

การพัฒนาดัชนีเชิงปริมาณสำหรับประเมินระดับการกระจายของสารเติมแต่ง
ในวัสดุผสมโดยการทดลองด้วยคอมพิวเตอร์



นาย เมธี สุภาวิดา

สถาบันวิทยบริการ

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิศวกรรมศาสตรมหาบัณฑิต

สาขาวิชาวิศวกรรมเคมี ภาควิชาวิศวกรรมเคมี

บัณฑิตวิทยาลัย จุฬาลงกรณ์มหาวิทยาลัย

ปีการศึกษา 2540

ISBN 974-637-197-5

ลิขสิทธิ์ของบัณฑิตวิทยาลัย จุฬาลงกรณ์มหาวิทยาลัย

23 ธ.ค. 2545

11758484X

**DEVELOPMENT OF QUANTITATIVE INDICES FOR EVALUATING THE
DEGREE OF DISPERSION OF ADDITIVES IN COMPOUNDED
MATERIALS USING COMPUTER EXPERIMENTS**

Mr. Mathee Suphawita

**A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Engineering in Chemical Engineering**

Department of Chemical Engineering

Graduate School

Chulalongkorn University

Academic Year 1997

ISBN 974-637-197-5

Thesis Title Development of Quantitative Indices for Evaluating The
Degree of Dispersion of Additives in Compounded
Materials Using Computer Experiments

By Mr. Mathee Suphawita

Department Chemical Engineering

Thesis Advisor Professor Wiwut Tanthapanichakoon, Ph.D.

Thesis Co-advisor Assistant Professor Tawatchai Charinpanitkul, Dr. Eng.


Accepted by the Graduate School, Chulalongkorn University, in Partial
Fulfillment of the Requirements for the Master's Degree.

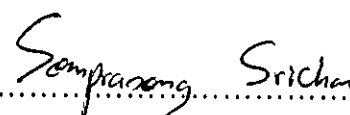

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พิมพ์ต้นฉบับบทความวิจัยวิทยานิพนธ์ภายในกรอบสี่เหลี่ยมนี้เพียงแผ่นเดียว

เมธี สุภาวิตา: การพัฒนาดัชนีเชิงปริมาณสำหรับประเมินระดับการกระจายของสารเติมแต่งในวัสดุผสม โดยการทดลองด้วยคอมพิวเตอร์ (DEVELOPMENT OF QUANTITATIVE INDICES FOR EVALUATING THE DEGREE OF DISPERSION OF ADDITIVES IN COMPOUNDED MATERIALS USING COMPUTER EXPERIMENTS) อ. ที่ปรึกษา: ศ. ดร. วิวัฒน์ ตัณฑะพานิชกุล, อ. ที่ปรึกษาร่วม: ผศ. ดร. ชวิชัย ขรินพานิชกุล, 221 หน้า. ISBN 974-637-197-5

จุดประสงค์ของงานวิทยานิพนธ์นี้ คือการศึกษาและเสนอดัชนีเชิงปริมาณที่เหมาะสมสำหรับประเมินระดับการกระจายตัวของสารเติมแต่งองค์ประกอบเดียว และสององค์ประกอบ ในสารประกอบและของผสมอย่างมีระเบียบ (Ordered mixture) ดัชนีที่น่าสนใจคือ ระดับของการผสม (Degree of mixedness), มิติแฟร็กทัลแบบพื้นที่ และแบบนับ (Area-based and count-based fractal dimension) และเลขโคออร์ดิเนชัน การจำลองด้วยคอมพิวเตอร์นำมาใช้เพื่อจำลองกรณีต่างๆของการกระจายตัวแบบจุดมคตินิตต่างๆ และแบบผสมของมัน ในระบบสารเติมแต่งองค์ประกอบเดียว ในกรณีของระบบที่มีสององค์ประกอบ ยังมีการแปรเปลี่ยนอัตราส่วนของความเข้มข้น อัตราส่วนของขนาดอนุภาค และความน่าจะเป็นในการเกาะของอนุภาค B บนผิวของอนุภาค A ด้วย

จากการศึกษาพบว่า แฟร็กทัลแบบพื้นที่ (Area-based fractal dimension) และ แบบนับ (Count-based fractal dimension) ไม่เปลี่ยนแปลงเมื่ออัตราส่วนของขนาดอนุภาคเพิ่มขึ้น ดังนั้นดัชนีเชิงปริมาณทั้งสอง จึงเป็นดัชนีที่เหมาะสมที่ใช้ประเมินระดับการกระจายตัวของสารเติมแต่งทั้งในระบบขององค์ประกอบเดียว และสององค์ประกอบ การศึกษานี้ยังแสดงให้เห็นว่าดัชนีทั้งสองสามารถใช้หาชนิดของการกระจายตัว และความน่าจะเป็นในการเกาะได้อย่างไร

สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

ภาควิชา วิศวกรรมเคมี
สาขาวิชา วิศวกรรมเคมี
ปีการศึกษา 2540

ลายมือชื่อนิสิต เมธี สุภาวิตา
ลายมือชื่ออาจารย์ที่ปรึกษา ศ. ดร. วิวัฒน์ ตัณฑะพานิชกุล
ลายมือชื่ออาจารย์ที่ปรึกษาร่วม ผศ. ดร. ชวิชัย ขรินพานิชกุล

C717004 : MAJOR CHEMICAL ENGINEERING

KEY WORD: QUANTITATIVE INDICES / DEGREE OF DISPERSION/ADDITIVES

MATHEE SUPHAWITA: DEVELOPMENT OF QUANTITATIVE INDICES FOR EVALUATING THE DEGREE OF DISPERSION OF ADDITIVES IN COMPOUNDED MATERIALS USING COMPUTER EXPERIMENTS. THESIS ADVISOR: PROF. WIWAT TANTHAPANICHAKOON, Ph.D. THESIS CO-ADVISOR: ASSIT. PROF. TAWATCHAI CHARINPANITKUL, Dr. Eng. 221 pp. ISBN 974-637-197-5

The objective of the present thesis is to study and propose some suitable quantitative indices for evaluating the degree of dispersion of single and binary additives in compounded materials and ordered mixtures. The indices of interest are the degree of mixedness, the area-based and count-based fractal dimensions and the coordination number. Computer simulations are used to simulate various ideal cases of dispersion and their combination in the single additive systems. For the binary systems, the concentration ratio, the particle size ratio and the adhesion probability of B onto A are also varied.

It is found that both the area-based and count-based fractal dimensions do not change when the particle size ratio increases, so they are suitable quantitative indices for evaluating the degree of dispersion of both single and binary additives systems. The investigation also shows how these indices can be used to characterize the type of dispersion and estimate the adhesion probability.



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ภาควิชา.....วิศวกรรมเคมี

สาขาวิชา.....วิศวกรรมเคมี

ปีการศึกษา.....2540

ลายมือชื่อนิสิต..... M. Suphawita

ลายมือชื่ออาจารย์ที่ปรึกษา..... Prof. ทานตะวัน

ลายมือชื่ออาจารย์ที่ปรึกษาร่วม..... T. Charinpanitkul

ACKNOWLEDGEMENT

The author would like to extend his sincere thanks to his advisor, Professor Wiwut Tanthapanichakoon, and co-advisor, Assistant Professor Tawatchai Charinpanitkul, for their inspiring guidance, advice, and helpful suggestions throughout this work. Their comments and suggestions help widen his perspectives in both knowledge and practical applications.

The author wishes to express his gratitude to Associate Professor Kroekchai Sukanjanajtee and Dr. Somprasong Srichai for their stimulative comments and participation as thesis committee and Ms. Nattaporn Tonanon for advice in presentation.

Furthermore, the author is very grateful to the National Science and Technology Development Agency (NSTDA) for providing his monthly scholarship and to MTEC for funding the research project headed by Professor Wiwut Tanthapanichakoon, which this work is a part of.

Besides, the author wishes to convey his most sincere gratitude to his family for their inspiration and support.

Finally, many thanks go to his friends and all those who have encouraged him over the years of his study.

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NOMENCLATURE

A	total area of the subdivision of interest [L^2]
A_i	area occupied by the additive particles in the i-th subdivision [L^2]
D	particle diameter [-]
D_A	particle diameter of core particle (particle A) [-]
D_B	particle diameter of adhering particle (particle B) [-]
$D_S(n)$	coefficient of deviation [-]
F_A	area-based fractal dimension [-]
F_A^*	normalized area-based fractal dimension [-]
F_C	count-based fractal dimension [-]
F_C^*	normalized count-based fractal dimension [-]
M	degree of mixedness
n^{-1}	similarity ratio [-]
n	number of times of sample division [-]
N_A	number of core particles (particle A) [-]
N_B	number of adhering particles (particle B) [-]
$N(n)$	the counted number of subsections that contain some additive particles [-]
R	radius of additive particle B [L]
$\bar{S}(n)$	mean area ratio of $S_i(n)$ [-]
$S_i(n)$	area ratio of additive particles [-]
X, Y	the position of an additive particle in the matrix [L,L]
XRND	uniform random number between zero and unity [-]
XRNG	normal random number (zero mean, unity variance) [-]
X', Y'	the position of particle B adhering onto A [L,L]
X_i	composition of key component in the spot sample [-]
\bar{X}_C	charged composition of key component [-]

\bar{X}_s	sample mean of X_i [-]
YRND	uniform random number between zero and unity [-]
YRNG	normal random number (zero mean, unity variance) [-]

Greek

θ	the angle of particle B from the x-axis [radian]
σ_s	standard deviation of $S_i(n)$ [-]
σ_0^2	variance of composition of key component in a completely segregated system [-]
σ_s^2	variance of sample subsection [-]
α_{AB}	adhesion probability [-]

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