VARIABLE=MOLE-DENSITY
1012          DEFINE FMPSD1 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD1  &
1013            VARIABLE=MOLE-FLOW
1014          DEFINE FMPSD2 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD2  &
1015            VARIABLE=MOLE-FLOW
1016          DEFINE FMPSD3 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD3  &
1017            VARIABLE=MOLE-FLOW
1018          DEFINE FMPSD4 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD4  &
1019            VARIABLE=MOLE-FLOW
1020          DEFINE FMPSD5 STREAM-VAR STREAM=S11 SUBSTREAM=CIPSD5  &
1021            VARIABLE=MOLE-FLOW
1022          DEFINE MOFRAC MOLE-FRAC STREAM=S11 SUBSTREAM=MIXED  &
1023            COMPONENT=O2
1024          DEFINE MDMIX STREAM-VAR STREAM=S11 SUBSTREAM=MIXED  &
1025            VARIABLE=MOLE-DENSITY
1026           VECTOR-DEF PSD1 SUBS-ATTR STREAM=S11 SUBSTREAM=CIPSD1
&
1027            ATTRIBUTE=PSD1
1028           VECTOR-DEF PSD2 SUBS-ATTR STREAM=S11 SUBSTREAM=CIPSD2
&
1029            ATTRIBUTE=PSD2
1030           VECTOR-DEF PSD3 SUBS-ATTR STREAM=S11 SUBSTREAM=CIPSD3
&
1031            ATTRIBUTE=PSD3
1032           VECTOR-DEF PSD4 SUBS-ATTR STREAM=S11 SUBSTREAM=CIPSD4
&
1033            ATTRIBUTE=PSD4
1034           VECTOR-DEF PSD5 SUBS-ATTR STREAM=S11 SUBSTREAM=CIPSD5
&
1035            ATTRIBUTE=PSD5
1036          DEFINE FCBSD1 MASS-FLOW STREAM=S11 SUBSTREAM=CIPSD1  &
1037            COMPONENT=C
1038          DEFINE FCBSD2 MASS-FLOW STREAM=S11 SUBSTREAM=CIPSD2  &
1039            COMPONENT=C
1040          DEFINE FCBSD3 MASS-FLOW STREAM=S11 SUBSTREAM=CIPSD3  &
1041            COMPONENT=C
1042          DEFINE FCBSD4 MASS-FLOW STREAM=S11 SUBSTREAM=CIPSD4  &
1043            COMPONENT=C
1044          DEFINE FCBSD5 MASS-FLOW STREAM=S11 SUBSTREAM=CIPSD5  &
1045            COMPONENT=C
1046          DEFINE DMIX STREAM-VAR STREAM=S11 SUBSTREAM=MIXED  &
1047            VARIABLE=MASS-DENSITY
1048          DEFINE FMIX STREAM-VAR STREAM=S11 SUBSTREAM=MIXED  &
1049            VARIABLE=MASS-FLOW
1050          DEFINE VISCO STREAM-PROP STREAM=S11 PROPERTY=PS-1
1051          DEFINE BEDV BLOCK-VAR BLOCK=P11-7 VARIABLE=VOL  &
1052            SENTENCE=PARAM
```

```
  1053         DEFINE BEDVU1 BLOCK-VAR BLOCK=P11-17 VARIABLE=VOL  &
  1054             SENTENCE=PARAM
  1055         DEFINE BEDP BLOCK-VAR BLOCK=P11-17 VARIABLE=PRES  &
  1056             SENTENCE=PARAM
  1057         DEFINE FMAIR1 STREAM-VAR STREAM=AIR1 SUBSTREAM=MIXED  &
  1058             VARIABLE=MOLE-FLOW
  1059         DEFINE FMAIR2 STREAM-VAR STREAM=AIR2 SUBSTREAM=MIXED  &
  1060             VARIABLE=MOLE-FLOW
  1061         DEFINE FMAIR3 STREAM-VAR STREAM=AIR3 SUBSTREAM=MIXED  &
  1062             VARIABLE=MOLE-FLOW
  1063         DEFINE BEDVU2 BLOCK-VAR BLOCK=P11-26 VARIABLE=VOL  &
  1064             SENTENCE=PARAM
  1065         DEFINE CONO2 BLOCK-VAR BLOCK=P11-17 VARIABLE=VALUE-LIST
&
  1066             SENTENCE=REAL ELEMENT=29
  1067          DEFINE VIS BLOCK-VAR BLOCK=P11-17 VARIABLE=VALUE-LIST
&
  1068             SENTENCE=REAL ELEMENT=108
  1069     F     OPEN (7,FILE='C-2.txt')
  1070     F
  1071     F
  1072     C     TOTAL MASS FLOW RATE OF SUBSTREAM CIPSD
  1073     F     FTOTAL =   FCPSD1 + FCPSD2 + FCPSD3 + FCPSD4 + FCPSD5
  1074     F    .         + FNPSD1 + FNPSD2 + FNPSD3 + FNPSD4 + FNPSD5
  1075     F    .         + FLIME
  1076      F      WRITE (7,*) 'TOTAL MASS FLOW RATE OF CIPSD (kg/s)',
FTOTAL
  1077     F
  1078     C     MEAN MASS DENSITY OF TOTAL FLOW TO RCSTR
  1079      F      DENS = 1/FTOTAL * (FCPSD1*DPSD1  + FCPSD2*DPSD2  +
FCPSD3*DPSD3
  1080     F     .                 +  FCPSD4*DPSD4  + FCPSD5*DPSD5
  1081      F    .                    +  FNPSD1*DNPSD1 + FNPSD2*DNPSD2 +
FNPSD3*DNPSD3
  1082     F     .                 +  FNPSD4*DNPSD4 + FNPSD5*DNPSD5
  1083     F     .                 +  FLIME*DLIME)
  1084     F     WRITE (7,*) 'MEAN MASS DENSITY (Kg/m^3)',DENS
  1085     F
  1086     C     VOLUMETRIC FLOW RATE OF TOTAL FLOW TO RCSTR
  1087     F     VFSUM = FTOTAL/DENS
  1088       F       WRITE (7,*) 'VOLUMETRIC FLOW RATE OF TOTAL FLOW
(m^3/s)', VFSUM
  1089     F
  1090     C     DEFINED MOLAR DENSITY TO EXTERNAL SUBROUTINE
  1091     F     DCIPNU(1) = DMPSD1
  1092     F     DCIPNU(2) = DMPSD2
  1093     F     DCIPNU(3) = DMPSD3
  1094     F     DCIPNU(4) = DMPSD4
  1095     F     DCIPNU(5) = DMPSD5
  1096     F
  1097     C     DEFINED MOLAR FLOW RATE TO EXTERNAL SUBROUTINE
  1098     F     FMOLU1(1) = FMPSD1
  1099     F     FMOLU1(2) = FMPSD2
  1100     F     FMOLU1(3) = FMPSD3
  1101     F     FMOLU1(4) = FMPSD4
```

```
 1102    F     FMOLU1(5) = FMPSD5
 1103    F
 1104    C     CONCENTRATION OF OXYGEN
 1105    F     CONO2 = MOFRAC*MDMIX
 1106    F     WRITE (7,*) 'CONCENTRATION ',CONO2
 1107    F
 1108    C     VISCOSITY OF FLUID
 1109    F     VIS = VISCO
 1110    F
 1111                                                                  C
*=================================================================*
 1112    C                    PREPARE WEIGHT FRACTION OF PSD
 1113                                                                  C
*=================================================================*
 1114    F     DO 5 I=1,5
 1115    F     W2PSD(I,1) = PSD1(I)
 1116    F     W2PSD(I,2) = PSD2(I)
 1117    F     W2PSD(I,3) = PSD3(I)
 1118    F     W2PSD(I,4) = PSD4(I)
 1119    F   5 W2PSD(I,5) = PSD5(I)
 1120    F     WRITE (7,6) ((W2PSD(I,J),J=1,5),I=1,5)
 1121    F   6 FORMAT(2X, 'W2PSD',/5(1X,E10.3))
 1122    F
 1123                                                                  C
*=================================================================*
 1124     C         MASS FLOW RATE OF CARBON FOR EACH COMPONENT IN
INPUT STREAM
 1125                                                                  C
*=================================================================*
 1126    F     FBSD2(1) = FCBSD1
 1127    F     FBSD2(2) = FCBSD2
 1128    F     FBSD2(3) = FCBSD3
 1129    F     FBSD2(4) = FCBSD4
 1130    F     FBSD2(5) = FCBSD5
 1131    F
 1132                                                                  C
*=================================================================*
 1133    C                                  LOWER REGION
 1134                                                                  C
*=================================================================*
 1135    C      WRITE (7,*)'AREA',AREA
 1136       C          WRITE (7,*) 'VOLUMETRIC FLOW RATE OF AIR
(m^3/s)',VFAIR1
 1137    C      WRITE (7,*) 'AIR VELOCITY (m/s)',VAIR1
 1138    C      WRITE (7,*)'MEAN VOIDAGE OF DENSE BED',VVOID(1)
 1139    F
 1140                                                                  C
*=================================================================*
 1141    C                                  UPPER REGION
 1142                                                                  C
*=================================================================*
 1143    F
 1144    C     VOLUMETRIC FLOW RATE FOR MIXED STREAM (m^3/s)
 1145    F     FVMIX = FMIX/DMIX
 1146    F
```

```
C     AIR VELOCITY (m/s)
F     VAIRU1 = FVMIX/AREA
F     WRITE (7,*) 'AIRVELOCITY TO UPPER REGION', VAIRU1
F
C     NET SOLIDS CIRCULATION FLUX (Kg/(m^2.s))
F     GS = 50.0
F
C     ACCELERATION DUE TO GRAVITY (m/s^2)
F     G  = 9.81
F
F     WRITE (7,*) 'DP',DP
C     DIMENSION LESS (DP STAR)  (m)
      F        DPSAT  =  DP  *  (  DMIX*(DENS-DMIX)*G/VISCO**2.
)**(1./3.)
F     WRITE (7,*) 'DIMENSIONLESS (DP STAR)',DPSAT
F
C     TERMINAL VELOCITY OF PARTICLE (m/s)
        F          UTSAT  =    1./(18./DPSAT**2.  +  (2.335-
1.744*PHIS)/DPSAT**0.5)
F     WRITE (7,*) 'UTSAT',UTSAT
F
      F        UT  =   UTSAT/(  DMIX**2./(VISCO*(DENS-DMIX)*G)
)**(1./3.)
F     WRITE (7,*) 'TERMINAL VELOCITY OF PARTICLE (M/S)',UT
F
C     EQUIVALENT DIAMETER (m)
F     BEDD = 4.*AREA/(4.*BEDW)
C      WRITE (7,*) 'BEDD (M)',BEDD
F
C     BED LENGTH (m)
F     BEDL(1) = BEDV/AREA
F     BEDL(2) = BEDVU1/AREA
F     BEDL(3) = BEDVU2/AREA
F     BEDL(4) = BEDLT - ( BEDL(1) + BEDL(2) + BEDL(3) )
F     WRITE (7,*) 'BEDL(I)',(BEDL(I),I=1,4)
F
C     TOTAL GAS CONCENTRATION (Kmole/m^3)
C     GAS CONSTANT (atm cm^3)/(gmole K)
F     R = 82.056
F     CONC = BEDP*1000./(101325.*R*BEDT2)
C      WRITE (7,*) 'CONC',CONC
F     WRITE (7,*) 'TEMP',BEDT2
C      WRITE (7,*) 'PRES',BEDP
F
C     SUPERFICIAL GAS VELOCITY (m/s)
F     UGAS(1) = FMAIR1/(AREA*CONC)
F     UGAS(2) = UGAS(1) + FMAIR2/(AREA*CONC)
F     UGAS(3) = UGAS(2) + FMAIR3/(AREA*CONC)
F     UGAS(4) = UGAS(3)
F     WRITE (7,*) 'UGAS(I)',(UGAS(I),I=1,4)
F
C     FROUDE NUMBER
F     FR = UGAS(4)/(G*BEDD)**0.5
F     WRITE (7,*) 'FR',FR
F
```

```
  1199    C     PARTICLE FROUDE NUMBER
  1200    F     FRT = UT/(G*BEDD)**0.5
  1201    F     WRITE (7,*) 'FRT',FRT
  1202    F
  1203    C     MEAN AXIAL VOIDAGE IN THE FULLY DEVELOPED ZONE
  1204    F     PHI = 1. + 5.6/FR + 0.47*FRT**0.41
  1205    F     VVOID(4) = 1./( 1. + PHI*GS/(UGAS(4)*DENS) )
  1206    F     WRITE (7,*) 'PHI',PHI
  1207    F     WRITE (7,*) 'VVOID(4)',VVOID(4)
  1208    F
  1209    C     DECAY CONSTANT
  1210    F     A = 5./UGAS(4)
  1211    F     WRITE (7,*) 'DECAY RATIO',A
  1212    F
  1213    C     LENGTH OF THE ACCELERATION ZONE
  1214     F      BEDZ = (-1./A) * DLOG( (VOIDS-VVOID(4)) / (VOIDS-
VVOID(1)) )
  1215    F     WRITE (7,*) 'BEDZ',BEDZ
  1216    F
  1217    C     HEIGHT IN CFBC AT ANY INTERVAL
  1218    F     BDL(1) = BEDV/AREA
  1219    F     BDL(2) = BEDZ/3.
  1220    F     BDL(3) = 2.*BEDZ/3.
  1221    F     BDL(4) = BEDLT - ( BEDZ+BDL(1) )
  1222    F     WRITE (7,*) 'BDL(I)',(BDL(I),I=1,4)
  1223    F
  1224    F     BEDVV(1) = BEDV
  1225    F     BEDVV(2) = AREA*BDL(2)
  1226    F     BEDVV(3) = AREA*BDL(3)
  1227    F     BEDVV(4) = AREA*BDL(4)
  1228    F     WRITE (7,*) 'BEDVV(I)',(BEDVV(I),I=1,4)
  1229    F
  1230    C     VOIDAGE AT ANOTHER INTERVAL
  1231    F     VVOID(2) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(1))
  1232    F    .          * ( DEXP(-A*BDL(2)) - 1. )
  1233    F     VVOID(3) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(2))
  1234    F    .           * ( DEXP(-A*BEDZ) - DEXP(-A*BDL(2)) )
  1235    F     WRITE (7,*) 'VVOID(2)',VVOID(2)
  1236    F     WRITE (7,*) 'VVOID(3)',VVOID(3)
  1237    F
  1238    C     VOLUME OF BED AT ANY INTERVAL
  1239    F
  1240    C      VOID1  = VVOID(1)
  1241    C      VOIDU1 = VVOID(2)
  1242    C      VOIDU2 = VVOID(3)
  1243    C      VOIDU3 = VVOID(4)
  1244    C       VOIDU1 = 0.8
  1245    F
  1246    F
  1247    C      BEDVU1 = BEDVV(2)
  1248    C      BEDVU2 = BEDVV(3)
  1249    C      BEDVU3 = BEDVV(4)
  1250        EXECUTE BEFORE BLOCK P11-17
  1251
  1252    CALCULATOR C-3
```

```
1253    F     COMMON /USER5/  AREA, VFAIR1, VAIR1, VVOID,
1254    F    .                BEDW, BEDVV
1255    F     COMMON /USER9/  DCINU2, FMOLU2, W3PSD, FBSD3, DP2
1256    F     COMMON /USER10/ VAIRU2, VVOID2, BEDVV2
1257    F     COMMON /USER16/ BEDT3
1258    F
1259    F     REAL*8 DCINU2(5), FMOLU2(5), W3PSD(5,5),
1260    F    .       VVOID2(4), BEDVV2(4), FBSD3(5),
1261    F    .       BEDL(4),   UGAS(4),   VVOID(4),
1262    F    .       BDL(4)
1263    F
1264    F     DATA PHIS/0.806/, BEDLT/21.84/, VOIDS/0.999/
1265    F
1266         DEFINE FCPSD1 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD1  &
1267             VARIABLE=MASS-FLOW
1268         DEFINE FCPSD2 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD2  &
1269             VARIABLE=MASS-FLOW
1270         DEFINE FCPSD3 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD3  &
1271             VARIABLE=MASS-FLOW
1272         DEFINE FCPSD4 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD4  &
1273             VARIABLE=MASS-FLOW
1274         DEFINE FCPSD5 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD5  &
1275             VARIABLE=MASS-FLOW
1276         DEFINE FNPSD1 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD1  &
1277             VARIABLE=MASS-FLOW
1278         DEFINE FNPSD2 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD2  &
1279             VARIABLE=MASS-FLOW
1280         DEFINE FNPSD3 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD3  &
1281             VARIABLE=MASS-FLOW
1282         DEFINE FNPSD4 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD4  &
1283             VARIABLE=MASS-FLOW
1284         DEFINE FNPSD5 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD5  &
1285             VARIABLE=MASS-FLOW
1286         DEFINE FLIME STREAM-VAR STREAM=S15 SUBSTREAM=CISOLID  &
1287             VARIABLE=MASS-FLOW
1288         DEFINE DPSD1 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD1  &
1289             VARIABLE=MASS-DENSITY
1290         DEFINE DPSD2 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD2  &
1291             VARIABLE=MASS-DENSITY
1292         DEFINE DPSD3 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD3  &
1293             VARIABLE=MASS-DENSITY
1294         DEFINE DPSD4 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD4  &
1295             VARIABLE=MASS-DENSITY
1296         DEFINE DPSD5 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD5  &
1297             VARIABLE=MASS-DENSITY
1298         DEFINE DNPSD1 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD1  &
1299             VARIABLE=MASS-DENSITY
1300         DEFINE DNPSD2 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD2  &
1301             VARIABLE=MASS-DENSITY
1302         DEFINE DNPSD3 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD3  &
1303             VARIABLE=MASS-DENSITY
1304         DEFINE DNPSD4 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD4  &
1305             VARIABLE=MASS-DENSITY
1306         DEFINE DNPSD5 STREAM-VAR STREAM=S15 SUBSTREAM=NCPSD5  &
1307             VARIABLE=MASS-DENSITY
```

```
 1308         DEFINE DLIME STREAM-VAR STREAM=S15 SUBSTREAM=CISOLID  &
 1309             VARIABLE=MASS-DENSITY
 1310         DEFINE DMPSD1 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD1  &
 1311             VARIABLE=MOLE-DENSITY
 1312         DEFINE DMPSD2 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD2  &
 1313             VARIABLE=MOLE-DENSITY
 1314         DEFINE DMPSD3 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD3  &
 1315             VARIABLE=MOLE-DENSITY
 1316         DEFINE DMPSD4 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD4  &
 1317             VARIABLE=MOLE-DENSITY
 1318         DEFINE DMPSD5 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD5  &
 1319             VARIABLE=MOLE-DENSITY
 1320         DEFINE FMPSD1 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD1  &
 1321             VARIABLE=MOLE-FLOW
 1322         DEFINE FMPSD2 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD2  &
 1323             VARIABLE=MOLE-FLOW
 1324         DEFINE FMPSD3 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD3  &
 1325             VARIABLE=MOLE-FLOW
 1326         DEFINE FMPSD4 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD4  &
 1327             VARIABLE=MOLE-FLOW
 1328         DEFINE FMPSD5 STREAM-VAR STREAM=S15 SUBSTREAM=CIPSD5  &
 1329             VARIABLE=MOLE-FLOW
 1330         DEFINE MOFRAC MOLE-FRAC STREAM=S15 SUBSTREAM=MIXED  &
 1331             COMPONENT=O2
 1332         DEFINE MDMIX STREAM-VAR STREAM=S15 SUBSTREAM=MIXED  &
 1333             VARIABLE=MOLE-DENSITY
 1334         DEFINE CONO2 BLOCK-VAR BLOCK=P11-26 VARIABLE=VALUE-LIST
&
 1335             SENTENCE=REAL ELEMENT=29
 1336         DEFINE VISCO STREAM-PROP STREAM=S15 PROPERTY=PS-1
 1337           DEFINE VIS BLOCK-VAR BLOCK=P11-26 VARIABLE=VALUE-LIST
&
 1338             SENTENCE=REAL ELEMENT=108
 1339           VECTOR-DEF PSD1 SUBS-ATTR STREAM=S15 SUBSTREAM=CIPSD1
&
 1340             ATTRIBUTE=PSD1
 1341           VECTOR-DEF PSD2 SUBS-ATTR STREAM=S15 SUBSTREAM=CIPSD2
&
 1342             ATTRIBUTE=PSD2
 1343           VECTOR-DEF PSD3 SUBS-ATTR STREAM=S15 SUBSTREAM=CIPSD3
&
 1344             ATTRIBUTE=PSD3
 1345           VECTOR-DEF PSD4 SUBS-ATTR STREAM=S15 SUBSTREAM=CIPSD4
&
 1346             ATTRIBUTE=PSD4
 1347           VECTOR-DEF PSD5 SUBS-ATTR STREAM=S15 SUBSTREAM=CIPSD5
&
 1348             ATTRIBUTE=PSD5
 1349         DEFINE VFSUM BLOCK-VAR BLOCK=P11-26 VARIABLE=VALUE-LIST
&
 1350             SENTENCE=REAL ELEMENT=1
 1351         DEFINE DMIX STREAM-VAR STREAM=S15 SUBSTREAM=MIXED  &
 1352             VARIABLE=MASS-DENSITY
 1353         DEFINE FMIX STREAM-VAR STREAM=S15 SUBSTREAM=MIXED  &
 1354             VARIABLE=MASS-FLOW
```

```
  1355         DEFINE FCBSD1 MASS-FLOW STREAM=S15 SUBSTREAM=CIPSD1  &
  1356             COMPONENT=C
  1357         DEFINE FCBSD2 MASS-FLOW STREAM=S15 SUBSTREAM=CIPSD2  &
  1358             COMPONENT=C
  1359         DEFINE FCBSD3 MASS-FLOW STREAM=S15 SUBSTREAM=CIPSD3  &
  1360             COMPONENT=C
  1361         DEFINE FCBSD4 MASS-FLOW STREAM=S15 SUBSTREAM=CIPSD4  &
  1362             COMPONENT=C
  1363         DEFINE FCBSD5 MASS-FLOW STREAM=S15 SUBSTREAM=CIPSD5  &
  1364             COMPONENT=C
  1365         DEFINE BEDV BLOCK-VAR BLOCK=P11-7 VARIABLE=VOL  &
  1366             SENTENCE=PARAM
  1367         DEFINE BEDVU1 BLOCK-VAR BLOCK=P11-17 VARIABLE=VOL  &
  1368             SENTENCE=PARAM
  1369         DEFINE BEDVU2 BLOCK-VAR BLOCK=P11-26 VARIABLE=VOL  &
  1370             SENTENCE=PARAM
  1371         DEFINE BEDP BLOCK-VAR BLOCK=P11-26 VARIABLE=PRES  &
  1372             SENTENCE=PARAM
  1373         DEFINE FMAIR1 STREAM-VAR STREAM=AIR1 SUBSTREAM=MIXED  &
  1374             VARIABLE=MOLE-FLOW
  1375         DEFINE FMAIR2 STREAM-VAR STREAM=AIR2 SUBSTREAM=MIXED  &
  1376             VARIABLE=MOLE-FLOW
  1377         DEFINE FMAIR3 STREAM-VAR STREAM=AIR3 SUBSTREAM=MIXED  &
  1378             VARIABLE=MOLE-FLOW
  1379     F     OPEN (7,FILE='C-3.txt')
  1380     F
  1381     F
  1382     C     TOTAL MASS FLOW RATE OF SUBSTREAM CIPSD
  1383     F     FTOTAL =   FCPSD1 + FCPSD2 + FCPSD3 + FCPSD4 + FCPSD5
  1384     F    .         + FNPSD1 + FNPSD2 + FNPSD3 + FNPSD4 + FNPSD5
  1385     F    .         + FLIME
  1386      F      WRITE (7,*) 'TOTAL MASS FLOW RATE OF CIPSD (kg/s)',
FTOTAL
  1387     F
  1388     C     MEAN MASS DENSITY OF TOTAL FLOW TO RCSTR
  1389      F      DENS = 1/FTOTAL * (FCPSD1*DPSD1  + FCPSD2*DPSD2  +
FCPSD3*DPSD3
  1390     F    .                 +  FCPSD4*DPSD4  + FCPSD5*DPSD5
  1391      F   .                   +  FNPSD1*DNPSD1 + FNPSD2*DNPSD2 +
FNPSD3*DNPSD3
  1392     F    .                 +  FNPSD4*DNPSD4 + FNPSD5*DNPSD5
  1393     F    .                 +  FLIME*DLIME)
  1394     F     WRITE (7,*) 'MEAN MASS DENSITY (Kg/m^3)',DENS
  1395     F
  1396     C     VOLUMETRIC FLOW RATE OF TOTAL FLOW TO RCSTR
  1397     F     VFSUM = FTOTAL/DENS
  1398       F       WRITE (7,*) 'VOLUMETRIC FLOW RATE OF TOTAL FLOW
(m^3/s)', VFSUM
  1399     F
  1400     C     DEFINED MOLAR DENSITY TO EXTERNAL SUBROUTINE
  1401     F     DCINU2(1) = DMPSD1
  1402     F     DCINU2(2) = DMPSD2
  1403     F     DCINU2(3) = DMPSD3
  1404     F     DCINU2(4) = DMPSD4
  1405     F     DCINU2(5) = DMPSD5
```

```
 1406    F
 1407    C     DEFINED MOLAR FLOW RATE TO EXTERNAL SUBROUTINE
 1408    F     FMOLU2(1) = FMPSD1
 1409    F     FMOLU2(2) = FMPSD2
 1410    F     FMOLU2(3) = FMPSD3
 1411    F     FMOLU2(4) = FMPSD4
 1412    F     FMOLU2(5) = FMPSD5
 1413    F
 1414    C     CONCENTRATION OF OXYGEN
 1415    F     CONO2 = MOFRAC*MDMIX
 1416    F     WRITE (7,*) 'CONCENTRATION ',CONO2
 1417    F
 1418    C     VISCOSITY OF FLUID
 1419    F     VIS = VISCO
 1420    F
 1421                                                                  C
*=================================================================*
 1422    C                     PREPARE WEIGHT FRACTION OF PSD
 1423                                                                  C
*=================================================================*
 1424    F     DO 5 I=1,5
 1425    F     W3PSD(I,1) = PSD1(I)
 1426    F     W3PSD(I,2) = PSD2(I)
 1427    F     W3PSD(I,3) = PSD3(I)
 1428    F     W3PSD(I,4) = PSD4(I)
 1429    F   5 W3PSD(I,5) = PSD5(I)
 1430    F     WRITE (7,6) ((W3PSD(I,J),J=1,5),I=1,5)
 1431    F   6 FORMAT(2X, 'W3PSD',/5(1X,E10.3))
 1432    F
 1433                                                                  C
*=================================================================*
 1434     C         MASS FLOW RATE OF CARBON FOR EACH COMPONENT IN
INPUT STREAM
 1435                                                                  C
*=================================================================*
 1436    F     FBSD3(1) = FCBSD1
 1437    F     FBSD3(2) = FCBSD2
 1438    F     FBSD3(3) = FCBSD3
 1439    F     FBSD3(4) = FCBSD4
 1440    F     FBSD3(5) = FCBSD5
 1441    F
 1442                                                                  C
*=================================================================*
 1443    C                                 UPPER REGION
 1444                                                                  C
*=================================================================*
 1445    F
 1446    C     VOLUMETRIC FLOW RATE FOR MIXED STREAM (m^3/s)
 1447    F     FVMIX = FMIX/DMIX
 1448    F
 1449    C     AIR VELOCITY (m/s)
 1450    F     VAIRU2 = FVMIX/AREA
 1451    F     WRITE (7,*) 'AIRVELOCITY TO UPPER REGION', VAIRU2
 1452    F
 1453    C     NET SOLIDS CIRCULATION FLUX (Kg/(m^2.s))
```

```
 1454    F     GS = 50.0
 1455    F
 1456    C     ACCELERATION DUE TO GRAVITY (m/s^2)
 1457    F     G  = 9.81
 1458    F
 1459    F     WRITE (7,*) 'DP2',DP2
 1460    F
 1461    C     DIMENSION LESS (DP STAR)  (m)
 1462       F        DPSAT  =  DP2  *  (  DMIX*(DENS-DMIX)*G/VISCO**2.
)**(1./3.)
 1463    F     WRITE (7,*) 'DIMENSIONLESS (DP STAR)',DPSAT
 1464    F
 1465    C     TERMINAL VELOCITY OF PARTICLE (m/s)
 1466         F           UTSAT  =    1./(18./DPSAT**2.  +  (2.335-
1.744*PHIS)/DPSAT**0.5)
 1467    F     WRITE (7,*) 'UTSAT',UTSAT
 1468    F
 1469       F        UT  =   UTSAT/(  DMIX**2./(VISCO*(DENS-DMIX)*G)
)**(1./3.)
 1470    F     WRITE (7,*) 'TERMINAL VELOCITY OF PARTICLE (M/S)',UT
 1471    F
 1472    C     EQUIVALENT DIAMETER (m)
 1473    F     BEDD = 4.*AREA/(4.*BEDW)
 1474    C      WRITE (7,*) 'BEDD (M)',BEDD
 1475    F
 1476    C     BED LENGTH (m)
 1477    F     BEDL(1) = BEDV/AREA
 1478    F     BEDL(2) = BEDVU1/AREA
 1479    F     BEDL(3) = BEDVU2/AREA
 1480    F     BEDL(4) = BEDLT - ( BEDL(1) + BEDL(2) + BEDL(3) )
 1481    F     WRITE (7,*) 'BEDL(I)',(BEDL(I),I=1,4)
 1482    F
 1483    C     TOTAL GAS CONCENTRATION (Kmole/m^3)
 1484    C     GAS CONSTANT (atm cm^3)/(gmole K)
 1485    F     R = 82.056
 1486    F     CONC = BEDP*1000./(101325.*R*BEDT3)
 1487    F     WRITE (7,*) 'TEMP',BEDT3
 1488    F
 1489    C     SUPERFICIAL GAS VELOCITY (m/s)
 1490    F     UGAS(1) = FMAIR1/(AREA*CONC)
 1491    F     UGAS(2) = UGAS(1) + FMAIR2/(AREA*CONC)
 1492    F     UGAS(3) = UGAS(2) + FMAIR3/(AREA*CONC)
 1493    F     UGAS(4) = UGAS(3)
 1494    F     WRITE (7,*) 'UGAS(I)',(UGAS(I),I=1,4)
 1495    F
 1496    C     FROUDE NUMBER
 1497    F     FR = UGAS(4)/(G*BEDD)**0.5
 1498    F     WRITE (7,*) 'FR',FR
 1499    F
 1500    C     PARTICLE FROUDE NUMBER
 1501    F     FRT = UT/(G*BEDD)**0.5
 1502    F     WRITE (7,*) 'FRT',FRT
 1503    F
 1504    C     MEAN AXIAL VOIDAGE IN THE FULLY DEVELOPED ZONE
 1505    F     PHI = 1. + 5.6/FR + 0.47*FRT**0.41
```

```
  1506    F     VVOID2(4) = 1./( 1. + PHI*GS/(UGAS(4)*DENS) )
  1507    F     WRITE (7,*) 'PHI',PHI
  1508    F     WRITE (7,*) 'VVOID2(4)',VVOID2(4)
  1509    F
  1510    C     DECAY CONSTANT
  1511    F     A = 5./UGAS(4)
  1512    F     WRITE (7,*) 'DECAY RATIO',A
  1513    F
  1514    C     LENGTH OF THE ACCELERATION ZONE
  1515     F      BEDZ = (-1./A) * DLOG( (VOIDS-VVOID2(4)) / (VOIDS-
VVOID(1)) )
  1516    F     WRITE (7,*) 'BEDZ',BEDZ
  1517    F
  1518    C     HEIGHT IN CFBC AT ANY INTERVAL
  1519    F     BDL(1) = BEDV/AREA
  1520    F     BDL(2) = BEDZ/3.
  1521    F     BDL(3) = 2.*BEDZ/3.
  1522    F     BDL(4) = BEDLT - ( BEDZ+BDL(1) )
  1523    F     WRITE (7,*) 'BDL(I)',(BDL(I),I=1,4)
  1524    F
  1525    F     BEDVV2(1) = BEDV
  1526    F     BEDVV2(2) = AREA*BDL(2)
  1527    F     BEDVV2(3) = AREA*BDL(3)
  1528    F     BEDVV2(4) = AREA*BDL(4)
  1529    F     WRITE (7,*) 'BEDVV(I)',(BEDVV2(I),I=1,4)
  1530    F
  1531    C     VOIDAGE AT ANOTHER INTERVAL
  1532    F     VVOID2(2) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(1))
  1533    F    .          * ( DEXP(-A*BDL(2)) - 1. )
  1534    F     VVOID2(3) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(2))
  1535    F    .          * ( DEXP(-A*BEDZ) - DEXP(-A*BDL(2)) )
  1536    F     WRITE (7,*) 'VVOID2(2)',VVOID2(2)
  1537    F     WRITE (7,*) 'VVOID2(3)',VVOID2(3)
  1538        EXECUTE BEFORE BLOCK P11-26
  1539
  1540    CALCULATOR C-4
  1541    F     COMMON /USER5/  AREA, VFAIR1, VAIR1, VVOID,
  1542    F    .                BEDW, BEDVV
  1543    F     COMMON /USER12/  DCINU3, FMOLU3, W4PSD, FBSD4, DP3
  1544    F     COMMON /USER13/ VAIRU3, VVOID3, BEDVV3
  1545    F     COMMON /USER17/ BEDT4
  1546    F     COMMON /USER23/ UGAS
  1547    F
  1548    F     REAL*8 DCINU3(5), FMOLU3(5), W4PSD(5,5),
  1549    F    .       FBSD4(5),  VVOID(4),  VVOID3(4),
  1550    F    .       BEDVV3(4), BEDL(4),   UGAS(4),
  1551    F    .       BDL(4)
  1552    F
  1553    F     DATA PHIS/0.806/, BEDLT/21.84/, VOIDS/0.999/
  1554        DEFINE FCPSD1 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD1  &
  1555            VARIABLE=MASS-FLOW
  1556        DEFINE FCPSD2 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD2  &
  1557            VARIABLE=MASS-FLOW
  1558        DEFINE FCPSD3 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD3  &
  1559            VARIABLE=MASS-FLOW
```

```
1560        DEFINE FCPSD4 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD4  &
1561            VARIABLE=MASS-FLOW
1562        DEFINE FCPSD5 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD5  &
1563            VARIABLE=MASS-FLOW
1564        DEFINE FNPSD1 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD1  &
1565            VARIABLE=MASS-FLOW
1566        DEFINE FNPSD2 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD2  &
1567            VARIABLE=MASS-FLOW
1568        DEFINE FNPSD3 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD3  &
1569            VARIABLE=MASS-FLOW
1570        DEFINE FNPSD4 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD4  &
1571            VARIABLE=MASS-FLOW
1572        DEFINE FNPSD5 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD5  &
1573            VARIABLE=MASS-FLOW
1574        DEFINE FLIME STREAM-VAR STREAM=S19 SUBSTREAM=CISOLID  &
1575            VARIABLE=MASS-FLOW
1576        DEFINE DPSD1 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD1  &
1577            VARIABLE=MASS-DENSITY
1578        DEFINE DPSD2 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD2  &
1579            VARIABLE=MASS-DENSITY
1580        DEFINE DPSD3 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD3  &
1581            VARIABLE=MASS-DENSITY
1582        DEFINE DPSD4 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD4  &
1583            VARIABLE=MASS-DENSITY
1584        DEFINE DPSD5 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD5  &
1585            VARIABLE=MASS-DENSITY
1586        DEFINE DNPSD1 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD1  &
1587            VARIABLE=MASS-DENSITY
1588        DEFINE DNPSD2 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD2  &
1589            VARIABLE=MASS-DENSITY
1590        DEFINE DNPSD3 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD3  &
1591            VARIABLE=MASS-DENSITY
1592        DEFINE DNPSD4 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD4  &
1593            VARIABLE=MASS-DENSITY
1594        DEFINE DNPSD5 STREAM-VAR STREAM=S19 SUBSTREAM=NCPSD5  &
1595            VARIABLE=MASS-DENSITY
1596        DEFINE DLIME STREAM-VAR STREAM=S19 SUBSTREAM=CISOLID  &
1597            VARIABLE=MASS-DENSITY
1598       DEFINE VFSUM BLOCK-VAR BLOCK=P11-35 VARIABLE=VALUE-LIST
&
1599            SENTENCE=REAL ELEMENT=1
1600        DEFINE DMPSD1 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD1  &
1601            VARIABLE=MOLE-DENSITY
1602        DEFINE DMPSD2 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD2  &
1603            VARIABLE=MOLE-DENSITY
1604        DEFINE DMPSD3 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD3  &
1605            VARIABLE=MOLE-DENSITY
1606        DEFINE DMPSD4 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD4  &
1607            VARIABLE=MOLE-DENSITY
1608        DEFINE DMPSD5 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD5  &
1609            VARIABLE=MOLE-DENSITY
1610        DEFINE FMPSD1 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD1  &
1611            VARIABLE=MOLE-FLOW
1612        DEFINE FMPSD2 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD2  &
1613            VARIABLE=MOLE-FLOW
```

```
DEFINE FMPSD3 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD3  &
    VARIABLE=MOLE-FLOW
DEFINE FMPSD4 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD4  &
    VARIABLE=MOLE-FLOW
DEFINE FMPSD5 STREAM-VAR STREAM=S19 SUBSTREAM=CIPSD5  &
    VARIABLE=MOLE-FLOW
DEFINE MOFRAC MOLE-FRAC STREAM=S19 SUBSTREAM=MIXED  &
    COMPONENT=O2
DEFINE MDMIX STREAM-VAR STREAM=S19 SUBSTREAM=MIXED  &
    VARIABLE=MOLE-DENSITY
DEFINE CONO2 BLOCK-VAR BLOCK=P11-35 VARIABLE=VALUE-LIST
&
    SENTENCE=REAL ELEMENT=29
DEFINE VISCO STREAM-PROP STREAM=S19 PROPERTY=PS-1
 DEFINE VIS BLOCK-VAR BLOCK=P11-35 VARIABLE=VALUE-LIST
&
    SENTENCE=REAL ELEMENT=108
 VECTOR-DEF PSD1 SUBS-ATTR STREAM=S19 SUBSTREAM=CIPSD1
&
    ATTRIBUTE=PSD1
 VECTOR-DEF PSD2 SUBS-ATTR STREAM=S19 SUBSTREAM=CIPSD2
&
    ATTRIBUTE=PSD2
 VECTOR-DEF PSD3 SUBS-ATTR STREAM=S19 SUBSTREAM=CIPSD3
&
    ATTRIBUTE=PSD3
 VECTOR-DEF PSD4 SUBS-ATTR STREAM=S19 SUBSTREAM=CIPSD4
&
    ATTRIBUTE=PSD4
 VECTOR-DEF PSD5 SUBS-ATTR STREAM=S19 SUBSTREAM=CIPSD5
&
    ATTRIBUTE=PSD5
DEFINE FCBSD1 MASS-FLOW STREAM=S19 SUBSTREAM=CIPSD1  &
    COMPONENT=C
DEFINE FCBSD2 MASS-FLOW STREAM=S19 SUBSTREAM=CIPSD2  &
    COMPONENT=C
DEFINE FCBSD3 MASS-FLOW STREAM=S19 SUBSTREAM=CIPSD3  &
    COMPONENT=C
DEFINE FCBSD4 MASS-FLOW STREAM=S19 SUBSTREAM=CIPSD4  &
    COMPONENT=C
DEFINE FCBSD5 MASS-FLOW STREAM=S19 SUBSTREAM=CIPSD5  &
    COMPONENT=C
DEFINE FMIX STREAM-VAR STREAM=S19 SUBSTREAM=MIXED  &
    VARIABLE=MASS-FLOW
DEFINE DMIX STREAM-VAR STREAM=S19 SUBSTREAM=MIXED  &
    VARIABLE=MASS-DENSITY
DEFINE BEDV BLOCK-VAR BLOCK=P11-7 VARIABLE=VOL  &
    SENTENCE=PARAM
DEFINE BEDVU1 BLOCK-VAR BLOCK=P11-17 VARIABLE=VOL  &
    SENTENCE=PARAM
DEFINE BEDVU2 BLOCK-VAR BLOCK=P11-26 VARIABLE=VOL  &
    SENTENCE=PARAM
DEFINE BEDP BLOCK-VAR BLOCK=P11-35 VARIABLE=PRES  &
    SENTENCE=PARAM
DEFINE FMAIR1 STREAM-VAR STREAM=AIR1 SUBSTREAM=MIXED  &
```

```
  1662            VARIABLE=MOLE-FLOW
  1663         DEFINE FMAIR2 STREAM-VAR STREAM=AIR2 SUBSTREAM=MIXED  &
  1664            VARIABLE=MOLE-FLOW
  1665         DEFINE FMAIR3 STREAM-VAR STREAM=AIR3 SUBSTREAM=MIXED  &
  1666            VARIABLE=MOLE-FLOW
  1667     F      OPEN (7,FILE='C-4.txt')
  1668     F
  1669     F
  1670     C      TOTAL MASS FLOW RATE OF SUBSTREAM CIPSD
  1671     F      FTOTAL =   FCPSD1 + FCPSD2 + FCPSD3 + FCPSD4 + FCPSD5
  1672     F     .         + FNPSD1 + FNPSD2 + FNPSD3 + FNPSD4 + FNPSD5
  1673     F     .         + FLIME
  1674      F       WRITE (7,*) 'TOTAL MASS FLOW RATE OF CIPSD (kg/s)',
FTOTAL
  1675     F
  1676     C      MEAN MASS DENSITY OF TOTAL FLOW TO RCSTR
  1677      F       DENS = 1/FTOTAL * (FCPSD1*DPSD1   + FCPSD2*DPSD2   +
FCPSD3*DPSD3
  1678     F     .                  +  FCPSD4*DPSD4  + FCPSD5*DPSD5
  1679      F     .                    +  FNPSD1*DNPSD1 + FNPSD2*DNPSD2 +
FNPSD3*DNPSD3
  1680     F     .                  +  FNPSD4*DNPSD4 + FNPSD5*DNPSD5
  1681     F     .                  +  FLIME*DLIME)
  1682     F      WRITE (7,*) 'MEAN MASS DENSITY (Kg/m^3)',DENS
  1683     F
  1684     C      VOLUMETRIC FLOW RATE OF TOTAL FLOW TO RCSTR
  1685     F      VFSUM = FTOTAL/DENS
  1686       F        WRITE  (7,*)  'VOLUMETRIC  FLOW  RATE  OF  TOTAL  FLOW
(m^3/s)', VFSUM
  1687     F
  1688     C      DEFINED MOLAR DENSITY TO EXTERNAL SUBROUTINE
  1689     F      DCINU3(1) = DMPSD1
  1690     F      DCINU3(2) = DMPSD2
  1691     F      DCINU3(3) = DMPSD3
  1692     F      DCINU3(4) = DMPSD4
  1693     F      DCINU3(5) = DMPSD5
  1694     F
  1695     C      DEFINED MOLAR FLOW RATE TO EXTERNAL SUBROUTINE
  1696     F      FMOLU3(1) = FMPSD1
  1697     F      FMOLU3(2) = FMPSD2
  1698     F      FMOLU3(3) = FMPSD3
  1699     F      FMOLU3(4) = FMPSD4
  1700     F      FMOLU3(5) = FMPSD5
  1701     F
  1702     C      CONCENTRATION OF OXYGEN
  1703     F      CONO2 = MOFRAC*MDMIX
  1704     F      WRITE (7,*) 'CONCENTRATION ',CONO2
  1705     F
  1706     C      VISCOSITY OF FLUID
  1707     F      VIS = VISCO
  1708     F
  1709                                                                    C
*=============================================================*
  1710     C                     PREPARE WEIGHT FRACTION OF PSD
```

```
  1711                                                                  C
*================================================================*
  1712    F     DO 5 I=1,5
  1713    F     W4PSD(I,1) = PSD1(I)
  1714    F     W4PSD(I,2) = PSD2(I)
  1715    F     W4PSD(I,3) = PSD3(I)
  1716    F     W4PSD(I,4) = PSD4(I)
  1717    F   5 W4PSD(I,5) = PSD5(I)
  1718    F     WRITE (7,6) ((W4PSD(I,J),J=1,5),I=1,5)
  1719    F   6 FORMAT(2X, 'W4PSD',/5(1X,E10.3))
  1720    F
  1721                                                                  C
*================================================================*
  1722     C         MASS FLOW RATE OF CARBON FOR EACH COMPONENT IN
INPUT STREAM
  1723                                                                  C
*================================================================*
  1724    F     FBSD4(1) = FCBSD1
  1725    F     FBSD4(2) = FCBSD2
  1726    F     FBSD4(3) = FCBSD3
  1727    F     FBSD4(4) = FCBSD4
  1728    F     FBSD4(5) = FCBSD5
  1729    F
  1730                                                                  C
*================================================================*
  1731    C                                 UPPER REGION
  1732                                                                  C
*================================================================*
  1733    F
  1734    C     VOLUMETRIC FLOW RATE FOR MIXED STREAM (m^3/s)
  1735    F     FVMIX = FMIX/DMIX
  1736    F
  1737    C     AIR VELOCITY (m/s)
  1738    F     VAIRU3 = FVMIX/AREA
  1739    F     WRITE (7,*) 'AIRVELOCITY TO UPPER REGION', VAIRU3
  1740    F
  1741    C     NET SOLIDS CIRCULATION FLUX (Kg/(m^2.s))
  1742    F     GS = 50.0
  1743    F
  1744    C     ACCELERATION DUE TO GRAVITY (m/s^2)
  1745    F     G  = 9.81
  1746    F
  1747    F     WRITE (7,*) 'DP3',DP3
  1748    F
  1749    C     DIMENSION LESS (DP STAR)  (m)
  1750       F        DPSAT  =  DP3  *  (  DMIX*(DENS-DMIX)*G/VISCO**2.
)**(1./3.)
  1751    F     WRITE (7,*) 'DIMENSIONLESS (DP STAR)',DPSAT
  1752    F
  1753    C     TERMINAL VELOCITY OF PARTICLE (m/s)
  1754         F           UTSAT  =    1./(18./DPSAT**2.  +  (2.335-
1.744*PHIS)/DPSAT**0.5)
  1755    F     WRITE (7,*) 'UTSAT',UTSAT
  1756    F
```

```
  1757       F         UT  =   UTSAT/(  DMIX**2./(VISCO*(DENS-DMIX)*G)
)**(1./3.)
  1758     F     WRITE (7,*) 'TERMINAL VELOCITY OF PARTICLE (M/S)',UT
  1759     F
  1760     C     EQUIVALENT DIAMETER (m)
  1761     F     BEDD = 4.*AREA/(4.*BEDW)
  1762     F     WRITE (7,*) 'BEDD (M)',BEDD
  1763     F
  1764     C     BED LENGTH (m)
  1765     F     BEDL(1) = BEDV/AREA
  1766     F     BEDL(2) = BEDVU1/AREA
  1767     F     BEDL(3) = BEDVU2/AREA
  1768     F     BEDL(4) = BEDLT - ( BEDL(1) + BEDL(2) + BEDL(3) )
  1769     F     WRITE (7,*) 'BEDL(I)',(BEDL(I),I=1,4)
  1770     F
  1771     C     TOTAL GAS CONCENTRATION (Kmole/m^3)
  1772     C     GAS CONSTANT (atm cm^3)/(gmole K)
  1773     F     R = 82.056
  1774     F     CONC = BEDP*1000./(101325.*R*BEDT4)
  1775     F     WRITE (7,*) 'TEMP',BEDT4
  1776     F
  1777     C     SUPERFICIAL GAS VELOCITY (m/s)
  1778     F     UGAS(1) = FMAIR1/(AREA*CONC)
  1779     F     UGAS(2) = UGAS(1) + FMAIR2/(AREA*CONC)
  1780     F     UGAS(3) = UGAS(2) + FMAIR3/(AREA*CONC)
  1781     F     UGAS(4) = UGAS(3)
  1782     F     WRITE (7,*) 'UGAS(I)',(UGAS(I),I=1,4)
  1783     F
  1784     C     FROUDE NUMBER
  1785     F     FR = UGAS(4)/(G*BEDD)**0.5
  1786     F     WRITE (7,*) 'FR',FR
  1787     F
  1788     C     PARTICLE FROUDE NUMBER
  1789     F     FRT = UT/(G*BEDD)**0.5
  1790     F     WRITE (7,*) 'FRT',FRT
  1791     F
  1792     C     MEAN AXIAL VOIDAGE IN THE FULLY DEVELOPED ZONE
  1793     F     PHI = 1. + 5.6/FR + 0.47*FRT**0.41
  1794     F     VVOID3(4) = 1./( 1. + PHI*GS/(UGAS(4)*DENS) )
  1795     F     WRITE (7,*) 'PHI',PHI
  1796     F     WRITE (7,*) 'VVOID3(4)',VVOID3(4)
  1797     F
  1798     C     DECAY CONSTANT
  1799     F     A = 5./UGAS(4)
  1800     F     WRITE (7,*) 'DECAY RATIO',A
  1801     F
  1802     C     LENGTH OF THE ACCELERATION ZONE
  1803      F      BEDZ = (-1./A) * DLOG( (VOIDS-VVOID3(4)) / (VOIDS-
VVOID(1)) )
  1804     F     WRITE (7,*) 'BEDZ',BEDZ
  1805     F
  1806     C     HEIGHT IN CFBC AT ANY INTERVAL
  1807     F     BDL(1) = BEDV/AREA
  1808     F     BDL(2) = BEDZ/3.
  1809     F     BDL(3) = 2.*BEDZ/3.
```

```
1810    F     BDL(4) = BEDLT - ( BEDZ+BDL(1) )
1811    F     WRITE (7,*) 'BDL(I)',(BDL(I),I=1,4)
1812    F
1813    F     BEDVV3(1) = BEDV
1814    F     BEDVV3(2) = AREA*BDL(2)
1815    F     BEDVV3(3) = AREA*BDL(3)
1816    F     BEDVV3(4) = AREA*BDL(4)
1817    F     WRITE (7,*) 'BEDVV(I)',(BEDVV3(I),I=1,4)
1818    F
1819    C     VOIDAGE AT ANOTHER INTERVAL
1820    F     VVOID3(2) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(1))
1821    F    .          * ( DEXP(-A*BDL(2)) - 1. )
1822    F     VVOID3(3) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(2))
1823    F    .          * ( DEXP(-A*BEDZ) - DEXP(-A*BDL(2)) )
1824    F     WRITE (7,*) 'VVOID3(2)',VVOID3(2)
1825    F     WRITE (7,*) 'VVOID3(3)',VVOID3(3)
1826        EXECUTE BEFORE BLOCK P11-35
1827
1828    CALCULATOR C-5
1829    F     COMMON /USER5/ AREA, VFAIR1, VAIR1, VVOID,
1830    F    .               BEDW, BEDVV
1831    F     COMMON /USER10/ VAIRU2, VVOID2, BEDVV2
1832    F     COMMON /USER13/ VAIRU3, VVOID3, BEDVV3
1833    F     COMMON /USER14/ VOIDM,  BEDVM,  BEDL
1834    F
1835    F     REAL*8 VVOID(4),  BEDVV(4),  VVOID2(4),
1836    F    .       BEDVV2(4), VVOID3(4), BEDVV3(4),
1837    F    .       VOIDM(3),  BEDVM(3),  BEDL(4)
1838    F
1839    F
1840        DEFINE FLOW STREAM-VAR STREAM=AIR1 SUBSTREAM=MIXED  &
1841          VARIABLE=MASS-FLOW
1842        DEFINE BEDV BLOCK-VAR BLOCK=P11-7 VARIABLE=VOL  &
1843          SENTENCE=PARAM
1844    F     OPEN (7,FILE='C-5.txt')
1845    F
1846    F     WRITE (7,*) 'VVOID',(VVOID(I),I=1,4)
1847    F     WRITE (7,*) 'BEDVV',(BEDVV(I),I=1,4)
1848    F     WRITE (7,*) 'VVOID2',(VVOID2(I),I=1,4)
1849    F     WRITE (7,*) 'BEDVV2',(BEDVV2(I),I=1,4)
1850    F     WRITE (7,*) 'VVOID3',(VVOID3(I),I=1,4)
1851    F     WRITE (7,*) 'BEDVV3',(BEDVV3(I),I=1,4)
1852    F
1853    F
1854                                                                C
*=============================================================*
1855    C                                   UPPER REGION
1856                                                                C
*=============================================================*
1857    F
1858    C     FIRST INTERVAL
1859    F     VOIDM(1) = ( VVOID(2) + VVOID2(2) + VVOID3(2) )/3.
1860    F     BEDVM(1) = ( BEDVV(2) + BEDVV2(2) + BEDVV3(2) )/3.
1861    F
1862    C     SECOND INTERVAL
```

```
  1863    F     VOIDM(2) = ( VVOID(3) + VVOID2(3) + VVOID3(3) )/3.
  1864    F     BEDVM(2) = ( BEDVV(3) + BEDVV2(3) + BEDVV3(3) )/3.
  1865    F
  1866    C     THIRD INTERVAL
  1867    F     VOIDM(3) = ( VVOID(4) + VVOID2(4) + VVOID3(4) )/3.
  1868    F     BEDVM(3) = ( BEDVV(4) + BEDVV2(4) + BEDVV3(4) )/3.
  1869    F
  1870          F            WRITE   (7,*)   'MEAN   VOID   AT   EACH
INTERVAL',(VOIDM(I),I=1,3)
  1871          F           WRITE   (7,*)   'MEAN   VOLUME   AT   EACH
INTERVAL',(BEDVM(I),I=1,3)
  1872    F
  1873    C     THE HEIGHT OF EACH ZONE
  1874    F     BEDL(1) = BEDV/AREA
  1875    F     BEDL(2) = BEDVM(1)/AREA
  1876    F     BEDL(3) = BEDVM(2)/AREA
  1877    F     BEDL(4) = BEDVM(3)/AREA
  1878        EXECUTE AFTER BLOCK P11-35
  1879
  1880    CALCULATOR C-6
  1881        DEFINE DMIX STREAM-VAR STREAM=S7 SUBSTREAM=MIXED  &
  1882           VARIABLE=MOLE-DENSITY
  1883        DEFINE MOFRAC MOLE-FRAC STREAM=S7 SUBSTREAM=MIXED  &
  1884           COMPONENT=O2
  1885         DEFINE CONO2 BLOCK-VAR BLOCK=P11-8 VARIABLE=VALUE-LIST
&
  1886           SENTENCE=REAL ELEMENT=1
  1887             DEFINE  FN2  MOLE-FLOW  STREAM=S7  SUBSTREAM=MIXED
COMPONENT=N2
  1888             DEFINE  FO2  MOLE-FLOW  STREAM=S7  SUBSTREAM=MIXED
COMPONENT=O2
  1889         DEFINE FMN2 BLOCK-VAR BLOCK=P11-8 VARIABLE=VALUE-LIST
&
  1890           SENTENCE=REAL ELEMENT=2
  1891         DEFINE FMO2 BLOCK-VAR BLOCK=P11-8 VARIABLE=VALUE-LIST
&
  1892           SENTENCE=REAL ELEMENT=3
  1893    F     OPEN (7,FILE='C-6.txt')
  1894    F
  1895    C     CONCENTRATION OF O2
  1896    F     CONO2 = MOFRAC*DMIX
  1897    F     WRITE (7,*) 'CONCENTRATION OF O2',CONO2
  1898    F
  1899    F     FMN2 = FN2
  1900    F     FMO2 = FO2
  1901        EXECUTE BEFORE BLOCK P11-8
  1902
  1903    CALCULATOR C-7
  1904        DEFINE DMIX STREAM-VAR STREAM=S8-1 SUBSTREAM=MIXED  &
  1905           VARIABLE=MOLE-DENSITY
  1906        DEFINE MOFNO MOLE-FRAC STREAM=S8-1 SUBSTREAM=MIXED  &
  1907           COMPONENT=NO
  1908         DEFINE CONNO BLOCK-VAR BLOCK=P11-9 VARIABLE=VALUE-LIST
&
  1909           SENTENCE=REAL ELEMENT=1
```

```
 1910         DEFINE FN2 MOLE-FLOW STREAM=S8-1 SUBSTREAM=MIXED  &
 1911             COMPONENT=N2
 1912         DEFINE FO2 MOLE-FLOW STREAM=S8-1 SUBSTREAM=MIXED  &
 1913             COMPONENT=O2
 1914          DEFINE FMN2 BLOCK-VAR BLOCK=P11-9 VARIABLE=VALUE-LIST
&
 1915             SENTENCE=REAL ELEMENT=2
 1916          DEFINE FMO2 BLOCK-VAR BLOCK=P11-9 VARIABLE=VALUE-LIST
&
 1917             SENTENCE=REAL ELEMENT=3
 1918     F     OPEN (7,FILE='C-7.txt')
 1919     F
 1920     C     CONCENTRATION OF NO
 1921     F     CONNO = MOFNO*DMIX
 1922     F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
 1923     F
 1924     F     FMN2 = FN2
 1925     F     FMO2 = FO2
 1926         EXECUTE BEFORE BLOCK P11-9
 1927
 1928     CALCULATOR C-8
 1929         DEFINE DMIX STREAM-VAR STREAM=S8-2 SUBSTREAM=MIXED  &
 1930             VARIABLE=MOLE-DENSITY
 1931         DEFINE MOFNO MOLE-FRAC STREAM=S8-2 SUBSTREAM=MIXED  &
 1932             COMPONENT=NO
 1933         DEFINE CONNO BLOCK-VAR BLOCK=P11-10 VARIABLE=VALUE-LIST
&
 1934             SENTENCE=REAL ELEMENT=1
 1935         DEFINE FNO MOLE-FLOW STREAM=S8-2 SUBSTREAM=MIXED  &
 1936             COMPONENT=NO
 1937         DEFINE FC1 MOLE-FLOW STREAM=S8-2 SUBSTREAM=CIPSD1  &
 1938             COMPONENT=C
 1939         DEFINE FC2 MOLE-FLOW STREAM=S8-2 SUBSTREAM=CIPSD2  &
 1940             COMPONENT=C
 1941         DEFINE FC3 MOLE-FLOW STREAM=S8-2 SUBSTREAM=CIPSD3  &
 1942             COMPONENT=C
 1943         DEFINE FC4 MOLE-FLOW STREAM=S8-2 SUBSTREAM=CIPSD4  &
 1944             COMPONENT=C
 1945         DEFINE FC5 MOLE-FLOW STREAM=S8-2 SUBSTREAM=CIPSD5  &
 1946             COMPONENT=C
 1947          DEFINE FMNO BLOCK-VAR BLOCK=P11-10 VARIABLE=VALUE-LIST
&
 1948             SENTENCE=REAL ELEMENT=2
 1949          DEFINE FMC1 BLOCK-VAR BLOCK=P11-10 VARIABLE=VALUE-LIST
&
 1950             SENTENCE=REAL ELEMENT=3
 1951          DEFINE FMC2 BLOCK-VAR BLOCK=P11-10 VARIABLE=VALUE-LIST
&
 1952             SENTENCE=REAL ELEMENT=4
 1953          DEFINE FMC3 BLOCK-VAR BLOCK=P11-10 VARIABLE=VALUE-LIST
&
 1954             SENTENCE=REAL ELEMENT=5
 1955          DEFINE FMC4 BLOCK-VAR BLOCK=P11-10 VARIABLE=VALUE-LIST
&
 1956             SENTENCE=REAL ELEMENT=6
```

```
  1957         DEFINE FMC5 BLOCK-VAR BLOCK=P11-10 VARIABLE=VALUE-LIST
&
  1958           SENTENCE=REAL ELEMENT=7
  1959     F     OPEN (7,FILE='C-8.txt')
  1960     F
  1961     C     CONCENTRATION OF NO
  1962     F     CONNO = MOFNO*DMIX
  1963     F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  1964     F
  1965     F     FMNO = FNO
  1966     F     FMC1 = FC1
  1967     F     FMC2 = FC2
  1968     F     FMC3 = FC3
  1969     F     FMC4 = FC4
  1970     F     FMC5 = FC5
  1971         EXECUTE BEFORE BLOCK P11-10
  1972
  1973     CALCULATOR C-9
  1974         DEFINE DMIX STREAM-VAR STREAM=S8-3 SUBSTREAM=MIXED  &
  1975           VARIABLE=MOLE-DENSITY
  1976         DEFINE MOFNO MOLE-FRAC STREAM=S8-3 SUBSTREAM=MIXED  &
  1977           COMPONENT=NO
  1978         DEFINE CONNO BLOCK-VAR BLOCK=P11-11 VARIABLE=VALUE-LIST
&
  1979           SENTENCE=REAL ELEMENT=1
  1980         DEFINE FNO MOLE-FLOW STREAM=S8-3 SUBSTREAM=MIXED  &
  1981           COMPONENT=NO
  1982         DEFINE FCO MOLE-FLOW STREAM=S8-3 SUBSTREAM=MIXED  &
  1983           COMPONENT=CO
  1984         DEFINE FMNO BLOCK-VAR BLOCK=P11-11 VARIABLE=VALUE-LIST
&
  1985           SENTENCE=REAL ELEMENT=2
  1986         DEFINE FMCO BLOCK-VAR BLOCK=P11-11 VARIABLE=VALUE-LIST
&
  1987           SENTENCE=REAL ELEMENT=3
  1988     F     OPEN (7,FILE='C-9.txt')
  1989     F
  1990     C     CONCENTRATION OF CO
  1991     F     CONNO = MOFNO*DMIX
  1992     F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  1993     F
  1994     F     FMNO = FNO
  1995     F     FMCO = FCO
  1996         EXECUTE BEFORE BLOCK P11-11
  1997
  1998     CALCULATOR C-10
  1999         DEFINE DMIX STREAM-VAR STREAM=S8-4 SUBSTREAM=MIXED  &
  2000           VARIABLE=MOLE-DENSITY
  2001         DEFINE MOFN2O MOLE-FRAC STREAM=S8-4 SUBSTREAM=MIXED  &
  2002           COMPONENT=N2O
  2003          DEFINE CONN2O BLOCK-VAR BLOCK=P11-12 VARIABLE=VALUE-
LIST  &
  2004           SENTENCE=REAL ELEMENT=1
  2005         DEFINE FN2O MOLE-FLOW STREAM=S8-4 SUBSTREAM=MIXED  &
  2006           COMPONENT=N2O
```

```
  2007         DEFINE FC1 MOLE-FLOW STREAM=S8-4 SUBSTREAM=CIPSD1  &
  2008             COMPONENT=C
  2009         DEFINE FC2 MOLE-FLOW STREAM=S8-4 SUBSTREAM=CIPSD2  &
  2010             COMPONENT=C
  2011         DEFINE FC3 MOLE-FLOW STREAM=S8-4 SUBSTREAM=CIPSD3  &
  2012             COMPONENT=C
  2013         DEFINE FC4 MOLE-FLOW STREAM=S8-4 SUBSTREAM=CIPSD4  &
  2014             COMPONENT=C
  2015         DEFINE FC5 MOLE-FLOW STREAM=S8-4 SUBSTREAM=CIPSD5  &
  2016             COMPONENT=C
  2017         DEFINE FMN2O BLOCK-VAR BLOCK=P11-12 VARIABLE=VALUE-LIST
&
  2018             SENTENCE=REAL ELEMENT=2
  2019          DEFINE FMC1 BLOCK-VAR BLOCK=P11-12 VARIABLE=VALUE-LIST
&
  2020             SENTENCE=REAL ELEMENT=3
  2021          DEFINE FMC2 BLOCK-VAR BLOCK=P11-12 VARIABLE=VALUE-LIST
&
  2022             SENTENCE=REAL ELEMENT=4
  2023          DEFINE FMC3 BLOCK-VAR BLOCK=P11-12 VARIABLE=VALUE-LIST
&
  2024             SENTENCE=REAL ELEMENT=5
  2025          DEFINE FMC4 BLOCK-VAR BLOCK=P11-12 VARIABLE=VALUE-LIST
&
  2026             SENTENCE=REAL ELEMENT=6
  2027          DEFINE FMC5 BLOCK-VAR BLOCK=P11-12 VARIABLE=VALUE-LIST
&
  2028             SENTENCE=REAL ELEMENT=7
  2029     F      OPEN (7,FILE='C-10.txt')
  2030     F
  2031     C      CONCENTRATION OF N2O
  2032     F      CONN2O = MOFN2O*DMIX
  2033     F      WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2034     F
  2035     F      FMN2O = FN2O
  2036     F      FMC1 = FC1
  2037     F      FMC2 = FC2
  2038     F      FMC3 = FC3
  2039     F      FMC4 = FC4
  2040     F      FMC5 = FC5
  2041         EXECUTE BEFORE BLOCK P11-12
  2042
  2043     CALCULATOR C-11
  2044         DEFINE DMIX STREAM-VAR STREAM=S8-5 SUBSTREAM=MIXED  &
  2045             VARIABLE=MOLE-DENSITY
  2046         DEFINE MOFCO MOLE-FRAC STREAM=S8-5 SUBSTREAM=MIXED  &
  2047             COMPONENT=CO
  2048         DEFINE CONCO BLOCK-VAR BLOCK=P11-13 VARIABLE=VALUE-LIST
&
  2049             SENTENCE=REAL ELEMENT=1
  2050         DEFINE MOFN2O MOLE-FRAC STREAM=S8-5 SUBSTREAM=MIXED  &
  2051             COMPONENT=N2O
  2052           DEFINE CONN2O BLOCK-VAR BLOCK=P11-13 VARIABLE=VALUE-
LIST  &
  2053             SENTENCE=REAL ELEMENT=2
```

```
  2054         DEFINE FN2O MOLE-FLOW STREAM=S8-5 SUBSTREAM=MIXED  &
  2055             COMPONENT=N2O
  2056         DEFINE FCO MOLE-FLOW STREAM=S8-5 SUBSTREAM=MIXED  &
  2057             COMPONENT=CO
  2058         DEFINE FMN2O BLOCK-VAR BLOCK=P11-41 VARIABLE=VALUE-LIST
&
  2059             SENTENCE=REAL ELEMENT=3
  2060          DEFINE FMCO BLOCK-VAR BLOCK=P11-13 VARIABLE=VALUE-LIST
&
  2061             SENTENCE=REAL ELEMENT=4
  2062     F     OPEN (7,FILE='C-11.txt')
  2063     F
  2064     C     CONCENTRATION OF CO
  2065     F     CONCO = MOFCO*DMIX
  2066     F     WRITE (7,*) 'CONCENTRATION OF CO',CONCO
  2067     F
  2068     C     CONCENTRATION OF N2O
  2069     F     CONN2O = MOFN2O*DMIX
  2070     F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2071     F
  2072     F     FMN2O = FN2O
  2073     F     FMCO = FCO
  2074         EXECUTE BEFORE BLOCK P11-13
  2075
  2076     CALCULATOR C-12
  2077         DEFINE DMIX STREAM-VAR STREAM=S8-6 SUBSTREAM=MIXED  &
  2078             VARIABLE=MOLE-DENSITY
  2079         DEFINE MOFN2O MOLE-FRAC STREAM=S8-6 SUBSTREAM=MIXED  &
  2080             COMPONENT=N2O
  2081           DEFINE CONN2O BLOCK-VAR BLOCK=P11-14 VARIABLE=VALUE-
LIST  &
  2082             SENTENCE=REAL ELEMENT=1
  2083         DEFINE FN2O MOLE-FLOW STREAM=S8-6 SUBSTREAM=MIXED  &
  2084             COMPONENT=N2O
  2085         DEFINE FMN2O BLOCK-VAR BLOCK=P11-14 VARIABLE=VALUE-LIST
&
  2086             SENTENCE=REAL ELEMENT=2
  2087     F     OPEN (7,FILE='C-12.txt')
  2088     F
  2089     C     CONCENTRATION OF N2O
  2090     F     CONN2O = MOFN2O*DMIX
  2091     F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2092     F
  2093     F     FMN2O = FN2O
  2094         EXECUTE BEFORE BLOCK P11-14
  2095
  2096     CALCULATOR C-13
  2097         DEFINE DMIX STREAM-VAR STREAM=S12 SUBSTREAM=MIXED  &
  2098             VARIABLE=MOLE-DENSITY
  2099         DEFINE MOFRAC MOLE-FRAC STREAM=S12 SUBSTREAM=MIXED  &
  2100             COMPONENT=O2
  2101         DEFINE CONO2 BLOCK-VAR BLOCK=P11-18 VARIABLE=VALUE-LIST
&
  2102             SENTENCE=REAL ELEMENT=1
  2103         DEFINE FN2 MOLE-FLOW STREAM=S12 SUBSTREAM=MIXED  &
```

```
  2104           COMPONENT=N2
  2105        DEFINE FO2 MOLE-FLOW STREAM=S12 SUBSTREAM=MIXED  &
  2106           COMPONENT=O2
  2107         DEFINE FMN2 BLOCK-VAR BLOCK=P11-18 VARIABLE=VALUE-LIST
&
  2108           SENTENCE=REAL ELEMENT=2
  2109         DEFINE FMO2 BLOCK-VAR BLOCK=P11-18 VARIABLE=VALUE-LIST
&
  2110           SENTENCE=REAL ELEMENT=3
  2111    F     OPEN (7,FILE='C-13.txt')
  2112    F
  2113    C     CONCENTRATION OF O2
  2114    F     CONO2 = MOFRAC*DMIX
  2115    F     WRITE (7,*) 'CONCENTRATION OF O2',CONO2
  2116    F
  2117    F     FMN2 = FN2
  2118    F     FMO2 = FO2
  2119        EXECUTE BEFORE BLOCK P11-18
  2120
  2121    CALCULATOR C-14
  2122        DEFINE DMIX STREAM-VAR STREAM=S13-1 SUBSTREAM=MIXED  &
  2123           VARIABLE=MOLE-DENSITY
  2124        DEFINE MOFNO MOLE-FRAC STREAM=S13-1 SUBSTREAM=MIXED  &
  2125           COMPONENT=NO
  2126        DEFINE CONNO BLOCK-VAR BLOCK=P11-19 VARIABLE=VALUE-LIST
&
  2127           SENTENCE=REAL ELEMENT=1
  2128        DEFINE FN2 MOLE-FLOW STREAM=S13-1 SUBSTREAM=MIXED  &
  2129           COMPONENT=N2
  2130        DEFINE FNO MOLE-FLOW STREAM=S13-1 SUBSTREAM=MIXED  &
  2131           COMPONENT=NO
  2132         DEFINE FMN2 BLOCK-VAR BLOCK=P11-19 VARIABLE=VALUE-LIST
&
  2133           SENTENCE=REAL ELEMENT=2
  2134         DEFINE FMNO BLOCK-VAR BLOCK=P11-19 VARIABLE=VALUE-LIST
&
  2135           SENTENCE=REAL ELEMENT=3
  2136    F     OPEN (7,FILE='C-14.txt')
  2137    F
  2138    C     CONCENTRATION OF NO
  2139    F     CONNO = MOFNO*DMIX
  2140    F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  2141    F
  2142    F     FMN2 = FN2
  2143    F     FMNO = FNO
  2144        EXECUTE BEFORE BLOCK P11-19
  2145
  2146    CALCULATOR C-15
  2147        DEFINE DMIX STREAM-VAR STREAM=S13-2 SUBSTREAM=MIXED  &
  2148           VARIABLE=MOLE-DENSITY
  2149        DEFINE MOFNO MOLE-FRAC STREAM=S13-2 SUBSTREAM=MIXED  &
  2150           COMPONENT=NO
  2151        DEFINE CONNO BLOCK-VAR BLOCK=P11-20 VARIABLE=VALUE-LIST
&
  2152           SENTENCE=REAL ELEMENT=1
```

```
 2153         DEFINE FNO MOLE-FLOW STREAM=S13-2 SUBSTREAM=MIXED  &
 2154             COMPONENT=NO
 2155         DEFINE FC1 MOLE-FLOW STREAM=S13-2 SUBSTREAM=CIPSD1  &
 2156             COMPONENT=C
 2157         DEFINE FC2 MOLE-FLOW STREAM=S13-2 SUBSTREAM=CIPSD2  &
 2158             COMPONENT=C
 2159         DEFINE FC3 MOLE-FLOW STREAM=S13-2 SUBSTREAM=CIPSD3  &
 2160             COMPONENT=C
 2161         DEFINE FC4 MOLE-FLOW STREAM=S13-2 SUBSTREAM=CIPSD4  &
 2162             COMPONENT=C
 2163         DEFINE FC5 MOLE-FLOW STREAM=S13-2 SUBSTREAM=CIPSD5  &
 2164             COMPONENT=C
 2165          DEFINE FMNO BLOCK-VAR BLOCK=P11-20 VARIABLE=VALUE-LIST
&
 2166             SENTENCE=REAL ELEMENT=2
 2167          DEFINE FMC1 BLOCK-VAR BLOCK=P11-20 VARIABLE=VALUE-LIST
&
 2168             SENTENCE=REAL ELEMENT=3
 2169          DEFINE FMC2 BLOCK-VAR BLOCK=P11-20 VARIABLE=VALUE-LIST
&
 2170             SENTENCE=REAL ELEMENT=4
 2171          DEFINE FMC3 BLOCK-VAR BLOCK=P11-20 VARIABLE=VALUE-LIST
&
 2172             SENTENCE=REAL ELEMENT=5
 2173          DEFINE FMC4 BLOCK-VAR BLOCK=P11-20 VARIABLE=VALUE-LIST
&
 2174             SENTENCE=REAL ELEMENT=6
 2175          DEFINE FMC5 BLOCK-VAR BLOCK=P11-20 VARIABLE=VALUE-LIST
&
 2176             SENTENCE=REAL ELEMENT=7
 2177     F     OPEN (7,FILE='C-15.txt')
 2178     F
 2179     C     CONCENTRATION OF NO
 2180     F     CONNO = MOFNO*DMIX
 2181     F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
 2182     F
 2183     F     FMNO = FNO
 2184     F     FMC1 = FC1
 2185     F     FMC2 = FC2
 2186     F     FMC3 = FC3
 2187     F     FMC4 = FC4
 2188     F     FMC5 = FC5
 2189         EXECUTE BEFORE BLOCK P11-20
 2190
 2191     CALCULATOR C-16
 2192         DEFINE DMIX STREAM-VAR STREAM=S13-3 SUBSTREAM=MIXED  &
 2193             VARIABLE=MOLE-DENSITY
 2194         DEFINE MOFNO MOLE-FRAC STREAM=S13-3 SUBSTREAM=MIXED  &
 2195             COMPONENT=NO
 2196          DEFINE CONNO BLOCK-VAR BLOCK=P11-21 VARIABLE=VALUE-LIST
&
 2197             SENTENCE=REAL ELEMENT=1
 2198         DEFINE FNO MOLE-FLOW STREAM=S13-3 SUBSTREAM=MIXED  &
 2199             COMPONENT=NO
 2200         DEFINE FCO MOLE-FLOW STREAM=S13-3 SUBSTREAM=MIXED  &
```

```
  2201           COMPONENT=CO
  2202         DEFINE FMNO BLOCK-VAR BLOCK=P11-21 VARIABLE=VALUE-LIST
&
  2203           SENTENCE=REAL ELEMENT=2
  2204         DEFINE FMCO BLOCK-VAR BLOCK=P11-21 VARIABLE=VALUE-LIST
&
  2205           SENTENCE=REAL ELEMENT=3
  2206    F     OPEN (7,FILE='C-16.txt')
  2207    F
  2208    C     CONCENTRATION OF NO
  2209    F     CONNO = MOFNO*DMIX
  2210    F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  2211    F
  2212    F     FMNO = FNO
  2213    F     FMCO = FCO
  2214        EXECUTE BEFORE BLOCK P11-21
  2215
  2216    CALCULATOR C-17
  2217        DEFINE DMIX STREAM-VAR STREAM=S13-4 SUBSTREAM=MIXED  &
  2218           VARIABLE=MOLE-DENSITY
  2219        DEFINE MOFN2O MOLE-FRAC STREAM=S13-4 SUBSTREAM=MIXED  &
  2220           COMPONENT=N2O
  2221         DEFINE CONN2O BLOCK-VAR BLOCK=P11-22 VARIABLE=VALUE-
LIST  &
  2222           SENTENCE=REAL ELEMENT=1
  2223        DEFINE FN2O MOLE-FLOW STREAM=S13-4 SUBSTREAM=MIXED  &
  2224           COMPONENT=N2O
  2225        DEFINE FC1 MOLE-FLOW STREAM=S13-4 SUBSTREAM=CIPSD1  &
  2226           COMPONENT=C
  2227        DEFINE FC2 MOLE-FLOW STREAM=S13-4 SUBSTREAM=CIPSD2  &
  2228           COMPONENT=C
  2229        DEFINE FC3 MOLE-FLOW STREAM=S13-4 SUBSTREAM=CIPSD3  &
  2230           COMPONENT=C
  2231        DEFINE FC4 MOLE-FLOW STREAM=S13-4 SUBSTREAM=CIPSD4  &
  2232           COMPONENT=C
  2233        DEFINE FC5 MOLE-FLOW STREAM=S13-4 SUBSTREAM=CIPSD5  &
  2234           COMPONENT=C
  2235        DEFINE FMN2O BLOCK-VAR BLOCK=P11-22 VARIABLE=VALUE-LIST
&
  2236           SENTENCE=REAL ELEMENT=2
  2237         DEFINE FMC1 BLOCK-VAR BLOCK=P11-22 VARIABLE=VALUE-LIST
&
  2238           SENTENCE=REAL ELEMENT=3
  2239         DEFINE FMC2 BLOCK-VAR BLOCK=P11-22 VARIABLE=VALUE-LIST
&
  2240           SENTENCE=REAL ELEMENT=4
  2241         DEFINE FMC3 BLOCK-VAR BLOCK=P11-22 VARIABLE=VALUE-LIST
&
  2242           SENTENCE=REAL ELEMENT=5
  2243         DEFINE FMC4 BLOCK-VAR BLOCK=P11-22 VARIABLE=VALUE-LIST
&
  2244           SENTENCE=REAL ELEMENT=6
  2245         DEFINE FMC5 BLOCK-VAR BLOCK=P11-22 VARIABLE=VALUE-LIST
&
  2246           SENTENCE=REAL ELEMENT=7
```

```
  2247    F     OPEN (7,FILE='C-17.txt')
  2248    F
  2249    C     CONCENTRATION OF N2O
  2250    F     CONN2O = MOFN2O*DMIX
  2251    F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2252    F
  2253    F     FMN2O = FN2O
  2254    F     FMC1 = FC1
  2255    F     FMC2 = FC2
  2256    F     FMC3 = FC3
  2257    F     FMC4 = FC4
  2258    F     FMC5 = FC5
  2259        EXECUTE BEFORE BLOCK P11-22
  2260
  2261    CALCULATOR C-18
  2262        DEFINE DMIX STREAM-VAR STREAM=S13-5 SUBSTREAM=MIXED  &
  2263            VARIABLE=MOLE-DENSITY
  2264        DEFINE MOFCO MOLE-FRAC STREAM=S13-5 SUBSTREAM=MIXED  &
  2265            COMPONENT=CO
  2266        DEFINE CONCO BLOCK-VAR BLOCK=P11-23 VARIABLE=VALUE-LIST
&
  2267            SENTENCE=REAL ELEMENT=1
  2268        DEFINE MOFN2O MOLE-FRAC STREAM=S13-5 SUBSTREAM=MIXED  &
  2269            COMPONENT=N2O
  2270          DEFINE CONN2O BLOCK-VAR BLOCK=P11-23 VARIABLE=VALUE-
LIST  &
  2271            SENTENCE=REAL ELEMENT=2
  2272        DEFINE FN2O MOLE-FLOW STREAM=S13-5 SUBSTREAM=MIXED  &
  2273            COMPONENT=N2O
  2274        DEFINE FCO MOLE-FLOW STREAM=S13-5 SUBSTREAM=MIXED  &
  2275            COMPONENT=CO
  2276        DEFINE FMN2O BLOCK-VAR BLOCK=P11-23 VARIABLE=VALUE-LIST
&
  2277            SENTENCE=REAL ELEMENT=3
  2278         DEFINE FMCO BLOCK-VAR BLOCK=P11-23 VARIABLE=VALUE-LIST
&
  2279            SENTENCE=REAL ELEMENT=4
  2280    F     OPEN (7,FILE='C-18.txt')
  2281    F
  2282    C     CONCENTRATION OF CO
  2283    F     CONCO = MOFCO*DMIX
  2284    F     WRITE (7,*) 'CONCENTRATION OF CO',CONCO
  2285    F
  2286    C     CONCENTRATION OF N2O
  2287    F     CONN2O = MOFN2O*DMIX
  2288    F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2289    F
  2290    F     FMN2O = FN2O
  2291    F     FMCO = FCO
  2292        EXECUTE BEFORE BLOCK P11-23
  2293
  2294    CALCULATOR C-19
  2295        DEFINE DMIX STREAM-VAR STREAM=S13-6 SUBSTREAM=MIXED  &
  2296            VARIABLE=MOLE-DENSITY
  2297        DEFINE MOFN2O MOLE-FRAC STREAM=S13-6 SUBSTREAM=MIXED  &
```

```
  2298           COMPONENT=N2O
  2299         DEFINE CONN2O BLOCK-VAR BLOCK=P11-24 VARIABLE=VALUE-
LIST  &
  2300           SENTENCE=REAL ELEMENT=1
  2301       DEFINE FN2O MOLE-FLOW STREAM=S13-6 SUBSTREAM=MIXED  &
  2302           COMPONENT=N2O
  2303       DEFINE FMN2O BLOCK-VAR BLOCK=P11-24 VARIABLE=VALUE-LIST
&
  2304           SENTENCE=REAL ELEMENT=2
  2305    F     OPEN (7,FILE='C-12.txt')
  2306    F
  2307    C     CONCENTRATION OF N2O
  2308    F     CONN2O = MOFN2O*DMIX
  2309    F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2310    F
  2311    F     FMN2O = FN2O
  2312        EXECUTE BEFORE BLOCK P11-24
  2313
  2314    CALCULATOR C-20
  2315        DEFINE DMIX STREAM-VAR STREAM=S16 SUBSTREAM=MIXED  &
  2316           VARIABLE=MOLE-DENSITY
  2317        DEFINE MOFRAC MOLE-FRAC STREAM=S16 SUBSTREAM=MIXED  &
  2318           COMPONENT=O2
  2319        DEFINE CONO2 BLOCK-VAR BLOCK=P11-27 VARIABLE=VALUE-LIST
&
  2320           SENTENCE=REAL ELEMENT=1
  2321        DEFINE FN2 MOLE-FLOW STREAM=S16 SUBSTREAM=MIXED  &
  2322           COMPONENT=N2
  2323        DEFINE FO2 MOLE-FLOW STREAM=S16 SUBSTREAM=MIXED  &
  2324           COMPONENT=O2
  2325         DEFINE FMN2 BLOCK-VAR BLOCK=P11-27 VARIABLE=VALUE-LIST
&
  2326           SENTENCE=REAL ELEMENT=2
  2327         DEFINE FMO2 BLOCK-VAR BLOCK=P11-27 VARIABLE=VALUE-LIST
&
  2328           SENTENCE=REAL ELEMENT=3
  2329    F     OPEN (7,FILE='C-20.txt')
  2330    F
  2331    C     CONCENTRATION OF O2
  2332    F     CONO2 = MOFRAC*DMIX
  2333    F     WRITE (7,*) 'CONCENTRATION OF O2',CONO2
  2334    F
  2335    F     FMN2 = FN2
  2336    F     FMO2 = FO2
  2337        EXECUTE BEFORE BLOCK P11-27
  2338
  2339    CALCULATOR C-21
  2340        DEFINE DMIX STREAM-VAR STREAM=S17-1 SUBSTREAM=MIXED  &
  2341           VARIABLE=MOLE-DENSITY
  2342        DEFINE MOFNO MOLE-FRAC STREAM=S17-1 SUBSTREAM=MIXED  &
  2343           COMPONENT=NO
  2344        DEFINE CONNO BLOCK-VAR BLOCK=P11-28 VARIABLE=VALUE-LIST
&
  2345           SENTENCE=REAL ELEMENT=1
  2346        DEFINE FN2 MOLE-FLOW STREAM=S17-1 SUBSTREAM=MIXED  &
```

```
  2347           COMPONENT=N2
  2348        DEFINE FNO MOLE-FLOW STREAM=S17-1 SUBSTREAM=MIXED  &
  2349           COMPONENT=NO
  2350         DEFINE FMN2 BLOCK-VAR BLOCK=P11-28 VARIABLE=VALUE-LIST
&
  2351           SENTENCE=REAL ELEMENT=2
  2352         DEFINE FMNO BLOCK-VAR BLOCK=P11-28 VARIABLE=VALUE-LIST
&
  2353           SENTENCE=REAL ELEMENT=3
  2354    F     OPEN (7,FILE='C-21.txt')
  2355    F
  2356    C     CONCENTRATION OF NO
  2357    F     CONNO = MOFNO*DMIX
  2358    F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  2359    F
  2360    F     FMN2 = FN2
  2361    F     FMNO = FNO
  2362        EXECUTE BEFORE BLOCK P11-28
  2363
  2364    CALCULATOR C-22
  2365        DEFINE DMIX STREAM-VAR STREAM=S17-2 SUBSTREAM=MIXED  &
  2366           VARIABLE=MOLE-DENSITY
  2367        DEFINE MOFNO MOLE-FRAC STREAM=S17-2 SUBSTREAM=MIXED  &
  2368           COMPONENT=NO
  2369        DEFINE CONNO BLOCK-VAR BLOCK=P11-29 VARIABLE=VALUE-LIST
&
  2370           SENTENCE=REAL ELEMENT=1
  2371        DEFINE FNO MOLE-FLOW STREAM=S17-2 SUBSTREAM=MIXED  &
  2372           COMPONENT=NO
  2373        DEFINE FC1 MOLE-FLOW STREAM=S17-2 SUBSTREAM=CIPSD1  &
  2374           COMPONENT=C
  2375        DEFINE FC2 MOLE-FLOW STREAM=S17-2 SUBSTREAM=CIPSD2  &
  2376           COMPONENT=C
  2377        DEFINE FC3 MOLE-FLOW STREAM=S17-2 SUBSTREAM=CIPSD3  &
  2378           COMPONENT=C
  2379        DEFINE FC4 MOLE-FLOW STREAM=S17-2 SUBSTREAM=CIPSD4  &
  2380           COMPONENT=C
  2381        DEFINE FC5 MOLE-FLOW STREAM=S17-2 SUBSTREAM=CIPSD5  &
  2382           COMPONENT=C
  2383         DEFINE FMNO BLOCK-VAR BLOCK=P11-29 VARIABLE=VALUE-LIST
&
  2384           SENTENCE=REAL ELEMENT=2
  2385         DEFINE FMC1 BLOCK-VAR BLOCK=P11-29 VARIABLE=VALUE-LIST
&
  2386           SENTENCE=REAL ELEMENT=3
  2387         DEFINE FMC2 BLOCK-VAR BLOCK=P11-29 VARIABLE=VALUE-LIST
&
  2388           SENTENCE=REAL ELEMENT=4
  2389         DEFINE FMC3 BLOCK-VAR BLOCK=P11-29 VARIABLE=VALUE-LIST
&
  2390           SENTENCE=REAL ELEMENT=5
  2391         DEFINE FMC4 BLOCK-VAR BLOCK=P11-29 VARIABLE=VALUE-LIST
&
  2392           SENTENCE=REAL ELEMENT=6
```

```
  2393          DEFINE FMC5 BLOCK-VAR BLOCK=P11-29 VARIABLE=VALUE-LIST
&
  2394             SENTENCE=REAL ELEMENT=7
  2395     F      OPEN (7,FILE='C-22.txt')
  2396     F
  2397     C      CONCENTRATION OF NO
  2398     F      CONNO = MOFNO*DMIX
  2399     F      WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  2400     F
  2401     F      FMNO = FNO
  2402     F      FMC1 = FC1
  2403     F      FMC2 = FC2
  2404     F      FMC3 = FC3
  2405     F      FMC4 = FC4
  2406     F      FMC5 = FC5
  2407          EXECUTE BEFORE BLOCK P11-29
  2408
  2409     CALCULATOR C-23
  2410          DEFINE DMIX STREAM-VAR STREAM=S17-3 SUBSTREAM=MIXED  &
  2411             VARIABLE=MOLE-DENSITY
  2412          DEFINE MOFNO MOLE-FRAC STREAM=S17-3 SUBSTREAM=MIXED  &
  2413             COMPONENT=NO
  2414          DEFINE CONNO BLOCK-VAR BLOCK=P11-30 VARIABLE=VALUE-LIST
&
  2415             SENTENCE=REAL ELEMENT=1
  2416          DEFINE FNO MOLE-FLOW STREAM=S17-3 SUBSTREAM=MIXED  &
  2417             COMPONENT=NO
  2418          DEFINE FCO MOLE-FLOW STREAM=S17-3 SUBSTREAM=MIXED  &
  2419             COMPONENT=CO
  2420          DEFINE FMNO BLOCK-VAR BLOCK=P11-30 VARIABLE=VALUE-LIST
&
  2421             SENTENCE=REAL ELEMENT=2
  2422          DEFINE FMCO BLOCK-VAR BLOCK=P11-30 VARIABLE=VALUE-LIST
&
  2423             SENTENCE=REAL ELEMENT=3
  2424     F      OPEN (7,FILE='C-23.txt')
  2425     F
  2426     C      CONCENTRATION OF NO
  2427     F      CONNO = MOFNO*DMIX
  2428     F      WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  2429     F
  2430     F      FMNO = FNO
  2431     F      FMCO = FCO
  2432          EXECUTE BEFORE BLOCK P11-30
  2433
  2434     CALCULATOR C-24
  2435          DEFINE DMIX STREAM-VAR STREAM=S17-4 SUBSTREAM=MIXED  &
  2436             VARIABLE=MOLE-DENSITY
  2437          DEFINE MOFN2O MOLE-FRAC STREAM=S17-4 SUBSTREAM=MIXED  &
  2438             COMPONENT=N2O
  2439           DEFINE CONN2O BLOCK-VAR BLOCK=P11-31 VARIABLE=VALUE-
LIST  &
  2440             SENTENCE=REAL ELEMENT=1
  2441          DEFINE FN2O MOLE-FLOW STREAM=S17-4 SUBSTREAM=MIXED  &
  2442             COMPONENT=N2O
```

```
  2443         DEFINE FC1 MOLE-FLOW STREAM=S17-4 SUBSTREAM=CIPSD1  &
  2444             COMPONENT=C
  2445         DEFINE FC2 MOLE-FLOW STREAM=S17-4 SUBSTREAM=CIPSD2  &
  2446             COMPONENT=C
  2447         DEFINE FC3 MOLE-FLOW STREAM=S17-4 SUBSTREAM=CIPSD3  &
  2448             COMPONENT=C
  2449         DEFINE FC4 MOLE-FLOW STREAM=S17-4 SUBSTREAM=CIPSD4  &
  2450             COMPONENT=C
  2451         DEFINE FC5 MOLE-FLOW STREAM=S17-4 SUBSTREAM=CIPSD5  &
  2452             COMPONENT=C
  2453         DEFINE FMN2O BLOCK-VAR BLOCK=P11-31 VARIABLE=VALUE-LIST
&
  2454             SENTENCE=REAL ELEMENT=2
  2455          DEFINE FMC1 BLOCK-VAR BLOCK=P11-31 VARIABLE=VALUE-LIST
&
  2456             SENTENCE=REAL ELEMENT=3
  2457          DEFINE FMC2 BLOCK-VAR BLOCK=P11-31 VARIABLE=VALUE-LIST
&
  2458             SENTENCE=REAL ELEMENT=4
  2459          DEFINE FMC3 BLOCK-VAR BLOCK=P11-31 VARIABLE=VALUE-LIST
&
  2460             SENTENCE=REAL ELEMENT=5
  2461          DEFINE FMC4 BLOCK-VAR BLOCK=P11-31 VARIABLE=VALUE-LIST
&
  2462             SENTENCE=REAL ELEMENT=6
  2463          DEFINE FMC5 BLOCK-VAR BLOCK=P11-31 VARIABLE=VALUE-LIST
&
  2464             SENTENCE=REAL ELEMENT=7
  2465     F      OPEN (7,FILE='C-24.txt')
  2466     F
  2467     C      CONCENTRATION OF N2O
  2468     F      CONN2O = MOFN2O*DMIX
  2469     F      WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2470     F
  2471     F      FMN2O = FN2O
  2472     F      FMC1 = FC1
  2473     F      FMC2 = FC2
  2474     F      FMC3 = FC3
  2475     F      FMC4 = FC4
  2476     F      FMC5 = FC5
  2477         EXECUTE BEFORE BLOCK P11-31
  2478
  2479     CALCULATOR C-25
  2480         DEFINE DMIX STREAM-VAR STREAM=S17-5 SUBSTREAM=MIXED  &
  2481             VARIABLE=MOLE-DENSITY
  2482         DEFINE MOFCO MOLE-FRAC STREAM=S17-5 SUBSTREAM=MIXED  &
  2483             COMPONENT=CO
  2484         DEFINE CONCO BLOCK-VAR BLOCK=P11-32 VARIABLE=VALUE-LIST
&
  2485             SENTENCE=REAL ELEMENT=1
  2486         DEFINE MOFN2O MOLE-FRAC STREAM=S17-5 SUBSTREAM=MIXED  &
  2487             COMPONENT=N2O
  2488           DEFINE CONN2O BLOCK-VAR BLOCK=P11-32 VARIABLE=VALUE-
LIST  &
  2489             SENTENCE=REAL ELEMENT=2
```

```
  2490         DEFINE FN2O MOLE-FLOW STREAM=S17-5 SUBSTREAM=MIXED  &
  2491             COMPONENT=N2O
  2492         DEFINE FCO MOLE-FLOW STREAM=S17-5 SUBSTREAM=MIXED  &
  2493             COMPONENT=CO
  2494         DEFINE FMN2O BLOCK-VAR BLOCK=P11-32 VARIABLE=VALUE-LIST
&
  2495             SENTENCE=REAL ELEMENT=3
  2496          DEFINE FMCO BLOCK-VAR BLOCK=P11-32 VARIABLE=VALUE-LIST
&
  2497             SENTENCE=REAL ELEMENT=4
  2498     F     OPEN (7,FILE='C-18.txt')
  2499     F
  2500     C     CONCENTRATION OF CO
  2501     F     CONCO = MOFCO*DMIX
  2502     F     WRITE (7,*) 'CONCENTRATION OF CO',CONCO
  2503     F
  2504     C     CONCENTRATION OF N2O
  2505     F     CONN2O = MOFN2O*DMIX
  2506     F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2507     F
  2508     F     FMN2O = FN2O
  2509     F     FMCO = FCO
  2510         EXECUTE BEFORE BLOCK P11-32
  2511
  2512     CALCULATOR C-26
  2513         DEFINE DMIX STREAM-VAR STREAM=S17-6 SUBSTREAM=MIXED  &
  2514             VARIABLE=MOLE-DENSITY
  2515         DEFINE MOFN2O MOLE-FRAC STREAM=S17-6 SUBSTREAM=MIXED  &
  2516             COMPONENT=N2O
  2517           DEFINE CONN2O BLOCK-VAR BLOCK=P11-33 VARIABLE=VALUE-
LIST  &
  2518             SENTENCE=REAL ELEMENT=1
  2519         DEFINE FN2O MOLE-FLOW STREAM=S17-6 SUBSTREAM=MIXED  &
  2520             COMPONENT=N2O
  2521         DEFINE FMN2O BLOCK-VAR BLOCK=P11-33 VARIABLE=VALUE-LIST
&
  2522             SENTENCE=REAL ELEMENT=2
  2523     F     OPEN (7,FILE='C-12.txt')
  2524     F
  2525     C     CONCENTRATION OF N2O
  2526     F     CONN2O = MOFN2O*DMIX
  2527     F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2528     F
  2529     F     FMN2O = FN2O
  2530         EXECUTE BEFORE BLOCK P11-33
  2531
  2532     CALCULATOR C-27
  2533         DEFINE DMIX STREAM-VAR STREAM=S20 SUBSTREAM=MIXED  &
  2534             VARIABLE=MOLE-DENSITY
  2535         DEFINE MOFRAC MOLE-FRAC STREAM=S20 SUBSTREAM=MIXED  &
  2536             COMPONENT=O2
  2537         DEFINE CONO2 BLOCK-VAR BLOCK=P11-36 VARIABLE=VALUE-LIST
&
  2538             SENTENCE=REAL ELEMENT=1
  2539         DEFINE FN2 MOLE-FLOW STREAM=S20 SUBSTREAM=MIXED  &
```

```
  2540           COMPONENT=N2
  2541        DEFINE FO2 MOLE-FLOW STREAM=S20 SUBSTREAM=MIXED  &
  2542           COMPONENT=O2
  2543         DEFINE FMN2 BLOCK-VAR BLOCK=P11-36 VARIABLE=VALUE-LIST
&
  2544           SENTENCE=REAL ELEMENT=2
  2545         DEFINE FMO2 BLOCK-VAR BLOCK=P11-36 VARIABLE=VALUE-LIST
&
  2546           SENTENCE=REAL ELEMENT=3
  2547    F     OPEN (7,FILE='C-27.txt')
  2548    F
  2549    C     CONCENTRATION OF O2
  2550    F     CONO2 = MOFRAC*DMIX
  2551    F     WRITE (7,*) 'CONCENTRATION OF O2',CONO2
  2552    F     FMN2 = FN2
  2553    F     FMO2 = FO2
  2554        EXECUTE BEFORE BLOCK P11-36
  2555
  2556    CALCULATOR C-28
  2557        DEFINE DMIX STREAM-VAR STREAM=S21-1 SUBSTREAM=MIXED  &
  2558           VARIABLE=MOLE-DENSITY
  2559        DEFINE MOFNO MOLE-FRAC STREAM=S21-1 SUBSTREAM=MIXED  &
  2560           COMPONENT=NO
  2561        DEFINE CONNO BLOCK-VAR BLOCK=P11-37 VARIABLE=VALUE-LIST
&
  2562           SENTENCE=REAL ELEMENT=1
  2563        DEFINE FN2 MOLE-FLOW STREAM=S21-1 SUBSTREAM=MIXED  &
  2564           COMPONENT=N2
  2565        DEFINE FNO MOLE-FLOW STREAM=S21-1 SUBSTREAM=MIXED  &
  2566           COMPONENT=NO
  2567         DEFINE FMN2 BLOCK-VAR BLOCK=P11-37 VARIABLE=VALUE-LIST
&
  2568           SENTENCE=REAL ELEMENT=2
  2569         DEFINE FMNO BLOCK-VAR BLOCK=P11-37 VARIABLE=VALUE-LIST
&
  2570           SENTENCE=REAL ELEMENT=3
  2571    F     OPEN (7,FILE='C-28.txt')
  2572    F
  2573    C     CONCENTRATION OF NO
  2574    F     CONNO = MOFNO*DMIX
  2575    F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  2576    F
  2577    F     FMN2 = FN2
  2578    F     FMNO = FNO
  2579        EXECUTE BEFORE BLOCK P11-37
  2580
  2581    CALCULATOR C-29
  2582        DEFINE DMIX STREAM-VAR STREAM=S21-2 SUBSTREAM=MIXED  &
  2583           VARIABLE=MOLE-DENSITY
  2584        DEFINE MOFNO MOLE-FRAC STREAM=S21-2 SUBSTREAM=MIXED  &
  2585           COMPONENT=NO
  2586        DEFINE CONNO BLOCK-VAR BLOCK=P11-38 VARIABLE=VALUE-LIST
&
  2587           SENTENCE=REAL ELEMENT=1
  2588        DEFINE FNO MOLE-FLOW STREAM=S21-2 SUBSTREAM=MIXED  &
```

```
  2589           COMPONENT=NO
  2590         DEFINE FMNO BLOCK-VAR BLOCK=P11-38 VARIABLE=VALUE-LIST
&
  2591           SENTENCE=REAL ELEMENT=2
  2592        DEFINE FC1 MOLE-FLOW STREAM=S21-2 SUBSTREAM=CIPSD1  &
  2593           COMPONENT=C
  2594        DEFINE FC2 MOLE-FLOW STREAM=S21-2 SUBSTREAM=CIPSD2  &
  2595           COMPONENT=C
  2596        DEFINE FC3 MOLE-FLOW STREAM=S21-2 SUBSTREAM=CIPSD3  &
  2597           COMPONENT=C
  2598        DEFINE FC4 MOLE-FLOW STREAM=S21-2 SUBSTREAM=CIPSD4  &
  2599           COMPONENT=C
  2600        DEFINE FC5 MOLE-FLOW STREAM=S21-2 SUBSTREAM=CIPSD5  &
  2601           COMPONENT=C
  2602         DEFINE FMC1 BLOCK-VAR BLOCK=P11-38 VARIABLE=VALUE-LIST
&
  2603           SENTENCE=REAL ELEMENT=3
  2604         DEFINE FMC2 BLOCK-VAR BLOCK=P11-38 VARIABLE=VALUE-LIST
&
  2605           SENTENCE=REAL ELEMENT=4
  2606         DEFINE FMC3 BLOCK-VAR BLOCK=P11-38 VARIABLE=VALUE-LIST
&
  2607           SENTENCE=REAL ELEMENT=5
  2608         DEFINE FMC4 BLOCK-VAR BLOCK=P11-38 VARIABLE=VALUE-LIST
&
  2609           SENTENCE=REAL ELEMENT=6
  2610         DEFINE FMC5 BLOCK-VAR BLOCK=P11-38 VARIABLE=VALUE-LIST
&
  2611           SENTENCE=REAL ELEMENT=7
  2612    F     OPEN (7,FILE='C-29.txt')
  2613    F
  2614    C     CONCENTRATION OF NO
  2615    F     CONNO = MOFNO*DMIX
  2616    F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  2617    F
  2618    F     FMNO = FNO
  2619    F     FMC1 = FC1
  2620    F     FMC2 = FC2
  2621    F     FMC3 = FC3
  2622    F     FMC4 = FC4
  2623    F     FMC5 = FC5
  2624        EXECUTE BEFORE BLOCK P11-38
  2625
  2626    CALCULATOR C-30
  2627        DEFINE DMIX STREAM-VAR STREAM=S21-3 SUBSTREAM=MIXED  &
  2628           VARIABLE=MOLE-DENSITY
  2629        DEFINE MOFNO MOLE-FRAC STREAM=S21-3 SUBSTREAM=MIXED  &
  2630           COMPONENT=NO
  2631        DEFINE CONNO BLOCK-VAR BLOCK=P11-39 VARIABLE=VALUE-LIST
&
  2632           SENTENCE=REAL ELEMENT=1
  2633        DEFINE FNO MOLE-FLOW STREAM=S21-3 SUBSTREAM=MIXED  &
  2634           COMPONENT=NO
  2635        DEFINE FCO MOLE-FLOW STREAM=S21-3 SUBSTREAM=MIXED  &
  2636           COMPONENT=CO
```

```
  2637         DEFINE FMNO BLOCK-VAR BLOCK=P11-39 VARIABLE=VALUE-LIST
&
  2638            SENTENCE=REAL ELEMENT=2
  2639         DEFINE FMCO BLOCK-VAR BLOCK=P11-39 VARIABLE=VALUE-LIST
&
  2640            SENTENCE=REAL ELEMENT=3
  2641    F     OPEN (7,FILE='C-30.txt')
  2642    F
  2643    C     CONCENTRATION OF NO
  2644    F     CONNO = MOFNO*DMIX
  2645    F     WRITE (7,*) 'CONCENTRATION OF NO',CONNO
  2646    F
  2647    F     FMNO = FNO
  2648    F     FMCO = FCO
  2649        EXECUTE BEFORE BLOCK P11-39
  2650
  2651    CALCULATOR C-31
  2652        DEFINE DMIX STREAM-VAR STREAM=S21-4 SUBSTREAM=MIXED  &
  2653            VARIABLE=MOLE-DENSITY
  2654        DEFINE MOFN2O MOLE-FRAC STREAM=S21-4 SUBSTREAM=MIXED  &
  2655            COMPONENT=N2O
  2656          DEFINE CONN2O BLOCK-VAR BLOCK=P11-40 VARIABLE=VALUE-
LIST  &
  2657            SENTENCE=REAL ELEMENT=1
  2658        DEFINE FN2O MOLE-FLOW STREAM=S21-4 SUBSTREAM=MIXED  &
  2659            COMPONENT=N2O
  2660        DEFINE FC1 MOLE-FLOW STREAM=S21-4 SUBSTREAM=CIPSD1  &
  2661            COMPONENT=C
  2662        DEFINE FC2 MOLE-FLOW STREAM=S21-4 SUBSTREAM=CIPSD2  &
  2663            COMPONENT=C
  2664        DEFINE FC3 MOLE-FLOW STREAM=S21-4 SUBSTREAM=CIPSD3  &
  2665            COMPONENT=C
  2666        DEFINE FC4 MOLE-FLOW STREAM=S21-4 SUBSTREAM=CIPSD4  &
  2667            COMPONENT=C
  2668        DEFINE FC5 MOLE-FLOW STREAM=S21-4 SUBSTREAM=CIPSD5  &
  2669            COMPONENT=C
  2670        DEFINE FMN2O BLOCK-VAR BLOCK=P11-40 VARIABLE=VALUE-LIST
&
  2671            SENTENCE=REAL ELEMENT=2
  2672         DEFINE FMC1 BLOCK-VAR BLOCK=P11-40 VARIABLE=VALUE-LIST
&
  2673            SENTENCE=REAL ELEMENT=3
  2674         DEFINE FMC2 BLOCK-VAR BLOCK=P11-40 VARIABLE=VALUE-LIST
&
  2675            SENTENCE=REAL ELEMENT=4
  2676         DEFINE FMC3 BLOCK-VAR BLOCK=P11-40 VARIABLE=VALUE-LIST
&
  2677            SENTENCE=REAL ELEMENT=5
  2678         DEFINE FMC4 BLOCK-VAR BLOCK=P11-40 VARIABLE=VALUE-LIST
&
  2679            SENTENCE=REAL ELEMENT=6
  2680         DEFINE FMC5 BLOCK-VAR BLOCK=P11-40 VARIABLE=VALUE-LIST
&
  2681            SENTENCE=REAL ELEMENT=7
  2682    F     OPEN (7,FILE='C-31.txt')
```

```
  2683    F
  2684    C     CONCENTRATION OF N2O
  2685    F     CONN2O = MOFN2O*DMIX
  2686    F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2687    F
  2688    F     FMN2O = FN2O
  2689    F     FMC1 = FC1
  2690    F     FMC2 = FC2
  2691    F     FMC3 = FC3
  2692    F     FMC4 = FC4
  2693    F     FMC5 = FC5
  2694        EXECUTE BEFORE BLOCK P11-40
  2695
  2696    CALCULATOR C-32
  2697        DEFINE DMIX STREAM-VAR STREAM=S21-5 SUBSTREAM=MIXED  &
  2698            VARIABLE=MOLE-DENSITY
  2699        DEFINE MOFCO MOLE-FRAC STREAM=S21-5 SUBSTREAM=MIXED  &
  2700            COMPONENT=CO
  2701        DEFINE CONCO BLOCK-VAR BLOCK=P11-41 VARIABLE=VALUE-LIST
&
  2702            SENTENCE=REAL ELEMENT=1
  2703        DEFINE MOFN2O MOLE-FRAC STREAM=S21-5 SUBSTREAM=MIXED  &
  2704            COMPONENT=N2O
  2705          DEFINE CONN2O BLOCK-VAR BLOCK=P11-41 VARIABLE=VALUE-
LIST  &
  2706            SENTENCE=REAL ELEMENT=2
  2707        DEFINE FN2O MOLE-FLOW STREAM=S21-5 SUBSTREAM=MIXED  &
  2708            COMPONENT=N2O
  2709        DEFINE FCO MOLE-FLOW STREAM=S21-5 SUBSTREAM=MIXED  &
  2710            COMPONENT=CO
  2711        DEFINE FMN2O BLOCK-VAR BLOCK=P11-41 VARIABLE=VALUE-LIST
&
  2712            SENTENCE=REAL ELEMENT=3
  2713         DEFINE FMCO BLOCK-VAR BLOCK=P11-41 VARIABLE=VALUE-LIST
&
  2714            SENTENCE=REAL ELEMENT=4
  2715    F     OPEN (7,FILE='C-32.txt')
  2716    F
  2717    C     CONCENTRATION OF CO
  2718    F     CONCO = MOFCO*DMIX
  2719    F     WRITE (7,*) 'CONCENTRATION OF CO',CONCO
  2720    F
  2721    C     CONCENTRATION OF N2O
  2722    F     CONN2O = MOFN2O*DMIX
  2723    F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2724    F
  2725    F     FMN2O = FN2O
  2726    F     FMCO = FCO
  2727        EXECUTE BEFORE BLOCK P11-41
  2728
  2729    CALCULATOR C-33
  2730    F
  2731    F
  2732    F     COMMON /USER14/ VOIDM,  BEDVM,  BEDL
  2733    F
```

```
  2734    F     REAL*8 BEDL(4)
  2735         DEFINE DMIX STREAM-VAR STREAM=S21-6 SUBSTREAM=MIXED  &
  2736             VARIABLE=MOLE-DENSITY
  2737         DEFINE MOFN2O MOLE-FRAC STREAM=S21-6 SUBSTREAM=MIXED  &
  2738             COMPONENT=N2O
  2739           DEFINE CONN2O BLOCK-VAR BLOCK=P11-42 VARIABLE=VALUE-
LIST  &
  2740             SENTENCE=REAL ELEMENT=1
  2741         DEFINE FN2O MOLE-FLOW STREAM=S21-6 SUBSTREAM=MIXED  &
  2742             COMPONENT=N2O
  2743         DEFINE FMN2O BLOCK-VAR BLOCK=P11-42 VARIABLE=VALUE-LIST
&
  2744             SENTENCE=REAL ELEMENT=2
  2745    F     OPEN (7,FILE='C-33.txt')
  2746    F
  2747    C     CONCENTRATION OF N2O
  2748    F     CONN2O = MOFN2O*DMIX
  2749    F     WRITE (7,*) 'CONCENTRATION OF N2O',CONN2O
  2750      F       WRITE  (7,*)  'BEDL',  BEDL(1),  BEDL(2),  BEDL(3),
BEDL(4)
  2751    F
  2752    F     FMN2O = FN2O
  2753         EXECUTE BEFORE BLOCK P11-42
  2754
  2755    CALCULATOR C-34
  2756    F     COMMON /USER5/ AREA, VFAIR1, VAIR1, VVOID,
  2757    F    .               BEDW
  2758    F     COMMON /USER14/ VOIDM,  BEDVM,  BEDL
  2759    F     COMMON /USER23/ UGAS, RSO2, YSO2, TAVE, XCAO
  2760    F     COMMON /USER24/ CONC, DMEAN, A1, ALPHA, VCAO
  2761    F
  2762    F     REAL*8 VOIDM(3), BEDVM(3), BEDL(4),  UGAS(4),
  2763    F    .       RSO2(5),  YSO2(5),  FRACL(5), TAVE(4),
  2764    F    .       XCAO(5),  SIZE(5),  WDR(5),   ETASO2(5)
  2765    F
  2766    F
  2767    F     DATA FRACL/0.02,0.07,0.45,0.405,0.055/
  2768    F     DATA SIZE/2.5E-5,7.5E-5,1.5E-4,3.5E-4,7.5E-4/
  2769    F     DATA R/82.05/,SIGMP/0.001/,RKV/8E-4/
  2770    F     DATA EPSI/0.52/
  2771         DEFINE MFAIR1 STREAM-VAR STREAM=AIR1 SUBSTREAM=MIXED  &
  2772             VARIABLE=MOLE-FLOW
  2773         DEFINE MFAIR2 STREAM-VAR STREAM=AIR2 SUBSTREAM=MIXED  &
  2774             VARIABLE=MOLE-FLOW
  2775         DEFINE MFAIR3 STREAM-VAR STREAM=AIR3 SUBSTREAM=MIXED  &
  2776             VARIABLE=MOLE-FLOW
  2777         DEFINE MFSO2 MOLE-FLOW STREAM=S8-7 SUBSTREAM=MIXED  &
  2778             COMPONENT=SO2
  2779           DEFINE FLIME STREAM-VAR STREAM=LIME SUBSTREAM=CISOLID
&
  2780             VARIABLE=MASS-FLOW
  2781         DEFINE RECAO MASS-FLOW STREAM=RESOLID SUBSTREAM=CISOLID
&
  2782             COMPONENT=CAO
  2783         DEFINE BEDV BLOCK-VAR BLOCK=P11-7 VARIABLE=VOL  &
```

```
  2784           SENTENCE=PARAM
  2785        DEFINE BEDP BLOCK-VAR BLOCK=P11-7 VARIABLE=PRES  &
  2786           SENTENCE=PARAM
  2787        DEFINE BEDT BLOCK-VAR BLOCK=P11-7 VARIABLE=TEMP  &
  2788           SENTENCE=PARAM
  2789         DEFINE DLIME STREAM-VAR STREAM=LIME SUBSTREAM=CISOLID
&
  2790           VARIABLE=MASS-DENSITY
  2791         DEFINE DMLIME STREAM-VAR STREAM=LIME SUBSTREAM=CISOLID
&
  2792           VARIABLE=MOLE-DENSITY
  2793        DEFINE ETAL BLOCK-VAR BLOCK=P11-15 VARIABLE=CONV  &
  2794           SENTENCE=CONV ID1=2
  2795    F     OPEN (7,FILE='SO2.txt')
  2796    F
  2797    C     TOTAL GAS CONCENTRATION (Kmol/m3)
  2798    F     CONC = BEDP*1000/(101325.*R*BEDT)
  2799    F     WRITE (7,*) 'CONC=',CONC
  2800    F
  2801    C     RATE OF SO2 AT LOWER REGION Kmol/(s m3)
  2802    F     RSO2(1) = MFSO2/BEDV
  2803    F     YSO2(1) = 0.5
  2804    F
  2805    C     CALCULATE MEAN RADIUS OF SORBENT (m.)
  2806    F     DO 5 I = 1,5
  2807    F   5 WDR(I) = FRACL(I)/SIZE(I)
  2808    F
  2809    F     SUMWDR = 0.
  2810    F     DO 10 I = 1,5
  2811    F  10 SUMWDR = SUMWDR + WDR(I)
  2812    F
  2813    F     RMEAN = 1/SUMWDR
  2814    F     WRITE (7,*) 'RMEAN', RMEAN
  2815    F
  2816    C     CHANGE RADIUS TO DIAMETER IN cm.
  2817    F     DMEAN = RMEAN*2*100.
  2818    F     WRITE (7,*) 'DMEAN', DMEAN, 'cm.'
  2819    F
  2820    C      DO 15 I = 1,4
  2821    F
  2822    F     A1 = 3.33E-4*DEXP(-0.0113*DMEAN)
  2823    F     WRITE (7,*) 'A1=',A1
  2824    F
  2825    F     ALPHA = 35.*DMEAN**0.3
  2826    F     WRITE (7,*) 'ALPHA=',ALPHA
  2827    F
  2828    C     MEAN RESIDENCE TIME
  2829    F     TAVE(1) = DLIME*SIGMP*AREA*BEDL(1)/FLIME
  2830    F     WRITE (7,*) 'TAVE=',TAVE(1)
  2831    F     WRITE (7,*) 'AREA',AREA,'DLIME',DLIME,'FLIME',FLIME
  2832    F
  2833                F        20    XCAO1    =    TAVE(1)-1./A1*DLOG(
1.+6.*ALPHA*CONC*YSO2(1)/(DMEAN*RKV)
  2834    F    .         *(DEXP(A1*TAVE(1)) -1.) )
  2835    F
```

```
F     XCAO2 = DMEAN/(6*ALPHA*CONC*YSO2(1)) - 1./RKV
F
C      VCAO = 1./DMLIME
F     VCAO = 1.69E-2
F     XCAO(1) = (VCAO/(1.-EPSI)) * (XCAO1/XCAO2)
F     WRITE (7,*) 'XCAO=', XCAO(1)
F
F     RSO21 = (VCAO*FLIME/(1-EPSI*AREA*BEDL(1)*100.))
F    .        *XCAO1/XCAO2
F     WRITE (7,*) 'RSO21=',RSO21
F
F     YSO2JN = (BEDL(1)*(RSO2(1)-RSO21)/(CONC*UGAS(1)))
F     WRITE (7,*) 'RSO2(1)', RSO2(1)
F     WRITE (7,*) 'YSO2JN=',YSO2JN
F
F     IF(ABS((YSO2JN-YSO2(1))/YSO2JN).LE.1E-4) GOTO 25
F     YSO2(1) = YSO2JN
F     GOTO 20
F
F  25 ETASO21 = YSO2(1)*CONC*UGAS(1)/(RSO2(1)*BEDL(1))
F     WRITE (7,*) 'ETASO21', ETASO21
F     ETASO2(1) = 1-ABS(ETASO21)
F
F     WRITE (7,*) 'UGAS(1)', UGAS(1)
F     WRITE (7,*) 'BEDL(1)', BEDL(1)
F     WRITE (7,*) 'YSO2(1)', YSO2(1)
F     WRITE (7,*) 'ETASO21', ETASO21
F     WRITE (7,*) 'ETASO2(1)', ETASO2(1)
F
F      ETAL  = ABS(ETASO2(1))
      EXECUTE BEFORE BLOCK P11-15

CALCULATOR C-35
F     COMMON /USER5/ AREA, VFAIR1, VAIR1, VVOID,
F    .               BEDW
F     COMMON /USER14/ VOIDM,  BEDVM,  BEDL
F     COMMON /USER23/ UGAS, RSO2, YSO2, TAVE, XCAO
F     COMMON /USER24/ CONC, DMEAN, A1, ALPHA, VCAO
F
F     REAL*8 VOIDM(3), BEDVM(3), BEDL(4),  UGAS(4),
F    .       RSO2(5),  YSO2(5),  FRACL(5), TAVE(4),
F    .       XCAO(5),  SIZE(5),  WDR(5),   ETASO2(5)
F
F
F     DATA FRACL/0.02,0.07,0.45,0.405,0.055/
F     DATA SIZE/2.5E-5,7.5E-5,1.5E-4,3.5E-4,7.5E-4/
F     DATA R/82.05/,SIGMP/0.001/,RKV/8E-4/
F     DATA EPSI/0.52/
      DEFINE ETAU1 BLOCK-VAR BLOCK=P11-25 VARIABLE=CONV  &
         SENTENCE=CONV ID1=1
       DEFINE DLIME STREAM-VAR STREAM=LIME SUBSTREAM=CISOLID
&
         VARIABLE=MASS-DENSITY
       DEFINE FLIME STREAM-VAR STREAM=S13-7 SUBSTREAM=CISOLID
&
```

```
  2889           VARIABLE=MASS-FLOW
  2890    F     OPEN (7,FILE='SO21.txt')
  2891    F
  2892    F     FX = 1- XCAO(1)
  2893    F     RSO2(2) = BEDL(1)*(RSO2(1)-RSO21)/BEDL(2)
  2894    F     WRITE (7,*) 'RSO2(2)', RSO2(2)
  2895    F
  2896    C     MEAN RESIDENCE TIME
  2897    F     TAVE(2) = DLIME*SIGMP*AREA*BEDL(2)/(FLIME*FX)
  2898    F     WRITE (7,*) 'TAVE=',TAVE(2)
  2899    F
  2900                F        20    XCAO1    =    TAVE(2)-1./A1*DLOG(
1.+6.*ALPHA*CONC*YSO2(1)/(DMEAN*RKV)
  2901    F    .         *(DEXP(A1*TAVE(2)) -1.) )
  2902    F
  2903    F     XCAO2 = DMEAN/(6*ALPHA*CONC*YSO2(1)) - 1./RKV
  2904    F
  2905    c      VCAO = 1./DMLIME
  2906    F      VCAO = 1.69E-2
  2907    F     XCAO(2) = VCAO/(1-EPSI) * XCAO1/XCAO2
  2908    F     WRITE (7,*) 'XCAO=',XCAO(1)
  2909    F
  2910    F     RSO21 = (VCAO*FLIME/(1-EPSI*AREA*BEDL(2)*100.))
  2911    F    .         *XCAO1/XCAO2
  2912    F     WRITE (7,*) 'RSO21=',RSO21
  2913    F
  2914    F     YSO2JN = ABS(BEDL(2)*(RSO2(2)-RSO21)/(CONC*UGAS(2)))
  2915    F     WRITE (7,*) 'YSO2JN=',YSO2JN
  2916    F
  2917    F     IF(ABS((YSO2JN-YSO2(2))/YSO2JN).LE.1E-4) GOTO 25
  2918    F     YSO2(2) = YSO2JN
  2919    F     GOTO 20
  2920    F
  2921    F  25 ETASO21 = YSO2(2)*CONC*UGAS(2)/(RSO2(2)*BEDL(2))
  2922    F     ETASO2(2) = 1-ABS(ETASO21)
  2923    F
  2924    F     WRITE (7,*) 'UGAS(2)', UGAS(2)
  2925    F     WRITE (7,*) 'BEDL(2)', BEDL(2)
  2926    F     WRITE (7,*) 'YSO2(2)', YSO2(2)
  2927    F     WRITE (7,*) 'ETASO21', ETASO21
  2928    F     WRITE (7,*) 'ETASO2(2)', ETASO2(2)
  2929    F
  2930    F     ETAU1 = ABS(ETASO2(2))
  2931         EXECUTE BEFORE BLOCK P11-25
  2932
  2933    CALCULATOR C-36
  2934    F     COMMON /USER5/ AREA, VFAIR1, VAIR1, VVOID,
  2935    F    .               BEDW
  2936    F     COMMON /USER14/ VOIDM,  BEDVM,  BEDL
  2937    F     COMMON /USER23/ UGAS, RSO2, YSO2, TAVE, XCAO
  2938    F     COMMON /USER24/ CONC, DMEAN, A1, ALPHA, VCAO
  2939    F
  2940    F     REAL*8 VOIDM(3), BEDVM(3), BEDL(4),  UGAS(4),
  2941    F    .       RSO2(5),  YSO2(5),  FRACL(5), TAVE(4),
  2942    F    .       XCAO(5),  SIZE(5),  WDR(5),   ETASO2(5)
```

```
  2943    F
  2944    F
  2945    F     DATA FRACL/0.02,0.07,0.45,0.405,0.055/
  2946    F     DATA SIZE/2.5E-5,7.5E-5,1.5E-4,3.5E-4,7.5E-4/
  2947    F     DATA R/82.05/,SIGMP/0.001/,RKV/8E-4/
  2948    F     DATA EPSI/0.52/
  2949        DEFINE ETAU2 BLOCK-VAR BLOCK=P11-34 VARIABLE=CONV  &
  2950           SENTENCE=CONV ID1=1
  2951         DEFINE DLIME STREAM-VAR STREAM=LIME SUBSTREAM=CISOLID
&
  2952           VARIABLE=MASS-DENSITY
  2953        DEFINE FLIME STREAM-VAR STREAM=S17-7 SUBSTREAM=CISOLID
&
  2954           VARIABLE=MASS-FLOW
  2955    F     OPEN (7,FILE='SO22.txt')
  2956    F
  2957    F     FX = 1- XCAO(2)
  2958    F     RSO2(3) = BEDL(2)*(RSO2(2)-RSO21)/BEDL(3)
  2959    F     WRITE (7,*) 'RSO2(3)', RSO2(3)
  2960    F
  2961    C     MEAN RESIDENCE TIME
  2962    F     TAVE(3) = DLIME*SIGMP*AREA*BEDL(3)/(FLIME*FX)
  2963    F     WRITE (7,*) 'TAVE=',TAVE(3)
  2964    F
  2965              F       20    XCAO1    =    TAVE(3)-1./A1*DLOG(
1.+6.*ALPHA*CONC*YSO2(2)/(DMEAN*RKV)
  2966    F    .        *(DEXP(A1*TAVE(3)) -1.) )
  2967    F
  2968    F     XCAO2 = DMEAN/(6*ALPHA*CONC*YSO2(2)) - 1./RKV
  2969    F
  2970    c      VCAO = 1./DMLIME
  2971    F     VCAO = 1.69E-2
  2972    F     XCAO(3) = VCAO/(1-EPSI) * XCAO1/XCAO2
  2973    F     WRITE (7,*) 'XCAO=',XCAO(3)
  2974    F
  2975    F     RSO21 = (VCAO*FLIME/(1-EPSI*AREA*BEDL(3)*100.))
  2976    F    .        *XCAO1/XCAO2
  2977    F     WRITE (7,*) 'RSO21=',RSO21
  2978    F
  2979    F     YSO2JN = ABS(BEDL(3)*(RSO2(3)-RSO21)/(CONC*UGAS(3)))
  2980    F     WRITE (7,*) 'YSO2JN=',YSO2JN
  2981    F
  2982    F     IF(ABS((YSO2JN-YSO2(3))/YSO2JN).LE.1E-4) GOTO 25
  2983    F     YSO2(3) = YSO2JN
  2984    F     GOTO 20
  2985    F
  2986    F  25 ETASO21 = YSO2(3)*CONC*UGAS(3)/(RSO2(3)*BEDL(3))
  2987    F     ETASO2(3) = 1-ABS(ETASO21)
  2988    F
  2989    F     WRITE (7,*) 'UGAS(3)', UGAS(3)
  2990    F     WRITE (7,*) 'BEDL(3)', BEDL(3)
  2991    F     WRITE (7,*) 'YSO2(3)', YSO2(3)
  2992    F     WRITE (7,*) 'ETASO21', ETASO21
  2993    F     WRITE (7,*) 'ETASO2(3)', ETASO2(3)
  2994    F
```

```
  2995    F     ETAU2 = ABS(ETASO2(3))
  2996        EXECUTE BEFORE BLOCK P11-34
  2997
  2998    CALCULATOR C-37
  2999    F     COMMON /USER5/ AREA, VFAIR1, VAIR1, VVOID,
  3000    F    .               BEDW
  3001    F     COMMON /USER14/ VOIDM,  BEDVM,  BEDL
  3002    F     COMMON /USER23/ UGAS, RSO2, YSO2, TAVE, XCAO
  3003    F     COMMON /USER24/ CONC, DMEAN, A1, ALPHA, VCAO
  3004    F
  3005    F     REAL*8 VOIDM(3), BEDVM(3), BEDL(4),  UGAS(4),
  3006    F    .       RSO2(5),  YSO2(5),  FRACL(5), TAVE(4),
  3007    F    .       XCAO(5),  SIZE(5),  WDR(5),   ETASO2(5)
  3008    F
  3009    F
  3010    F     DATA FRACL/0.02,0.07,0.45,0.405,0.055/
  3011    F     DATA SIZE/2.5E-5,7.5E-5,1.5E-4,3.5E-4,7.5E-4/
  3012    F     DATA R/82.05/,SIGMP/0.001/,RKV/8E-4/
  3013    F     DATA EPSI/0.52/
  3014        DEFINE ETAU3 BLOCK-VAR BLOCK=P11-43 VARIABLE=CONV  &
  3015           SENTENCE=CONV ID1=1
  3016         DEFINE DLIME STREAM-VAR STREAM=LIME SUBSTREAM=CISOLID
&
  3017           VARIABLE=MASS-DENSITY
  3018         DEFINE FLIME STREAM-VAR STREAM=S21-7 SUBSTREAM=CISOLID
&
  3019           VARIABLE=MASS-FLOW
  3020        DEFINE MFSO2 MOLE-FLOW STREAM=S21-7 SUBSTREAM=MIXED  &
  3021           COMPONENT=SO2
  3022    F     OPEN (7,FILE='SO23.txt')
  3023    F
  3024    F     FX = 1- XCAO(3)
  3025    F     RSO2(4) = BEDL(3)*(RSO2(3)-RSO21)/BEDL(4)
  3026    F     WRITE (7,*) 'RSO2(4)', RSO2(4)
  3027    F
  3028    C     MEAN RESIDENCE TIME
  3029    F     TAVE(4) = DLIME*SIGMP*AREA*BEDL(4)/(FLIME*FX)
  3030    F     WRITE (7,*) 'TAVE=',TAVE(4)
  3031    F
  3032          F      20    XCAO1    =    TAVE(4)-1./A1*DLOG(
1.+6.*ALPHA*CONC*YSO2(3)/(DMEAN*RKV)
  3033    F    .        *(DEXP(A1*TAVE(4)) -1.) )
  3034    F
  3035    F     XCAO2 = DMEAN/(6*ALPHA*CONC*YSO2(3)) - 1./RKV
  3036    F
  3037    c      VCAO = 1./DMLIME
  3038    F     VCAO = 1.69E-2
  3039    F     XCAO(4) = VCAO/(1-EPSI) * XCAO1/XCAO2
  3040    F     WRITE (7,*) 'XCAO=',XCAO(4)
  3041    F
  3042    F     RSO21 = (VCAO*FLIME/(1-EPSI*AREA*BEDL(4)*100.))
  3043    F    .        *XCAO1/XCAO2
  3044    F     WRITE (7,*) 'RSO21=',RSO21
  3045    F
  3046    F     YSO2JN = ABS(BEDL(4)*(RSO2(4)-RSO21)/(CONC*UGAS(4)))
```

```
3047    F     WRITE (7,*) 'YSO2JN=',YSO2JN
3048    F
3049    F     IF(ABS((YSO2JN-YSO2(4))/YSO2JN).LE.1E-4) GOTO 25
3050    F     YSO2(4) = YSO2JN
3051    F     GOTO 20
3052    F
3053    F  25 ETASO21 = YSO2(4)*CONC*UGAS(4)/(RSO2(4)*BEDL(4))
3054    F     ETASO2(4) = 1-ABS(ETASO21)
3055    F     WRITE (7,*) 'UGAS(4)', UGAS(4)
3056    F     WRITE (7,*) 'BEDL(4)', BEDL(4)
3057    F     WRITE (7,*) 'YSO2(4)', YSO2(4)
3058    F     WRITE (7,*) 'ETASO21', ETASO21
3059    F     WRITE (7,*) 'ETASO2(4)', ETASO2(4)
3060    F
3061    F     ETAU3 = ABS(ETASO2(4))
3062        EXECUTE BEFORE BLOCK P11-15
3063
3064    CONV-OPTIONS
3065        PARAM TEAR-METHOD=WEGSTEIN
3066        WEGSTEIN MAXIT=9999
3067        BROYDEN MAXIT=9999
3068
3069    STREAM-REPOR MOLEFLOW PROPERTIES=PS-1
3070
3071    REACTIONS R-1 USER
3072        PARAM SUBROUTINE=USRKI1 ORIGIN=SYSTEM
3073        REAC-DATA 1 PHASE=V
3074        REAC-DATA 2 PHASE=V
3075        REAC-DATA 3 PHASE=V
3076        REAC-DATA 4 PHASE=V
3077        REAC-DATA 5 PHASE=V
3078        REAC-DATA 6 PHASE=V
3079        STOIC 1 CIPSD1 C -2. / MIXED O2 -1. / CO 2.
3080        STOIC 2 CIPSD2 C -2. / MIXED O2 -1. / CO 2.
3081        STOIC 3 CIPSD3 C -2. / MIXED O2 -1. / CO 2.
3082        STOIC 4 CIPSD4 C -2. / MIXED O2 -1. / CO 2.
3083        STOIC 5 CIPSD5 C -2. / MIXED O2 -1. / CO 2.
3084        STOIC 6 MIXED CO -2. / O2 -1. / CO2 2.
3085
3086    REACTIONS R-2 USER
3087        PARAM SUBROUTINE=USRKI2
3088        REAC-DATA 1 PHASE=V
3089        REAC-DATA 2 PHASE=V
3090        REAC-DATA 3 PHASE=V
3091        REAC-DATA 4 PHASE=V
3092        REAC-DATA 5 PHASE=V
3093        REAC-DATA 6 PHASE=V
3094        STOIC 1 CIPSD1 C -2. / MIXED O2 -1. / CO 2.
3095        STOIC 2 CIPSD2 C -2. / MIXED O2 -1. / CO 2.
3096        STOIC 3 CIPSD3 C -2. / MIXED O2 -1. / CO 2.
3097        STOIC 4 CIPSD4 C -2. / MIXED O2 -1. / CO 2.
3098        STOIC 5 CIPSD5 C -2. / MIXED O2 -1. / CO 2.
3099        STOIC 6 MIXED CO -2. / O2 -1. / CO2 2.
3100
3101    REACTIONS R-3 USER
```

```
3102        PARAM SUBROUTINE=USRKI3
3103        REAC-DATA 1 PHASE=V
3104        REAC-DATA 2 PHASE=V
3105        REAC-DATA 3 PHASE=V
3106        REAC-DATA 4 PHASE=V
3107        REAC-DATA 5 PHASE=V
3108        REAC-DATA 6 PHASE=V
3109        STOIC 1 CIPSD1 C -2. / MIXED O2 -1. / CO 2.
3110        STOIC 2 CIPSD2 C -2. / MIXED O2 -1. / CO 2.
3111        STOIC 3 CIPSD3 C -2. / MIXED O2 -1. / CO 2.
3112        STOIC 4 CIPSD4 C -2. / MIXED O2 -1. / CO 2.
3113        STOIC 5 CIPSD5 C -2. / MIXED O2 -1. / CO 2.
3114        STOIC 6 MIXED CO -2. / O2 -1. / CO2 2.
3115
3116    REACTIONS R-4 USER
3117        PARAM SUBROUTINE=USRKI4
3118        REAC-DATA 1 PHASE=V
3119        REAC-DATA 2 PHASE=V
3120        REAC-DATA 3 PHASE=V
3121        REAC-DATA 4 PHASE=V
3122        REAC-DATA 5 PHASE=V
3123        REAC-DATA 6 PHASE=V
3124        STOIC 1 CIPSD1 C -2. / MIXED O2 -1. / CO 2.
3125        STOIC 2 CIPSD2 C -2. / MIXED O2 -1. / CO 2.
3126        STOIC 3 CIPSD3 C -2. / MIXED O2 -1. / CO 2.
3127        STOIC 4 CIPSD4 C -2. / MIXED O2 -1. / CO 2.
3128        STOIC 5 CIPSD5 C -2. / MIXED O2 -1. / CO 2.
3129        STOIC 6 MIXED CO -2. / O2 -1. / CO2 2.
3130
3131    REACTIONS R-5 USER
3132        PARAM SUBROUTINE=USRKI5
3133        REAC-DATA 1 PHASE=V
3134        STOIC 1 MIXED N2 -1. / O2 -1. / NO 2.
3135
3136    REACTIONS R-6 USER
3137        PARAM SUBROUTINE=USRKI6
3138        REAC-DATA 1 PHASE=V
3139        STOIC 1 MIXED N2 -1. / NO -2. / N2O 2.
3140
3141    REACTIONS R-7 USER
3142        PARAM SUBROUTINE=USRKI7
3143        REAC-DATA 1 PHASE=V
3144        REAC-DATA 2 PHASE=V
3145        REAC-DATA 3 PHASE=V
3146        REAC-DATA 4 PHASE=V
3147        REAC-DATA 5 PHASE=V
3148        STOIC 1 MIXED NO -2. / CIPSD1 C -2. / MIXED N2 1. /  &
3149            CO 2.
3150        STOIC 2 MIXED NO -2. / CIPSD2 C -2. / MIXED N2 1. /  &
3151            CO 2.
3152        STOIC 3 MIXED NO -2. / CIPSD3 C -2. / MIXED N2 1. /  &
3153            CO 2.
3154        STOIC 4 MIXED NO -2. / CIPSD4 C -2. / MIXED N2 1. /  &
3155            CO 2.
3156        STOIC 5 MIXED NO -2. / CIPSD5 C -2. / MIXED N2 1. /  &
```

```
3157            CO 2.
3158
3159    REACTIONS R-8 USER
3160        PARAM SUBROUTINE=USRKI8
3161        REAC-DATA 1 PHASE=V
3162        STOIC 1 MIXED NO -2. / CO -2. / N2 1. / CO2 2.
3163
3164    REACTIONS R-9 USER
3165        PARAM SUBROUTINE=USRKI9
3166        REAC-DATA 1 PHASE=V
3167        REAC-DATA 2 PHASE=V
3168        REAC-DATA 3 PHASE=V
3169        REAC-DATA 4 PHASE=V
3170        REAC-DATA 5 PHASE=V
3171        STOIC 1 MIXED N2O -1. / CIPSD1 C -1. / MIXED N2 1. /  &
3172            CO 1.
3173        STOIC 2 MIXED N2O -1. / CIPSD2 C -1. / MIXED N2 1. /  &
3174            CO 1.
3175        STOIC 3 MIXED N2O -1. / CIPSD3 C -1. / MIXED N2 1. /  &
3176            CO 1.
3177        STOIC 4 MIXED N2O -1. / CIPSD4 C -1. / MIXED N2 1. /  &
3178            CO 1.
3179        STOIC 5 MIXED N2O -1. / CIPSD5 C -1. / MIXED N2 1. /  &
3180            CO 1.
3181
3182    REACTIONS R-10 USER
3183        PARAM SUBROUTINE=USRK10
3184        REAC-DATA 1 PHASE=V
3185        STOIC 1 MIXED N2O -1. / CO -1. / N2 1. / CO2 1.
3186
3187    REACTIONS R-11 USER
3188        PARAM SUBROUTINE=USRK11
3189        REAC-DATA 1 PHASE=V
3190        STOIC 1 MIXED N2O -2. / O2 1. / N2 2.
3191
3192    REACTIONS R-12 USER
3193        PARAM SUBROUTINE=USRK12
3194        REAC-DATA 1 PHASE=V
3195        STOIC 1 MIXED N2 -1. / O2 -1. / NO 2.
3196
3197    REACTIONS R-13 USER
3198        PARAM SUBROUTINE=USRK13
3199        REAC-DATA 1 PHASE=V
3200        STOIC 1 MIXED N2 -1. / NO -2. / N2O 2.
3201
3202    REACTIONS R-14 USER
3203        PARAM SUBROUTINE=USRK14
3204        REAC-DATA 1 PHASE=V
3205        REAC-DATA 2 PHASE=V
3206        REAC-DATA 3 PHASE=V
3207        REAC-DATA 4 PHASE=V
3208        REAC-DATA 5 PHASE=V
3209        STOIC 1 MIXED NO -2. / CIPSD1 C -2. / MIXED N2 1. /  &
3210            CO 2.
3211        STOIC 2 MIXED NO -2. / CIPSD2 C -2. / MIXED N2 1. /  &
```

```
3212            CO 2.
3213        STOIC 3 MIXED NO -2. / CIPSD3 C -2. / MIXED N2 1. /  &
3214            CO 2.
3215        STOIC 4 MIXED NO -2. / CIPSD4 C -2. / MIXED N2 1. /  &
3216            CO 2.
3217        STOIC 5 MIXED NO -2. / CIPSD5 C -2. / MIXED N2 1. /  &
3218            CO 2.
3219
3220    REACTIONS R-15 USER
3221        PARAM SUBROUTINE=USRK15
3222        REAC-DATA 1 PHASE=V
3223        STOIC 1 MIXED NO -2. / CO -2. / N2 1. / CO2 2.
3224
3225    REACTIONS R-16 USER
3226        PARAM SUBROUTINE=USRK16
3227        REAC-DATA 1 PHASE=V
3228        REAC-DATA 2 PHASE=V
3229        REAC-DATA 3 PHASE=V
3230        REAC-DATA 4 PHASE=V
3231        REAC-DATA 5 PHASE=V
3232        STOIC 1 MIXED N2O -1. / CIPSD1 C -1. / MIXED N2 1. /  &
3233            CO 1.
3234        STOIC 2 MIXED N2O -1. / CIPSD2 C -1. / MIXED N2 1. /  &
3235            CO 1.
3236        STOIC 3 MIXED N2O -1. / CIPSD3 C -1. / MIXED N2 1. /  &
3237            CO 1.
3238        STOIC 4 MIXED N2O -1. / CIPSD4 C -1. / MIXED N2 1. /  &
3239            CO 1.
3240        STOIC 5 MIXED N2O -1. / CIPSD5 C -1. / MIXED N2 1. /  &
3241            CO 1.
3242
3243    REACTIONS R-17 USER
3244        PARAM SUBROUTINE=USRK17
3245        REAC-DATA 1 PHASE=V
3246        STOIC 1 MIXED N2O -1. / CO -1. / N2 1. / CO2 1.
3247
3248    REACTIONS R-18 USER
3249        PARAM SUBROUTINE=USRK18
3250        REAC-DATA 1 PHASE=V
3251        STOIC 1 MIXED N2O -2. / N2 2. / O2 1.
3252
3253    REACTIONS R-19 USER
3254        PARAM SUBROUTINE=USRK19
3255        REAC-DATA 1 PHASE=V
3256        STOIC 1 MIXED N2 -1. / O2 -1. / NO 2.
3257
3258    REACTIONS R-20 USER
3259        PARAM SUBROUTINE=USRK20
3260        REAC-DATA 1 PHASE=V
3261        STOIC 1 MIXED N2 -1. / NO -2. / N2O 2.
3262
3263    REACTIONS R-21 USER
3264        PARAM SUBROUTINE=USRK21
3265        REAC-DATA 1 PHASE=V
3266        REAC-DATA 2 PHASE=V
```

```
3267        REAC-DATA 3 PHASE=V
3268        REAC-DATA 4 PHASE=V
3269        REAC-DATA 5 PHASE=V
3270        STOIC 1 MIXED NO -2. / CIPSD1 C -2. / MIXED N2 1. /  &
3271            CO 2.
3272        STOIC 2 MIXED NO -2. / CIPSD2 C -2. / MIXED N2 1. /  &
3273            CO 2.
3274        STOIC 3 MIXED NO -2. / CIPSD3 C -2. / MIXED N2 1. /  &
3275            CO 2.
3276        STOIC 4 MIXED NO -2. / CIPSD4 C -2. / MIXED N2 1. /  &
3277            CO 2.
3278        STOIC 5 MIXED NO -2. / CIPSD5 C -2. / MIXED N2 1. /  &
3279            CO 2.
3280
3281    REACTIONS R-22 USER
3282        PARAM SUBROUTINE=USRK22
3283        REAC-DATA 1 PHASE=V
3284        STOIC 1 MIXED NO -2. / CO -2. / N2 1. / CO2 2.
3285
3286    REACTIONS R-23 USER
3287        PARAM SUBROUTINE=USRK23
3288        REAC-DATA 1 PHASE=V
3289        REAC-DATA 2 PHASE=V
3290        REAC-DATA 3 PHASE=V
3291        REAC-DATA 4 PHASE=V
3292        REAC-DATA 5 PHASE=V
3293        STOIC 1 MIXED N2O -1. / CIPSD1 C -1. / MIXED N2 1. /  &
3294            CO 1.
3295        STOIC 2 MIXED N2O -1. / CIPSD2 C -1. / MIXED N2 1. /  &
3296            CO 1.
3297        STOIC 3 MIXED N2O -1. / CIPSD3 C -1. / MIXED N2 1. /  &
3298            CO 1.
3299        STOIC 4 MIXED N2O -1. / CIPSD4 C -1. / MIXED N2 1. /  &
3300            CO 1.
3301        STOIC 5 MIXED N2O -1. / CIPSD5 C -1. / MIXED N2 1. /  &
3302            CO 1.
3303
3304    REACTIONS R-24 USER
3305        PARAM SUBROUTINE=USRK24
3306        REAC-DATA 1 PHASE=V
3307        STOIC 1 MIXED N2O -1. / CO -1. / N2 1. / CO2 1.
3308
3309    REACTIONS R-25 USER
3310        PARAM SUBROUTINE=USRK25
3311        REAC-DATA 1 PHASE=V
3312        STOIC 1 MIXED N2O -2. / N2 2. / O2 1.
3313
3314    REACTIONS R-26 USER
3315        PARAM SUBROUTINE=USRK26
3316        REAC-DATA 1 PHASE=V
3317        STOIC 1 MIXED N2 -1. / O2 -1. / NO 2.
3318
3319    REACTIONS R-27 USER
3320        PARAM SUBROUTINE=USRK27
3321        REAC-DATA 1 PHASE=V
```

```
3322        STOIC 1 MIXED N2 -1. / NO -2. / N2O 2.
3323
3324    REACTIONS R-28 USER
3325        PARAM SUBROUTINE=USRK28
3326        REAC-DATA 1 PHASE=V
3327        REAC-DATA 2 PHASE=V
3328        REAC-DATA 3 PHASE=V
3329        REAC-DATA 4 PHASE=V
3330        REAC-DATA 5 PHASE=V
3331        STOIC 1 MIXED NO -2. / CIPSD1 C -2. / MIXED N2 1. /  &
3332            CO 2.
3333        STOIC 2 MIXED NO -2. / CIPSD2 C -2. / MIXED N2 1. /  &
3334            CO 2.
3335        STOIC 3 MIXED NO -2. / CIPSD3 C -2. / MIXED N2 1. /  &
3336            CO 2.
3337        STOIC 4 MIXED NO -2. / CIPSD4 C -2. / MIXED N2 1. /  &
3338            CO 2.
3339        STOIC 5 MIXED NO -2. / CIPSD5 C -2. / MIXED N2 1. /  &
3340            CO 2.
3341
3342    REACTIONS R-29 USER
3343        PARAM SUBROUTINE=USRK29
3344        REAC-DATA 1 PHASE=V
3345        STOIC 1 MIXED NO -2. / CO -2. / N2 1. / CO2 2.
3346
3347    REACTIONS R-30 USER
3348        PARAM SUBROUTINE=USRK30
3349        REAC-DATA 1 PHASE=V
3350        REAC-DATA 2 PHASE=V
3351        REAC-DATA 3 PHASE=V
3352        REAC-DATA 4 PHASE=V
3353        REAC-DATA 5 PHASE=V
3354        STOIC 1 MIXED N2O -1. / CIPSD1 C -1. / MIXED N2 1. /  &
3355            CO 1.
3356        STOIC 2 MIXED N2O -1. / CIPSD2 C -1. / MIXED N2 1. /  &
3357            CO 1.
3358        STOIC 3 MIXED N2O -1. / CIPSD3 C -1. / MIXED N2 1. /  &
3359            CO 1.
3360        STOIC 4 MIXED N2O -1. / CIPSD4 C -1. / MIXED N2 1. /  &
3361            CO 1.
3362        STOIC 5 MIXED N2O -1. / CIPSD5 C -1. / MIXED N2 1. /  &
3363            CO 1.
3364
3365    REACTIONS R-31 USER
3366        PARAM SUBROUTINE=USRK31
3367        REAC-DATA 1 PHASE=V
3368        STOIC 1 MIXED N2O -1. / CO -1. / N2 1. / CO2 1.
3369
3370    REACTIONS R-32 USER
3371        PARAM SUBROUTINE=USRK32
3372        REAC-DATA 1 PHASE=V
3373        STOIC 1 MIXED N2O -2. / N2 2. / O2 1.
```

Appendix E

PSD subroutine by addind Weibull distribution

```
*======================================================================*
C     User Subroutine for devolatilization
*======================================================================*

      Subroutine USRKI1  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*----------------------------------------------------------------------*

      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)



C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

      INTEGER IMISS, DMS_KCCIDC, DMS_KFORMC
      REAL*8  RMISS

      DIMENSION RLOW(62),   UPPER(61),  WSIZE(61), YW(61), SIZEPSD(61),
     .          RVN(61,61), DVN(61,61), SUM1(61),  ID(61), SUM2(61)



      OPEN (7,FILE='Devol.txt')
*======================================================================*
C     ORDER OF SUBSTREAM: MIXED, CIPSD, AND NCPSD
*======================================================================*

*======================================================================*
C                         LOWER AND UPPER BOUNDARY                     C
*======================================================================*
```

```
      DO 5 I = 1,62
5     RLOW(I) = 0.0

      DO 10 I = 1,61
10    UPPER(I) = 0.0

      RLOW(1)  = 0.0
          DO 15 I = 1,61

          UPPER(I) = ( 2.*REAL(I+1) - RLOW(I) )
              IF(UPPER(I).LT.0.) THEN
                  UPPER(I) = RLOW(I) + 1.
              END IF
15        RLOW(I+1)  = UPPER(I)
C15       WRITE (7,*) 'BOUNDARY FOR PSD',I, RLOW(I),UPPER(I)

C     APPLIED WEIBULL DISTRIBUTION
C     THIS CURVE WAS FIXED FROM THE EXPERIMENTS
      DO 20 I = 1,61
20    WSIZE(I) = 0.0

      DELTA  = 1.25E-4
      WSIZE(1) = 1.25E-4

      DO 25 I = 2,27
25    WSIZE(I) = WSIZE(I-1) + DELTA

C     DO 26 I = 1,27
C26   WRITE (7,*) 'INPUT SIZE FROM EXPERIMENTS', WSIZE(I)

C     WEIBULL DISTRIBUTION Y= 1-(EXP((-(X/B))^C)
C     B AND C ARE ADJUSTABLE PARAMETERS
      B = 2.13E-3
      C = 7.5

      DO 30 I = 1,27
30    YW(I) = 1-EXP(-((WSIZE(I)/B)**C))

C     DO 31 I = 1,27
C31   WRITE (7,*) 'CUMULATIVE FRACTION', WSIZE(I), YW(I)

C     CHANGE CUMALATIVE FRACTION TO SIZE DISTRIBUTION
      SIZEPSD(1) = YW(1)

      DO 35 I = 2,27
35    SIZEPSD(I) = YW(I)-YW(I-1)

      DO 36 I = 1,27
36    WRITE (7,*) 'PARTICLE SIZE DISTRIBUTION', WSIZE(I), SIZEPSD(I)

      DO 40 J = 1,61
      DO 40 I = 1,61
      RVN(I,J) = 0.0
40    DVN(I,J) = 0.0

      DO 45 J = 1,61
      DO 45 I = 1,61
          IF (WSIZE(J).GE.RLOW(I).AND.WSIZE(J).LT.UPPER(I)) THEN
              RVN(I,J) = WSIZE(J)
              DVN(I,J) = SIZEPSD(J)

                  IF (RVN(I,J).EQ.0.0) THEN
                      DVN(I,J) = 0.0
                  END IF
45        END IF

      DO 50 I = 1,61
50    SUM1(I) = 0.0

      DO 55 J = 1,61
```

```
      DO 55 I = 1,61
55    SUM1(J) = SUM1(J) + DVN(J,I)

      DO 51 I = 1,61
51    WRITE (7,*) 'INPUT', I, SUM1(I)

      DO 60 I = 1,500
60    RATES(I) = 0.0

C     SEND PARTICLE SIZE DISTRIBUTION TO ASPEN PLUS
      DO 65 I = 1,61
65    ID(I) = IDXSUB(2) - 1 + NCOMP_NCC + (I+9)

      DO 70 I = 1,61
70    SOUT(ID(I)) = SUM1(I)

      RETURN
      END
```

Appendix F

Shrinking particle model subroutine with wide PSD for RCSTR

```
*==========================================================================*
C     User Subroutine by apply Shrinking Particle Model
*==========================================================================*

      Subroutine USRKI2  (SOUT,   NSUBS,  IDXSUB, ITYPE,  NINT,
     .                    INT,    NREAL,  REAL,   IDS,    NPO,
     .                    NBOPST, NIWORK, IWORK,  NWORK,  WORK,
     .                    NC,     NR,     STOIC,  RATES,  FLUXM,
     .                    FLUXS,  XCURR,  NTCAT,  RATCAT, NTSSAT,
     .                    RATSSA, KCALL,  KFAIL,  KFLASH, NCOMP,
     .                    IDX,    Y,      X,      X1,     X2,
     .                    NRALL,  RATALL, NUSERV, USERV,  NINTR,
     .                    INTR,   NREALR, REALR,  NIWR,   IWR,
     .                    NWR,    WR,     NRL,    RATEL,  NRV,
     .                    RATEV,  VOID)
*--------------------------------------------------------------------------*

      IMPLICIT REAL*8 (A-H,O-Z)

      DIMENSION SOUT(500),          IDXSUB(NSUBS), ITYPE(NSUBS),
     .          INT(NINT),          REAL(NREAL),   IDS(2,1),
     .          NBOPST(6,NPO),      IWORK(NIWORK), WORK(NWORK),
     .          STOIC(NC,NSUBS,NR), RATES(500),    Y(NCOMP),
     .          IDX(NCOMP),         RATSSA(NTSSAT)

C     DECLARE VARIABLE USED IN DIMENSIONING
      INTEGER   NSUBS, NINT, NREAL, NPO, NIWORK, NWORK, NC, NR,
     .          NCOMP

      DATA EPSIC/0.30/, PIE/3.141592654/

#include "ppexec_user.cmn"
      EQUIVALENCE (RMISS, USER_RUMISS)
      EQUIVALENCE (IMISS, USER_IUMISS)

C     STREAM PROPERTIES
#include "dms_ncomp.cmn"

C     REACTOR VOLUME
#include "rxn_rcstrr.cmn"

C     GAS LAW CONSTANT (J/(Kg mole K))
#include "pputl_ppglob.cmn"

C     DECLARE LOCAL VARIABLES
      COMMON /USER1/ RADIUS, WPSD, FCBSD, FCBRS, DCIPN
      COMMON /USER2/ RWPSD, REWPSD, FMOLE
      COMMON /USER3/ RK0, Ea, RD
      COMMON /USER5/ AREA, VFAIR, VAIR, VVOID, BEDVV, DP
      COMMON /USER7/ RLOW, UPPER
      COMMON /USER19/ RF5, FIPSDF6
      COMMON /USER20/ RF2, FIPSDF3


      INTEGER IMISS, DMS_KCCIDC
      REAL*8  RMISS

      DIMENSION VVOID(4),      RLOW(62),     UPPER(61),   RWPSD(61),
     .          FCINV(61),     FCRINV(61),   FTOLINV(61), WPSDNEW(61),
     .          WPSD(61),      RM(61),       TAUD(61),    TAUR(61),
```

```
     .          SUMTAU(61),    R1PSD(61),    R2PSD(61),    RM1(61),
     .          RM2(61),       SRM(61),      RMEAN(61),    RC(61),

     .          RRC(61),       REWPSD(61),   UXB(61),      FUXB(61),
     .          FXB(61),       F(NCOMP_NCC), RC1(61),      XBN(61,61),
     .          RCN(61,61),    RC2(61),      SUM1(61),     XBN2(61,61),
     .          SIGMA(61),     RCN2(61),     XBN3(61),     FIPSD(61),
     .          UXBNR(61),     XBNNR(61),    WBYR1(61),    WBYR2(61),

     .          SWBYR(61),     FIRC(61),     FIPSDN(61),   RF(61,61),
     .          FIPSDF(61,61), SUM2(61),     SIGMA2(61),   RF2(61),
     .          FIPSDF2(61,61),FIPSDF3(61),  ID(61),       RMEANPSD(61),
     .          RF5(61),       FIPSDF6(61),  BEDVV(4)


      OPEN (7,FILE='KINETIC1.txt')

*-----------------------------------------------------------------------*
C     ORDER OF SUBSTREAM MIXED, CIPSD, AND NCPSD
*-----------------------------------------------------------------------*

C     MEAN RESIDENT TIME
      VFSUM = REAL(1)
      RTIME = RCSTRR_VOLRC*(1-VVOID(1)) / VFSUM
      WRITE (7,*) 'RESIDENT TIME (s)',RTIME

C     SUBSTITUTE SAND VOLUME
      RTIME = RTIME*.6
      WRITE (7,*) 'RESIDENT TIME2',RTIME

C     WRITE (7,*) 'VOLUMETRIC FLOW RATE OF TOTAL FLOW (m^3/s)', VFSUM
C     WRITE (7,*) 'VOID AT DENSE BED', VVOID(1)

C     DECLARE LOCAL OF CARBON
      IDXC   = DMS_KCCIDC('C')
C     WRITE (7,*) 'LOCAL ID. OF C    =',IDXC

C     DECLARE LOCAL OF OXYGEN
      IDXO2   = DMS_KCCIDC('O2')
C     WRITE (7,*) 'LOCAL ID. OF O2   =',IDXO2

C     DECLARE LOCAL OF CARBON MONOXIDE
      IDXCO   = DMS_KCCIDC('CO')
C     WRITE (7,*) 'LOCAL ID. OF CO   =',IDXCO

C     DECLARE LOCAL OF CARBON DIOXIDE
      IDXCO2  = DMS_KCCIDC('CO2')
C     WRITE (7,*) 'LOCAL ID. OF CO2  =',IDXCO2

C     DECLARE LOCAL OF WATER
      IDXH2O  = DMS_KCCIDC('H2O')
C     WRITE (7,*) 'LOCAL ID. OF H2O  =',IDXH2O

C     SET MISSING VALUE FOR RADIUS OF PARTICLES TO ZERO
      DO 10 I = 2,62
      IF (REAL(I).GT.1E34) THEN
      REAL(I) = 0.0
10    END IF

      DO 11 I = 64,185
      IF (REAL(I).GT.1E34) THEN
      REAL(I) = 0.0
11    END IF

*=======================================================================*
C                        LOWER AND UPPER BOUNDARY                       C
*=======================================================================*
      DO 16 I = 1,62
16    RLOW(I) = 0.0
```

```
      DO 17 I = 1,61
17    UPPER(I) = 0.0

      RLOW(1)  = 0.0
          DO 20 I = 1,61

          UPPER(I) = ( 2.*REAL(I+1) - RLOW(I) )
              IF(UPPER(I).LT.0.) THEN
                  UPPER(I) = RLOW(I) + 1.
              END IF
20        RLOW(I+1)  = UPPER(I)
C20       WRITE (7,*) 'BOUNDARY FOR PSD',I, RLOW(I),UPPER(I)

*=======================================================================*
C             CONCENTRATION OF OXYGEN IN SUBSTREAM MIXED                C
*=======================================================================*
C     CONCENTRATION (Kgmole/m^3)
      CONO2 = REAL(63)

C         IF (CONO2.EQ.0.0) THEN
C         CONO2 = 1E-15
C         END IF

      WRITE (7,*)'CONCENTRATION (Kgmole/m^3)        = ',CONO2

*=======================================================================*
C                     PROPETIES FOR CALCULATION                         C
*=======================================================================*

C     FREQUENCY FACTOR (m/(K s))
      RK0 = 59600.

C     ACTIVATED ENERGY (J/Kgmole)
      Ea = 1.492E8


C     DIFFUSIVITY (m^2/s)
      RD = 1.525E-4

*=======================================================================*
C                         PROPERTIES IN RCSTR                           C
*=======================================================================*
      TOTF = SOUT(NCOMP_NCC + 1)
      Tp   = SOUT(NCOMP_NCC + 2)
      PPAS = SOUT(NCOMP_NCC + 3)
      DEN  = SOUT(NCOMP_NCC + 8)
      WM   = SOUT(NCOMP_NCC + 9)
C     WRITE (7,*) 'TOTAL MOLE FLOW (Kgmole/s)       = ', TOTF
C     WRITE (7,*) 'TEMPERATURE (K)                  = ', Tp
C     WRITE (7,*) 'PRESSURE (Pa)                    = ', PPAS
C     WRITE (7,*) 'TOTAL MASS DENSITY (Kg/m^3)      = ', DEN
C     WRITE (7,*) 'MOLECULAR WEIGHT (Kg/Kgmole)     = ', WM

C     CONVERTED UNIT TO atm
      PATM = PPAS/1.01325E5
*-----------------------------------------------------------------------*

C     RATE CONSTANT

      RKCR = RK0 * Tp * DEXP( -Ea / (PPGLOB_RGAS*Tp) )
C     WRITE (7,*) 'GAS CONSTANT',PPGLOB_RGAS
      WRITE (7,*) 'RATE CONSTANT FOR LIGNITE',RKCR

*=======================================================================*
C                 NEW FRACTION FOR EACH INTERVAL                        C
*=======================================================================*

C     WEIGHT PARTICLE SIZE DISTRIBUTION FOR RECYCLE STREAM
      DO 49 I = 1,61
      IF(REWPSD(I).GT.1E34) THEN
```

```
      REWPSD(I) = 0.0
      END IF

      FCINV(I)   = 0.0
      FCRINV(I)  = 0.0
      FTOLINV(I) = 0.0
49    WPSDNEW(I) = 0.0

C     FLOW IN EACH INTERVAL BOTH INPUT AND RECYCLE
C     FCINV = INPUT, FCRINV = RECYCLE

      DO 998 I = 1,61
998   REAL(I+63) = RF5(I)

c     IF (FCBRS.EQ.0.0) THEN
c         FCBRS = 1E-15
c     END IF

      DO 999 I = 1,61
999   WRITE (7,*) 'REWPSD', I, REWPSD(I)

      WRITE (7,*) 'RECYCLE FLOW', FCBRS

      DO 50 I = 1,61
      FCINV(I)   = RWPSD(I) * FCBSD
      FCRINV(I)  = REWPSD(I) * FCBRS
50    FTOLINV(I) = FCINV(I) + FCRINV(I)

      DO 55 I = 1,61
      IF (FTOLINV(I).NE.0.) THEN
      R1PSD(I) = FCINV(I)/FTOLINV(I)
      R2PSD(I) = FCRINV(I)/FTOLINV(I)
55    END IF

C     NEW TOTAL FLOW
      FTOTAL = 0.0

      DO 56 I = 1,61
56    FTOTAL = FTOTAL + FTOLINV(I)

C     MEAN RADIUS BETWEEN INPUT AND RECYCLE STREAM
      WRITE (7,*) 'INPUT AND RECYCLE FLOW', FCBSD, FCBRS

      DO 57 I = 2,62
57    WRITE (7,*) 'INPUT RADIUS', I-1, REAL(I), FCINV(I-1)

      DO 58 I = 64,124
58    WRITE (7,*) 'RECYCLE RADIUS', I-63, REAL(I), FCRINV(I-63)

      DO 60 I = 1,61

      IF (REAL(I+1).EQ.0.0) THEN
          RM1(I) = 0.0
              ELSE
                  RM1(I) = R1PSD(I)/REAL(I+1)
60    END IF
C60   WRITE (7,*) 'RM1', I, RM1(I)

      DO 65 I = 1,61
      IF (REAL(I+63).EQ.0.0) THEN
          RM2(I) = 0.0
              ELSE
                  RM2(I) = R2PSD(I)/REAL(I+63)
65    END IF
C65   WRITE (7,*) 'RM2', I, RM2(I)

      DO 70 I = 1,61
      SRM(I) = RM1(I) + RM2(I)
          IF (SRM(I).NE.0.0) THEN
              REAL (I+124) = 1/SRM(I)
```

```
70    END IF
C70   WRITE (7,*) 'SRM', I,SRM(I)

      DO 75 I = 1,61
75    RMEAN(I) = 0.0

      DO 80 I = 1,61
80    RMEAN(I) = REAL(I+124)
C80   WRITE (7,*) 'RMEAN', I, RMEAN(I)

      DO 81 I = 1,61
81    RMEANPSD(I) = FTOLINV(I)/FTOTAL

      DO 82 I = 1,61
82    WRITE (7,*) 'RMEAN', REAL(I+1), RMEAN(I), RMEANPSD(I)

*=====================================================================*
C      TIME REQUIRED FOR COMPLETE CONVERSION (TAU) IN INPUT STREAM      C
*=====================================================================*
      DO 85 I = 1,61
      TAUD(I)   = 0.0
      TAUR(I)   = 0.0
85    SUMTAU(I) = 0.0


      IF (DCIPN.LE.1.0.OR.DCIPN.GE.1E34) THEN
      DCIPN = 187.33
      END IF

      WRITE (7,*) 'DCIPN, RD', DCIPN, RD
      WRITE (7,*) 'CONO2', CONO2
      WRITE (7,*) 'REAL(186)', REAL(186)
      WRITE (7,*) 'VAIR, DEN', VAIR, DEN

      DO 90 I = 1,61
      IF (RMEANPSD(I).NE.0.0) THEN

C     FOR SMALL PARTICLE

          IF (RMEAN(I).LE.1E-5) THEN

C     TAUD IS TIME IN FILM DIFFUSION CONTROLS
C     TAUR IS TIME IN REACTION CONTROLS FOR SMALL PARTICLE

              TAUD(I) = DCIPN * RMEAN(I)**2./ (4.*RD*CONO2)
              TAUR(I) = DCIPN * RMEAN(I) /(2.*RKCR*CONO2)

          ELSE

C     FOR LARGE PARTICLE

C     TAUD IN FILM DIFFUSION CONTROLS
C     TAUR IN REACTION CONTROLS

              TAUD(I) = DCIPN*RMEAN(I)**(3./2.)/( 1.8*CONO2*RD
     .                  * ( REAL(186)/(DEN*RD) )**(1./3.)
     .                  * ( 2.*VAIR*DEN/REAL(186) )**(1./2.)  )
              TAUR(I) = DCIPN * RMEAN(I) /(2.*RKCR*CONO2)

          END IF

      END IF

90            SUMTAU(I) = TAUD(I) + TAUR(I)

      DO 91 I = 1,61
91    WRITE (7,*) 'TAUD, TAUR',I, TAUD(I), TAUR(I)

*---------------------------------------------------------------------*
```

```
*=====================================================================*
C                    RESIDUAL RADIUS AFTER BURNING                    C
*=====================================================================*
      DO 95 I = 1,61
          IF (TAUD(I).LE.TAUR(I)) THEN
C     FOR REACTION CONTROLLING
                RC(I) =  RMEAN(I) - 2.*RTIME*RKCR*CONO2
     .                       / DCIPN
            ELSE

C     FOR DIFFUSION CONTROLLING
                IF (RMEAN(I).LE.5E-5) THEN

C     CALCULATED FOR SMALL PARTICLES
                RRC(I) = RMEAN(I)**3 - 6.*CONO2*RD*RTIME
     .                                  *RMEAN(I) / DCIPN


                    IF (RRC(I).GT.0.) THEN
                        RC(I) = RRC(I)**(1./3.)
                    END IF

                ELSE

                 RRC(I) = RMEAN(I)**3 - ( 1.8*RTIME*CONO2*RD
     .                       *RMEAN(I)**(3./2.)
     .                       *( REAL(186)/(DEN*RD) )**(1./3.)
     .                       *( 2.*VAIR*DEN/REAL(186) )**(1./2.) )
     .                       / DCIPN

                    IF (RRC(I).GT.0.) THEN
                        RC(I) = RRC(I)**(1./3.)
                    END IF

                END IF
            END IF

      IF (RC(I).LT.0.) THEN
      RC(I) = 0.0
95    END IF

      DO 96 I = 1,61
96    WRITE (7,*) 'RESIDUAL RADIUS AFTER BURNING', I, RC(I)

*=====================================================================*
C               CONVERSION FOR CHEMICAL CONTROLLING                   C
*=====================================================================*
C     FRACTION UNCONVERTED IN PARTICLES OF EACH SIZE

      DO 97 I = 1,61
      UXB(I) = 0.0
      FUXB(I) = 0.0
97    FXB(I) = 0.0

      DO 100 I = 1,61

          IF (TAUD(I).LE.TAUR(I)) THEN
                UXB(I) =   (1./4.)   * (SUMTAU(I)/RTIME)
     .                     - (1./20.)  * (SUMTAU(I)/RTIME)**2
     .                     + (1./120.) * (SUMTAU(I)/RTIME)**3

            ELSE
                UXB(I) =   (1./2.)   * (SUMTAU(I)/RTIME)
     .                     - (1./6.)   * (SUMTAU(I)/RTIME)**2
     .                     + (1./24.)  * (SUMTAU(I)/RTIME)**3

          END IF


          IF (UXB(I).GT.1.) THEN
```

```
              UXB(I) = 1.
100         END IF

C     CONVERTED AND UNCONVERTED FOR EACH STREAM

      DO 101 I = 1,61
101   WRITE (7,*) 'FRACTION UNCONVERTED SOLID, (UXB)', UXB(I)

      DO 601 I = 1,61
          FUXB(I) = UXB(I) * RMEANPSD(I)
              IF (FUXB(I).NE.0.0) THEN
                  FXB(I)  = 1.0-FUXB(I)
601           END IF

      DO 102 I = 1,61
102   WRITE (7,*) 'UNCONVERTED FOR EACH INTERVAL, (FUXB)',I, FUXB(I)

      DO 103 I = 1,61
103   WRITE (7,*) 'CONVERSION FOR EACH INTERVAL, (FXB)',I, FXB(I)

      TOTAL = 0.0

      DO 105 I = 1,61
105   TOTAL = TOTAL  + FUXB(I)

      XB = 1 - TOTAL

      WRITE (7,*) 'MEAN CONVERSION', XB
*-----------------------------------------------------------------------*

*=======================================================================*
C                      FIRST RATE OF COMBUSTION
*=======================================================================*
      R1 = FMOLE*XB/2.
C     WRITE (7,*) 'MOLAR FLOW', FMOLE
      WRITE (7,*) 'FIRST RATE OF COMBUSTION FOR MATERIAL', R1
*-----------------------------------------------------------------------*

*=======================================================================*
C                      SECOND RATE OF COMBUSTION
*=======================================================================*
C     CONVERT UNIT OF GAS LAW CONSTANT TO Kcal/(Kgmole K)
      RGASN  = PPGLOB_RGAS*0.239/1E3

C     CONVERT UNIT OF GAS LAW CONSTANT TO (atm cm^3)/(gmole K)
      RGASN1 = PPGLOB_RGAS*1E3/1.01325E5

C     MOLE FRACTION
      DO 110 I = 1,NCOMP_NCC
110   F(I) = SOUT(I)/TOTF

C     MOLAR DENSITY
      DENMOL = DEN/WM

      R2 = 1.18E13 * F(IDXCO) * F(IDXO2)**0.5 * F(IDXH2O)**0.5
     .     * (PATM/(RGASN1*Tp)) * DEXP(-25000./(RGASN*Tp)) * DENMOL
     .     * VVOID(1) * RCSTRR_VOLRC

      WRITE (7,*) 'SECOND RATE OF COMBUSTION', R2
*-----------------------------------------------------------------------*

*=======================================================================*
C                      REACTION RATES IN MIXED
*=======================================================================*
      DO 115 I = 1,NCOMP_NCC
115   RATES(I) = 0.0

C     FOR OXYGEN
      RATES(IDXO2) = - (R1 + R2)
C     WRITE (7,*) 'RATES O2 IN MIXED  = ', RATES(IDXO2)
```

```
C     FOR CARBON MONOXIDE
      RATES(IDXCO) = 2. * (R1 - R2)
C     WRITE (7,*) 'RATES CO IN MIXED  = ', RATES(IDXCO)

C     FOR CARBON DIOXIDE
      RATES(IDXCO2) = 2. * R2
C     WRITE (7,*) 'RATES CO2 IN MIXED = ', RATES(IDXCO2)

*=====================================================================*
C                     REACTION RATES IN CIPSD
*=====================================================================*
      L1 = NCOMP_NCC + 1
      L2 = L1 + NCOMP_NCC - 1


      DO 120 I = L1, L2
120   RATES(I) = 0.0

C     FOR CARBON
      CCPSD = IDXC + L1 - 1
      RATES(CCPSD) = -2.*R1
C     WRITE (7,*) 'RATES C IN CIPSD = ', RATES(CCPSD)

*=====================================================================*
C      ARRANGE NEW RADIUS AND FRACTION MATRIX FOR CONVERT PARTICLES

*=====================================================================*
      DO 125 J = 1,61
      DO 125 I = 1,61
      RCN(I,J) = 0.0
125   XBN(I,J) = 0.0

      DO 130 J = 1,61
      DO 130 I = 1,61
          IF (RC(J).GE.RLOW(I).AND.RC(J).LT.UPPER(I)) THEN
              RCN(I,J) = RC(J)
              XBN(I,J) = FXB(J)

                  IF (RCN(I,J).EQ.0.0) THEN
                      XBN(I,J) = 0.0
                  END IF
130       END IF



C     NORMALIZE WEIGHT FRACTION TO CALCULATE MEAN RADIUS FOR EACH INTERVAL
      DO 135 I = 1,61
      SUM1(I)  = 0.0
135   SIGMA(I) = 0.0

      DO 140 J = 1,61
      DO 140 I = 1,61
      SUM1(J) = SUM1(J) + XBN(J,I)

C     PREPARE MATRIX FOR NORMALIZED WEIGHT FRACTION
140   XBN2(I,J) = 0.0

      DO 145 J = 1,61
      DO 145 I = 1,61

          IF (SUM1(I).NE.0.0) THEN
              XBN2(I,J) = XBN(I,J)/SUM1(I)
145       END IF

*=====================================================================*
C     MEAN RADIUS FOR EACH INTERVAL OF CONVERTED PARTICLES
*=====================================================================*
      DO 150 I = 1,61
      RCN2(I)  = 0.0
```

```
      XBN3(I)  = 0.0
      UXBNR(I) = 0.0
150   XBNNR(I) = 0.0

      DO 155 J = 1,61
      DO 155 I = 1,61
          IF (RCN(J,I).NE.0.0) THEN
                  SIGMA(J) = SIGMA(J) + XBN2(J,I)/RCN(J,I)
155       END IF

      DO 160 I = 1,61
          IF (SIGMA(I).NE.0.0) THEN
              RCN2(I) = 1./SIGMA(I)
160       END IF

      DO 161 I = 1,61
161   WRITE (7,*) 'RADIUS OF CONVERTED PARTICLE', I,RCN2(I)

*=====================================================================*
C         NEW FRACTION FOR NEXT STEP OF CONVERT PARTICLES
*=====================================================================*
      SUM = 0.0
      DO 165 I = 1,61
165   SUM = SUM + SUM1(I)


      DO 170 I = 1,61
          IF (SUM.NE.0.0) THEN
              XBN3(I) = SUM1(I)/SUM
170       END IF

      DO 171 I = 1,61
171   WRITE (7,*) 'FRACTION OF CONVERTED PARTICLE', I,XBN3(I)

*=====================================================================*
C             MEAN RADIUS AND WEIGHT FRACTION FOR NEXT STEP
C               BOTH CONVERTED AND UNCONVERTED PARTICLES
*=====================================================================*
C     XBN3 = CONVERTED FRACTION, FUXB = UNCONVERTED FRACTION

C     NORMALIZE WEIGHT FRACTION FOR FIND MEAN RADIUS

C     SUMMATION OF FRACTION

      DO 175 I = 1,61
      FIPSD(I) = XBN3(I) + FUXB(I)

C     NORMALIZE XBN3 AND FUXB
          IF (FIPSD(I).NE.0.0) THEN
              UXBNR(I) = FUXB(I)/FIPSD(I)
              XBNNR(I) = XBN3(I)/FIPSD(I)
175       END IF

      DO 176 I = 1,61
176   WRITE (7,*) 'SUMMATION OF FRACTION', FIPSD(I)

      DO 177 I = 1,61
177   WRITE (7,*) 'NORMALIZED UXB', UXBNR(I)

      DO 178 I = 1,61
178   WRITE (7,*) 'NORMALIZED XBN', XBNNR(I)


C     FINAL RADIUS FOR NEXT STEP
      DO 180 I = 1,61
          IF (RMEAN(I).NE.0.0) THEN
              WBYR1(I) = UXBNR(I)/RMEAN(I)
          END IF

              IF (RCN2(I).NE.0.0) THEN
```

```
                WBYR2(I) = XBNNR(I)/RCN2(I)
              END IF

                    SWBYR(I) = WBYR1(I) + WBYR2(I)

              IF (SWBYR(I).NE.0.0) THEN
                  FIRC(I) = 1./SWBYR(I)
180           END IF

C     DO 181 I = 1,61
C181  WRITE (7,*) 'FINAL RADIUS FOR NEXT STEP', I, FIRC(I)
*-----------------------------------------------------------------------*
C     NEW FRACTION FOR NEXT STEP
C     NORMALIZE SUMMATION OF FRACTION
C     PREPARE MATRIX OF NEW FRACTION FOR NEXT STEP

      SUMFI = 0.0
      DO 185 I = 1,61
185   SUMFI = SUMFI + FIPSD(I)

      DO 190 I = 1,61
190   FIPSDN(I) = FIPSD(I)/SUMFI

C     DO 191 I = 1,61
C191  WRITE (7,*) 'FINAL WEIGHT FRACTION FOR THE NEXT STEP',I ,FIPSDN(I)

*=======================================================================*
C             ARRANGE FINAL RADIUS AND WEIGHT FRACTION
*=======================================================================*
      DO 195 J = 1,61
      DO 195 I = 1,61
      RF(I,J) = 0.0
195   FIPSDF(I,J) = 0.0

      DO 200 J = 1,61
      DO 200 I = 1,61
          IF (FIRC(J).GE.RLOW(I).AND.FIRC(J).LT.UPPER(I)) THEN
              RF(I,J) = FIRC(J)
              FIPSDF(I,J) = FIPSDN(J)

                  IF (RF(I,J).EQ.0.0) THEN
                      FIPSDF(I,J) = 0.0
                  END IF
200       END IF

C     NORMALIZE WEIGHT FRACTION TO CALCULATE MEAN RADIUS FOR EACH INTERVAL
      DO 205 I = 1,61
      SUM2(I)   = 0.0
205   SIGMA2(I) = 0.0

      DO 210 J = 1,61
      DO 210 I = 1,61
      SUM2(J) = SUM2(J) + FIPSDF(J,I)

C     PREPARE MATRIX FOR NORMALIZED WEIGHT FRACTION
210   FIPSDF2(I,J) = 0.0

      DO 215 J = 1,61
      DO 215 I = 1,61

          IF (SUM2(I).NE.0.0) THEN
              FIPSDF2(I,J) = FIPSDF(I,J)/SUM2(I)
215       END IF

*=======================================================================*
C     MEAN RADIUS FOR EACH INTERVAL OF CONVERTED PARTICLES
*=======================================================================*
      DO 220 I = 1,61
      RF2(I) = 0.0
220   FIPSDF3(I) = 0.0
```

```
      DO 225 J = 1,61
      DO 225 I = 1,61
          IF (RF(J,I).NE.0.0) THEN
                  SIGMA2(J) = SIGMA2(J) + FIPSDF2(J,I)/RF(J,I)
225       END IF

      DO 230 I = 1,61
          IF (SIGMA2(I).NE.0.0) THEN
              RF2(I) = 1./SIGMA2(I)
230       END IF

*=====================================================================*
C         NEW FRACTION FOR NEXT STEP OF CONVERT PARTICLES
*=====================================================================*
      SUM = 0.0
      DO 235 I = 1,61
235   SUM = SUM + SUM2(I)

      DO 240 I = 1,61
240   FIPSDF3(I) = SUM2(I)/SUM

      DO 241 I = 1,61
241   WRITE (7,*) 'SHRINKING CORE', I, RF2(I), FIPSDF3(I)
*---------------------------------------------------------------------*

C     INPUT WEIGHT FRACTION FOR NEXT STEP
      DO 245 I = 1,61
245   ID(I) = IDXSUB(2) - 1 + NCOMP_NCC + (I+9)

      DO 250 I = 1,61
250   SOUT(ID(I)) = FIPSDF3(I)

      RETURN
      END
```

Appendix G

ASPEN PLUS input file for laboratory scale

```
DYNAMICS
    DYNAMICS RESULTS=ON

TITLE 'PLEASE SEE DESCRIPTION'

IN-UNITS SI

DEF-STREAMS CONVEN ALL

DESCRIPTION "
    In block RCSTR (B3)
          REAL(1)        = Total volumetric flow rate to
RCSTR
          REAL(2-62)     = Radius of particle input stream
(m)
          REAL(63)       = Oxygen concentration
          REAL(64-124)   = Radius of particle recycle
stream (m)

          REAL(125-185)  = Mean radius of mixed particle
between input and
                           recycle stream (m)
          REAL(186)      = Viscosity of mixed stream

    "

DATABANKS PURE11  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
       NOASPENPCD

PROP-SOURCES PURE11  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
```

```
35        C C /
36        O2 O2 /
37        N2 N2 /
38        CO CO /
39        CO2 CO2 /
40        H2 H2 /
41        H2O H2O /
42        S S /
43        SO2 O2S /
44        NO NO /
45        N2O N2O /
46        ASH /
47        LIGNITE
48
49    FLOWSHEET
50        BLOCK B1 IN=LIGNITE OUT=S1
51        BLOCK B2 IN=S1 AIR OUT=1
52        BLOCK B3 IN=RESOLID S2 OUT=S3
53        BLOCK B4 IN=S3 OUT=S4
54        BLOCK B6 IN=S5 OUT=S6
55        BLOCK B5 IN=S4 OUT=S5
56        BLOCK B8 IN=S7 OUT=RESOLID BOTTOM FLUEGAS2
57        BLOCK B7 IN=S6 OUT=FLUEGAS S7
58        BLOCK B9 IN=1 OUT=S2
59
60    PROPERTIES PR-BM
61        PROPERTIES SOLIDS
62
63    NC-COMPS ASH PROXANAL ULTANAL SULFANAL
64
65    NC-PROPS ASH ENTHALPY HCOALGEN / DENSITY DCOALIGT
66
67    NC-COMPS LIGNITE PROXANAL ULTANAL SULFANAL
68
69    NC-PROPS LIGNITE ENTHALPY HCOALGEN / DENSITY DCOALIGT
70
71    DEF-SUBS-ATTR PSD PSD
```

```
    72        IN-UNITS ENG
    73        INTERVALS 61
    74        SIZE-LIMITS 0.0 <meter> / 4.9E-007 <meter> /  &
    75            5.8E-007 <meter> / 6.7E-007 <meter> / 7.8E-007
<meter> /  &
    76            9.1E-007 <meter> / 1.06E-006 <meter> / 1.24E-006
<meter> / &
    77            1.68E-006 <meter> / 1.95E-006 <meter> / 2.28E-006
<meter> / &
    78            2.65E-006 <meter> / 3.09E-006 <meter> / 3.6E-006
<meter> / &
    79            4.19E-006 <meter> / 4.88E-006 <meter> / 5.69E-006
<meter> / &
    80            6.63E-006 <meter> / 7.72E-006 <meter> / 9E-006
<meter> /  &
    81            1.048E-005 <meter> / 1.221E-005 <meter> /  &
    82            1.422E-005 <meter> / 1.657E-005 <meter> /  &
    83            1.931E-005 <meter> / 2.249E-005 <meter> /  &
    84            2.62E-005 <meter> / 3.053E-005 <meter> /  &
    85            3.556E-005 <meter> / 4.143E-005 <meter> /  &
    86            4.827E-005 <meter> / 5.623E-005 <meter> /  &
    87            6.551E-005 <meter> / 7.632E-005 <meter> /  &
    88            8.891E-005 <meter> / 0.00010358 <meter> /  &
    89            0.00012067 <meter> / 0.00014058 <meter> /  &
    90            0.00016377 <meter> / 0.0001908 <meter> /  &
    91            0.00022228 <meter> / 0.00025895 <meter> /  &
    92            0.00030168 <meter> / 0.00035146 <meter> /  &
    93            0.00040945 <meter> / 0.00047701 <meter> /  &
    94            0.00055571 <meter> / 0.00064741 <meter> /  &
    95            0.00075423 <meter> / 0.001 <meter> / 0.00125
<meter> /  &
    96            0.0015 <meter> / 0.00175 <meter> / 0.002 <meter> /
&
    97            0.00225 <meter> / 0.0025 <meter> / 0.00275 <meter>
/  &
    98            0.003 <meter> / 0.00325 <meter> / 0.0035 <meter> /
&
```

```
 99           0.00375 <meter> / 0.004 <meter>
100
101    DEF-STREAM-C CONVEN MIXED CIPSD NCPSD
102
103    PROP-SET PS-1 MUMX SUBSTREAM=MIXED PHASE=V
104
105    STREAM AIR
106        SUBSTREAM MIXED TEMP=25. <C> PRES=1. <atm>  &
107            VOLUME-FLOW=7. <l/min>
108        MOLE-FRAC O2 0.21 / N2 0.79
109
110    STREAM LIGNITE
111        SUBSTREAM NCPSD TEMP=25. <C> PRES=1. <atm>  &
112            MASS-FLOW=0.015 <gm/sec>
113        MASS-FRAC LIGNITE 1.
114        COMP-ATTR LIGNITE PROXANAL ( 20. 21. 39. 20. )
115        COMP-ATTR LIGNITE ULTANAL ( 20. 54.3 9.8 2.3 0. 3.7  &
116            9.9 )
117        COMP-ATTR LIGNITE SULFANAL ( 0. 0. 0. )
118        SUBS-ATTR PSD ( 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  &
119            0 0 0 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.  &
120            0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.  &
121            0. 0. 0. 0. 0. 0. 0. 0.048 0.262 0.428 0.167  &
122            0.071 0. 0. 0.024 )
123
124    BLOCK B2 RSTOIC
125        PARAM TEMP=850. <C> PRES=1. <atm> MAXIT=500
126        STOIC 1 CIPSD C -2. / MIXED O2 -1. / CO 2.
127        STOIC 2 CIPSD S -1. / MIXED O2 -1. / SO2 1.
128        STOIC 3 MIXED H2 -2. / O2 -1. / H2O 2.
129        CONV 1 CIPSD C 0.3
130        CONV 2 CIPSD S 0.8
131        CONV 3 MIXED H2 0.8
132
133    BLOCK B1 RYIELD
134        PARAM TEMP=850. <C> PRES=1. <atm> NPHASE=1 PHASE=V
135        MASS-YIELD CIPSD C 0.6815 / MIXED H2 0.0509 / N2  &
```

```
   136            0.0124 / S 0.0059 / O2 0.1189 / NCPSD ASH 0.1304
   137        BLOCK-OPTION FREE-WATER=NO
   138        COMP-ATTR NCPSD ASH PROXANAL ( 0. 0. 0. 100. )
   139        COMP-ATTR NCPSD ASH ULTANAL ( 100. 0. 0. 0. 0. 0. 0.  &
   140            )
   141        COMP-ATTR NCPSD ASH SULFANAL ( 0. 0. 0. )
   142        SUBS-ATTR 1 CIPSD PSD ( 0. 0. 0. 0. 0. 0. 0. 0. 0.  &
   143            0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.  &
   144            0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.  &
   145            0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.  &
   146            0.048 0.262 0.428 0.167 0.071 0. 0. 0.024 )
   147
   148    BLOCK B3 RCSTR
   149        USER-VECS NREAL=186
   150        REAL VALUE-LIST=* 2.45E-007 5.35E-007 6.25E-007 7.25E-
007  &
   151            8.45E-007 9.85E-007 1.15E-006 1.46E-006 1.815E-006
&
   152            2.115E-006 2.465E-006 2.87E-006 3.345E-006 3.895E-
006  &
   153            4.535E-006 5.285E-006 6.16E-006 7.175E-006 8.36E-
006  &
   154            9.74E-006 1.1345E-005 1.3215E-005 1.5395E-005
1.794E-005  &
   155            2.09E-005 2.4345E-005 2.8365E-005 3.3045E-005  &
   156            3.8495E-005 4.485E-005 5.225E-005 6.087E-005
7.0915E-005  &
   157            8.2615E-005 9.6245E-005 0.000112125 0.000130625  &
   158            0.000152175 0.000177285 0.00020654 0.000240615  &
   159            0.000280315 0.00032657 0.000380455 0.00044323
0.00051636  &
   160            0.00060156 0.00070082 0.000877115 0.001125 0.001375
&
   161            0.001625 0.001875 0.002125 0.002375 0.002625
0.002875  &
   162            0.003125 0.003375 0.003625 0.003875
```

```
   163        PARAM VOL=0.000147 TEMP=850. <C> PRES=1. <atm> MB-
MAXIT=500  &
   164            FLASH-MAXIT=500
   165        CONVERGENCE SOLVER=NEWTON
   166        REACTIONS RXN-IDS=R-1
   167
   168    BLOCK B4 RCSTR
   169        USER-VECS NREAL=186
   170        PARAM VOL=0.000147 TEMP=850. <C> PRES=1. <atm> MB-
MAXIT=500  &
   171            FLASH-MAXIT=500
   172        CONVERGENCE SOLVER=NEWTON
   173        REACTIONS RXN-IDS=R-2
   174
   175    BLOCK B5 RCSTR
   176        USER-VECS NREAL=186
   177        PARAM VOL=0.000245437 TEMP=850. <C> PRES=1. <atm>  &
   178            MB-MAXIT=500 FLASH-MAXIT=500
   179        CONVERGENCE SOLVER=NEWTON
   180        REACTIONS RXN-IDS=R-3
   181
   182    BLOCK B6 RCSTR
   183        USER-VECS NREAL=186
   184        PARAM VOL=0.000245437 TEMP=850. <C> PRES=1. <atm>  &
   185            MB-MAXIT=500 FLASH-MAXIT=500
   186        CONVERGENCE SOLVER=NEWTON
   187        REACTIONS RXN-IDS=R-4
   188
   189    BLOCK B9 RCSTR
   190        USER-VECS NREAL=186
   191        REAL VALUE-LIST=* 2.45E-007 5.35E-007 6.25E-007 7.25E-
007  &
   192            8.45E-007 9.85E-007 1.15E-006 1.46E-006 1.815E-006
&
   193            2.115E-006 2.465E-006 2.87E-006 3.345E-006 3.895E-
006  &
```

```
   194            4.535E-006 5.285E-006 6.16E-006 7.175E-006 8.36E-
006  &
   195            9.74E-006 1.1345E-005 1.3215E-005 1.5395E-005
1.794E-005  &
   196            2.09E-005 2.4345E-005 2.8365E-005 3.3045E-005  &
   197            3.8495E-005 4.485E-005 5.225E-005 6.087E-005
7.0915E-005  &
   198            8.2615E-005 9.6245E-005 0.00011212 0.00013062
0.00015217  &
   199            0.00017728 0.00020654 0.00024061 0.00028031
0.00032657  &
   200            0.00038045 0.00044323 0.00051636 0.00060156
0.00070082  &
   201            0.00087711 0.001125 0.001375 0.001625 0.001875
0.002125  &
   202            0.002375 0.002625 0.002875 0.003125 0.003375
0.003625  &
   203            0.003875
   204         PARAM VOL=0.000147 TEMP=850. <C> PRES=1. <atm>
   205         REACTIONS RXN-IDS=R-5
   206
   207    BLOCK B8 SSPLIT
   208         PARAM PRES=1. <atm>
   209         FRAC MIXED BOTTOM 0. / FLUEGAS2 1.
   210         FRAC CIPSD BOTTOM 0. / FLUEGAS2 0.28
   211         FRAC NCPSD BOTTOM 0.2 / FLUEGAS2 0.75
   212
   213    BLOCK B7 CYCLONE
   214         PARAM MODE=SIMULATION TYPE=USER
   215         SIMULATION DIAM=0.032
   216         DIMENSIONS LEN-CYLINDER=0.048 LEN-CONE=0.079 DIAM-
OVER=0.016  &
   217            LEN-OVER=0.008 WIDTH-INLET=0.006 HT-INLET=0.016  &
   218            DIAM-UNDER=0.012
   219
   220    EO-CONV-OPTI
   221
```

```
   222    CALCULATOR C-1
   223    F     COMMON /USER1/ RADIUS, WPSD, FCBSD, FCBRS,
   224    F    .               DCIPN
   225    F     COMMON /USER2/ RWPSD, REWPSD, FMOLE
   226    F     COMMON /USER5/ AREA, VFAIR, VAIR, VVOID, BEDVV, DP
   227    F
   228    F
   229    F     DATA RADIUS/0.0125/
   230    F     REAL*8 VVOID(4), WPSD(61), RWPSD(61), REWPSD(61),
BEDVV(4)
   231         DEFINE FCPSD STREAM-VAR STREAM=S2 SUBSTREAM=CIPSD  &
   232             VARIABLE=MASS-FLOW
   233         DEFINE FNPSD STREAM-VAR STREAM=S2 SUBSTREAM=NCPSD  &
   234             VARIABLE=MASS-FLOW
   235         DEFINE FRPSD STREAM-VAR STREAM=RESOLID SUBSTREAM=CIPSD
&
   236             VARIABLE=MASS-FLOW
   237         DEFINE FNRSD STREAM-VAR STREAM=RESOLID SUBSTREAM=NCPSD
&
   238             VARIABLE=MASS-FLOW
   239         DEFINE DPSD STREAM-VAR STREAM=S2 SUBSTREAM=CIPSD  &
   240             VARIABLE=MASS-DENSITY
   241         DEFINE DNPSD STREAM-VAR STREAM=S2 SUBSTREAM=NCPSD  &
   242             VARIABLE=MASS-DENSITY
   243         DEFINE DRPSD STREAM-VAR STREAM=RESOLID SUBSTREAM=CIPSD
&
   244             VARIABLE=MASS-DENSITY
   245         DEFINE DRNSD STREAM-VAR STREAM=RESOLID SUBSTREAM=NCPSD
&
   246             VARIABLE=MASS-DENSITY
   247         DEFINE VFSUM BLOCK-VAR BLOCK=B3 VARIABLE=VALUE-LIST  &
   248             SENTENCE=REAL ELEMENT=1
   249         DEFINE MDMIX STREAM-VAR STREAM=S2 SUBSTREAM=MIXED  &
   250             VARIABLE=MOLE-DENSITY
   251         DEFINE MOFRAC MOLE-FRAC STREAM=S2 SUBSTREAM=MIXED  &
   252             COMPONENT=O2
   253         DEFINE CONO2 BLOCK-VAR BLOCK=B3 VARIABLE=VALUE-LIST  &
```

```
   254            SENTENCE=REAL ELEMENT=63
   255         DEFINE FAIR STREAM-VAR STREAM=S2 SUBSTREAM=MIXED  &
   256            VARIABLE=MASS-FLOW
   257         DEFINE DAIR STREAM-VAR STREAM=S2 SUBSTREAM=MIXED  &
   258            VARIABLE=MASS-DENSITY
   259         DEFINE FCBSD MASS-FLOW STREAM=S2 SUBSTREAM=CIPSD  &
   260            COMPONENT=C
   261         DEFINE DMPSD STREAM-VAR STREAM=S2 SUBSTREAM=CIPSD  &
   262            VARIABLE=MOLE-DENSITY
   263         DEFINE VISCO STREAM-PROP STREAM=S2 PROPERTY=PS-1
   264         DEFINE VIS BLOCK-VAR BLOCK=B3 VARIABLE=VALUE-LIST  &
   265            SENTENCE=REAL ELEMENT=186
   266         VECTOR-DEF RPSD SUBS-ATTR STREAM=S2 SUBSTREAM=CIPSD  &
   267            ATTRIBUTE=PSD
   268         VECTOR-DEF PSD SUBS-ATTR STREAM=S2 SUBSTREAM=CIPSD  &
   269            ATTRIBUTE=PSD
   270         DEFINE FMPSD STREAM-VAR STREAM=S2 SUBSTREAM=CIPSD  &
   271            VARIABLE=MOLE-FLOW
   272         DEFINE VISCO1 STREAM-PROP STREAM=S2 PROPERTY=PS-1
   273     F     OPEN (7,FILE='C-1.txt')
   274     F
   275     F
   276     C     TOTAL MASS FLOW RATE OF SUBSTREAM CIPSD
   277     F
   278     F     FTOTAL = FCPSD + FNPSD + FRPSD + FNRSD
   279     F     WRITE (7,*) 'TOTAL MASS FLOW RATE OF CIPSD (kg/s)',
FTOTAL
   280     F
   281     C     MEAN MASS DENSITY OF TOTAL FLOW TO RCSTR
   282     F     FRAC = FCPSD*DPSD + FNPSD*DNPSD + FRPSD*DRPSD +
FNRSD*DRNSD
   283     F     DENS = 1/FTOTAL * FRAC
   284     F     WRITE (7,*) 'MEAN MASS DENSITY (Kg/m^3)',DENS
   285     F
   286     C     VOLUMETRIC FLOW RATE OF TOTAL FLOW TO RCSTR
   287     F     VFSUM = FTOTAL/DENS
```

```
   288    F     WRITE (7,*) 'VOLUMETRIC FLOW RATE OF TOTAL FLOW
(m^3/s)', VFSUM
   289    F
   290    C     CONCENTRATION OF OXYGEN
   291    F     DENMOL = MDMIX
   292    F     CONO2 = MOFRAC*MDMIX
   293    F     WRITE (7,*) 'CONCENTRATION ',CONO2
   294    F
   295    C
*===============================================================*
   296    C                                  LOWER REGION
   297    C
*===============================================================*
   298    C     SECTION AREA OF REACTOR
   299    F     PIE  = 3.141592654
   300    F     AREA = PIE*RADIUS**2
   301    F     WRITE (7,*)'AREA',AREA
   302    F
   303    C     AIR VOLUMETRIC FLOW RATE (m^3/s)
   304    F     VFAIR = FAIR/DAIR
   305    F     WRITE (7,*) 'VOLUMETRIC FLOW RATE OF AIR
(m^3/s)',VFAIR
   306    F
   307    C     AIR VELOCITY (m/s)
   308    F     VAIR = VFAIR/AREA
   309    F     WRITE (7,*) 'AIR VELOCITY (m/s)',VAIR
   310    F
   311    C     MEAN VOIDAGE OF DENSE BED
   312    C     FUNCTION BETWEEN VELOCITY AND 1-VOIDAGE
   313    F     VOI = -0.0884*DLOG(VAIR)+0.279
   314    F     VVOID(1) = 1.-VOI
   315    F     WRITE (7,*)'MEAN VOIDAGE OF DENSE BED',VVOID(1)
   316    F
   317    C
*===============================================================*
   318    C                    PREPARE WEIGHT FRACTION OF PSD
```

```
   319    C
*================================================================*
   320    C      DO 5 I=1,61
   321    C      WPSD(I) = PSD(I)
   322    C    5 WRITE (7,*) 'WPSD', WPSD(I)
   323    F
   324    F     DO 10 I=1,61
   325    F  10 RWPSD(I) = RPSD(I)
   326    F
   327    C     MOLAR DENSITY TO EXTERNAL SUBROUTINE
   328    F     DCIPN = DMPSD
   329    F
   330    F     WRITE (7,*) 'DCIPN', DCIPN
   331    F
   332    C     VISCOSITY OF MIXED STREAM
   333    F     VIS = VISCO1
   334    F     WRITE (7,*) 'VISCOSITY', VISCO, VISCO1, VIS
   335    F
   336    C     DEFINED MOLAR FLOW RATE TO EXTERNAL SUBROUTINE
   337    F     FMOLE = FMPSD
   338    F     WRITE (7,*) 'MOLE FLOW', FMOLE
   339    F
   340    F     FCBSD = FCPSD
   341    F     FCBRS = FRPSD
   342    F     WRITE (7,*) 'FLOW', FCBSD, FCBRS
   343        EXECUTE BEFORE BLOCK B3
   344
   345    CALCULATOR C-2
   346    F     COMMON /USER4/ DCIPNU, FMOLU, RW2PSD, FBSD2
   347    F     COMMON /USER5/ AREA, VFAIR, VAIR, VVOID, BEDVV, DP
   348    F     COMMON /USER6/ VAIRU1
   349    F     COMMON /USER14/ VOIDM, BEDVM, BEDL
   350    F
   351    F     REAL*8 RW2PSD(61), VVOID(4), BEDL(4), BDL(4),
   352    F    .       BEDVV(4), VOIDM(3), BEDVM(3)
   353    F     DATA PHIS/0.806/, BEDLT/1.6/, VOIDS/0.999/,
BEDD/0.025/
```

```
   354        DEFINE FCPSD STREAM-VAR STREAM=S3 SUBSTREAM=CIPSD  &
   355            VARIABLE=MASS-FLOW
   356        DEFINE FNPSD STREAM-VAR STREAM=S3 SUBSTREAM=NCPSD  &
   357            VARIABLE=MASS-FLOW
   358        DEFINE DPSD STREAM-VAR STREAM=S3 SUBSTREAM=CIPSD  &
   359            VARIABLE=MASS-DENSITY
   360        DEFINE DNPSD STREAM-VAR STREAM=S3 SUBSTREAM=NCPSD  &
   361            VARIABLE=MASS-DENSITY
   362        DEFINE DMPSD STREAM-VAR STREAM=S3 SUBSTREAM=CIPSD  &
   363            VARIABLE=MOLE-DENSITY
   364        DEFINE FMPSD STREAM-VAR STREAM=S3 SUBSTREAM=CIPSD  &
   365            VARIABLE=MOLE-FLOW
   366        DEFINE MOFRAC MOLE-FRAC STREAM=S3 SUBSTREAM=MIXED  &
   367            COMPONENT=O2
   368        DEFINE MDMIX STREAM-VAR STREAM=S3 SUBSTREAM=MIXED  &
   369            VARIABLE=MOLE-DENSITY
   370        VECTOR-DEF RPSD SUBS-ATTR STREAM=S3 SUBSTREAM=CIPSD  &
   371            ATTRIBUTE=PSD
   372        DEFINE FCBSD MASS-FLOW STREAM=S3 SUBSTREAM=CIPSD  &
   373            COMPONENT=C
   374        DEFINE FMIX STREAM-VAR STREAM=S3 SUBSTREAM=MIXED  &
   375            VARIABLE=MASS-FLOW
   376        DEFINE DMIX STREAM-VAR STREAM=S3 SUBSTREAM=MIXED  &
   377            VARIABLE=MASS-DENSITY
   378        DEFINE VFSUM BLOCK-VAR BLOCK=B4 VARIABLE=VALUE-LIST  &
   379            SENTENCE=REAL ELEMENT=1
   380        DEFINE VISCO STREAM-PROP STREAM=S3 PROPERTY=PS-1
   381        DEFINE BEDV BLOCK-VAR BLOCK=B3 VARIABLE=VOL
SENTENCE=PARAM
   382        DEFINE BEDVU1 BLOCK-VAR BLOCK=B4 VARIABLE=VOL  &
   383            SENTENCE=PARAM
   384        DEFINE BEDP BLOCK-VAR BLOCK=B4 VARIABLE=PRES
SENTENCE=PARAM
   385        DEFINE CONO2 BLOCK-VAR BLOCK=B4 VARIABLE=VALUE-LIST  &
   386            SENTENCE=REAL ELEMENT=63
   387        DEFINE BEDVU2 BLOCK-VAR BLOCK=B5 VARIABLE=VOL  &
   388            SENTENCE=PARAM
```

```
   389         DEFINE FMAIR STREAM-VAR STREAM=AIR SUBSTREAM=MIXED  &
   390             VARIABLE=MOLE-FLOW
   391         DEFINE VIS BLOCK-VAR BLOCK=B4 VARIABLE=VALUE-LIST  &
   392             SENTENCE=REAL ELEMENT=186
   393         DEFINE TEMP BLOCK-VAR BLOCK=B3 VARIABLE=TEMP
SENTENCE=PARAM
   394    F     OPEN (7,FILE='C-2.txt')
   395    F
   396    C     TOTAL MASS FLOW RATE OF SUBSTREAM CIPSD
   397    F     FTOTAL = FCPSD + FNPSD
   398    F     WRITE (7,*) 'TOTAL MASS FLOW RATE OF CIPSD (kg/s)',
FTOTAL
   399    F
   400    C     MEAN MASS DENSITY OF TOTAL FLOW TO RCSTR
   401    F     DENS = 1/FTOTAL * (FCPSD*DPSD + FNPSD*DNPSD)
   402    F     WRITE (7,*) 'MEAN MASS DENSITY (Kg/m^3)',DENS
   403    F
   404    C     VOLUMETRIC FLOW RATE OF TOTAL FLOW TO RCSTR
   405    F     VFSUM = FTOTAL/DENS
   406    F     WRITE (7,*) 'VOLUMETRIC FLOW RATE OF TOTAL FLOW
(m^3/s)', VFSUM
   407    F
   408    C     DEFINED MOLAR DENSITY TO EXTERNAL SUBROUTINE
   409    F     DCIPNU = DMPSD
   410    F
   411    C     DEFINED MOLAR FLOW RATE TO EXTERNAL SUBROUTINE
   412    F     FMOLU = FMPSD
   413    F
   414    C     OXYGEN CONCENTRATION
   415    F     CONO2 = MOFRAC*MDMIX
   416    F     WRITE (7,*) 'CONCENTRATION ',CONO2
   417    F
   418    C     VISCOSITY OF FLUID
   419    F     VIS = VISCO
   420    F     WRITE (7,*) 'VISCOSITY', VISCO
   421    F
```

```
   422    C
*================================================================*
   423    C                     PREPARE WEIGHT FRACTION OF PSD
   424    C
*================================================================*
   425    F     DO 5 I = 1,61
   426    F   5 RW2PSD(I) = RPSD(I)
   427    F
   428    C
*================================================================*
   429    C       MASS FLOW RATE OF CARBON IN INPUT STREAM
   430    C
*================================================================*
   431    F     FBSD2 = FCBSD
   432    F
   433    C
*================================================================*
   434    C                                LOWER REGION
   435    C
*================================================================*
   436    F     WRITE (7,*)'AREA',AREA
   437    F     WRITE (7,*) 'VOLUMETRIC FLOW RATE OF AIR
(m^3/s)',VFAIR
   438    F     WRITE (7,*) 'AIR VELOCITY (m/s)',VAIR
   439    F     WRITE (7,*)'MEAN VOIDAGE OF DENSE BED',VVOID(1)
   440    F
   441    C
*================================================================*
   442    C                                UPPER REGION
   443    C
*================================================================*
   444    C     VOLUMETRIC FLOW RATE FOR MIXED STREAM (m^3/s)
   445    F     FVMIX = FMIX/DMIX
   446    F
   447    C     AIR VELOCITY (m/s)
   448    F     VAIRU1 = FVMIX/AREA
   449    F     WRITE (7,*) 'AIR VELOCITY TO UPPER REGION', VAIRU1
```

```
   450    F
   451    C     NET SOLIDS CIRCULATION FLUX (Kg/(m^2.s))
   452    F     GS = 3.0
   453    F
   454    C     ACCELERATION DUE TO GRAVITY (m/s^2)
   455    F     G  = 9.81
   456    F
   457    C     DIMENSION LESS (DP STAR)  (m)
   458    F     IF (DP.EQ.0.0) THEN
   459    F     DP = 0.001
   460    F     END IF
   461    F     DPSAT = DP * ( DMIX*(DENS-DMIX)*G/VISCO**2.
)**(1./3.)
   462    F     WRITE (7,*) 'DP, DMIX', DP, DMIX
   463    F     WRITE (7,*) 'DIMENSIONLESS (DP STAR)',DPSAT
   464    F
   465    C     TERMINAL VELOCITY OF PARTICLE (m/s)
   466    F     UTSAT =  1./(18./DPSAT**2. + (2.335-
1.744*PHIS)/DPSAT**0.5)
   467    F     WRITE (7,*) 'UTSAT',UTSAT
   468    F
   469    F     UT =  UTSAT/( DMIX**2./(VISCO*(DENS-DMIX)*G)
)**(1./3.)
   470    F     WRITE (7,*) 'TERMINAL VELOCITY OF PARTICLE (M/S)',UT
   471    F
   472    C     BED LENGTH (m)
   473    F     BEDL(1) = BEDV/AREA
   474    F     BEDL(2) = BEDVU1/AREA
   475    F     BEDL(3) = BEDVU2/AREA
   476    F     BEDL(4) = BEDLT - ( BEDL(1) + BEDL(2) + BEDL(3) )
   477    F     WRITE (7,*) 'BEDL(I)',(BEDL(I),I=1,4)
   478    F
   479    C     TOTAL GAS CONCENTRATION (Kmole/m^3)
   480    C     GAS CONSTANT (atm cm^3)/(gmole K)
   481    F     R = 82.056
   482    F     BEDT2 = TEMP
   483    F     CONC = BEDP*1000./(101325.*R*BEDT2)
```

```
   484    F     WRITE (7,*) 'TEMP',BEDT2
   485    F     WRITE (7,*) 'CONC',CONC
   486    F     WRITE (7,*) 'PRES',BEDP
   487    F
   488    C     SUPERFICIAL GAS VELOCITY (m/s)
   489    F     UGAS = FMAIR/(AREA*CONC)
   490    F     WRITE (7,*) 'SUPERFICIAL GAS VELOCITY', UGAS
   491    F
   492    C     FROUDE NUMBER
   493    F     FR = UGAS/(G*BEDD)**0.5
   494    F     WRITE (7,*) 'FR',FR
   495    F
   496    C     PARTICLE FROUDE NUMBER
   497    F     FRT = UT/(G*BEDD)**0.5
   498    F     WRITE (7,*) 'FRT',FRT
   499    F
   500    C     MEAN AXIAL VOIDAGE IN THE FULLY DEVELOPED ZONE
   501    F     PHI = 1. + 5.6/FR + 0.47*FRT**0.41
   502    F     VVOID(4) = 1./( 1. + PHI*GS/(UGAS*DENS) )
   503    F     WRITE (7,*) 'PHI',PHI
   504    F     WRITE (7,*) 'VVOID(4)',VVOID(4)
   505    F
   506    C     DECAY CONSTANT
   507    F     A = 5./UGAS
   508    F     WRITE (7,*) 'DECAY RATIO, UGAS', A, UGAS
   509    F
   510    F     IF (VVOID(4).GE.VOIDS) THEN
   511    F     VVOID(4) = 0.99
   512    F     END IF
   513    F
   514    F     IF (VVOID(1).GE.VOIDS) THEN
   515    F     VVOID(1) = 0.99
   516    F     END IF
   517    F
   518    C     LENGTH OF THE ACCELERATION ZONE
   519    F     BEDZ = (-1./A) * DLOG( (VOIDS-VVOID(4)) / (VOIDS-
VVOID(1)) )
```

```
F     AAA = -DLOG( (VOIDS-VVOID(4)) / (VOIDS-VVOID(1)) )
F     WRITE (7,*) VOIDS, VVOID(4), VVOID(1)
F     WRITE (7,*) 'BEDZ', BEDZ, AAA
F
F     IF (BEDZ.GE.BEDLT) THEN
F     BEDZ = BEDLT - BEDL(1)
F     END IF
F
C     HEIGHT IN CFBC AT ANY INTERVAL
F     BDL(1) = BEDV/AREA
F     BDL(2) = BEDZ/3.
F     BDL(3) = 2.*BEDZ/3.
F     BDL(4) = BEDLT - ( BEDZ+BDL(1) )
F     WRITE (7,*) 'BDL(I)',(BDL(I),I=1,4)
F
F     BEDVV(1) = BEDV
F     BEDVV(2) = AREA*BDL(2)
F     BEDVV(3) = AREA*BDL(3)
F     BEDVV(4) = AREA*BDL(4)
F     WRITE (7,*) 'BEDVV(I)',(BEDVV(I),I=1,4)
F
C     VOIDAGE AT ANOTHER INTERVAL
F     VVOID(2) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(1))
F    .          * ( DEXP(-A*BDL(2)) - 1. )
F     VVOID(3) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(2))
F    .          * ( DEXP(-A*BEDZ) - DEXP(-A*BDL(2)) )
F     WRITE (7,*) 'VVOID(2)',VVOID(2)
F     WRITE (7,*) 'VVOID(3)',VVOID(3)
      EXECUTE BEFORE BLOCK B4

CALCULATOR C-3
F     COMMON /USER5/ AREA, VFAIR, VAIR, VVOID, BEDVV
F     COMMON /USER9/ DCINU2, FMOLU2, RW3PSD, FBSD3, DP2
F     COMMON /USER10/ VAIRU2, VVOID2, BEDVV2
F     COMMON /USER14/ VOIDM, BEDVM, BEDL
F
```

```
   556    F     REAL*8 RW3PSD(61), VVOID(4), BEDL(4), VVOID2(4),
BDL(4),
   557    F    .       BEDVV2(4), VOIDM(3), BEDVM(3)
   558    F
   559    F     DATA PHIS/0.806/, BEDLT/1.6/, VOIDS/0.999/,
BEDD/0.025/
   560         DEFINE FCPSD STREAM-VAR STREAM=S4 SUBSTREAM=CIPSD  &
   561             VARIABLE=MASS-FLOW
   562         DEFINE FNPSD STREAM-VAR STREAM=S4 SUBSTREAM=NCPSD  &
   563             VARIABLE=MASS-FLOW
   564         DEFINE DPSD STREAM-VAR STREAM=S4 SUBSTREAM=CIPSD  &
   565             VARIABLE=MASS-DENSITY
   566         DEFINE DNPSD STREAM-VAR STREAM=S4 SUBSTREAM=NCPSD  &
   567             VARIABLE=MASS-DENSITY
   568         DEFINE DMPSD STREAM-VAR STREAM=S4 SUBSTREAM=CIPSD  &
   569             VARIABLE=MOLE-DENSITY
   570         DEFINE FMPSD STREAM-VAR STREAM=S4 SUBSTREAM=CIPSD  &
   571             VARIABLE=MOLE-FLOW
   572         DEFINE MOFRAC MOLE-FRAC STREAM=S4 SUBSTREAM=MIXED  &
   573             COMPONENT=O2
   574         DEFINE MDMIX STREAM-VAR STREAM=S4 SUBSTREAM=MIXED  &
   575             VARIABLE=MOLE-DENSITY
   576         DEFINE VISCO STREAM-PROP STREAM=S4 PROPERTY=PS-1
   577         VECTOR-DEF RPSD SUBS-ATTR STREAM=S4 SUBSTREAM=CIPSD  &
   578             ATTRIBUTE=PSD
   579         DEFINE FCBSD MASS-FLOW STREAM=S4 SUBSTREAM=CIPSD  &
   580             COMPONENT=C
   581         DEFINE FMIX STREAM-VAR STREAM=S4 SUBSTREAM=MIXED  &
   582             VARIABLE=MASS-FLOW
   583         DEFINE DMIX STREAM-VAR STREAM=S4 SUBSTREAM=MIXED  &
   584             VARIABLE=MASS-DENSITY
   585         DEFINE BEDV BLOCK-VAR BLOCK=B3 VARIABLE=VOL
SENTENCE=PARAM
   586         DEFINE BEDVU1 BLOCK-VAR BLOCK=B4 VARIABLE=VOL  &
   587             SENTENCE=PARAM
   588         DEFINE BEDVU2 BLOCK-VAR BLOCK=B5 VARIABLE=VOL  &
   589             SENTENCE=PARAM
```

```
   590         DEFINE VFSUM BLOCK-VAR BLOCK=B5 VARIABLE=VALUE-LIST  &
   591             SENTENCE=REAL ELEMENT=1
   592         DEFINE CONO2 BLOCK-VAR BLOCK=B5 VARIABLE=VALUE-LIST  &
   593             SENTENCE=REAL ELEMENT=63
   594         DEFINE VIS BLOCK-VAR BLOCK=B5 VARIABLE=VALUE-LIST  &
   595             SENTENCE=REAL ELEMENT=186
   596         DEFINE TEMP BLOCK-VAR BLOCK=B4 VARIABLE=TEMP
SENTENCE=PARAM
   597         DEFINE BEDP BLOCK-VAR BLOCK=B5 VARIABLE=PRES
SENTENCE=PARAM
   598         DEFINE FMAIR STREAM-VAR STREAM=AIR SUBSTREAM=MIXED  &
   599             VARIABLE=MOLE-FLOW
   600     F     OPEN (7,FILE='C-3.txt')
   601     F
   602     F
   603     C     TOTAL MASS FLOW RATE OF SUBSTREAM CIPSD
   604     F     FTOTAL = FCPSD + FNPSD
   605     F     WRITE (7,*) 'TOTAL MASS FLOW RATE OF CIPSD (kg/s)',
FTOTAL
   606     F
   607     C     MEAN MASS DENSITY OF TOTAL FLOW TO RCSTR
   608     F     DENS = 1/FTOTAL * (FCPSD*DPSD + FNPSD*DNPSD)
   609     F     WRITE (7,*) 'MEAN MASS DENSITY (Kg/m^3)',DENS
   610     F
   611     C     VOLUMETRIC FLOW RATE OF TOTAL FLOW TO RCSTR
   612     F     VFSUM = FTOTAL/DENS
   613     F     WRITE (7,*) 'VOLUMETRIC FLOW RATE OF TOTAL FLOW
(m^3/s)', VFSUM
   614     F
   615     C     DEFINED MOLAR DENSITY TO EXTERNAL SUBROUTINE
   616     F     DCINU2 = DMPSD
   617     F
   618     C     DEFINED MOLAR FLOW RATE TO EXTERNAL SUBROUTINE
   619     F     FMOLU2 = FMPSD
   620     F
   621     C     OXYGEN CONCENTRATION
   622     F     CONO2 = MOFRAC*MDMIX
```

```
   623    F     WRITE (7,*) 'CONCENTRATION ',CONO2
   624    F
   625    C     VISCOSITY OF FLUID
   626    F     VIS = VISCO
   627    F     WRITE (7,*) 'VISCOSITY', VISCO
   628    F
   629    C
*================================================================*
   630    C                   PREPARE WEIGHT FRACTION OF PSD
   631    C
*================================================================*
   632    F     DO 5 I = 1,61
   633    F   5 RW3PSD(I) = RPSD(I)
   634    F
   635    C
*================================================================*
   636    C       MASS FLOW RATE OF CARBON IN INPUT STREAM
   637    C
*================================================================*
   638    F     FBSD3 = FCBSD
   639    F
   640    C
*================================================================*
   641    C                                  UPPER REGION
   642    C
*================================================================*
   643    F
   644    C     VOLUMETRIC FLOW RATE FOR MIXED STREAM (m^3/s)
   645    F     FVMIX = FMIX/DMIX
   646    F
   647    C     AIR VELOCITY (m/s)
   648    F     VAIRU2 = FVMIX/AREA
   649    F     WRITE (7,*) 'AIR VELOCITY TO UPPER REGION', VAIRU2
   650    F
   651    C     NET SOLIDS CIRCULATION FLUX (Kg/(m^2.s))
   652    F     GS = 3.0
   653    F
```

```
   654    C     ACCELERATION DUE TO GRAVITY (m/s^2)
   655    F     G  = 9.81
   656    F
   657    F     WRITE (7,*) 'DP2',DP2
   658    F
   659    C     DIMENSION LESS (DP STAR)  (m)
   660    F
   661    F     IF (DP2.EQ.0.0) THEN
   662    F     DP2 = 0.001
   663    F     END IF
   664    F
   665    F     DPSAT = DP2 * ( DMIX*(DENS-DMIX)*G/VISCO**2.
)**(1./3.)
   666    F     WRITE (7,*) 'DIMENSIONLESS (DP STAR)',DPSAT
   667    F
   668    C     TERMINAL VELOCITY OF PARTICLE (m/s)
   669    F     UTSAT =  1./(18./DPSAT**2. + (2.335-
1.744*PHIS)/DPSAT**0.5)
   670    F     WRITE (7,*) 'UTSAT',UTSAT
   671    F
   672    F     UT =  UTSAT/( DMIX**2./(VISCO*(DENS-DMIX)*G)
)**(1./3.)
   673    F     WRITE (7,*) 'TERMINAL VELOCITY OF PARTICLE (M/S)',UT
   674    F
   675    C     BED LENGTH (m)
   676    F     BEDL(1) = BEDV/AREA
   677    F     BEDL(2) = BEDVU1/AREA
   678    F     BEDL(3) = BEDVU2/AREA
   679    F     BEDL(4) = BEDLT - ( BEDL(1) + BEDL(2) + BEDL(3) )
   680    F     WRITE (7,*) 'BEDL(I)',(BEDL(I),I=1,4)
   681    F
   682    C     TOTAL GAS CONCENTRATION (Kmole/m^3)
   683    C     GAS CONSTANT (atm cm^3)/(gmole K)
   684    F     R = 82.056
   685    F     BEDT3 = TEMP
   686    F     CONC = BEDP*1000./(101325.*R*BEDT3)
   687    F     WRITE (7,*) 'TEMP', BEDT3
```

```
   688    F     WRITE (7,*) 'CONC', CONC
   689    F
   690    C     SUPERFICIAL GAS VELOCITY (m/s)
   691    F     UGAS = FMAIR/(AREA*CONC)
   692    F     WRITE (7,*) 'SUPERFICIAL GAS VELOCITY', UGAS
   693    F
   694    C     FROUDE NUMBER
   695    F     FR = UGAS/(G*BEDD)**0.5
   696    F     WRITE (7,*) 'FR',FR
   697    F
   698    C     PARTICLE FROUDE NUMBER
   699    F     FRT = UT/(G*BEDD)**0.5
   700    F     WRITE (7,*) 'FRT',FRT
   701    F
   702    C     MEAN AXIAL VOIDAGE IN THE FULLY DEVELOPED ZONE
   703    F     PHI = 1. + 5.6/FR + 0.47*FRT**0.41
   704    F     VVOID2(4) = 1./( 1. + PHI*GS/(UGAS*DENS) )
   705    F     WRITE (7,*) 'PHI',PHI
   706    F     WRITE (7,*) 'VVOID2(4)',VVOID2(4)
   707    F
   708    C     DECAY CONSTANT
   709    F     A = 5./UGAS
   710    F     WRITE (7,*) 'DECAY RATIO',A
   711    F
   712    F     IF (VVOID2(4).GE.VOIDS) THEN
   713    F     VVOID2(4) = 0.99
   714    F     END IF
   715    F
   716    F     IF (VVOID(1).GE.VOIDS) THEN
   717    F     VVOID(1) = 0.99
   718    F     END IF
   719    F
   720    C     LENGTH OF THE ACCELERATION ZONE
   721    F     BEDZ = (-1./A) * DLOG( (VOIDS-VVOID2(4)) / (VOIDS-
VVOID(1)) )
   722    F
   723    F     IF (BEDZ.GE.BEDLT) THEN
```

```
   724    F     BEDZ = BEDLT
   725    F     END IF
   726    F     WRITE (7,*) 'BEDZ',BEDZ
   727    F
   728    C     HEIGHT IN CFBC AT ANY INTERVAL
   729    F     BDL(1) = BEDV/AREA
   730    F     BDL(2) = BEDZ/3.
   731    F     BDL(3) = 2.*BEDZ/3.
   732    F     BDL(4) = BEDLT - ( BEDZ+BDL(1) )
   733    F     WRITE (7,*) 'BDL(I)',(BDL(I),I=1,4)
   734    F
   735    F     BEDVV2(1) = BEDV
   736    F     BEDVV2(2) = AREA*BDL(2)
   737    F     BEDVV2(3) = AREA*BDL(3)
   738    F     BEDVV2(4) = AREA*BDL(4)
   739    F     WRITE (7,*) 'BEDVV(I)',(BEDVV2(I),I=1,4)
   740    F
   741    C     VOIDAGE AT ANOTHER INTERVAL
   742    F     VVOID2(2) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(1))
   743    F    .          * ( DEXP(-A*BDL(2)) - 1. )
   744    F     VVOID2(3) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(2))
   745    F    .           * ( DEXP(-A*BEDZ) - DEXP(-A*BDL(2)) )
   746    F     WRITE (7,*) 'VVOID2(2)',VVOID2(2)
   747    F     WRITE (7,*) 'VVOID2(3)',VVOID2(3)
   748        EXECUTE BEFORE BLOCK B5
   749
   750    CALCULATOR C-4
   751    F     COMMON /USER5/ AREA, VFAIR, VAIR, VVOID, BEDVV
   752    F     COMMON /USER12/ DCINU3, FMOLU3, RW4PSD, FBSD4
   753    F     COMMON /USER13/ VAIRU3, VVOID3, BEDVV3
   754    F     COMMON /USER14/ VOIDM, BEDVM, BEDL
   755    F     COMMON /USER17/ BEDT4
   756    F     COMMON /USER18/ DP3
   757    F
   758    F     REAL*8 RW4PSD(61), VVOID(4), BEDL(4), VVOID3(4),
BDL(4),
   759    F    .       BEDVV3(4), VOIDM(3), BEDVM(3)
```

```
   760    F
   761    F     DATA PHIS/0.806/, BEDLT/1.6/, VOIDS/0.999/,
BEDD/0.025/
   762         DEFINE FCPSD STREAM-VAR STREAM=S5 SUBSTREAM=CIPSD  &
   763             VARIABLE=MASS-FLOW
   764         DEFINE FNPSD STREAM-VAR STREAM=S5 SUBSTREAM=NCPSD  &
   765             VARIABLE=MASS-FLOW
   766         DEFINE DPSD STREAM-VAR STREAM=S5 SUBSTREAM=CIPSD  &
   767             VARIABLE=MASS-DENSITY
   768         DEFINE DNPSD STREAM-VAR STREAM=S5 SUBSTREAM=NCPSD  &
   769             VARIABLE=MASS-DENSITY
   770         DEFINE DMPSD STREAM-VAR STREAM=S5 SUBSTREAM=CIPSD  &
   771             VARIABLE=MOLE-DENSITY
   772         DEFINE FMPSD STREAM-VAR STREAM=S5 SUBSTREAM=CIPSD  &
   773             VARIABLE=MOLE-FLOW
   774         DEFINE MOFRAC MOLE-FRAC STREAM=S5 SUBSTREAM=MIXED  &
   775             COMPONENT=O2
   776         DEFINE MDMIX STREAM-VAR STREAM=S5 SUBSTREAM=MIXED  &
   777             VARIABLE=MOLE-DENSITY
   778         DEFINE VISCO STREAM-PROP STREAM=S5 PROPERTY=PS-1
   779         VECTOR-DEF RPSD SUBS-ATTR STREAM=S5 SUBSTREAM=CIPSD  &
   780             ATTRIBUTE=PSD
   781         DEFINE FCBSD MASS-FLOW STREAM=S5 SUBSTREAM=CIPSD  &
   782             COMPONENT=C
   783         DEFINE FMIX STREAM-VAR STREAM=S5 SUBSTREAM=MIXED  &
   784             VARIABLE=MASS-FLOW
   785         DEFINE DMIX STREAM-VAR STREAM=S5 SUBSTREAM=MIXED  &
   786             VARIABLE=MASS-DENSITY
   787         DEFINE BEDV BLOCK-VAR BLOCK=B3 VARIABLE=VOL
SENTENCE=PARAM
   788         DEFINE BEDVU1 BLOCK-VAR BLOCK=B4 VARIABLE=VOL  &
   789             SENTENCE=PARAM
   790         DEFINE BEDVU2 BLOCK-VAR BLOCK=B5 VARIABLE=VOL  &
   791             SENTENCE=PARAM
   792         DEFINE VFSUM BLOCK-VAR BLOCK=B6 VARIABLE=VALUE-LIST  &
   793             SENTENCE=REAL ELEMENT=1
   794         DEFINE CONO2 BLOCK-VAR BLOCK=B6 VARIABLE=VALUE-LIST  &
```

```
   795            SENTENCE=REAL ELEMENT=63
   796         DEFINE VIS BLOCK-VAR BLOCK=B6 VARIABLE=VALUE-LIST  &
   797            SENTENCE=REAL ELEMENT=186
   798         DEFINE TEMP BLOCK-VAR BLOCK=B5 VARIABLE=TEMP
SENTENCE=PARAM
   799         DEFINE BEDP BLOCK-VAR BLOCK=B6 VARIABLE=PRES
SENTENCE=PARAM
   800         DEFINE FMAIR STREAM-VAR STREAM=AIR SUBSTREAM=MIXED  &
   801            VARIABLE=MOLE-FLOW
   802    F     OPEN (7,FILE='C-4.txt')
   803    F
   804    F
   805    C     TOTAL MASS FLOW RATE OF SUBSTREAM CIPSD
   806    F     FTOTAL = FCPSD + FNPSD
   807    F     WRITE (7,*) 'TOTAL MASS FLOW RATE OF CIPSD (kg/s)',
FTOTAL
   808    F
   809    C     MEAN MASS DENSITY OF TOTAL FLOW TO RCSTR
   810    F     DENS = 1/FTOTAL * (FCPSD*DPSD + FNPSD*DNPSD)
   811    F     WRITE (7,*) 'MEAN MASS DENSITY (Kg/m^3)',DENS
   812    F
   813    C     VOLUMETRIC FLOW RATE OF TOTAL FLOW TO RCSTR
   814    F     VFSUM = FTOTAL/DENS
   815    F     WRITE (7,*) 'VOLUMETRIC FLOW RATE OF TOTAL FLOW
(m^3/s)', VFSUM
   816    F
   817    C     DEFINED MOLAR DENSITY TO EXTERNAL SUBROUTINE
   818    F     DCINU3 = DMPSD
   819    F
   820    C     DEFINED MOLAR FLOW RATE TO EXTERNAL SUBROUTINE
   821    F     FMOLU3 = FMPSD
   822    F
   823    C     OXYGEN CONCENTRATION
   824    F     CONO2 = MOFRAC*MDMIX
   825    F     WRITE (7,*) 'CONCENTRATION ',CONO2
   826    F
   827    C     VISCOSITY OF FLUID
```

```
      F     VIS = VISCO
      F     WRITE (7,*) 'VISCOSITY', VISCO
      F
      C
*=================================================================*
      C                    PREPARE WEIGHT FRACTION OF PSD
      C
*=================================================================*
      F     DO 5 I = 1,61
      F   5 RW4PSD(I) = RPSD(I)
      F
      F
      C
*=================================================================*
      C       MASS FLOW RATE OF CARBON IN INPUT STREAM
      C
*=================================================================*
      F     FBSD4 = FCBSD
      F
      C
*=================================================================*
      C                                  UPPER REGION
      C
*=================================================================*
      F
      C     VOLUMETRIC FLOW RATE FOR MIXED STREAM (m^3/s)
      F     FVMIX = FMIX/DMIX
      F
      C     AIR VELOCITY (m/s)
      F     VAIRU3 = FVMIX/AREA
      F     WRITE (7,*) 'AIR VELOCITY TO UPPER REGION', VAIRU3
      F
      C     NET SOLIDS CIRCULATION FLUX (Kg/(m^2.s))
      F     GS = 3.0
      F
      C     ACCELERATION DUE TO GRAVITY (m/s^2)
      F     G  = 9.81
```

```
   859    F
   860    C     DIMENSION LESS (DP STAR)  (m)
   861    F
   862    F     WRITE (7,*) 'DP3', DP3
   863    F
   864    F     IF (DP3.EQ.0.0) THEN
   865    F     DP3 = 0.001
   866    F     END IF
   867    F     WRITE (7,*) 'DP3',DP3
   868    F
   869    F     DPSAT = DP3 * ( DMIX*(DENS-DMIX)*G/VISCO**2.
)**(1./3.)
   870    F     WRITE (7,*) 'DIMENSIONLESS (DP STAR)',DPSAT
   871    F
   872    C     TERMINAL VELOCITY OF PARTICLE (m/s)
   873    F     UTSAT =  1./(18./DPSAT**2. + (2.335-
1.744*PHIS)/DPSAT**0.5)
   874    F     WRITE (7,*) 'UTSAT',UTSAT
   875    F
   876    F     UT =  UTSAT/( DMIX**2./(VISCO*(DENS-DMIX)*G)
)**(1./3.)
   877    F     WRITE (7,*) 'TERMINAL VELOCITY OF PARTICLE (M/S)',UT
   878    F
   879    C     BED LENGTH (m)
   880    F     BEDL(1) = BEDV/AREA
   881    F     BEDL(2) = BEDVU1/AREA
   882    F     BEDL(3) = BEDVU2/AREA
   883    F     BEDL(4) = BEDLT - ( BEDL(1) + BEDL(2) + BEDL(3) )
   884    F     WRITE (7,*) 'BEDL(I)',(BEDL(I),I=1,4)
   885    F
   886    C     TOTAL GAS CONCENTRATION (Kmole/m^3)
   887    C     GAS CONSTANT (atm cm^3)/(gmole K)
   888    F     R = 82.056
   889    F     BEDT4 = TEMP
   890    F     CONC = BEDP*1000./(101325.*R*BEDT4)
   891    F     WRITE (7,*) 'TEMP',BEDT4
   892    F
```

```
   893    C     SUPERFICIAL GAS VELOCITY (m/s)
   894    F     UGAS = FMAIR/(AREA*CONC)
   895    F     WRITE (7,*) 'SUPERFICIAL GAS VELOCITY', UGAS
   896    F
   897    C     FROUDE NUMBER
   898    F     FR = UGAS/(G*BEDD)**0.5
   899    F     WRITE (7,*) 'FR',FR
   900    F
   901    C     PARTICLE FROUDE NUMBER
   902    F     FRT = UT/(G*BEDD)**0.5
   903    F     WRITE (7,*) 'FRT',FRT
   904    F
   905    C     MEAN AXIAL VOIDAGE IN THE FULLY DEVELOPED ZONE
   906    F     PHI = 1. + 5.6/FR + 0.47*FRT**0.41
   907    F     VVOID3(4) = 1./( 1. + PHI*GS/(UGAS*DENS) )
   908    F     WRITE (7,*) 'PHI',PHI
   909    F     WRITE (7,*) 'VVOID3(4)',VVOID3(4)
   910    F
   911    C     DECAY CONSTANT
   912    F     A = 5./UGAS
   913    F     WRITE (7,*) 'DECAY RATIO',A
   914    F
   915    F     IF (VVOID3(4).GE.VOIDS) THEN
   916    F     VVOID3(4) = 0.99
   917    F     END IF
   918    F
   919    F     IF (VVOID(1).GE.VOIDS) THEN
   920    F     VVOID(1) = 0.99
   921    F     END IF
   922    F
   923    C     LENGTH OF THE ACCELERATION ZONE
   924    F     BEDZ = (-1./A) * DLOG( (VOIDS-VVOID3(4)) / (VOIDS-
VVOID(1)) )
   925    F     WRITE (7,*) 'BEDZ',BEDZ
   926    F
   927    F     IF (BEDZ.GE.BEDLT) THEN
   928    F     BEDZ = BEDLT
```

```
F     END IF
F     WRITE (7,*) 'BEDZ',BEDZ
F
C     HEIGHT IN CFBC AT ANY INTERVAL
F     BDL(1) = BEDV/AREA
F     BDL(2) = BEDZ/3.
F     BDL(3) = 2.*BEDZ/3.
F     BDL(4) = BEDLT - ( BEDZ+BDL(1) )
F     WRITE (7,*) 'BDL(I)',(BDL(I),I=1,4)
F
F     BEDVV3(1) = BEDV
F     BEDVV3(2) = AREA*BDL(2)
F     BEDVV3(3) = AREA*BDL(3)
F     BEDVV3(4) = AREA*BDL(4)
F     WRITE (7,*) 'BEDVV(I)',(BEDVV3(I),I=1,4)
F
C     VOIDAGE AT ANOTHER INTERVAL
F     VVOID3(2) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(1))
F    .          * ( DEXP(-A*BDL(2)) - 1. )
F     VVOID3(3) = VOIDS + ( VOIDS-VVOID(1)) / (A*BDL(2))
F    .          * ( DEXP(-A*BEDZ) - DEXP(-A*BDL(2)) )
F     WRITE (7,*) 'VVOID3(2)',VVOID3(2)
F     WRITE (7,*) 'VVOID3(3)',VVOID3(3)
      EXECUTE BEFORE BLOCK B6

CALCULATOR C-5
F     COMMON /USER1/ RADIUS, WPSD, FCBSD, FCBRS, DCIPN
F     COMMON /USER5/ AREA, VFAIR, VAIR, VVOID, BEDVV
F     COMMON /USER10/ VAIRU2, VVOID2, BEDVV2
F     COMMON /USER13/ VAIRU3, VVOID3, BEDVV3
F     COMMON /USER14/ VOIDM, BEDVM, BEDL
F
F     REAL*8 VVOID(4),  BEDVV(4),  VVOID2(4),
F    .       BEDVV2(4), VVOID3(4), BEDVV3(4),
F    .       VOIDM(3),  BEDVM(3),  BEDL(4),
F    .       WPSD(61)
      DEFINE FLOW STREAM-VAR STREAM=AIR SUBSTREAM=MIXED  &
```

```
   966            VARIABLE=MASS-FLOW
   967        DEFINE BEDV BLOCK-VAR BLOCK=B3 VARIABLE=VOL
SENTENCE=PARAM
   968        DEFINE FRPSD MASS-FLOW STREAM=RESOLID SUBSTREAM=CIPSD
&
   969            COMPONENT=C
   970    F     OPEN (7,FILE='C-5.txt')
   971    F
   972    F     WRITE (7,*) 'VVOID',(VVOID(I),I=1,4)
   973    F     WRITE (7,*) 'BEDVV',(BEDVV(I),I=1,4)
   974    F     WRITE (7,*) 'VVOID2',(VVOID2(I),I=1,4)
   975    F     WRITE (7,*) 'BEDVV2',(BEDVV2(I),I=1,4)
   976    F     WRITE (7,*) 'VVOID3',(VVOID3(I),I=1,4)
   977    F     WRITE (7,*) 'BEDVV3',(BEDVV3(I),I=1,4)
   978    F
   979    C
*===============================================================*
   980    C                                  UPPER REGION
   981    C
*===============================================================*
   982    F
   983    C     FIRST INTERVAL
   984    F     VOIDM(1) = ( VVOID(2) + VVOID2(2) + VVOID3(2) )/3.
   985    F     BEDVM(1) = ( BEDVV(2) + BEDVV2(2) + BEDVV3(2) )/3.
   986    F
   987    C     SECOND INTERVAL
   988    F     VOIDM(2) = ( VVOID(3) + VVOID2(3) + VVOID3(3) )/3.
   989    F     BEDVM(2) = ( BEDVV(3) + BEDVV2(3) + BEDVV3(3) )/3.
   990    F
   991    C     THIRD INTERVAL
   992    F     VOIDM(3) = ( VVOID(4) + VVOID2(4) + VVOID3(4) )/3.
   993    F     BEDVM(3) = ( BEDVV(4) + BEDVV2(4) + BEDVV3(4) )/3.
   994    F
   995    F     WRITE (7,*) 'MEAN VOID AT EACH
INTERVAL',(VOIDM(I),I=1,3)
   996    F     WRITE (7,*) 'MEAN VOLUME AT EACH
INTERVAL',(BEDVM(I),I=1,3)
```

```
 997    F
 998    C     THE HEIGHT OF EACH ZONE
 999    F     BEDL(1) = BEDV/AREA
1000    F     BEDL(2) = BEDVM(1)/AREA
1001    F     BEDL(3) = BEDVM(2)/AREA
1002    F     BEDL(4) = BEDVM(3)/AREA
1003    F
1004    F     FCBRS = FRPSD
1005        EXECUTE AFTER BLOCK B6
1006
1007    CONV-OPTIONS
1008        PARAM TEAR-METHOD=WEGSTEIN
1009        WEGSTEIN MAXIT=501
1010
1011    TEAR
1012        TEAR RESOLID STATE=PH
1013
1014    STREAM-REPOR MOLEFLOW PROPERTIES=PS-1
1015
1016    REACTIONS R-1 USER
1017        PARAM SUBROUTINE=USRKI2 NREAL=1
1018        REAC-DATA 1 PHASE=V
1019        REAC-DATA 2 PHASE=V
1020        STOIC 1 CIPSD C -2. / MIXED O2 -1. / CO 2.
1021        STOIC 2 MIXED CO -2. / O2 -1. / CO2 2.
1022
1023    REACTIONS R-2 USER
1024        PARAM SUBROUTINE=USRKI3
1025        REAC-DATA 1 PHASE=V
1026        REAC-DATA 2 PHASE=V
1027        STOIC 1 CIPSD C -2. / MIXED O2 -1. / CO 2.
1028        STOIC 2 MIXED CO -2. / O2 -1. / CO2 2.
1029
1030    REACTIONS R-3 USER
1031        PARAM SUBROUTINE=USRKI4
1032        REAC-DATA 1 PHASE=V
1033        REAC-DATA 2 PHASE=V
```

```
1034        STOIC 1 CIPSD C -2. / MIXED O2 -1. / CO 2.
1035        STOIC 2 MIXED CO -2. / O2 -1. / CO2 2.
1036
1037    REACTIONS R-4 USER
1038        PARAM SUBROUTINE=USRKI5
1039        REAC-DATA 1 PHASE=V
1040        REAC-DATA 2 PHASE=V
1041        STOIC 1 CIPSD C -2. / MIXED O2 -1. / CO 2.
1042        STOIC 2 MIXED CO -2. / O2 -1. / CO2 2.
1043
1044    REACTIONS R-5 USER
1045        PARAM SUBROUTINE=USRKI1
1046        REAC-DATA 1 PHASE=V
1047        REAC-DATA 2 PHASE=V
1048        STOIC 1 CIPSD C -2. / MIXED O2 -1. / CO 2.
1049        STOIC 2 MIXED CO -2. / O2 -1. / CO2 2.
```

VITA

Mr. Natthapong Ngampradit was born on September 8, 1973 in Bangkok, Thailand. He graduated his Bachelor's degree of Engineering in Department of Chemical Engineering, Faculty of Engineering, Rangsit University in 1995. He graduated his Master's degree of Science in Department of Chemical Technology, Faculty of Science, Chulalongkorn University in 1998. He has continued his study in Ph.D. program at Department of Chemical Technology, Faculty of Science, Chulalongkorn University since 2000 and finished his study in 2005.