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APPENDIX A

METHEMATICAL APPROACH

A.1 Expected values and moments

For discrete random variable X with probability mass function, $f_x(x_i)$, the expected value of X is defined as

$$E(X) = \Sigma x_i f_x(x_i), \qquad if \ \Sigma |x_i| f_x(x_i) < \infty \tag{A1}$$

For continuous random variable it is similarly defined as

$$E(X) = \int x f(x) dx \tag{A2}$$

The expected value of X, $E(X)$, is commonly referred to as the mean of X.

Besides the mean, the variance is probably the most commonly used measure of a distribution. The variance of X (It is commonly denoted by var(X) or σ^2) may be expressed in terms of its mean and its second moment about zero as follows :

$$\text{var}(X) = E[X-E(X)]^2 = E(X^2)-[E(X)]^2 \tag{A3}$$

Clearly, the variance of a constant is zero.

For two random variables x_i and x_j the expected value,

$$E[\{x_i-E(x_i)\}\{x_j-E(x_j)\}] = cov(x_i,x_j) \tag{A4}$$

is known as the covariance of x_i and x_j . The covariance is measure of the statistical dependency of two random variables. It is zero, if the two random variables are independent of each other.

A.2 Runge-Kutta methods

The RK4 (fourth order Runge-Kutta) method has proves both computationally efficient and accurate, and it is obtained by a clever choice of these constants in approximating slopes at various points. Without derivation, we will state the method as follows.

The RK4 method of approximation is to define y_{k+1} in terms of y_k by:

$$y_{k+1} = y_k+(1/6)h[W_{k1}+2W_{k2}+2W_{k3}+W_{k4}], \quad \text{(A5)}$$

where

$$W_{k1} = f_k \quad \text{(A6)}$$

$$W_{k2} = f(x_k+h/2 , y_k+hW_{k1}/2) \quad \text{(A7)}$$

$$W_{k3} = f(x_k+h/2 , y_k+hW_{k2}/2) \quad \text{(A8)}$$

$$W_{k4} = f(x_k+h , y_k+hW_{k2}+W_{k3}) \quad \text{(A9)}$$

A.3 The method of Least-Squares analysis

Various criteria might be used to estimate the coefficients in a model from experimental data. For each p data points, we can define the error e_j as the difference between the observation Y_j, $j = 1, 2, ...,p$, and the predicted model response $y_j(x)$

$$Y_j - y_j = e_j \qquad j = 1, 2, ..., p \quad \text{(A10)}$$

The independent variables in the vector x can be difference variables or difference functions of the same variable, such as x, x^2, x^3, *etc.* The independent variables are assumed to be known exactly, or at least the error involved in each element of x is substantially less than that involved in Y. You might think that the overall sum of the errors could be the utility as an objective function (F), however, this idea is not appropriate because such an objective function allows positive and negative errors to cancel. A second criterion would be to sum the absolute values of the errors

$$f_1 = \sum_{j=1}^{p} |e_j| \quad or \quad = \sum_{j=1}^{p} e_j^2 \quad \text{(A11)}$$

Another would be to minimize the absolute value of the maximum error. For example, if the estimate function of y_i is

$$y_j = A\text{-}Bx_j \quad \text{(A12)}$$

Thus

$$\min_{A,B} F = \sum_{j=1}^{p} (Y_j - A - Bx_j)^2 \quad \text{(A13)}$$

$$\frac{\partial F}{\partial A} = -2\sum_{j=1}^{p}(Y_j - A - Bx_j) = 0 \tag{A14}$$

$$\sum_{j=1}^{p} Y_j = nA + B\sum_{j=1}^{p} x_j \tag{A15}$$

$$\frac{\partial F}{\partial B} = -2\sum_{j=1}^{p} x_j(Y_j - A - Bx_j) \tag{A16}$$

$$\sum_{j=1}^{p} x_j Y_j = A\sum_{j=1}^{p} x_j + B\sum_{j=1}^{p} x_j^{\,2} \tag{A17}$$

$\therefore$

$$B = \frac{\sum_{j=1}^{p} x_j Y_j - n\bar{x}\bar{Y}}{\sum_{j=1}^{p} x_j^2 - n\bar{x}^2} \tag{A18}$$

$$A = \bar{Y} - B\bar{x} \tag{A19}$$

A.4 Euler' s method

Euler' s method is an approach for approximating the solution of an initial value problem and is to define y_{k+1} in terms of y_k by:

$$Y_1 = Y_0 + (x_1 - x_0)f(x_0, Y_0) \tag{A20}$$

$$\vdots \qquad\qquad \vdots$$

$$Y_{k+1} = Y_k + (x_{k+1} - x_k)f(x_k, Y_k) \tag{A21}$$

or $$Y_{k+1} = Y_k + hf(x_k, Y_k) \tag{A22}$$

with

$$f(x,Y) = \frac{\partial Y}{\partial x} \quad ; Y(x_0) = y_0 \tag{A23}$$

A.5 Lagrange multiple method

Lagrange multiple method is the method to find out the solution of the optimization problem

The objective function is

$$\min_{x} f(x)$$

subject to

$$h(x) = 0 \tag{A24}$$

$$g(x) = 0 \tag{A25}$$

The Lagrangian Function can be written as

$$L(x, w1, w2) = f(x) + w1h(x) + w2g(x) \tag{A26}$$

and must differentiate equation (A26) with x, $w1$, $w2$

$$\frac{dL}{dx} = 0 \tag{A27}$$

$$\frac{dL}{dw1} = 0 \tag{A28}$$

$$\frac{dL}{dw2} = 0 \tag{A29}$$

then , can achieve the solution of x, $w1$,and $w2$

APPENDIX B

KINETIC MODEL AND SIMULATION RESULT

B.1 Kinetic model for MODEL I

The assumptions :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}$$

2. The hydrogen dose not break in free atom.
3. The product dose not be adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = 1/(1+K_{activity}\Sigma Ac)$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = K_{H2}C_{H2}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*,1996).

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA} and θ_{PD} in the rate equations. Obtain

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}K_{H2}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^2$$

$$-r_{Ac} = K1C_{Ac}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^2$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^2$$

$$-r_{MA} = K4C_{MA}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^2$$

$$-r_{PD} = K5C_{PD}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^2$$

B.2 The simulation result of the MODEL I

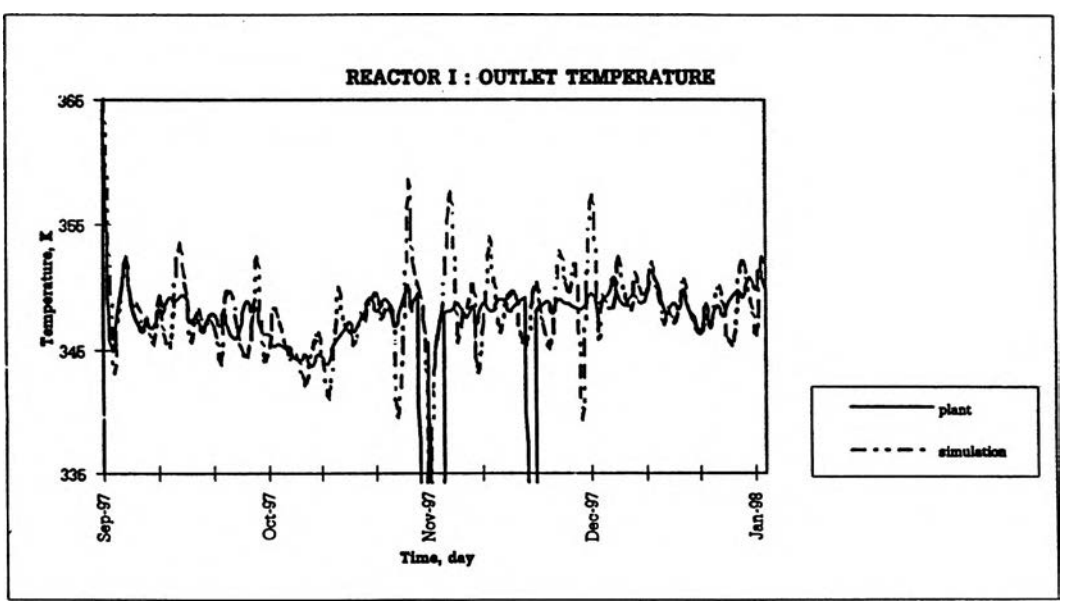

Figure B.1 MODEL I : Outlet temperature of reactor I with error 0.576%

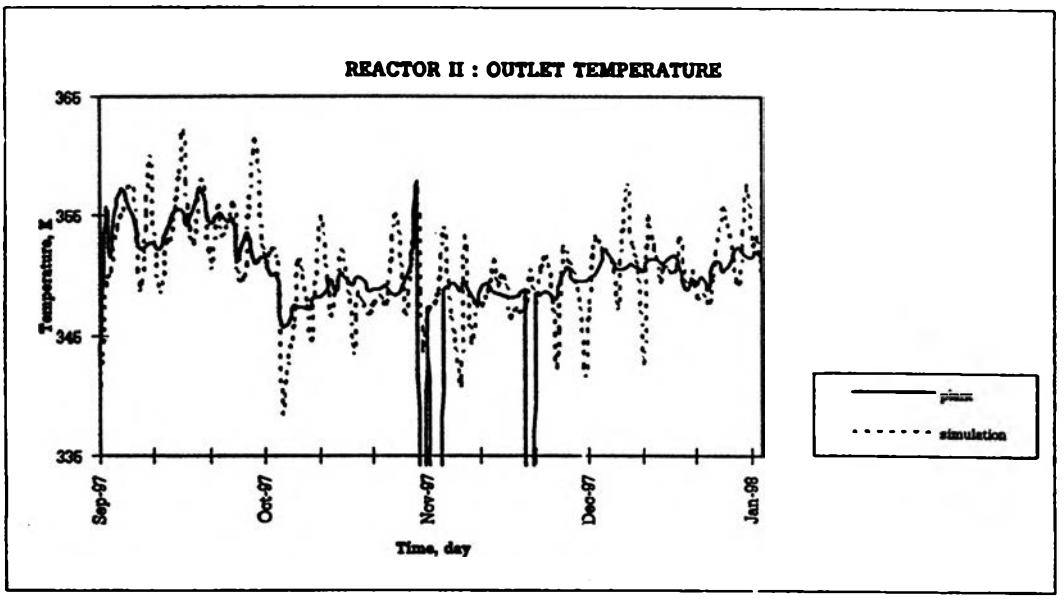

Figure B.2 MODEL I : Outlet temperature of reactor II with error 0.65%

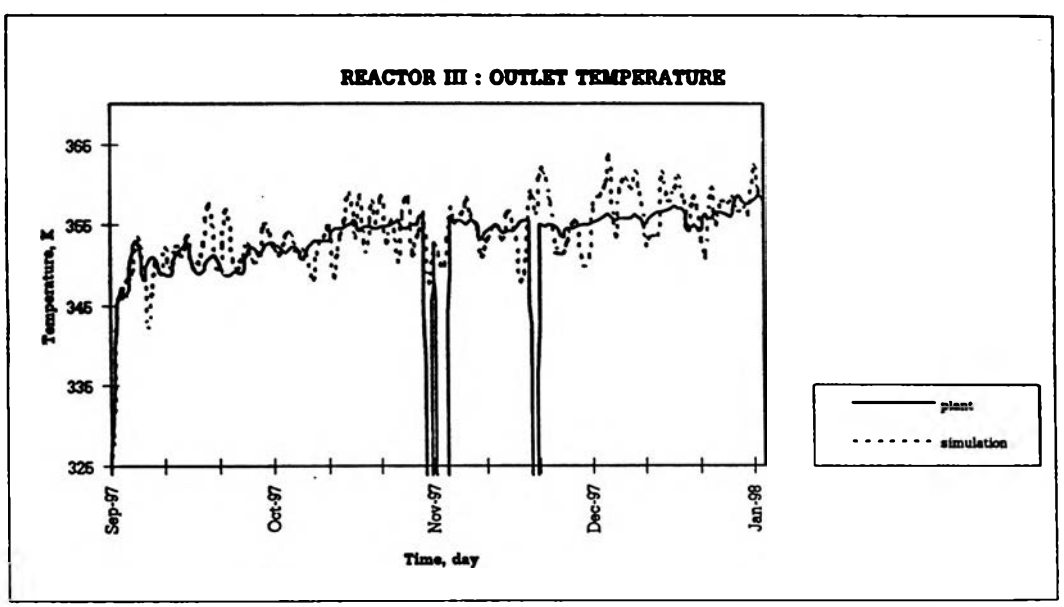

Figure B.3 MODEL I : Outlet temperature of reactor III with error 0.66%

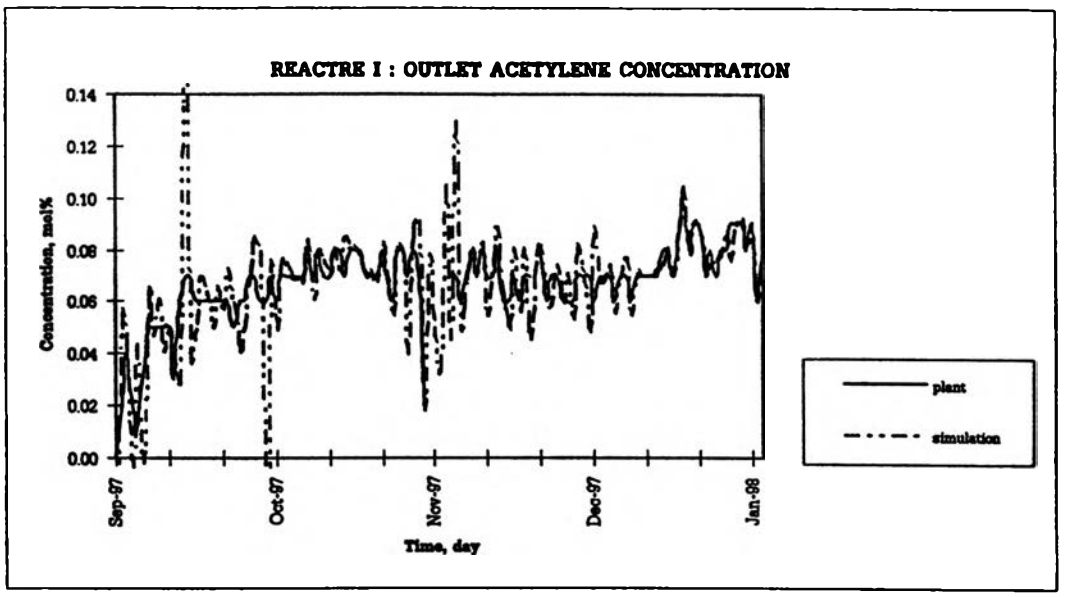

Figure B.4 MODEL I : Outlet acetylene concentration of reactor I with error 36.22%

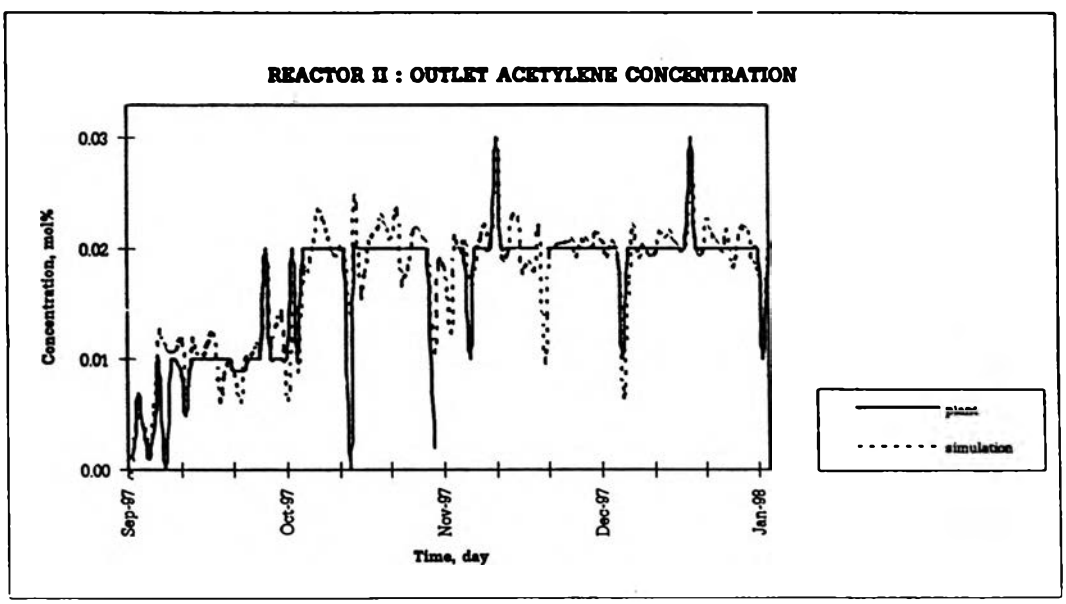

Figure B.5 MODEL I : Outlet acetylene concentration of reactor II with error 9.84%

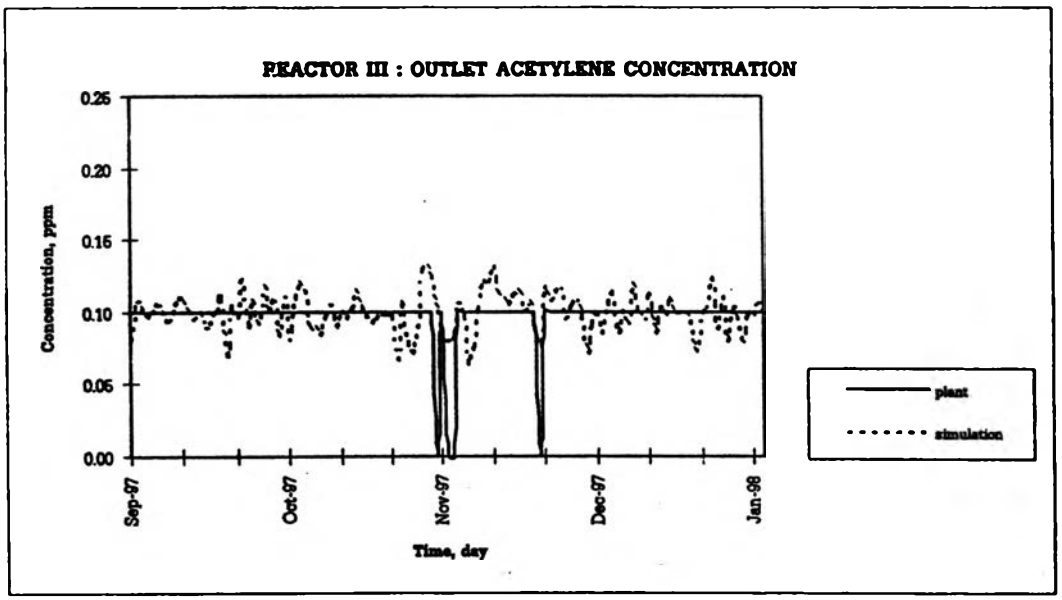

Figure B.6 MODEL I : Outlet acetylene concentration of reactor III with error **10.08%**

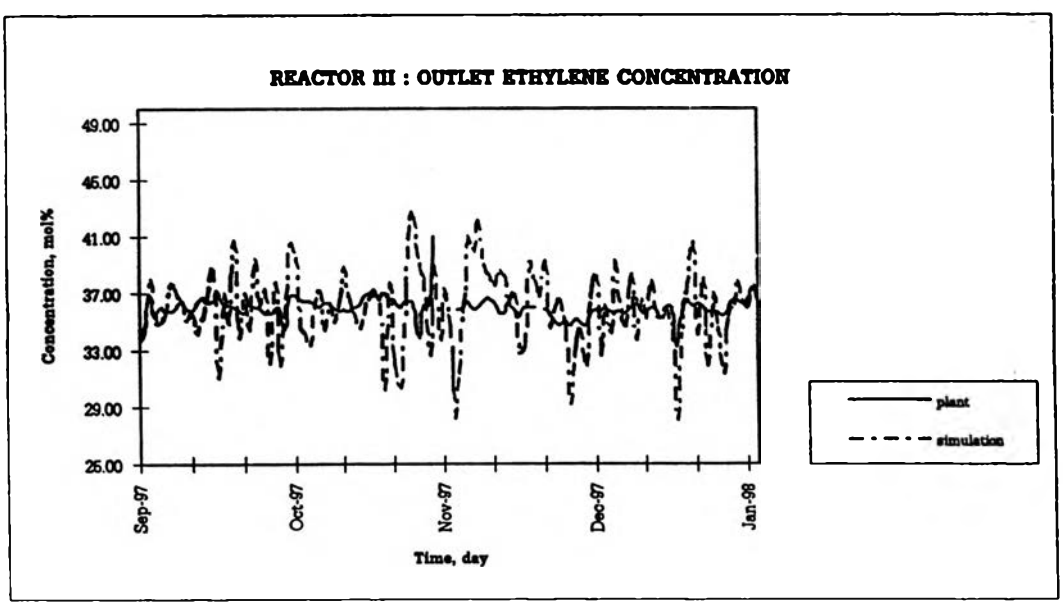

Figure B.7 MODEL I : Outlet ethylene concentration of reactor III with error 5.41%

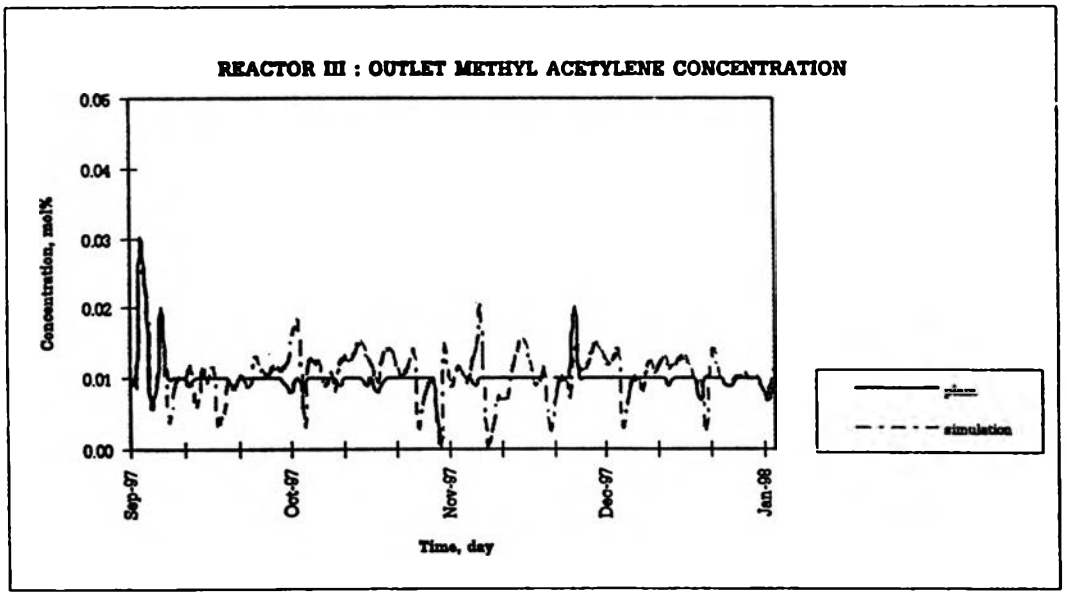

Figure B.8 MODEL I : Outlet methyl acetylene concentration of reactor III with error 25.52%

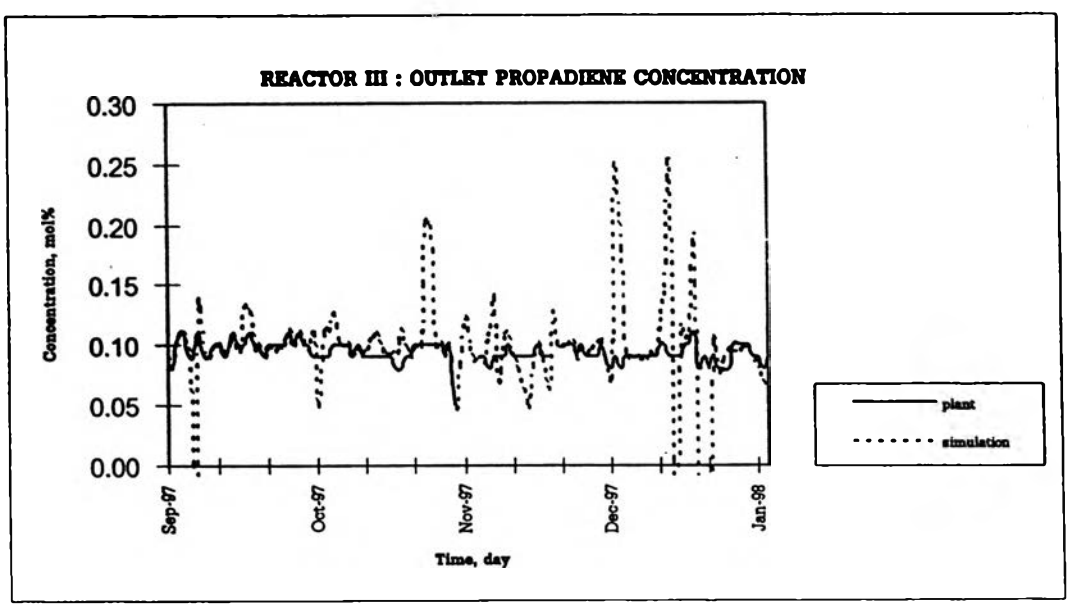

Figure B.9 MODEL I : Outlet propadiene concentration of reactor III with error 32.96%

B.3 Kinetic model for MODEL II

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}$$

2. The hydrogen does not break into free atom.
3. The product dose not be adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = K_{activity}EXP(E_{activity}/RT)C_{Ac}$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = K_{H2}C_{H2}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}K_{H2}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^2$$

$$-r_{Ac} = K1C_{Ac}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^2$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ K_{H2}C_{H2} + K_{CO}C_{CO})^2$$

$$-r_{MA} = K4C_{MA}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ K_{H2}C_{H2} + K_{CO}C_{CO})^2$$

$$-r_{PD} = K5C_{PD}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ K_{H2}C_{H2} + K_{CO}C_{CO})^2$$

B.4 The simulation result of the MODEL II

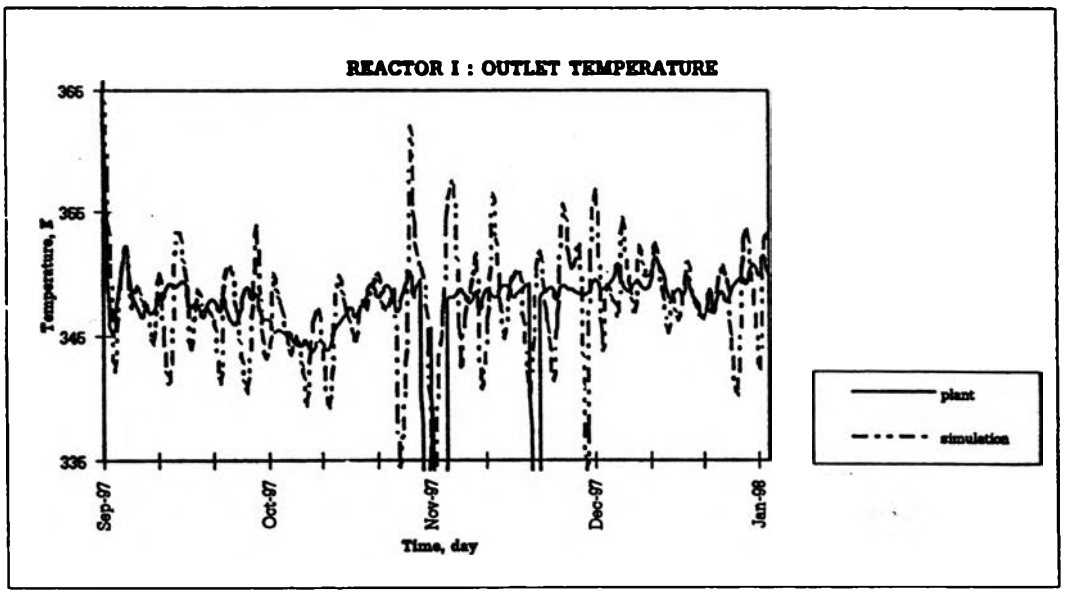

Figure B.10 MODEL II : Outlet temperature of reactor I with error 0.94%

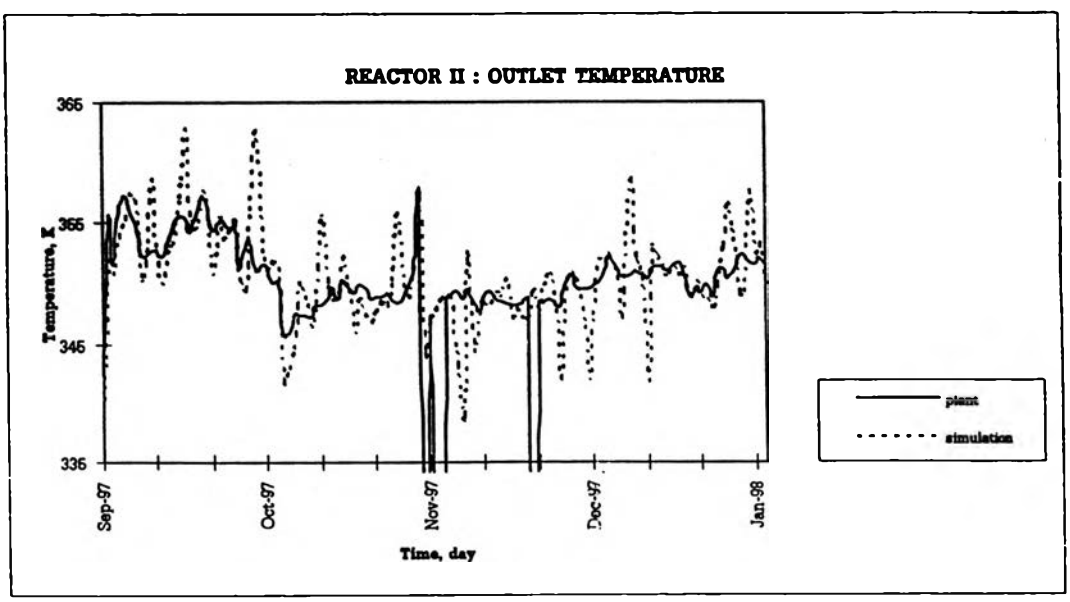

Figure B.11 MODEL II : Outlet temperature of reactor II with error 0.56%

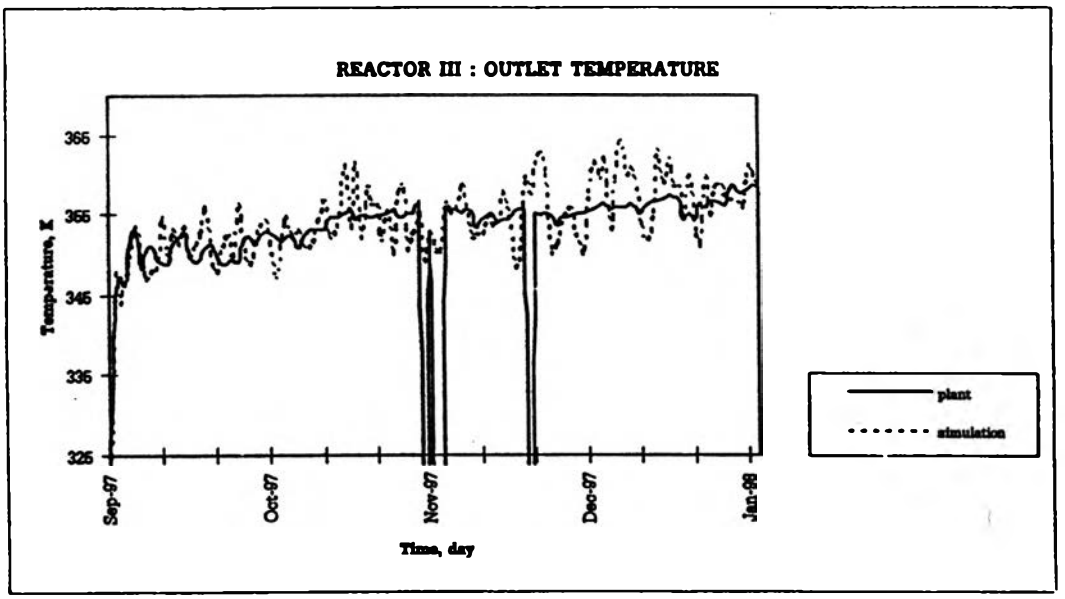

Figure B.12 MODEL II : Outlet temperature of reactor III with error 0.75%

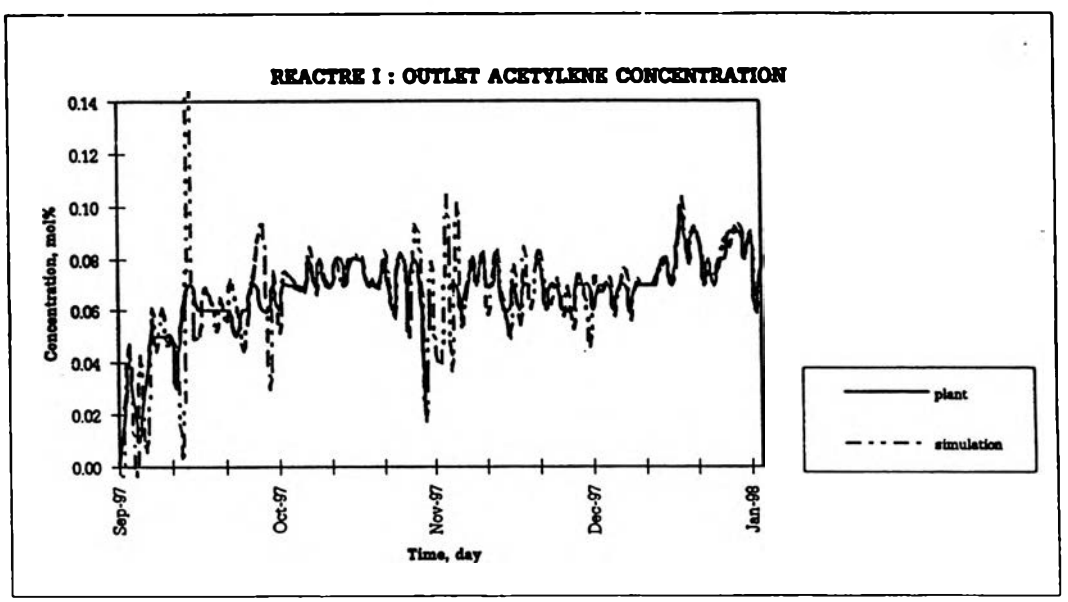

Figure B.13 MODEL II : Outlet acetylene concentration of reactor I with error 35.7%

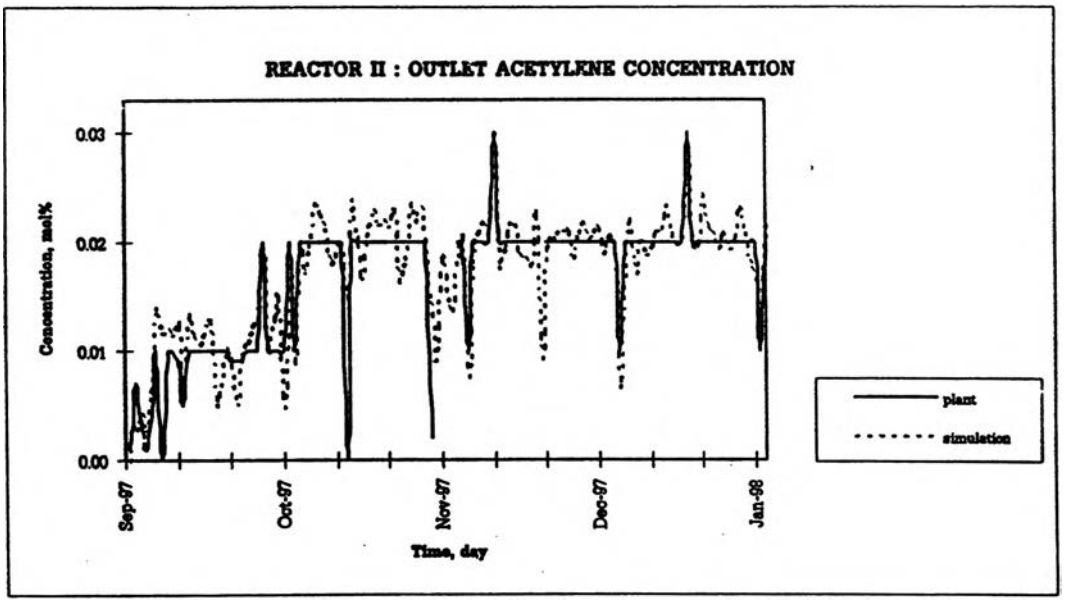

Figure B.14 MODEL II : Outlet acetylene concentration of reactor II with error 12.28%

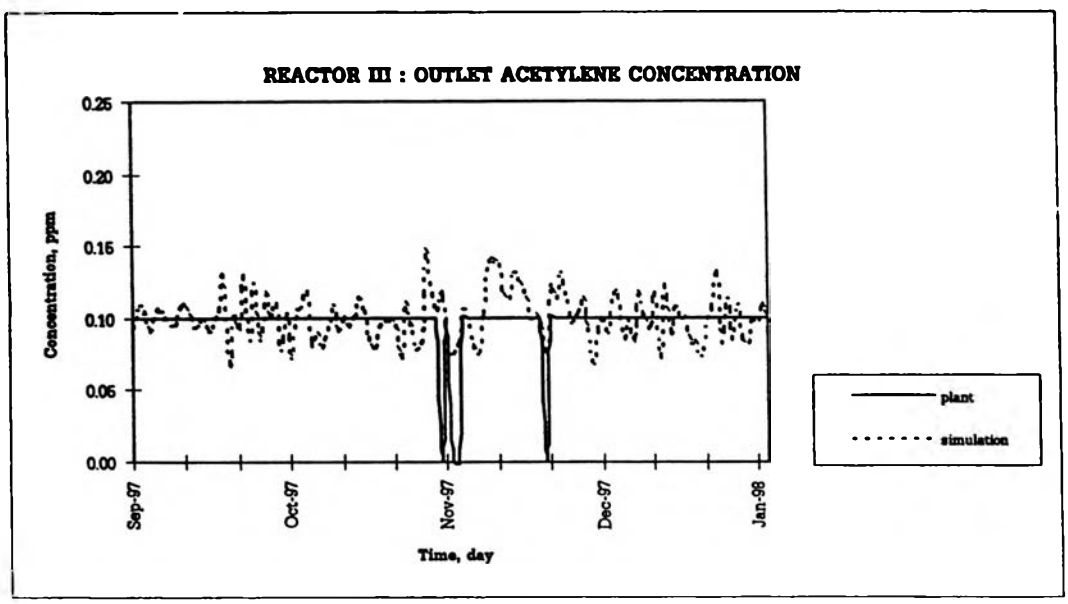

Figure B.15 MODEL II : Outlet acetylene concentration of reactor III with error 12.65%

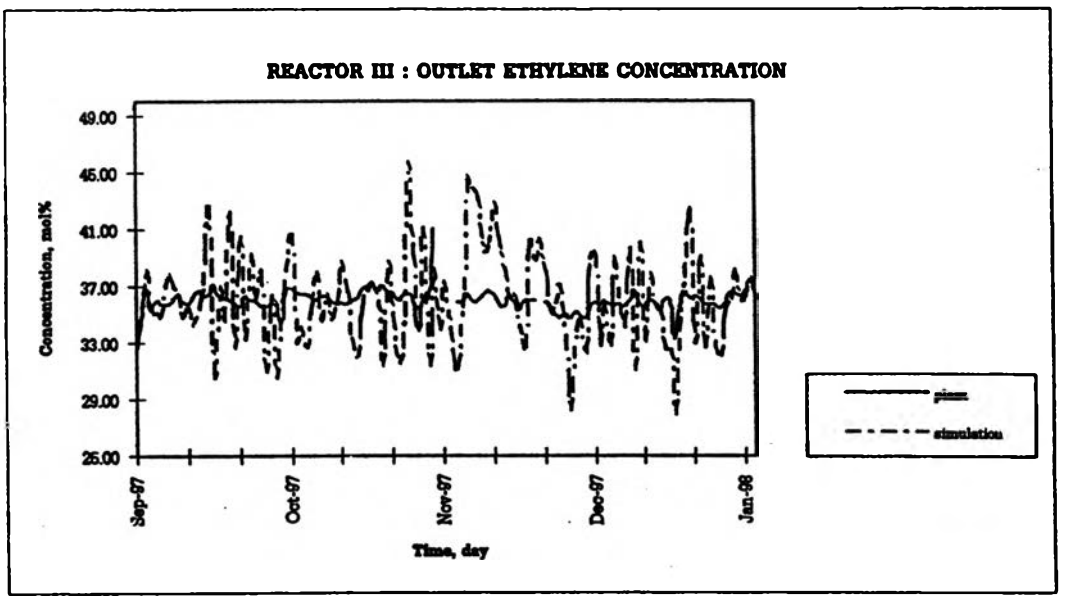

Figure B.16 MODEL II : Outlet ethylene concentration of reactor III with error 6.93%

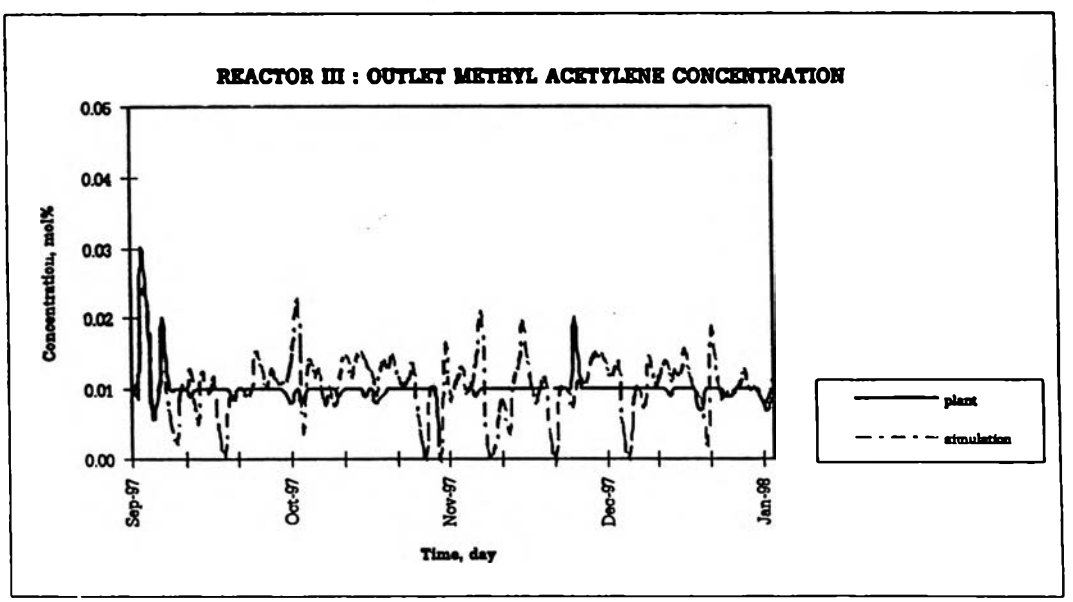

Figure B.17 MODEL II : Outlet methyl acetylene concentration of reactor III with error 30.92%

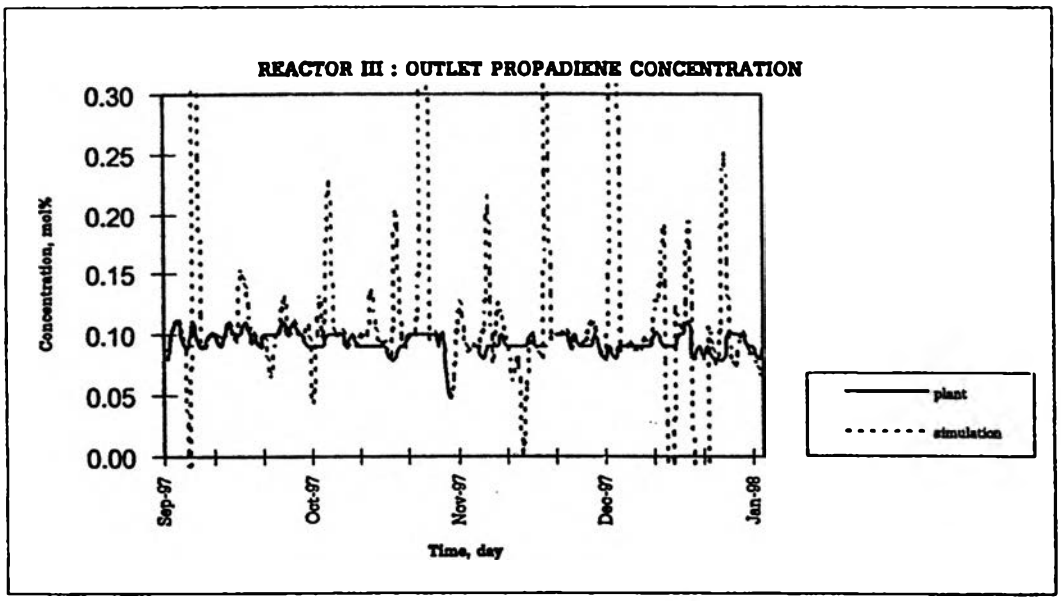

Figure B.18 MODEL II : Outlet propadiene concentration of reactor III with error **74.71%**

B.5 Kinetic model for MODEL III

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}(1-\Sigma\theta)$$

2. The hydrogen does not break into free atom.
3. The product is adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = 1/(1+K_{activity}\Sigma Ac)$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = K_{H2}C_{H2}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}K_{H2}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^3$$

$$-r_{Ac} = K1C_{Ac}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^3$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^3$$

$$-r_{MA} = K4C_{MA}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^3$$

$$-r_{PD} = K5C_{PD}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^3$$

B.6 The simulation result of the MODEL III

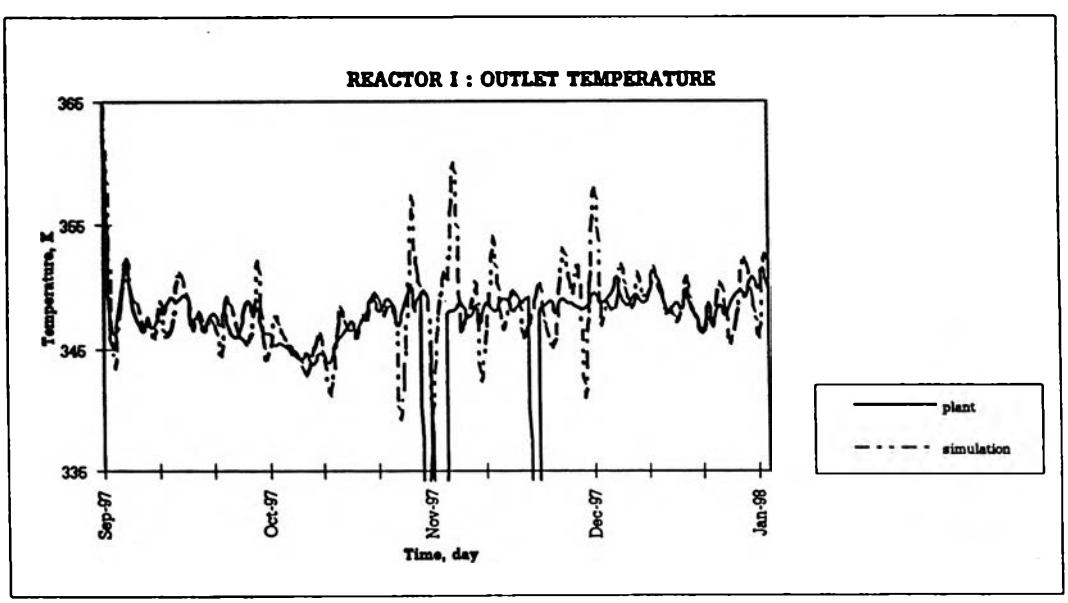

Figure B.19 MODEL III : Outlet temperature of reactor I with error 0.49%

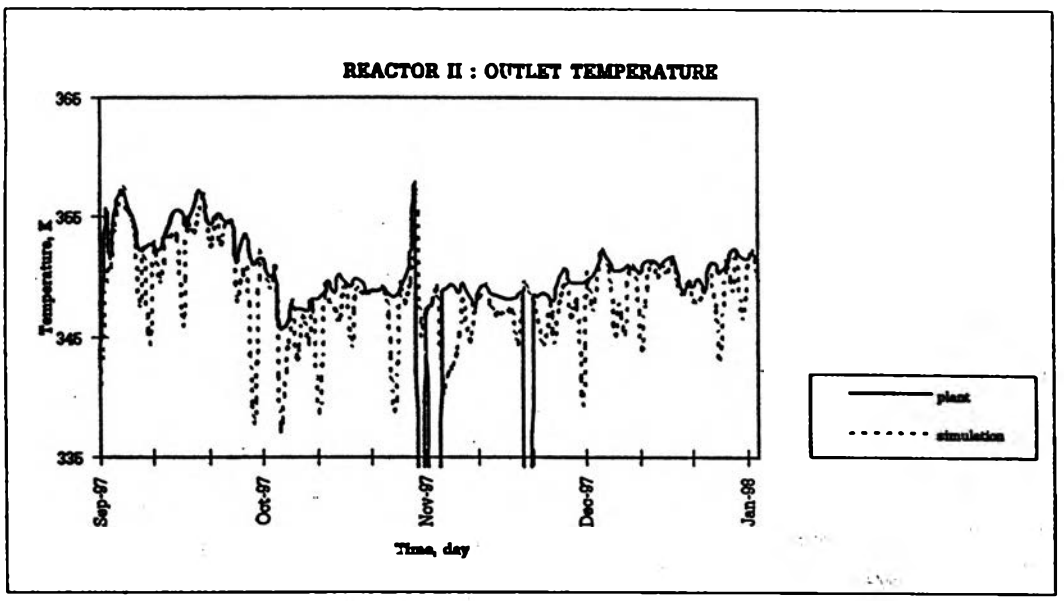

Figure B.20 MODEL III : Outlet temperature of reactor II with error 0.63%

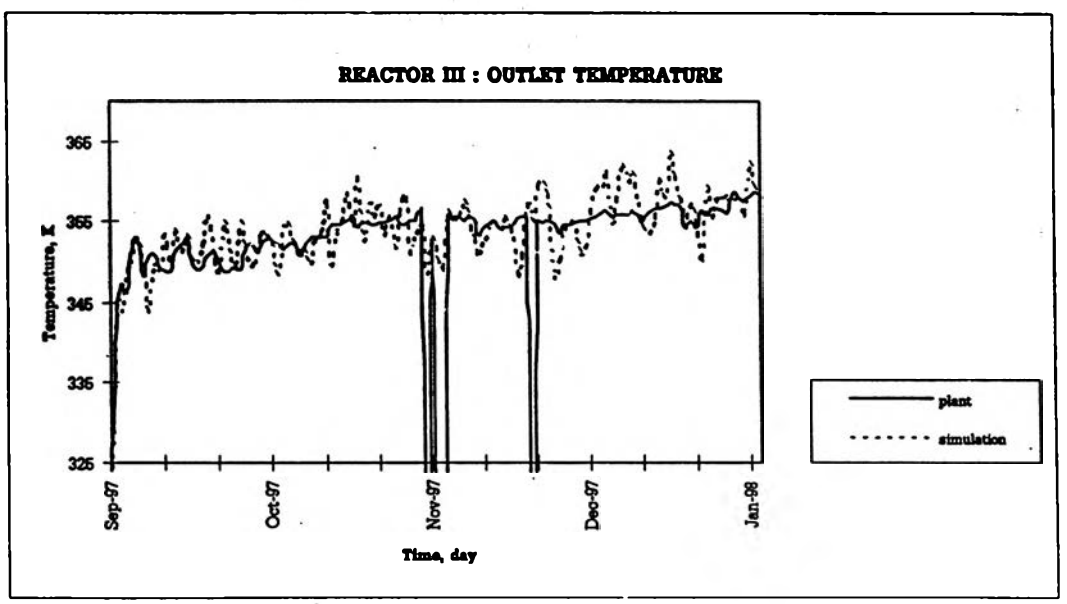

Figure B.21 MODEL III : Outlet temperature of reactor III with error 0.6%

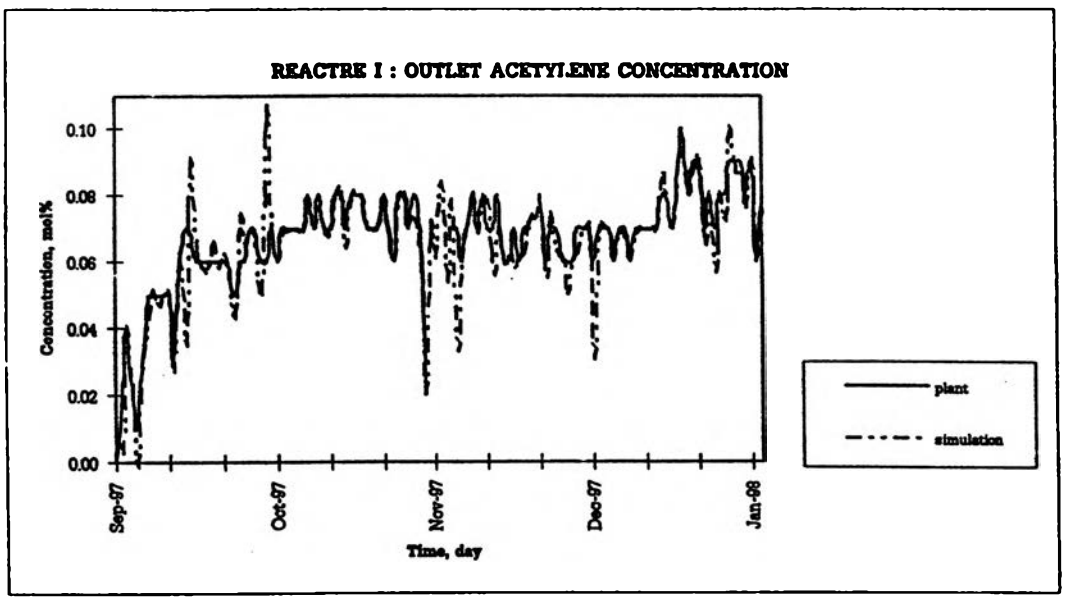

Figure B.22 MODEL III : Outlet acetylene concentration of reactor I with error 11.86%

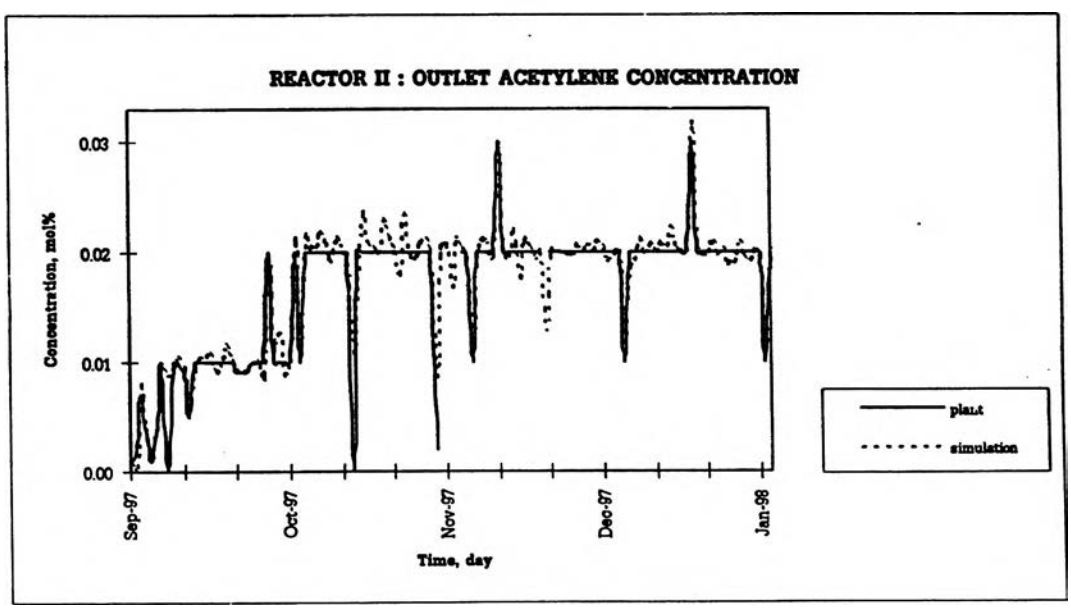

Figure B.23 MODEL III : Outlet acetylene concentration of reactor II with error 4.92%

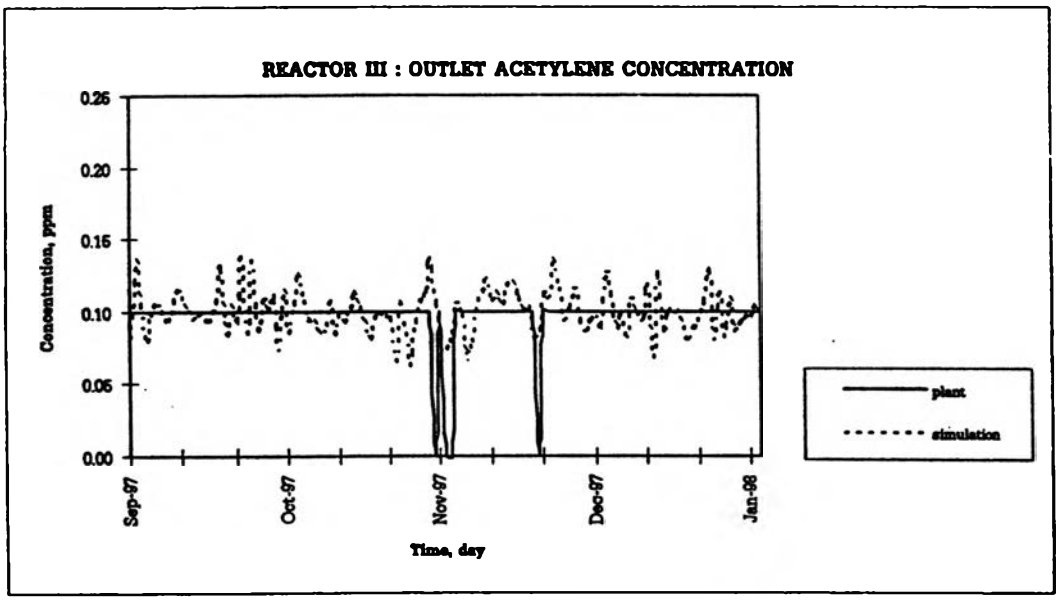

Figure B.24 MODEL III : Outlet acetylene concentration of reactor III with error 11.81%

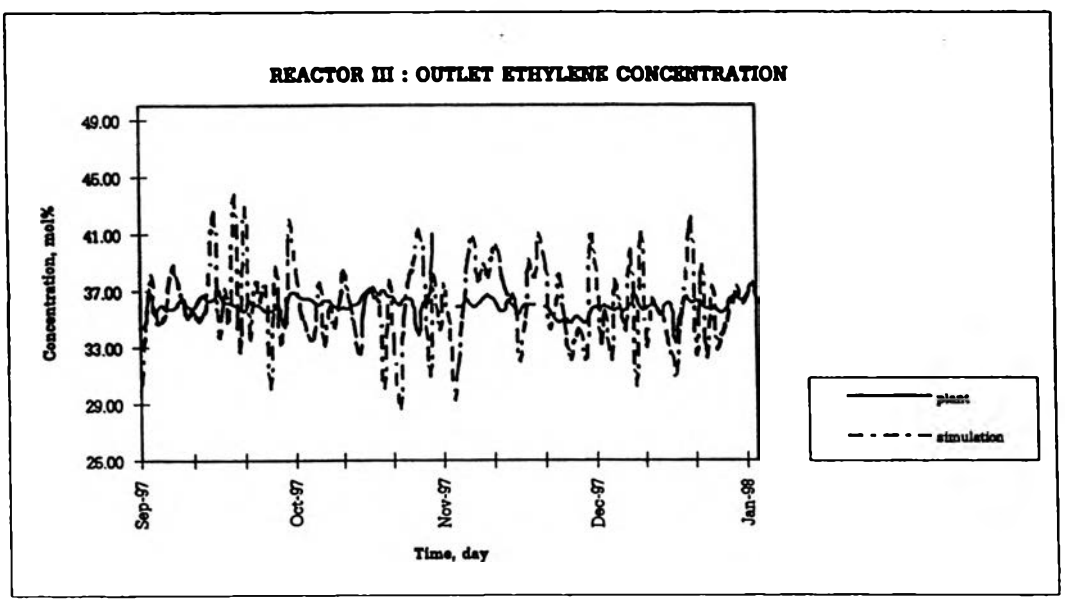

Figure B.25 MODEL III : Outlet ethylene concentration of reactor III with error 6.15%

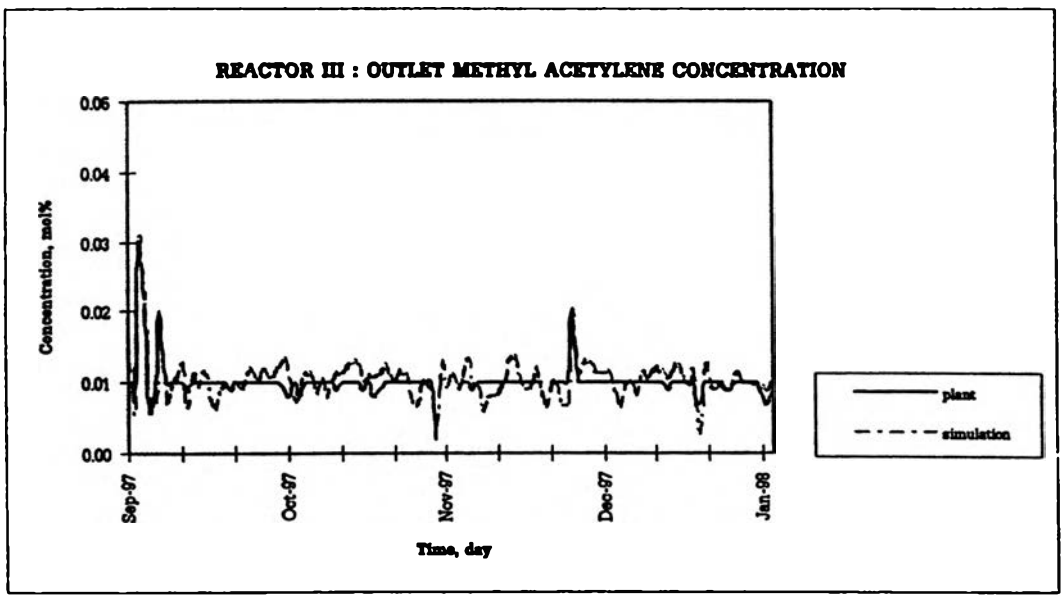

Figure B.26 MODEL III : Outlet methyl acetylene concentration of reactor III with error 16.34%

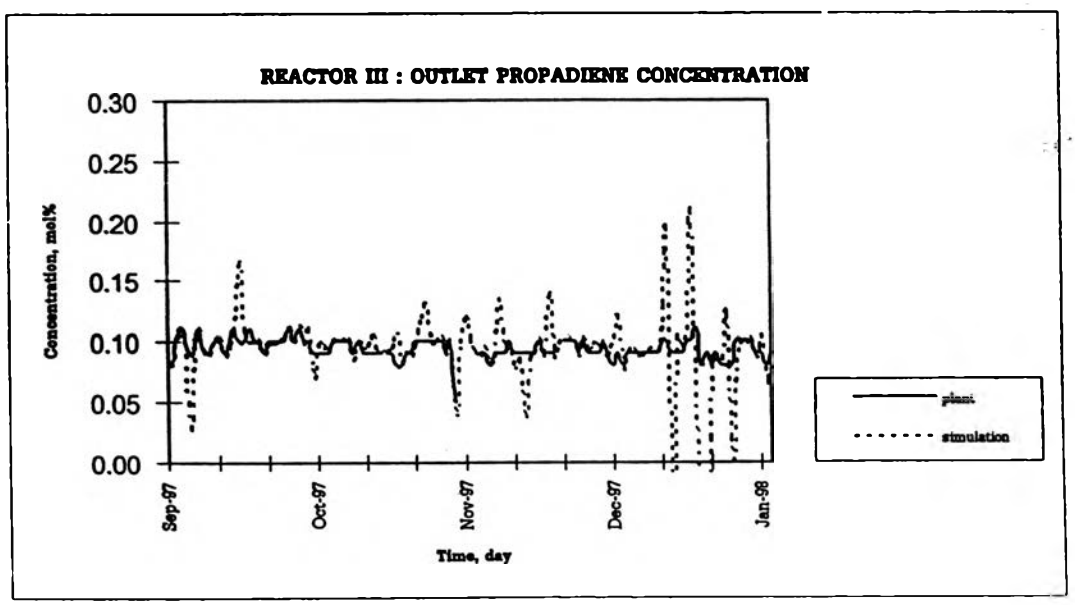

Figure B.27 MODEL III : Outlet propadiene concentration of reactor III with error 18.52%

B.7 Kinetic model for MODEL IV

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}(1-\Sigma\theta)$$

2. The hydrogen does not break into free atom.
3. The product is adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = K_{activity}EXP(E_{activity}/RT)C_{Ac}$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = K_{H2}C_{H2}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}K_{H2}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^3$$

$$-r_{Ac} = K1C_{Ac}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+K_{H2}C_{H2}+K_{CO}C_{CO})^3$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ K_{H2}C_{H2} + K_{CO}C_{CO})^3$$

$$-r_{MA} = K4C_{MA}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ K_{H2}C_{H2} + K_{CO}C_{CO})^3$$

$$-r_{PD} = K5C_{PD}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ K_{H2}C_{H2} + K_{CO}C_{CO})^3$$

B.8 The simulation result of the MODEL IV

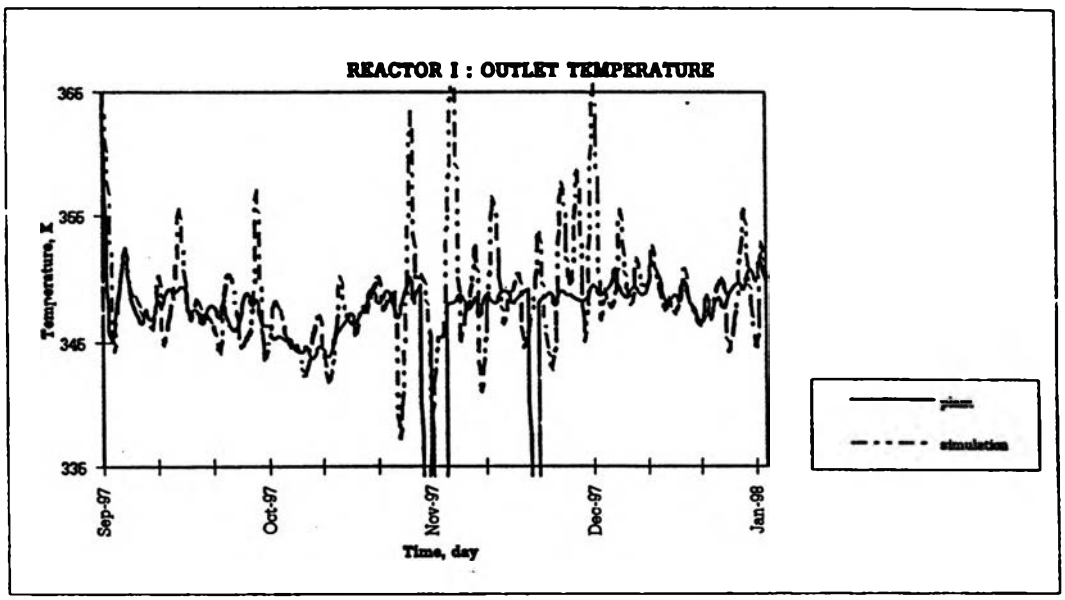

Figure B.28 MODEL IV : Outlet temperature of reactor I with error 0.74%

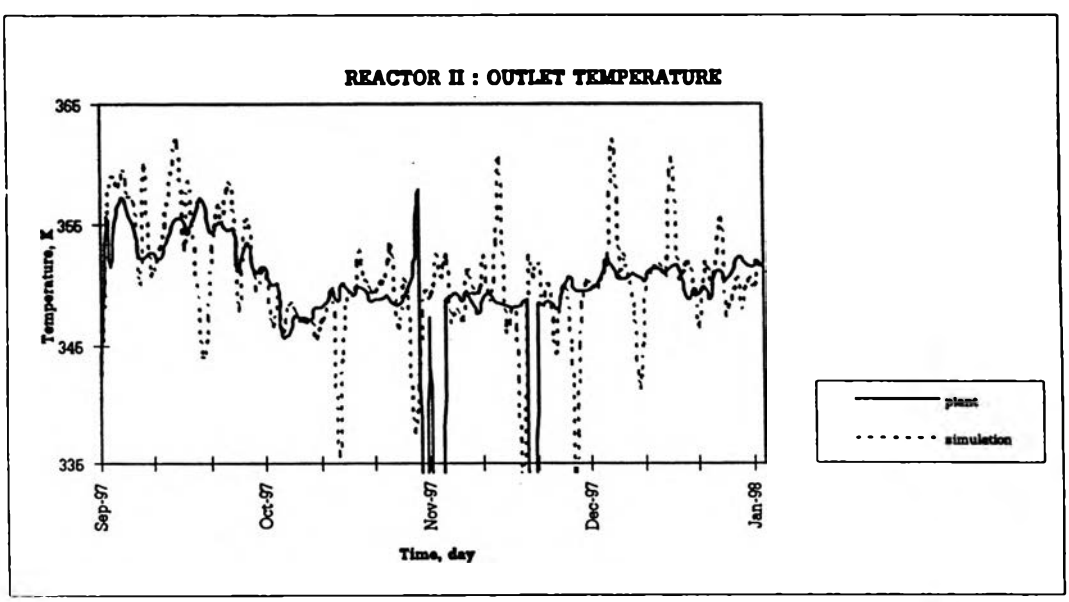

Figure B.29 MODEL IV : Outlet temperature of reactor II with error 0.79%

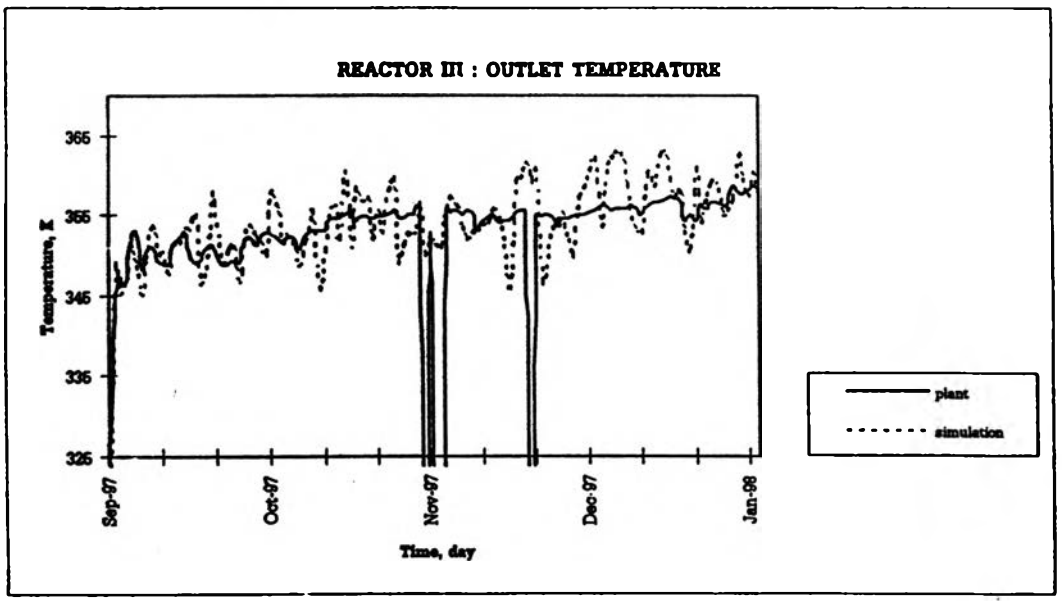

Figure B.30 MODEL IV : Outlet temperature of reactor III with error 0.76%

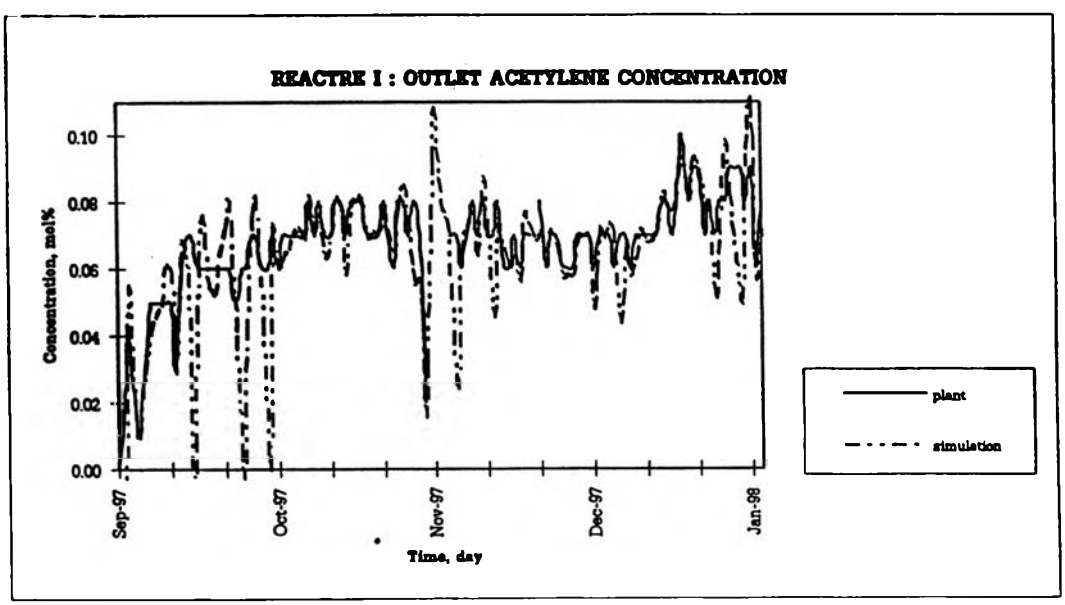

Figure B.31 MODEL IV : Outlet acetylene concentration of reactor I with error 20.74%

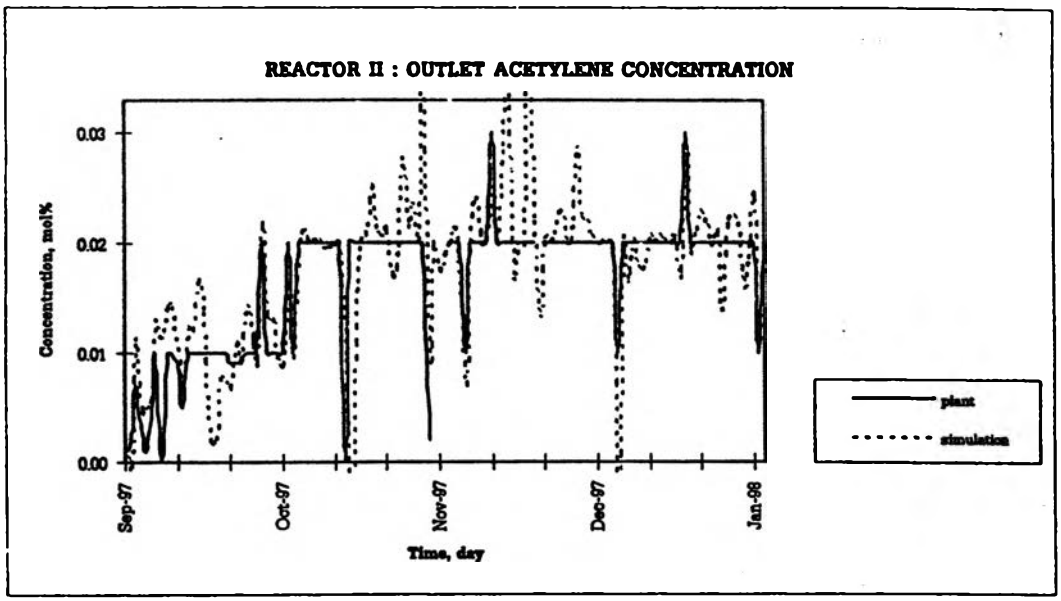

Figure B.32 MODEL IV : Outlet acetylene concentration of reactor II with error 18.92%

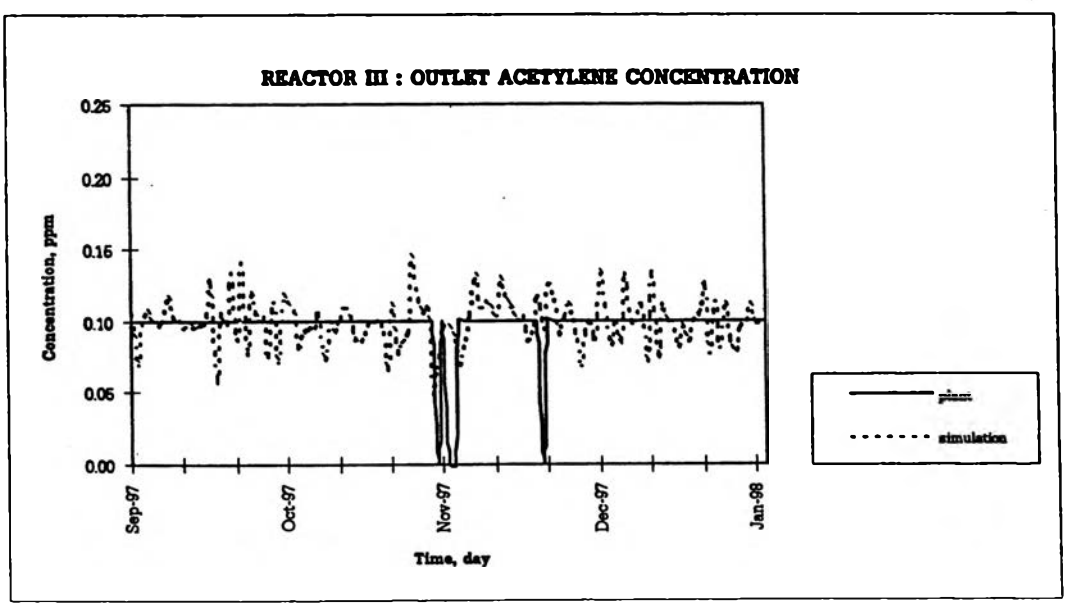

Figure B.33 MODEL IV : Outlet acetylene concentration of reactor III with error 12.62%

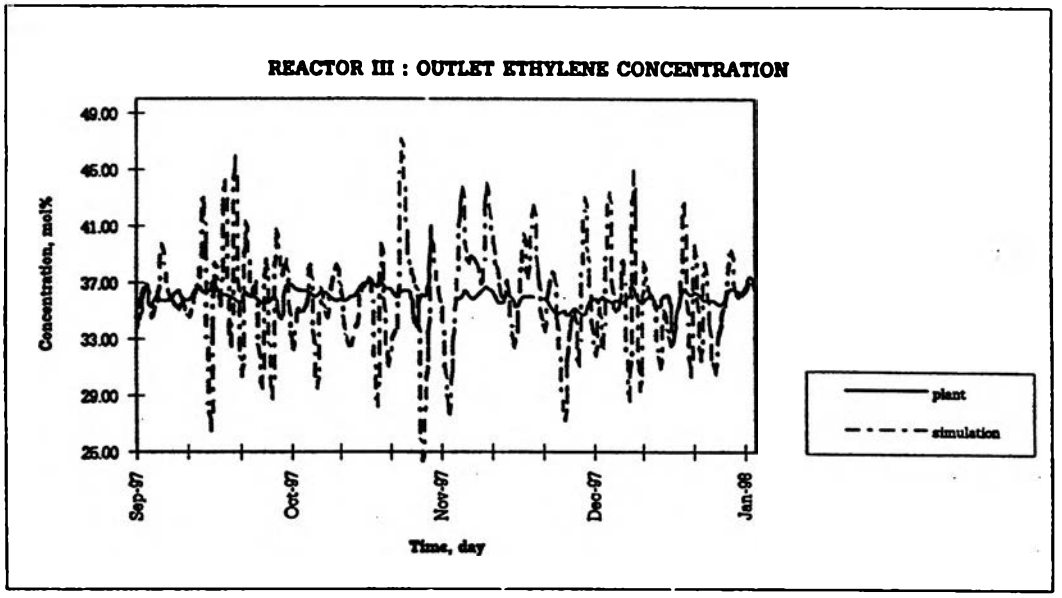

Figure B.34 MODEL IV : Outlet ethylene concentration of reactor III with error 8.03%

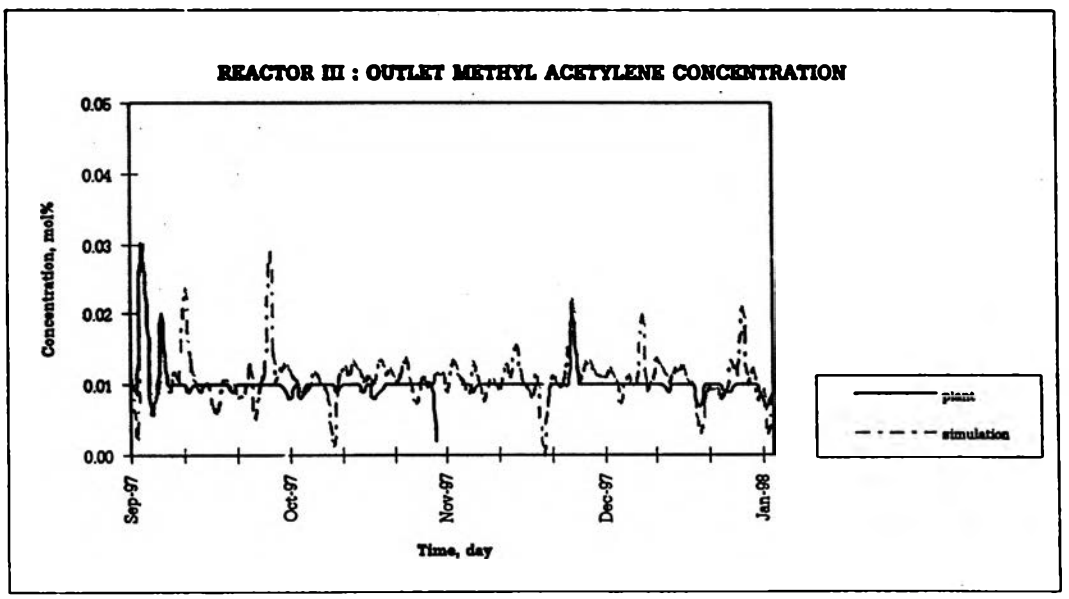

Figure B.35 MODEL IV : Outlet methyl acetylene concentration of reactor III with error 26.13%

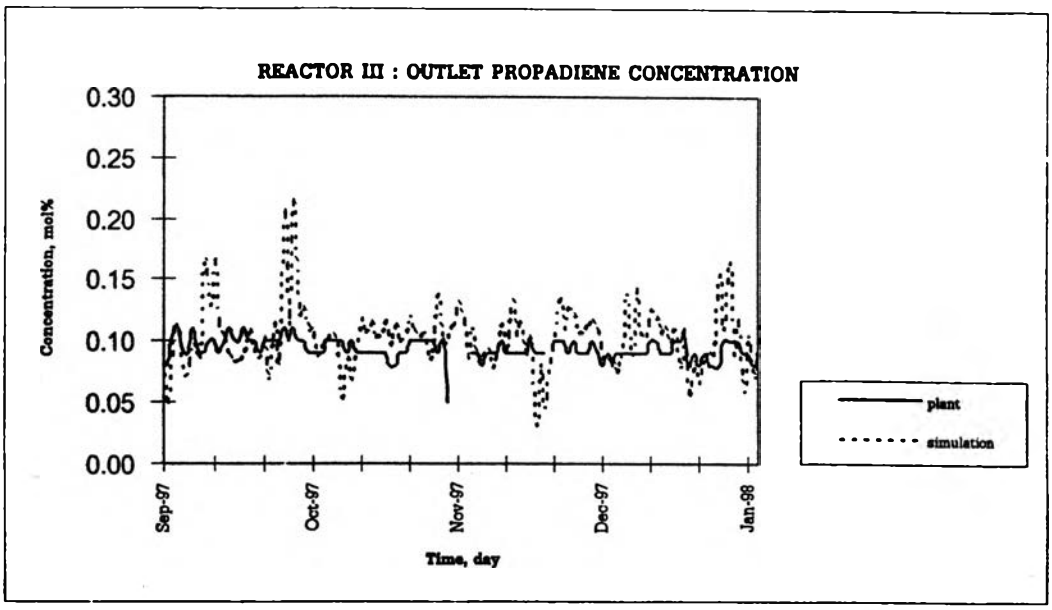

Figure B.36 MODEL IV : Outlet propadiene concentration of reactor III with error 21.45%

B.9 Kinetic model for MODEL VI

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}$$

2. The hydrogen breaks into free atom.
3. The product dose not be adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = K_{activity}EXP(E_{activity}/RT)C_{Ac}$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = (K_{H2}C_{H2})^{0.5}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}(K_{H2}C_{H2})^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^2$$

$$-r_{Ac} = K1C_{Ac}C_{H2}^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^2$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^2$$

$$-r_{MA} = K4C_{MA}C_{H2}^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^2$$

$$-r_{PD} = K5C_{PD}C_{H2}^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^2$$

B.10 The simulation result of the MODEL VI

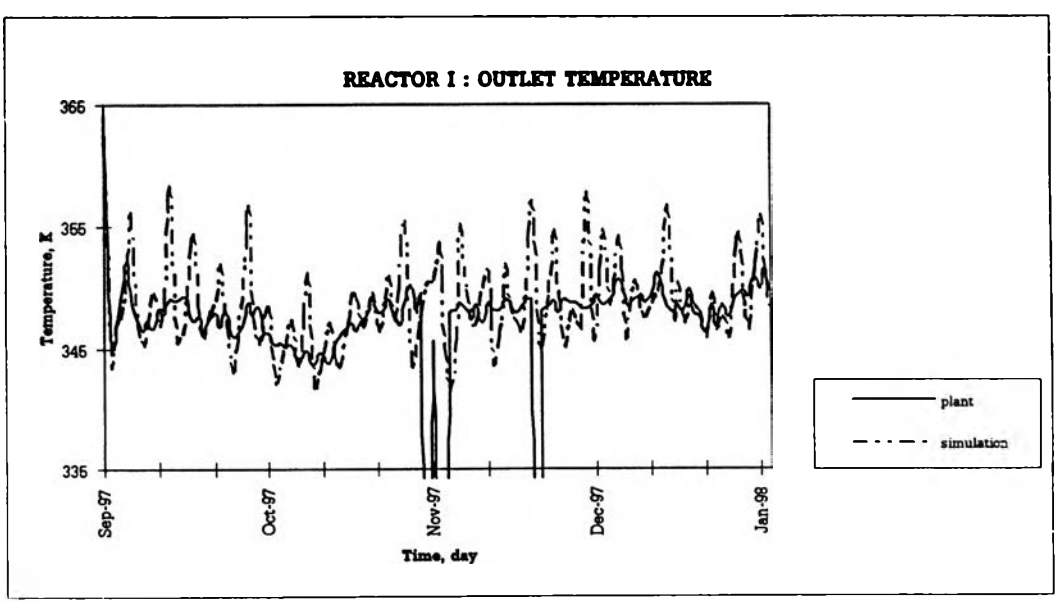

Figure B.37 MODEL VI : Outlet temperature of reactor I with error 0.67%

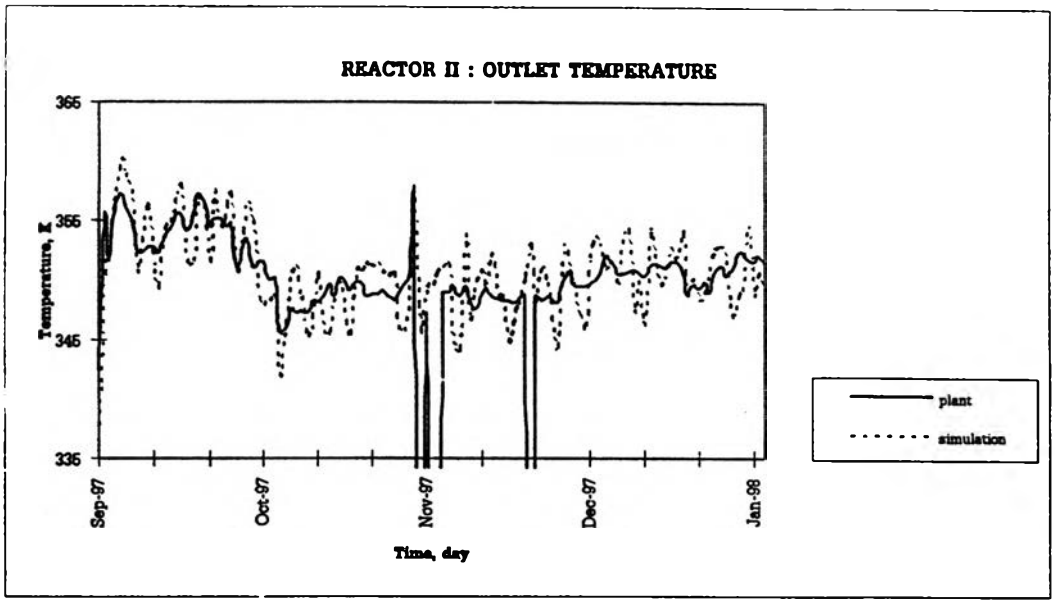

Figure B.38 MODEL VI : Outlet temperature of reactor II with error 0.59%

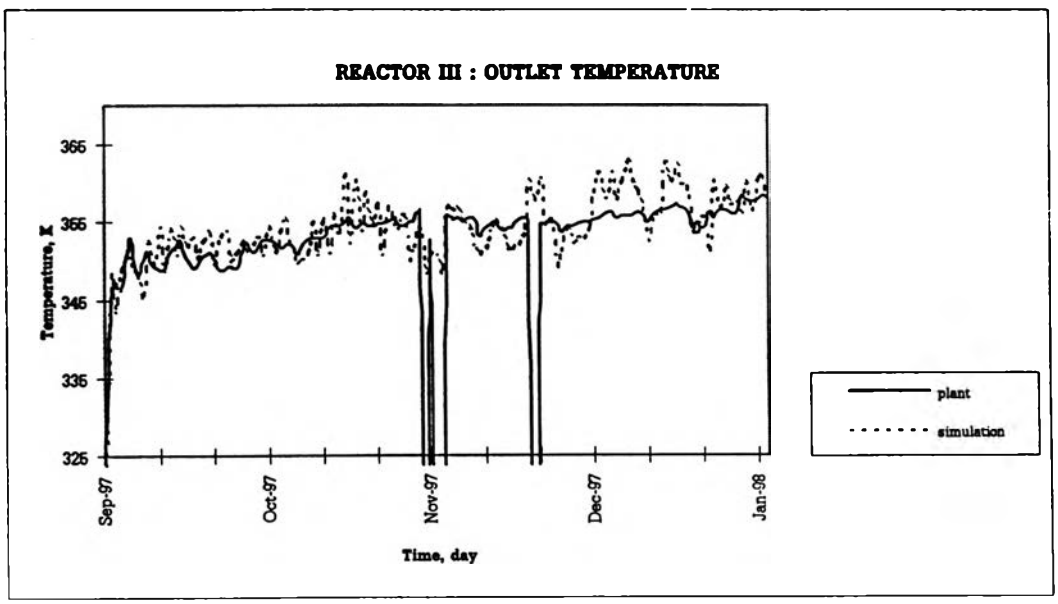

Figure B.39 MODEL VI : Outlet temperature of reactor III with error 0.68%

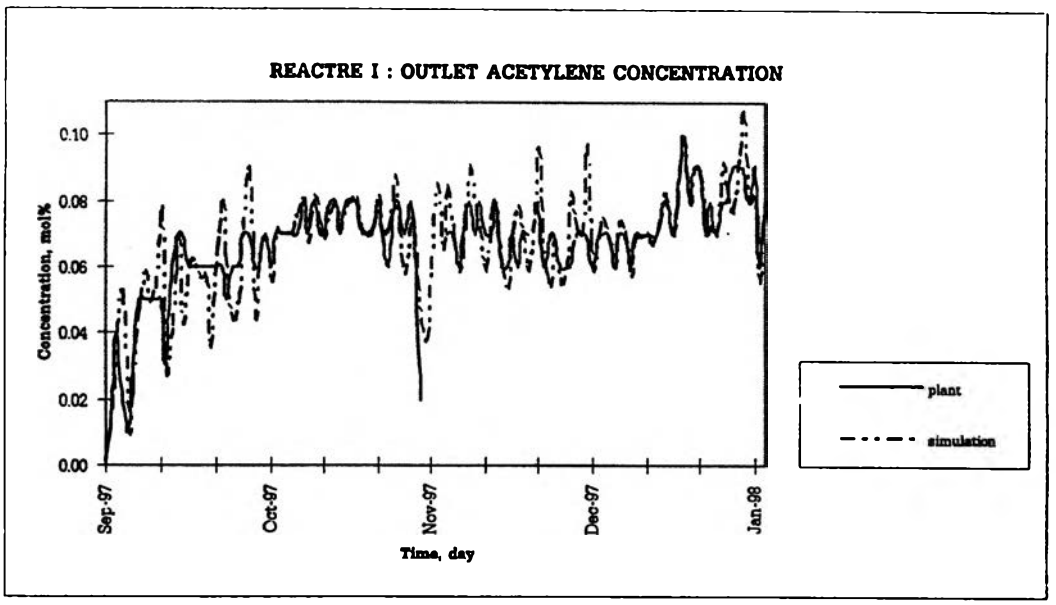

Figure B.40 MODEL VI : Outlet acetylene concentration of reactor I with error 12.64%

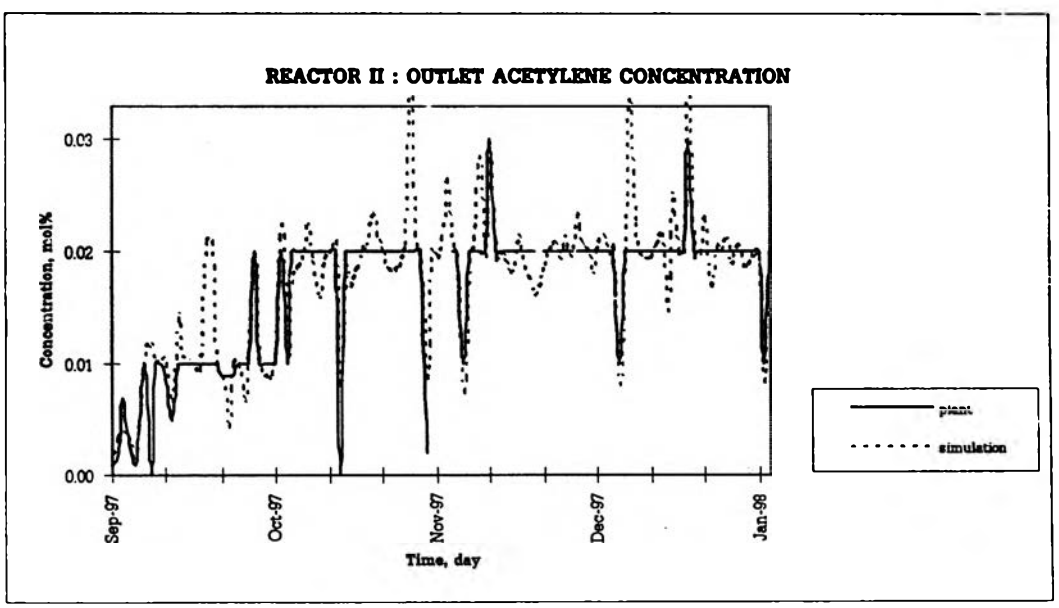

Figure B.41 MODEL VI : Outlet acetylene concentration of reactor II with error 11.87%

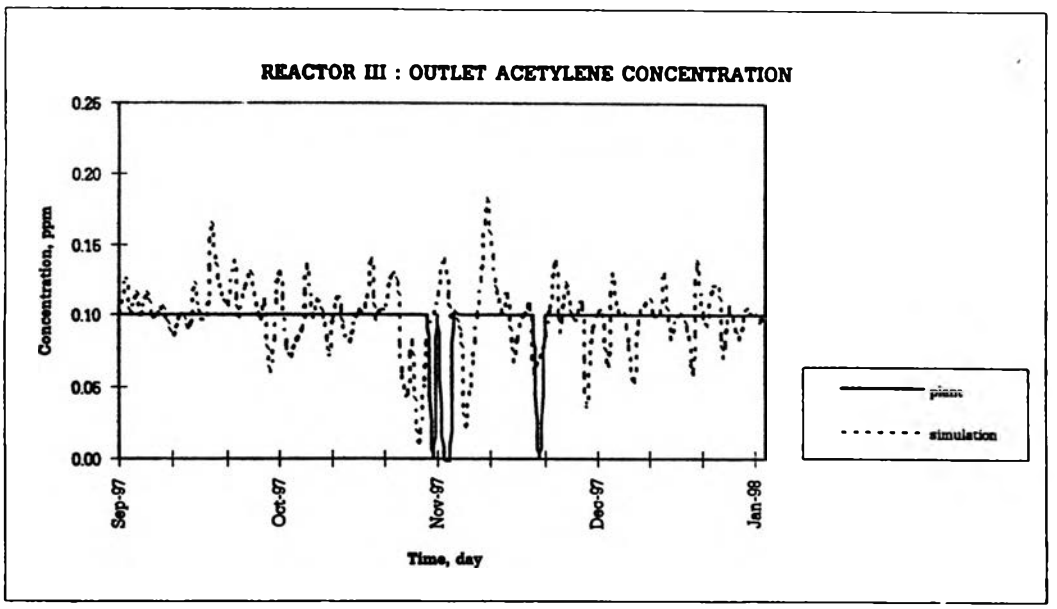

Figure B.42 MODEL VI : Outlet acetylene concentration of reactor III with error 16.92%

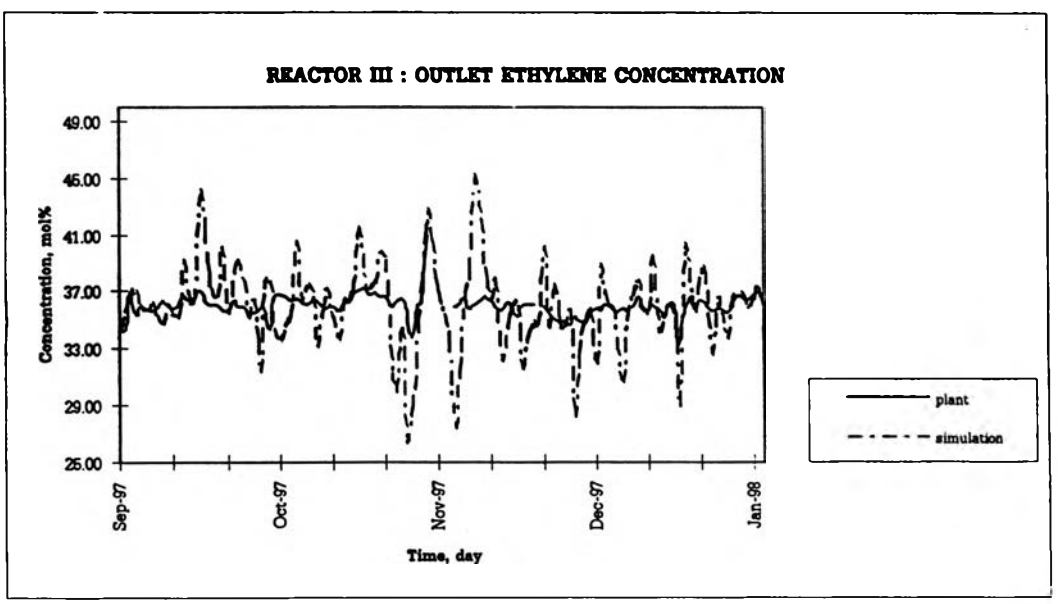

Figure B.43 MODEL VI : Outlet ethylene concentration of reactor III with error 5.16%

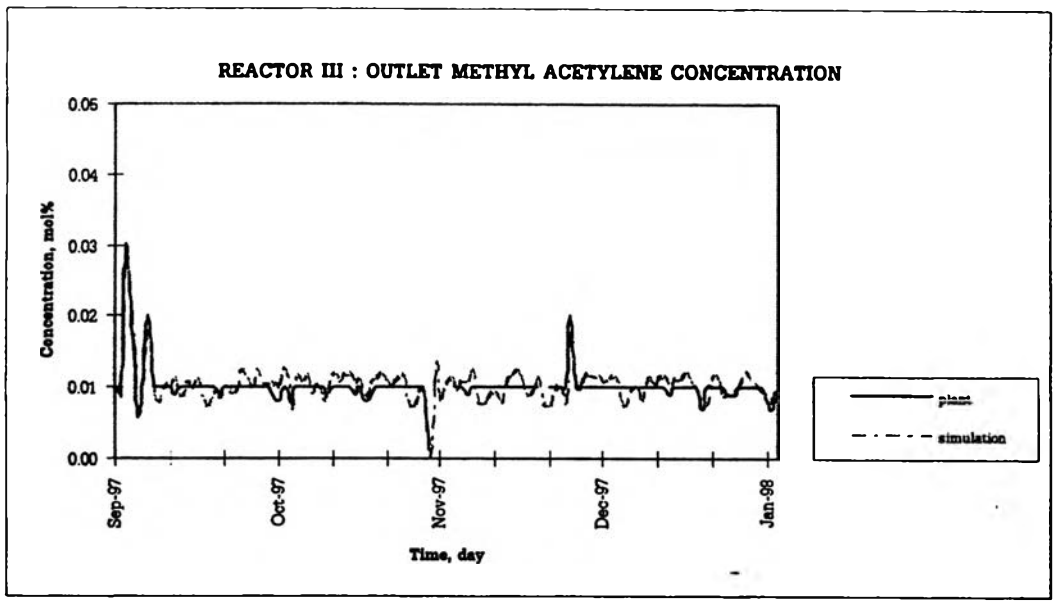

Figure B.44 MODEL VI : Outlet methyl acetylene concentration of reactor III with error 12.83%

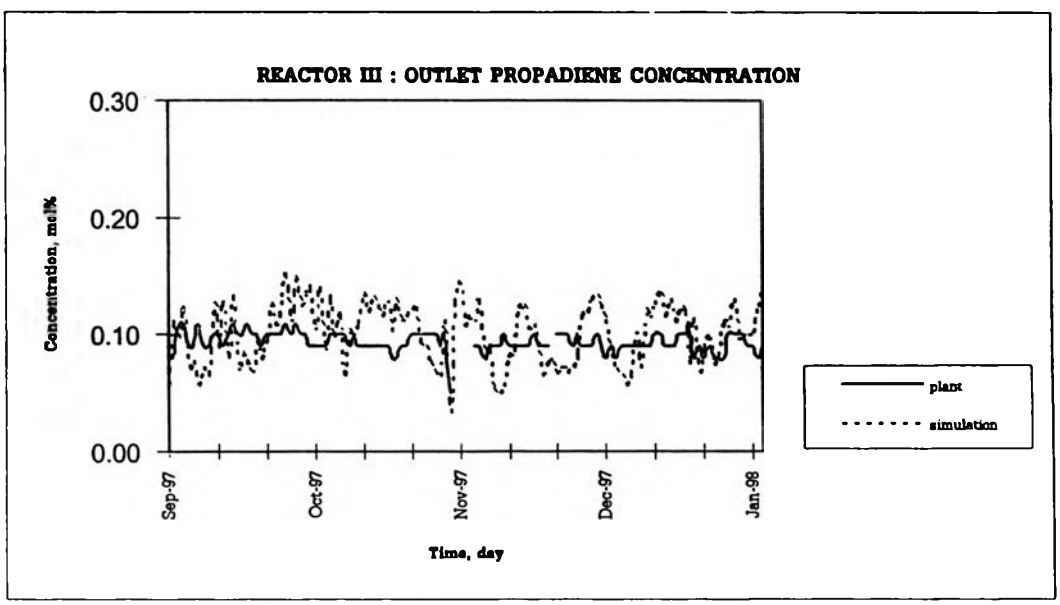

Figure B.45 MODEL VI : Outlet propadiene concentration of reactor III with error 25.02%

B.11 Kinetic model for MODEL VII

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}(1-\Sigma\theta)$$

2. The hydrogen breaks into free atom.
3. The product is adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = 1/(1+K_{activity}\Sigma Ac)$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = (K_{H2}C_{H2})^{0.5}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}(K_{H2}C_{H2})^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{3}$$

$$-r_{Ac} = K1C_{Ac}C_{H2}^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{3}$$

and

$$-r_{Eth} = K2C_{Eth}\, C_{H2}^{0.5}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^3$$

$$-r_{MA} = K4C_{MA}\, C_{H2}^{0.5}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^3$$

$$-r_{PD} = K5C_{PD}\, C_{H2}^{0.5}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^3$$

B.12 The simulation result of the MODEL VII

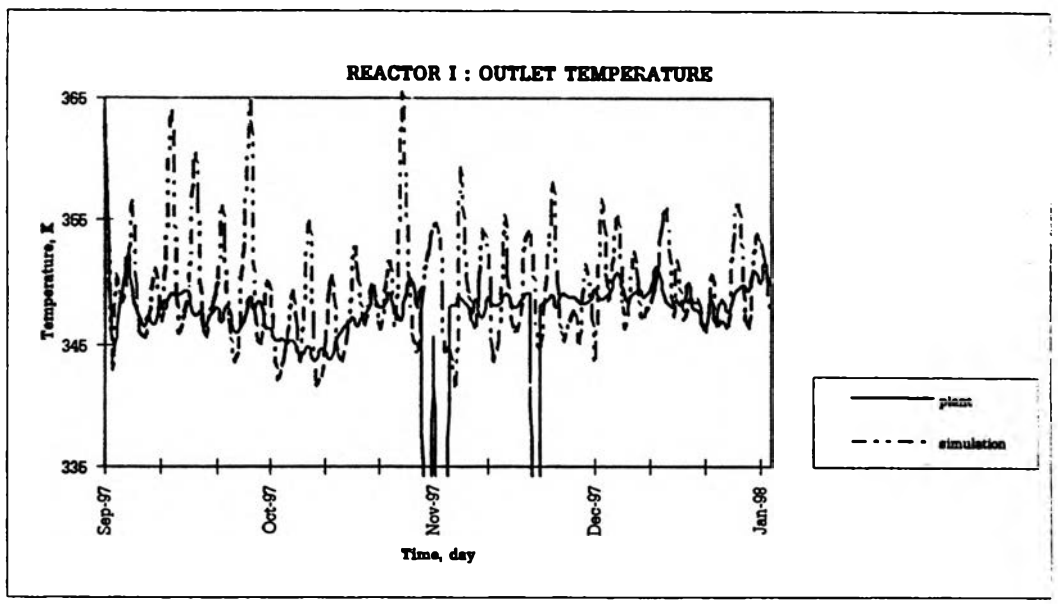

Figure B.46 MODEL VI : Outlet temperature of reactor I with error 0.94%

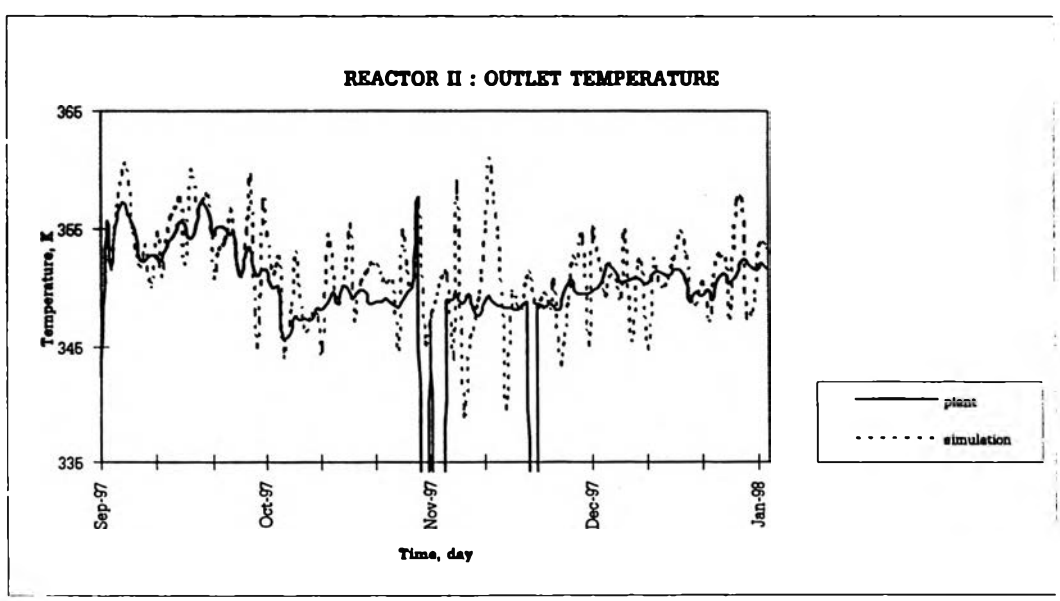

Figure B.47 MODEL VI : Outlet temperature of reactor II with error 0.75%

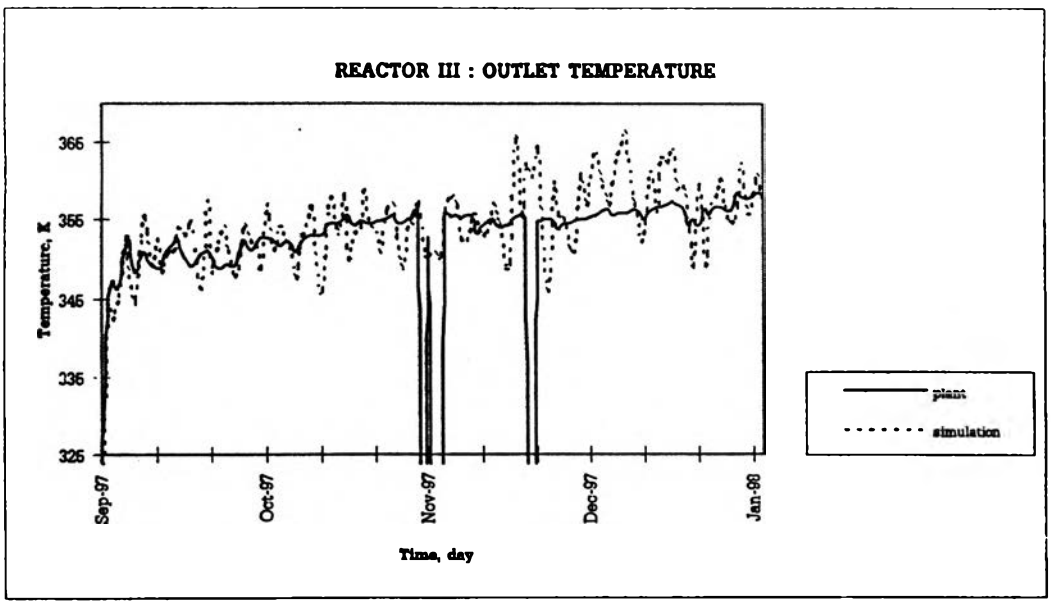

Figure B.48 MODEL VI : Outlet temperature of reactor III with error 0.84%

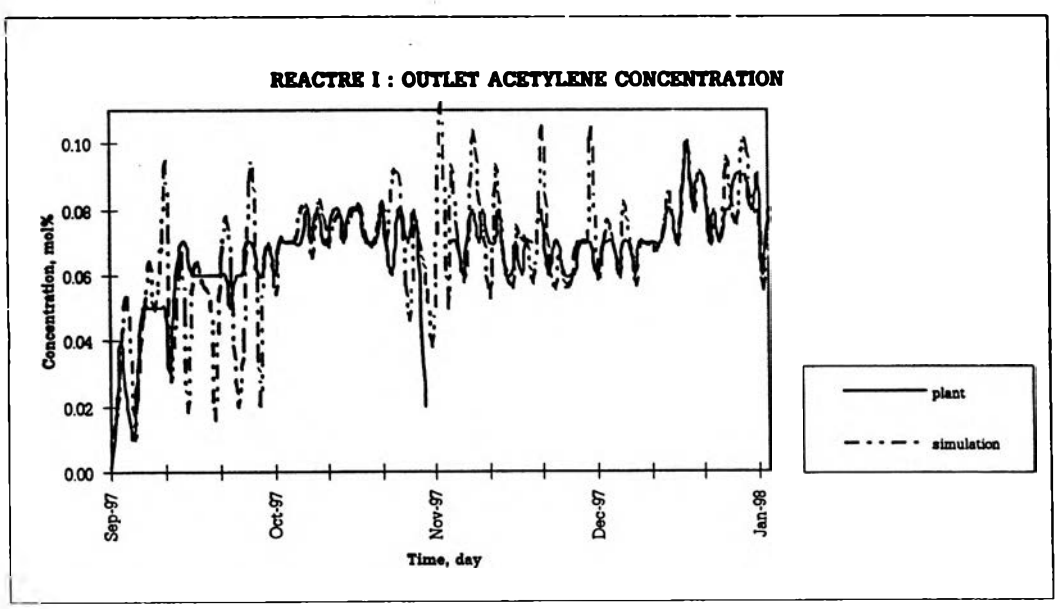

Figure B.49 MODEL VI : Outlet acetylene concentration of reactor I with error 21.76%

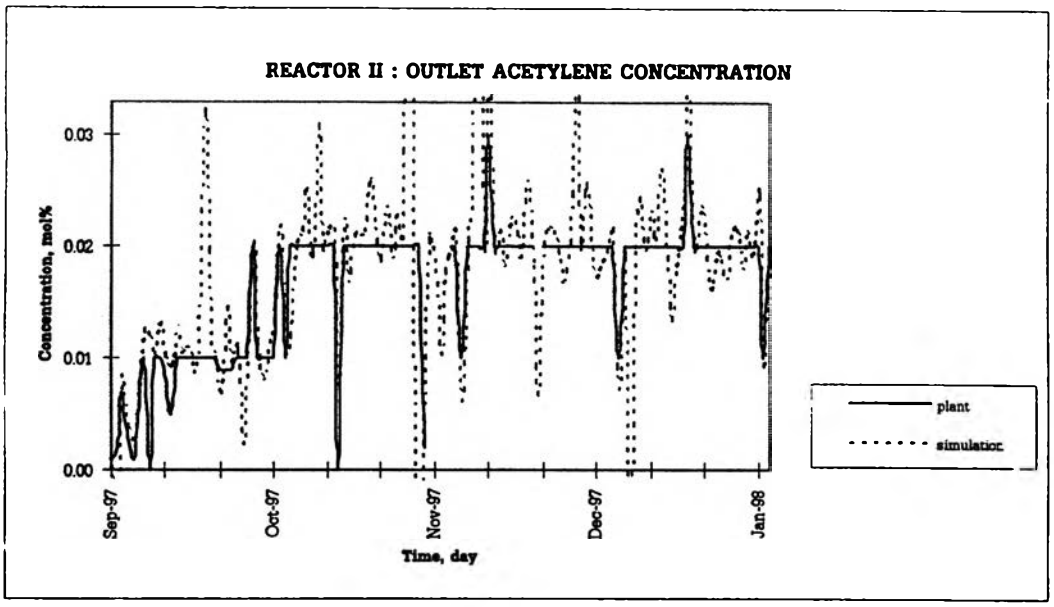

Figure B.50 MODEL VI : Outlet acetylene concentration of reactor II with error %

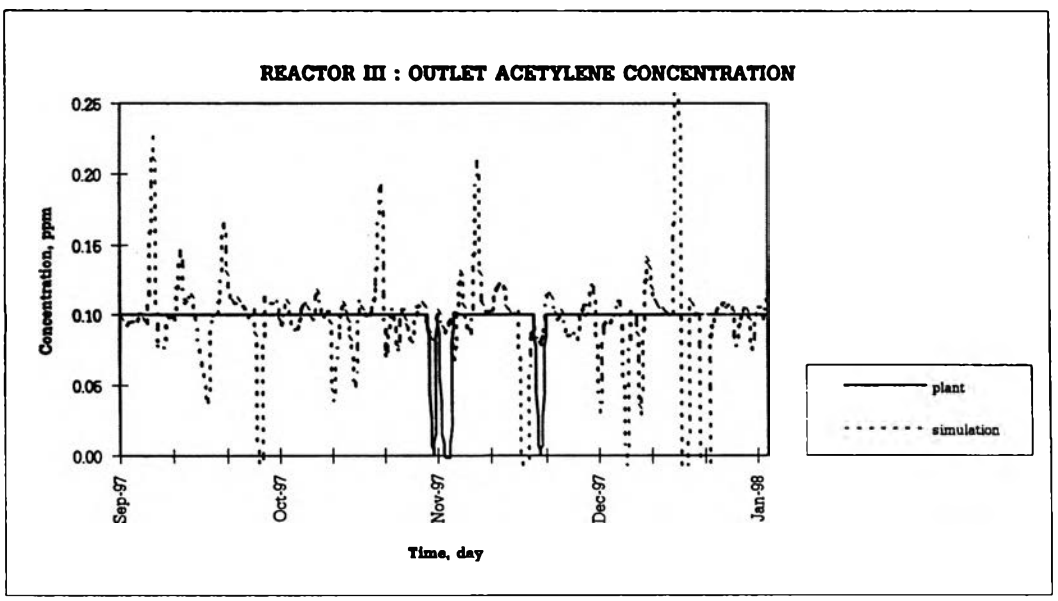

Figure B.51 MODEL VI : Outlet acetylene concentration of reactor III with error 37.99%

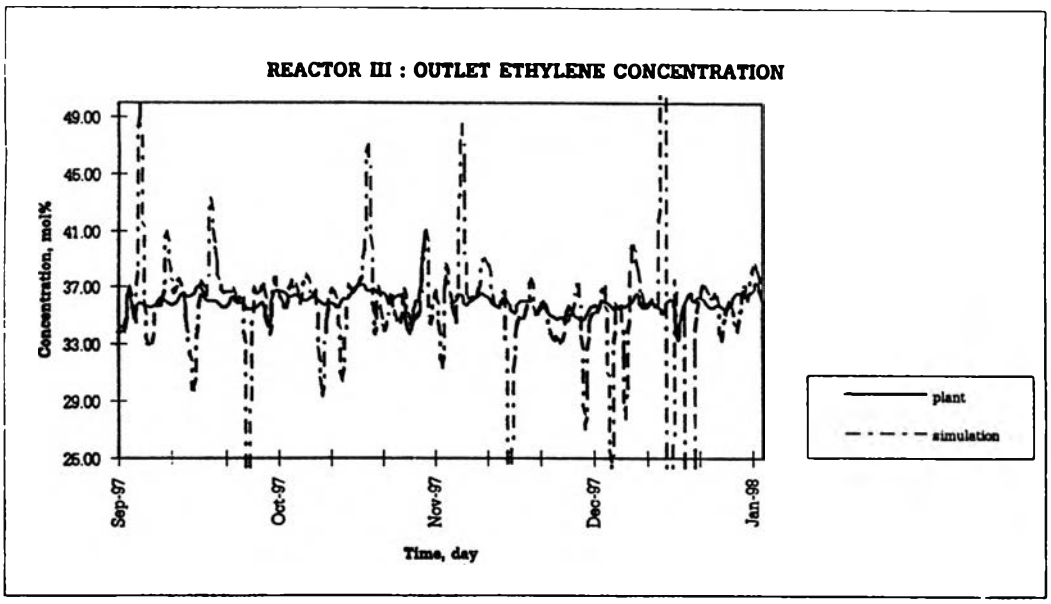

Figure B.52 MODEL VI : Outlet ethylene concentration of reactor III with error 11.46%

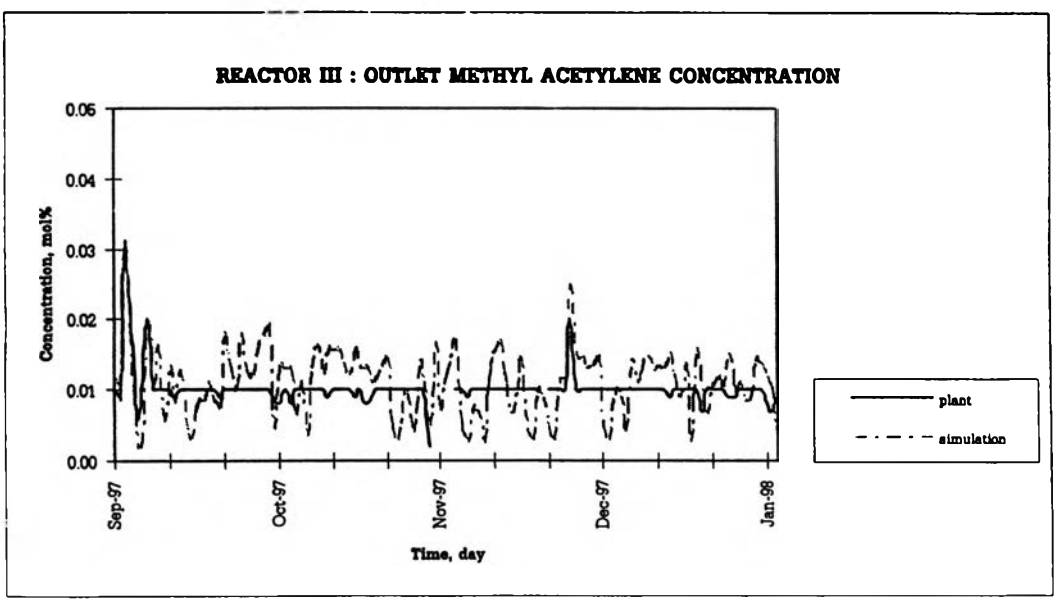

Figure B.53 MODEL VI : Outlet methyl acetylene concentration of reactor III with error 39.1%

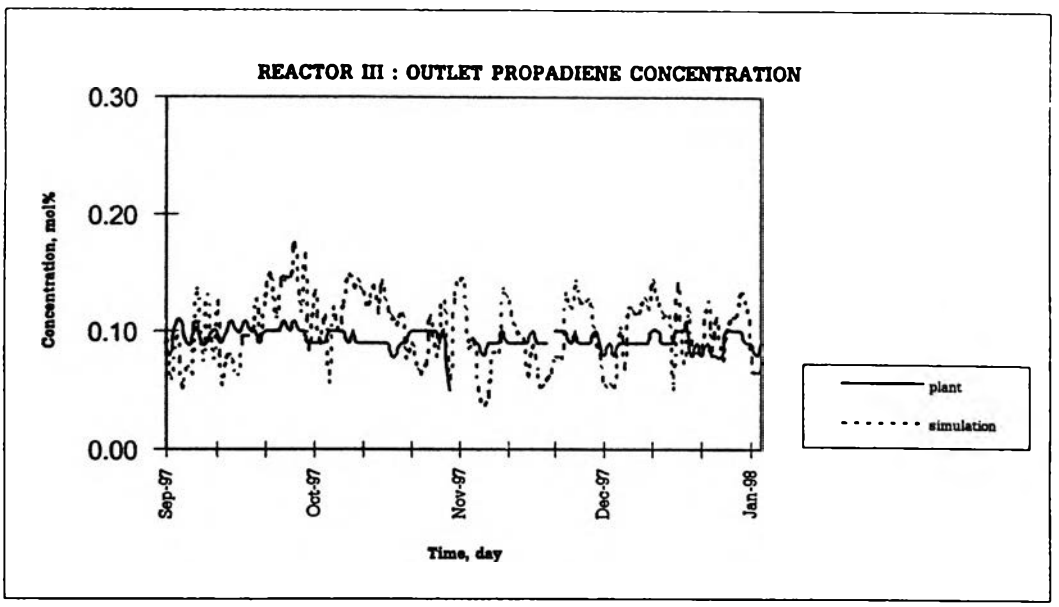

Figure B.54 MODEL VI : Outlet propadiene concentration of reactor III with error 27.67%

B.13 Kinetic model for MODEL VIII

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}(1-\Sigma\theta)$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}(1-\Sigma\theta)$$

2. The hydrogen breaks into free atom.
3. The product is adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = K_{activity}EXP(E_{activity}/RT)C_{Ac}$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = (K_{H2}C_{H2})^{0.5}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}(K_{H2}C_{H2})^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{3}$$

$$-r_{Ac} = K1C_{Ac}C_{H2}^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{3}$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{3}$$

$$-r_{MA} = K4C_{MA}C_{H2}^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{3}$$

$$-r_{PD} = K5C_{PD}C_{H2}^{0.5}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{3}$$

B.14 The simulation result of the MODEL VIII

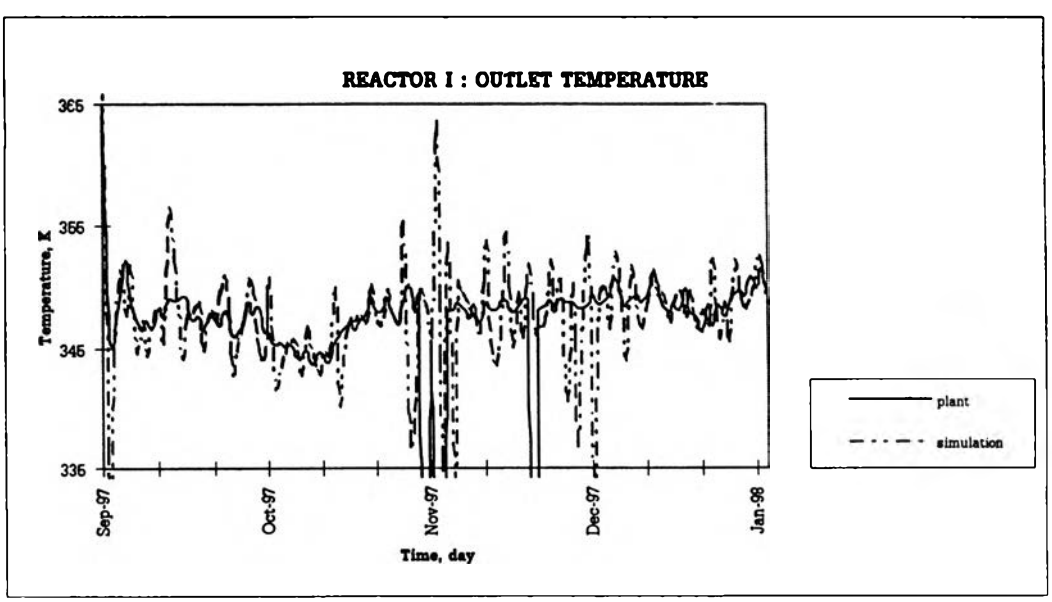

Figure B.55 MODEL VIII : Outlet temperature of reactor I with error 0.72%

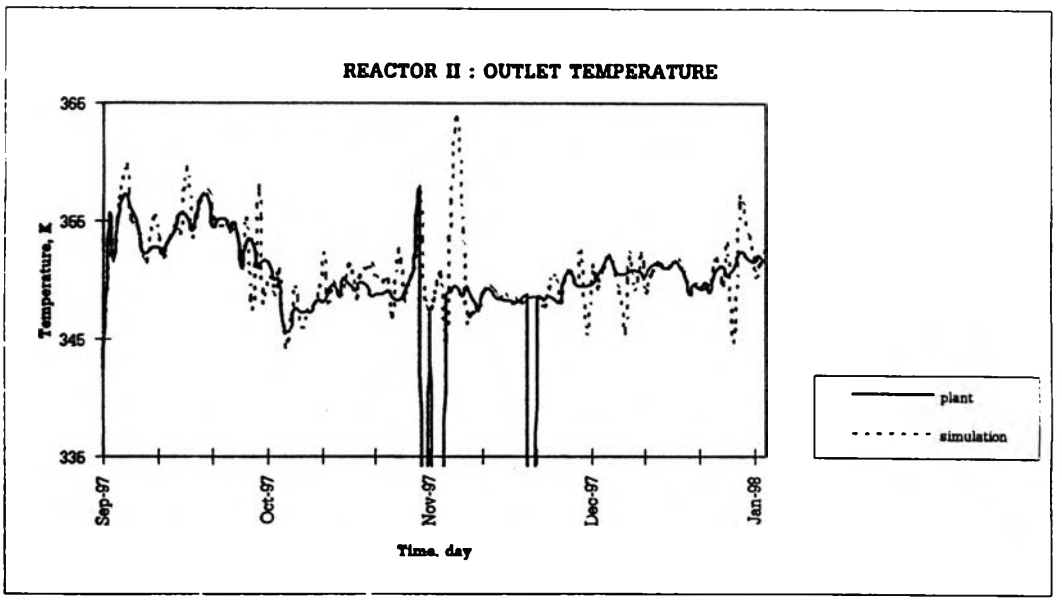

Figure B.56 MODEL VIII : Outlet temperature of reactor II with error 0.4%

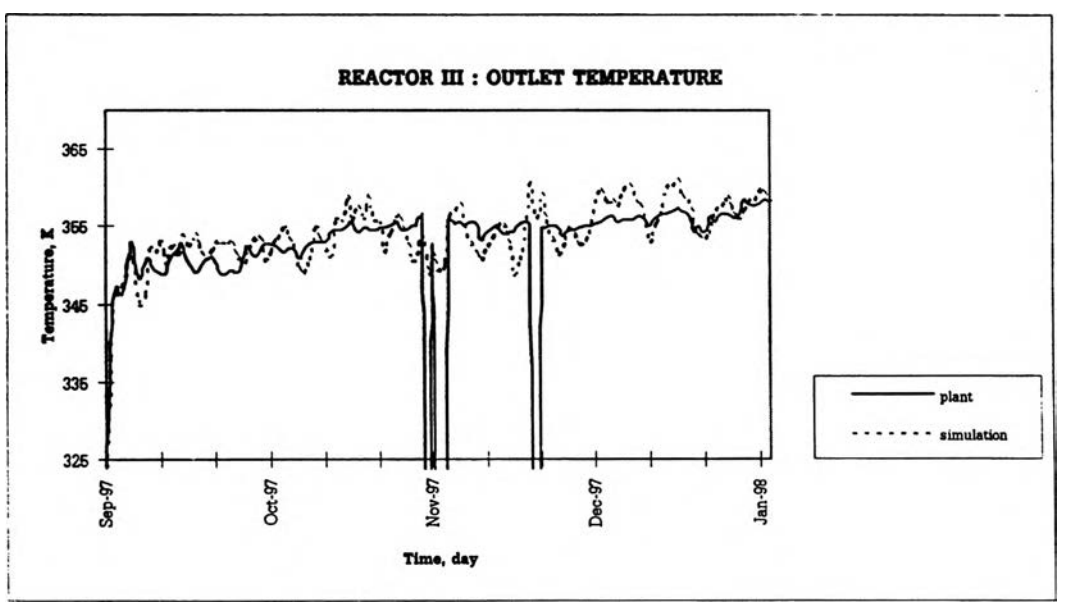

Figure B.57 MODEL VIII : Outlet temperature of reactor III with error 0.55%

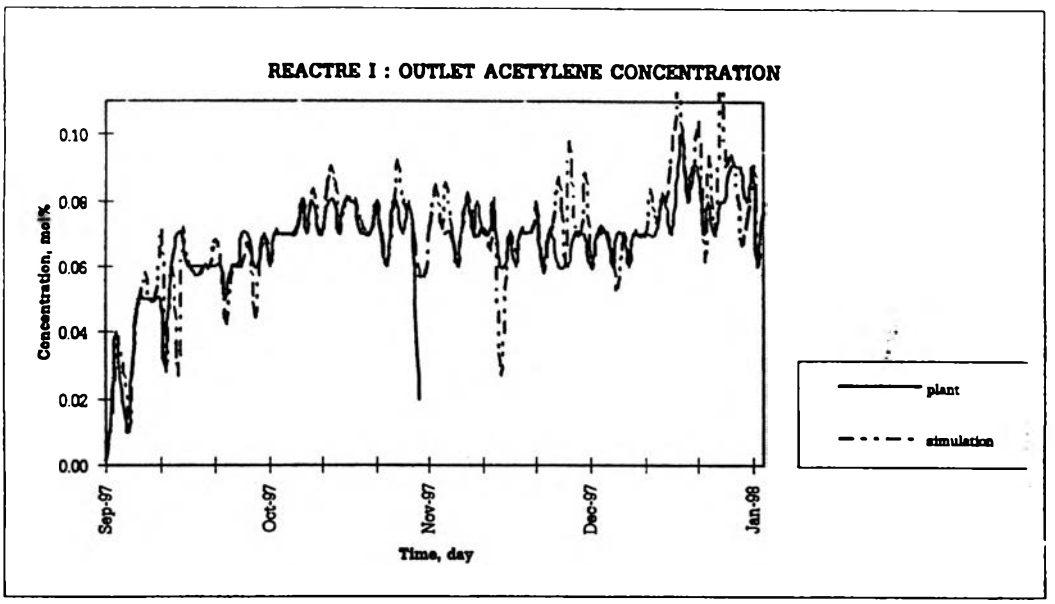

Figure B.58 MODEL VIII : Outlet acetylene concentration of reactor I with error 10.52%

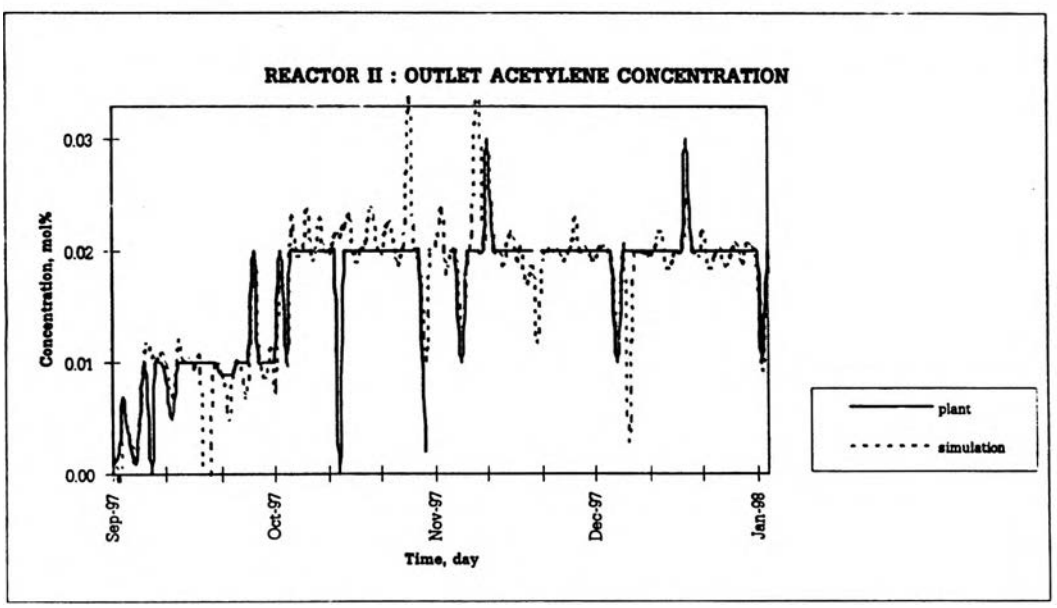

Figure B.59 MODEL VIII : Outlet acetylene concentration of reactor II with error 9.1%

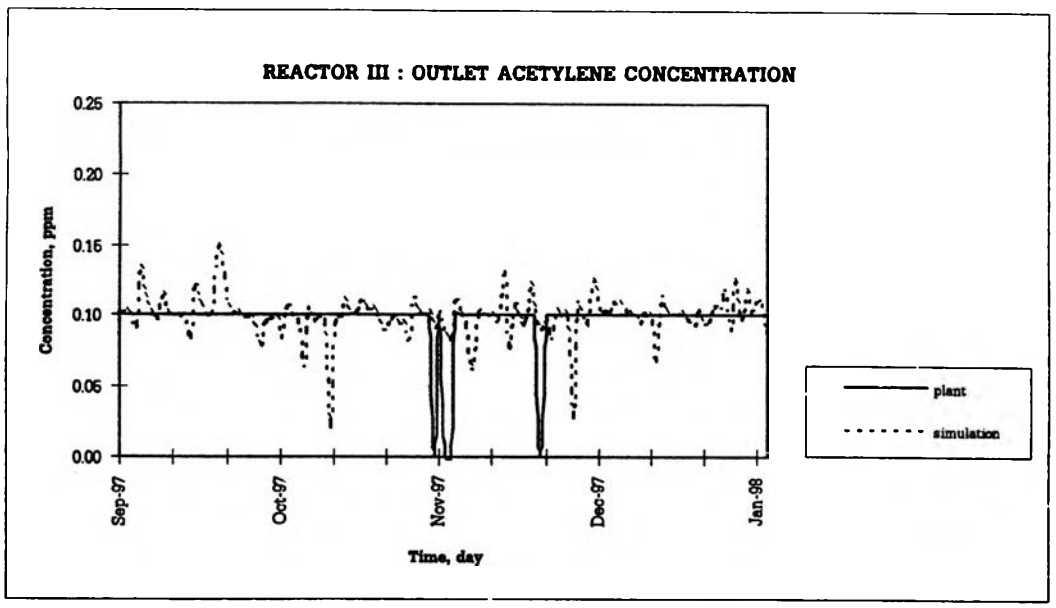

Figure B.60 MODEL VIII : Outlet acetylene concentration of reactor III with error 8.9%

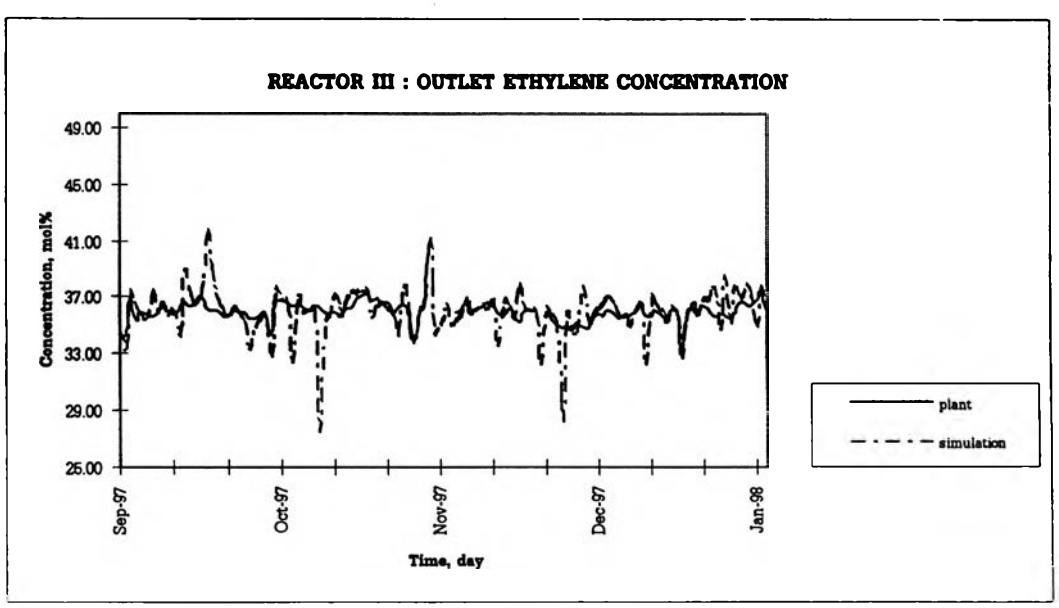

Figure B.61 MODEL VIII : Outlet ethylene concentration of reactor III with error 2.39%

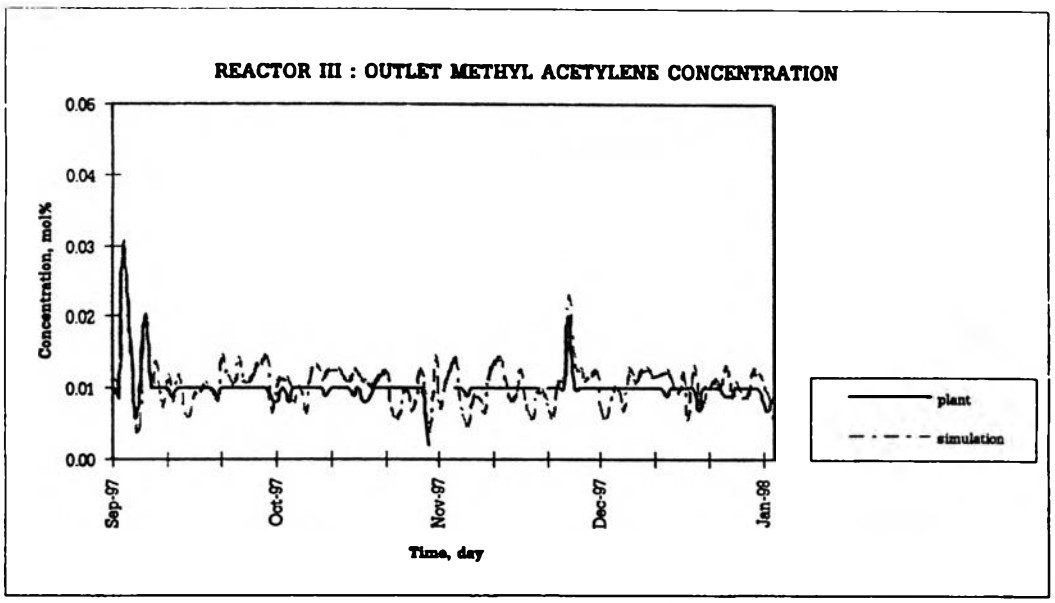

Figure B.62 MODEL VIII : Outlet methyl acetylene concentration of reactor III with error 22.27%

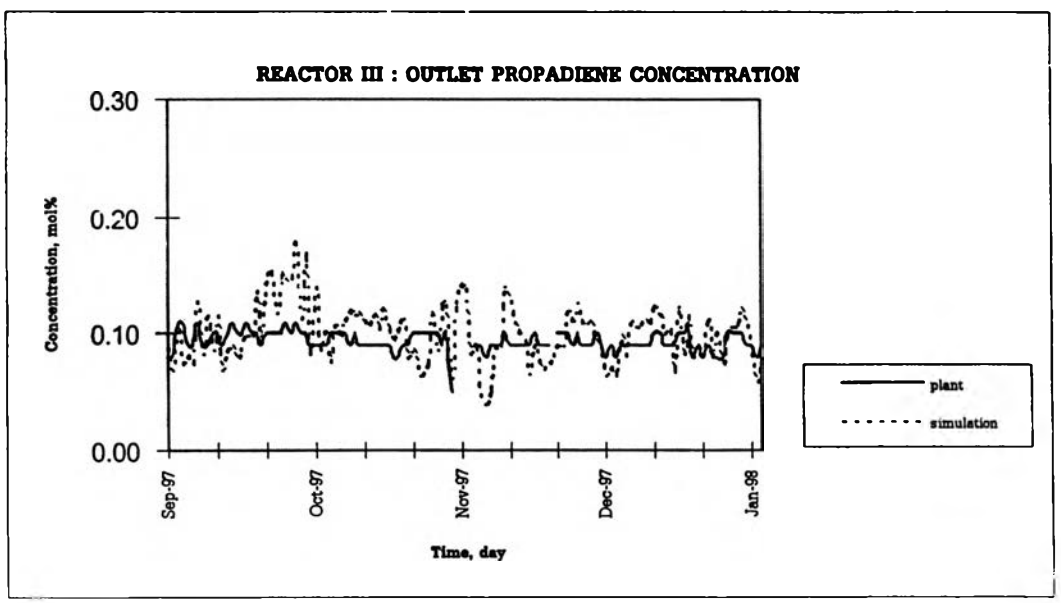

Figure B.63 MODEL VIII : Outlet propadiene concentration of reactor III with error 19.91%

B.15 Kinetic model for MODEL IX

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}^{2}$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}^{2}$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}^{2}$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}^{2}$$

2. The hydrogen breaks into free atom.
3. The product dose not be adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = 1/(1+K_{activity}\Sigma Ac)$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = (K_{H2}C_{H2})^{0.5}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}K_{H2}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{3}$$

$$-r_{Ac} = K1C_{Ac}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{3}$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^3$$

$$-r_{MA} = K4C_{MA}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^3$$

$$-r_{PD} = K5C_{PD}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^3$$

B.16 The simulation result of the MODEL IX

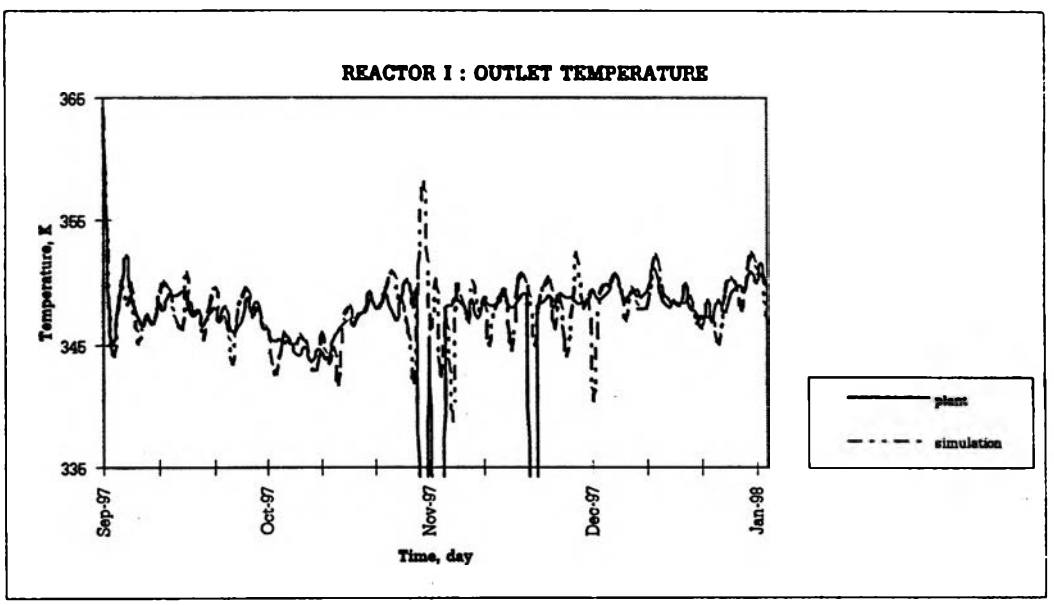

Figure B.64 MODEL IX : Outlet temperature of reactor I with error 0.37%

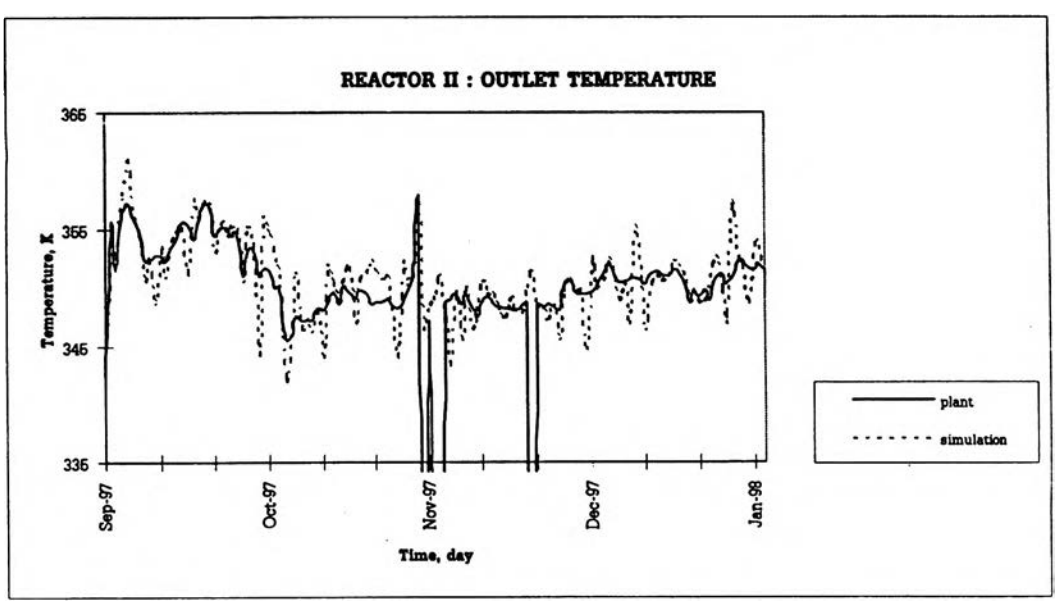

Figure B.65 MODEL IX : Outlet temperature of reactor II with error 0.43%

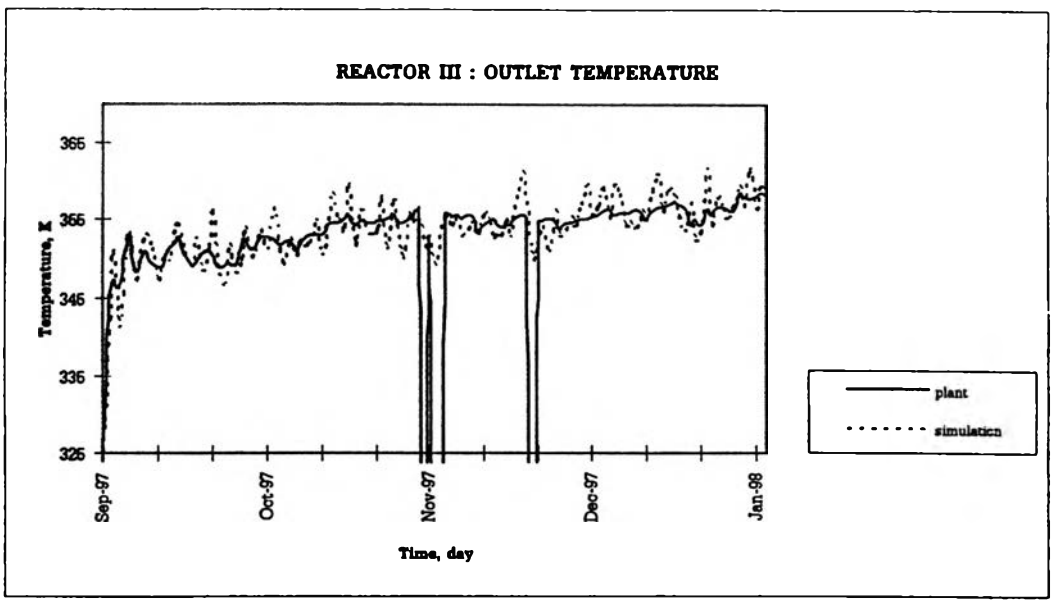

Figure B.66 MODEL IX : Outlet temperature of reactor III with error 0.49%

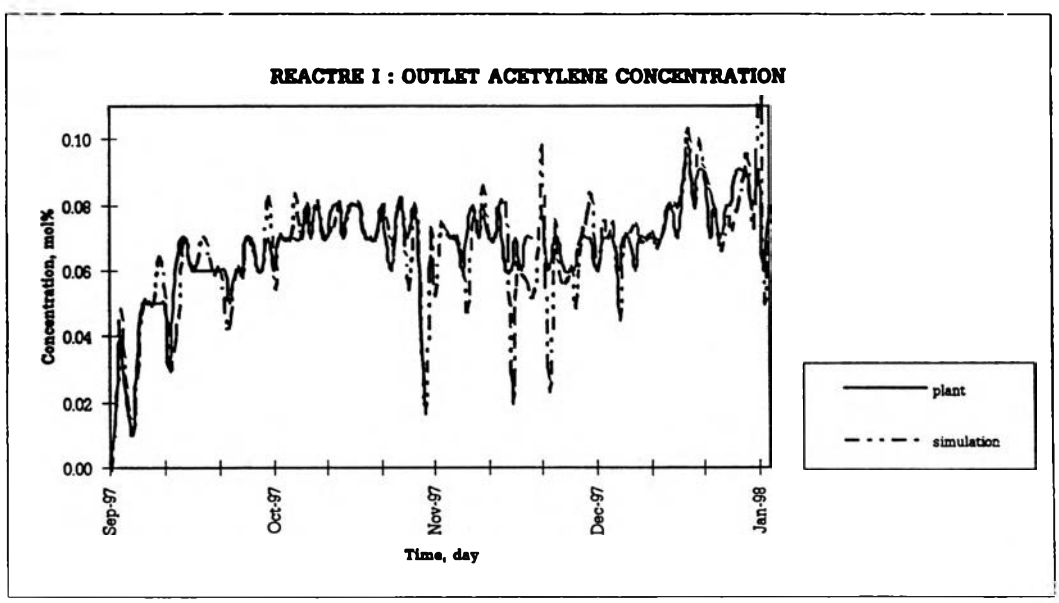

Figure B.67 MODEL IX : Outlet acetylene concentration of reactor I with error 8.97%

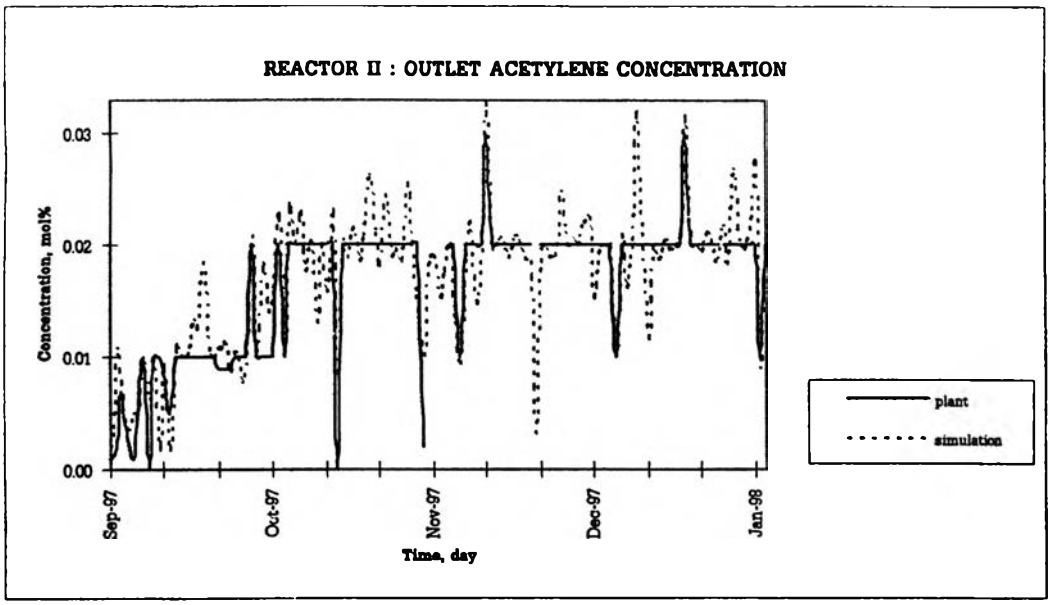

Figure B.68 MODEL IX : Outlet acetylene concentration of reactor II with error **11.56%**

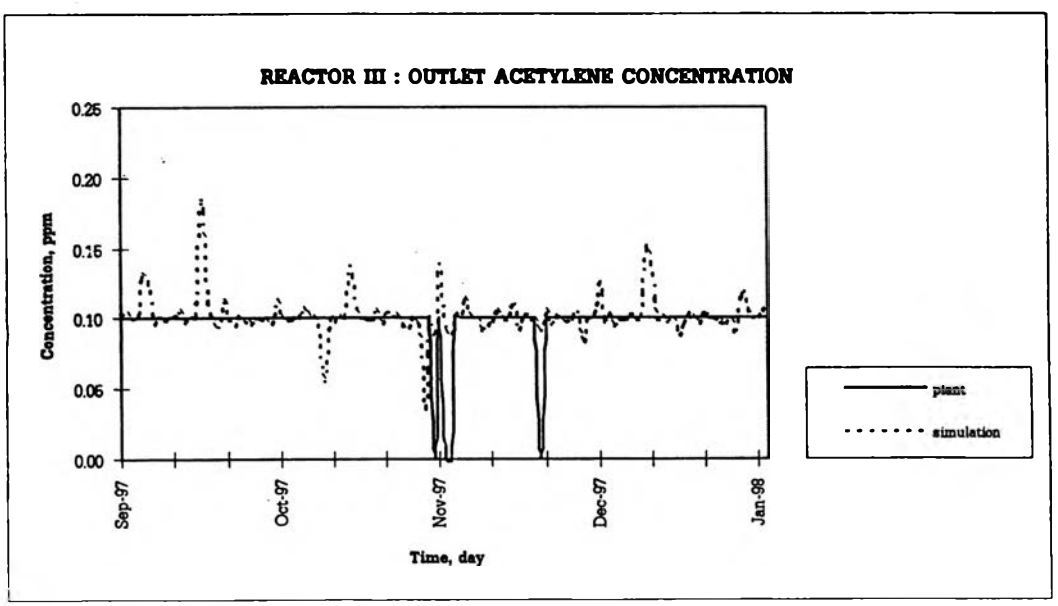

Figure B.69 MODEL IX : Outlet acetylene concentration of reactor III with error 6.65%

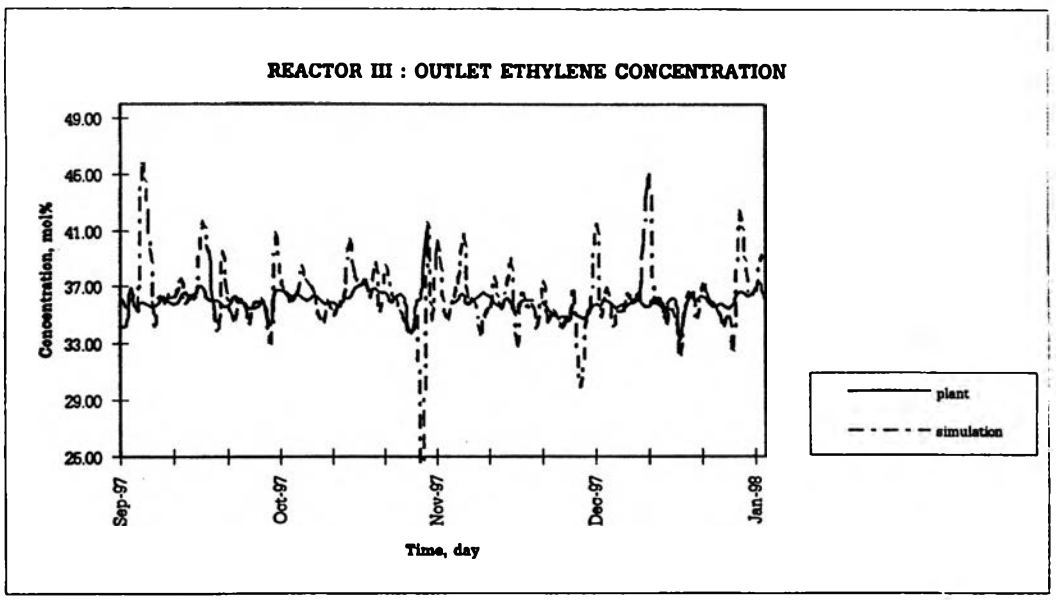

Figure B.70 MODEL IX : Outlet ethylene concentration of reactor III with error 4.12%

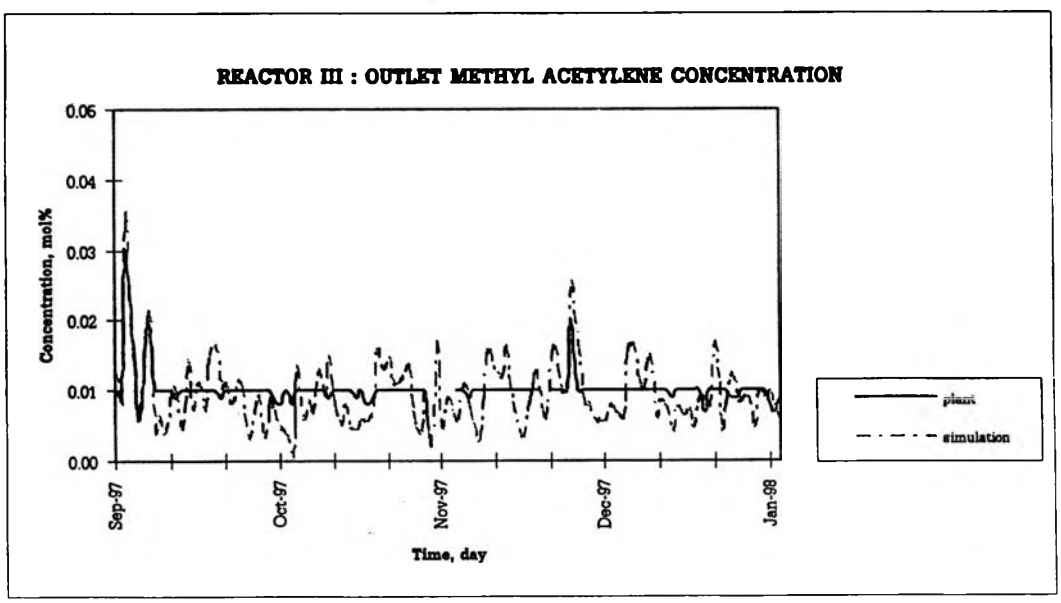

Figure B.71 MODEL IX : Outlet methyl acetylene concentration of reactor III with error 32.34%

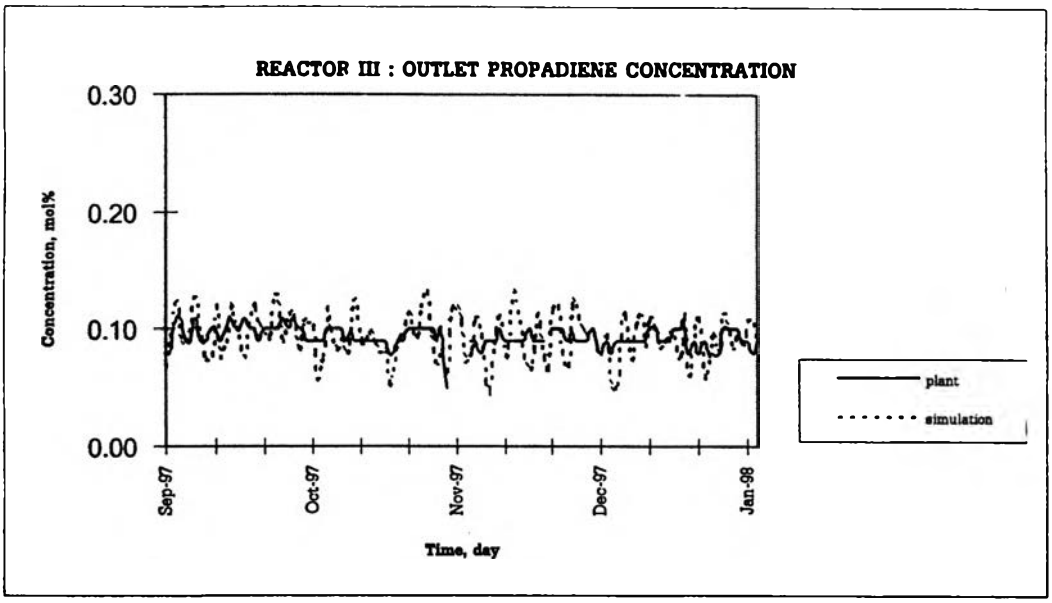

Figure B.72 MODEL IX : Outlet propadiene concentration of reactor III with error 16.09%

B.17 Kinetic model for MODEL X

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}^{2}$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}^{2}$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}^{2}$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}^{2}$$

2. The hydrogen breaks into free atom.
3. The product dose not be adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = K_{activity}EXP(E_{activity}/RT)C_{Ac}$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = (K_{H2}C_{H2})^{0.5}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}K_{H2}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^3$$

$$-r_{Ac} = K1C_{Ac}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^3$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^3$$

$$-r_{MA} = K4C_{MA}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^3$$

$$-r_{PD} = K5C_{PD}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^3$$

B.18 The simulation result of the MODEL X

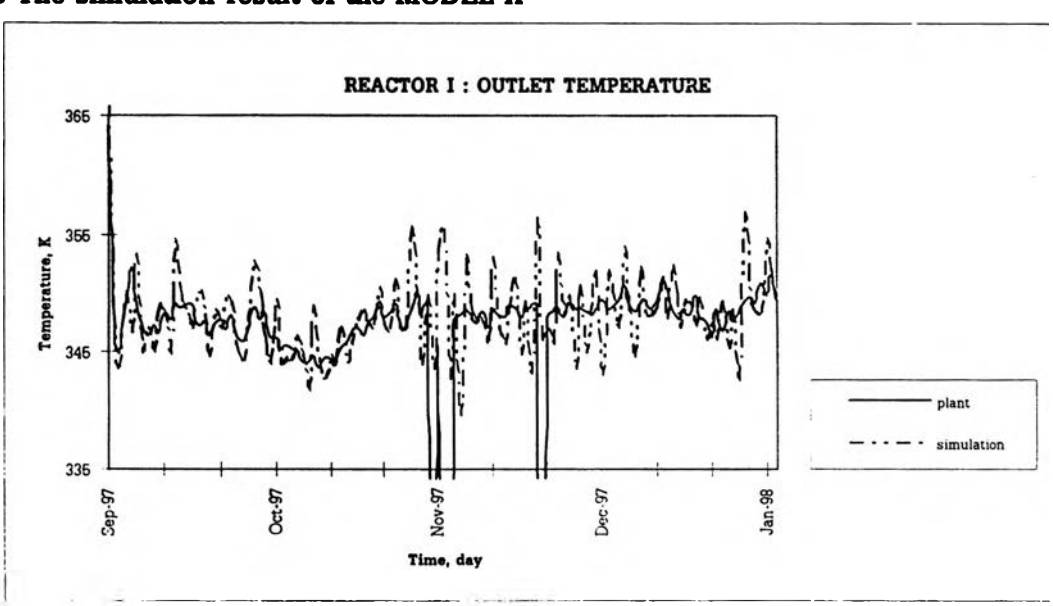

Figure B.73 MODEL X : Outlet temperature of reactor I with error 0.62%

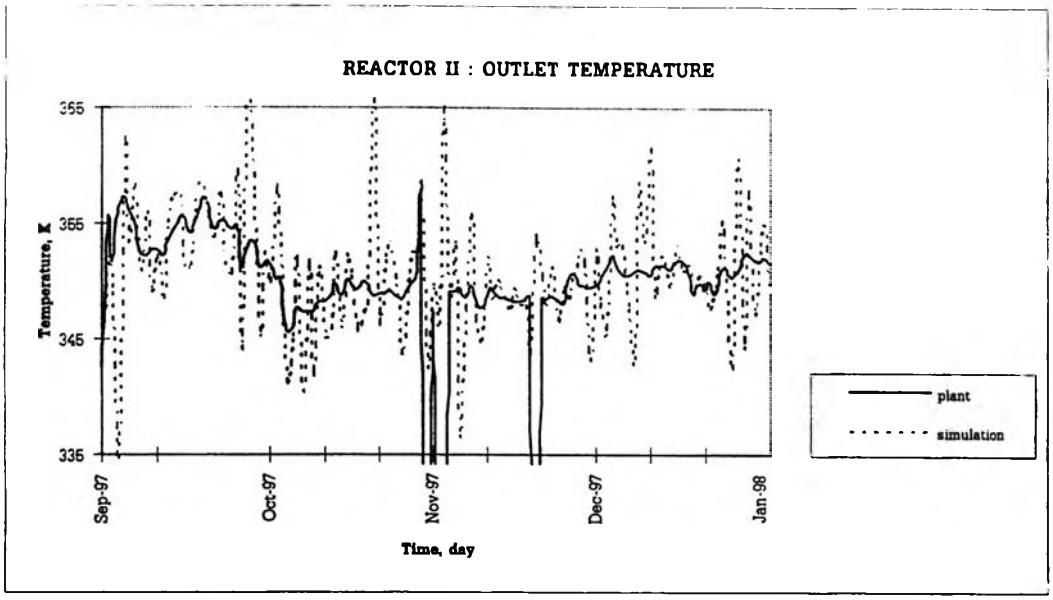

Figure B.74 MODEL X : Outlet temperature of reactor II with error 0.97%

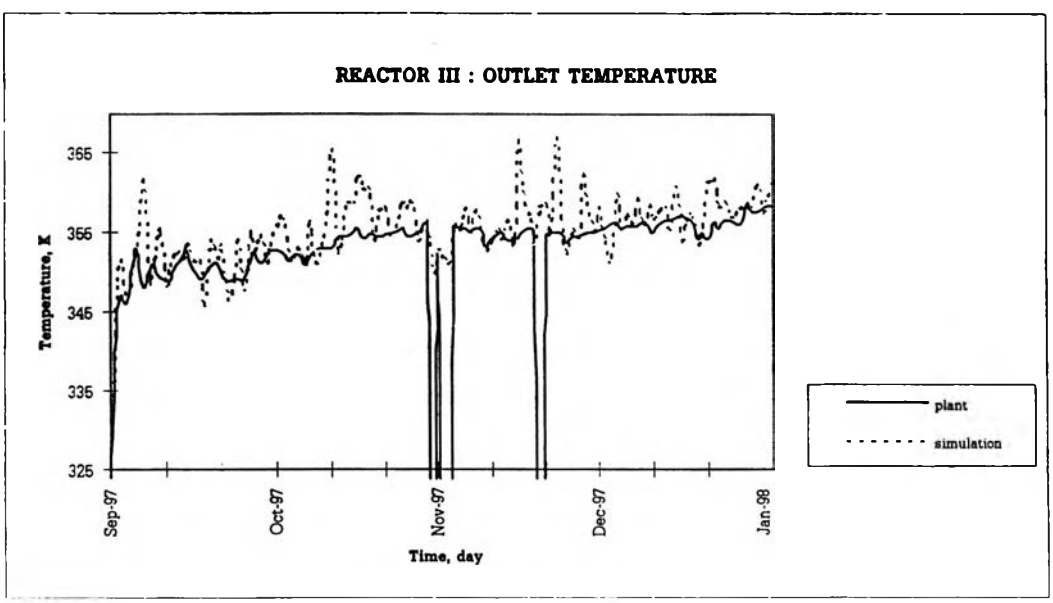

Figure B.75 MODEL X : Outlet temperature of reactor III with error 0.66%

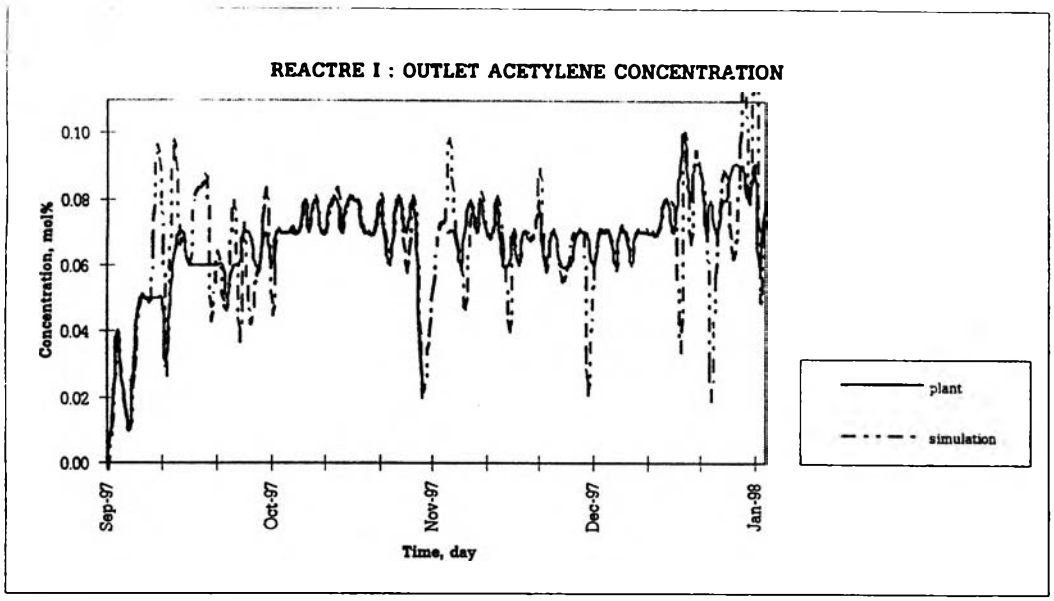

Figure B.76 MODEL X : Outlet acetylene concentration of reactor I with error 12.66%

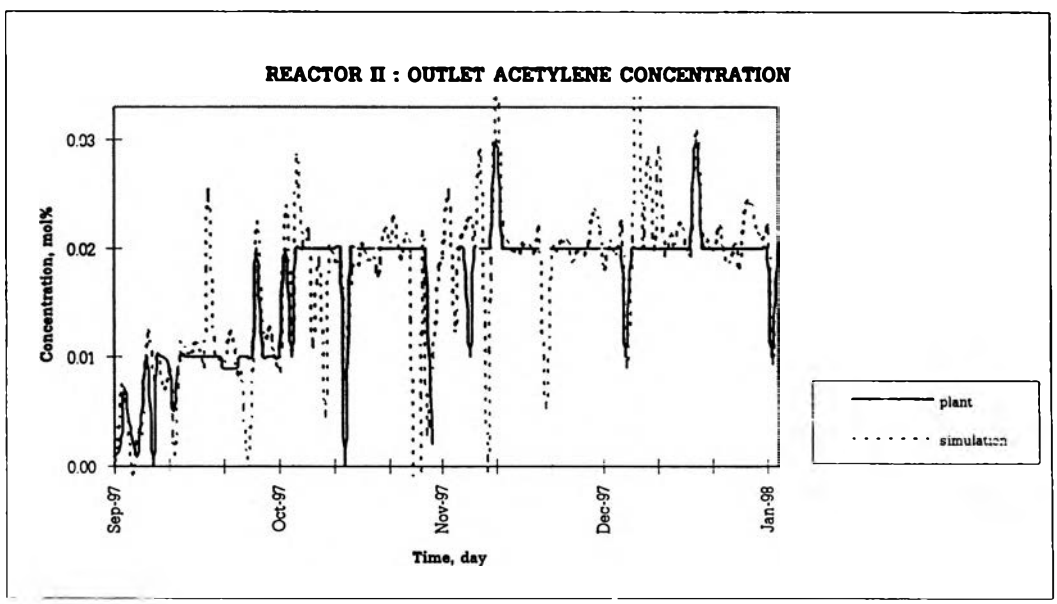

Figure B.77 MODEL X : Outlet acetylene concentration of reactor II with error 17.89%

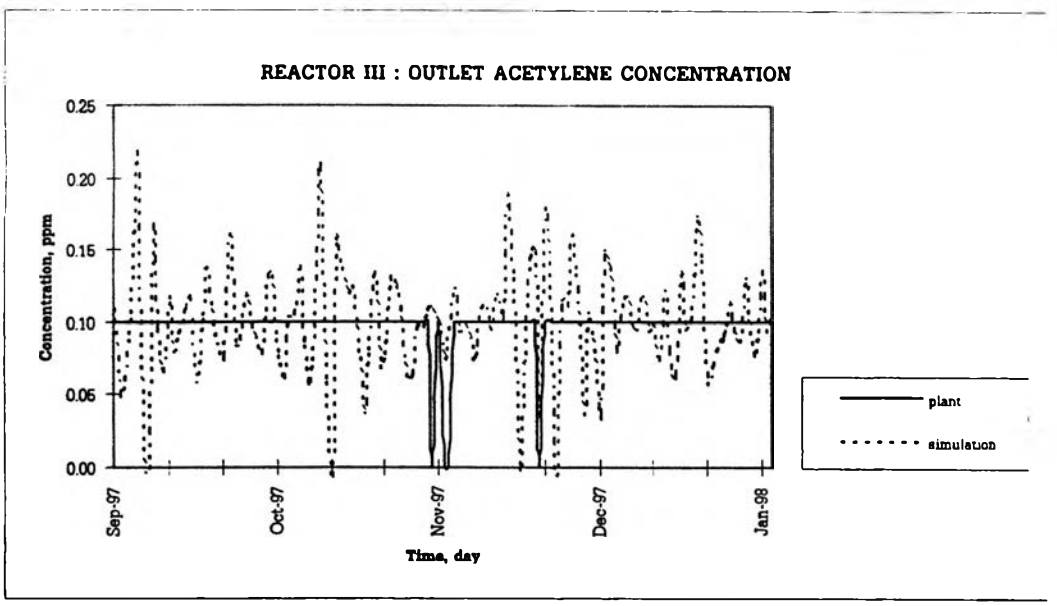

Figure B.78 MODEL X : Outlet acetylene concentration of reactor III with error 28.87%

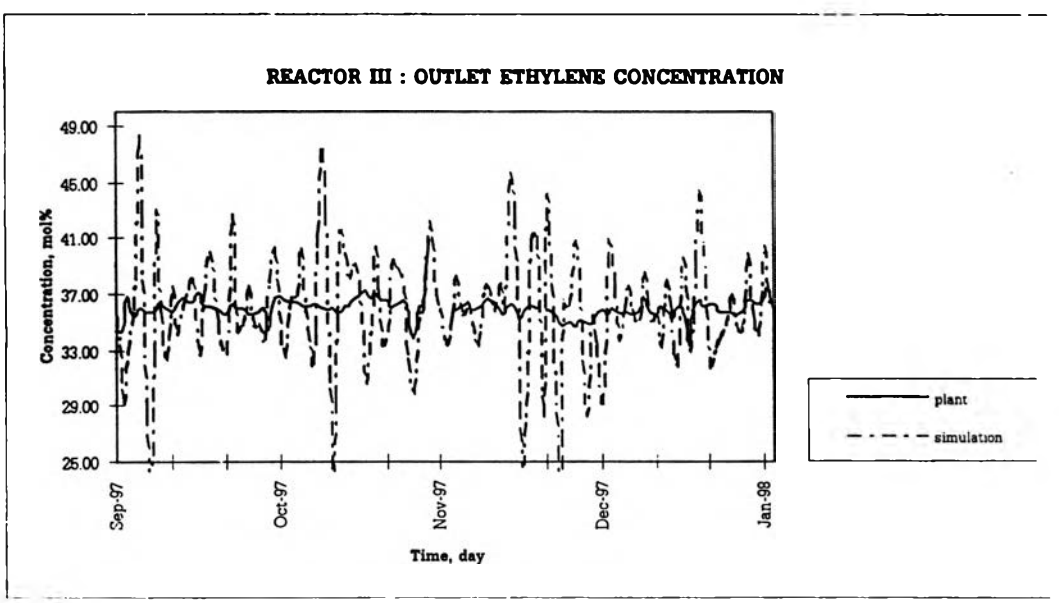

Figure B.79 MODEL X : Outlet ethylene concentration of reactor III with error 8.35%

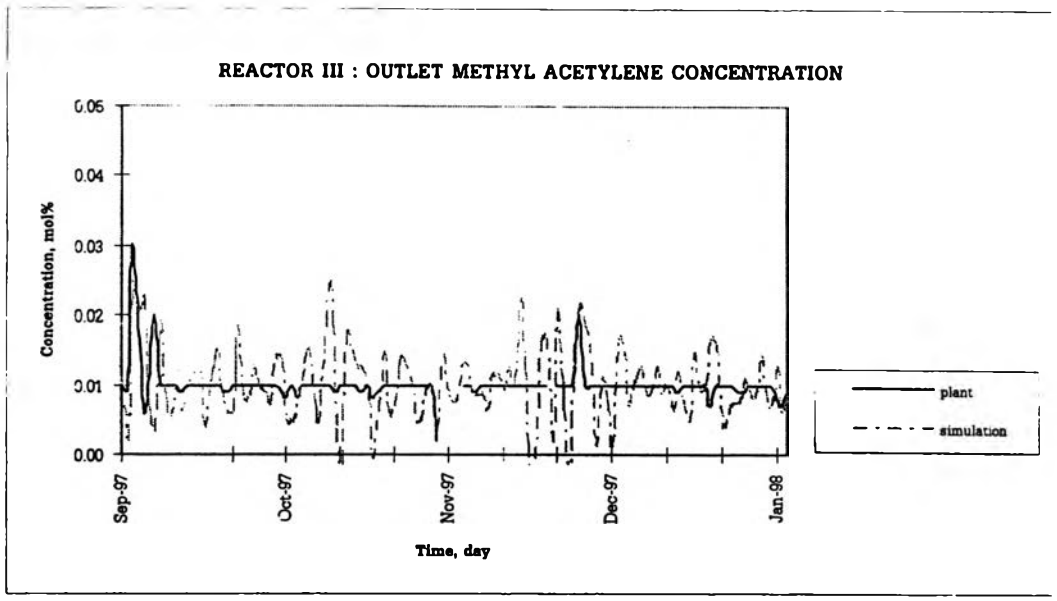

Figure B.80 MODEL X : Outlet methyl acetylene concentration of reactor III with error 41.02%

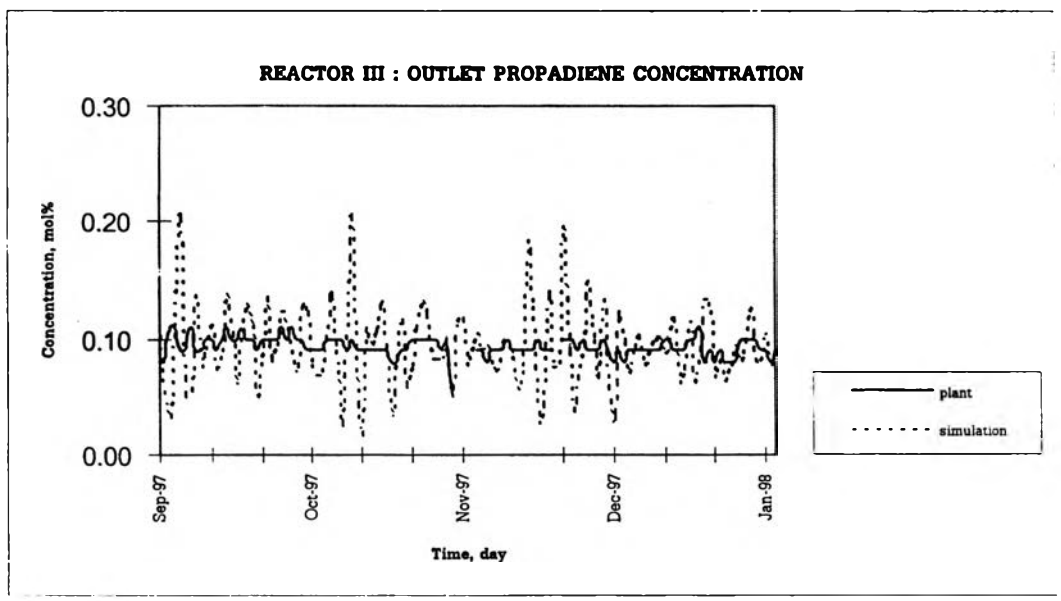

Figure B.81 MODEL X : Outlet propadiene concentration of reactor III with error 26.02%

B.19 Kinetic model for MODEL XI

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}^{2}(1-\Sigma\theta)$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}^{2}(1-\Sigma\theta)$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}^{2}(1-\Sigma\theta)$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}^{2}(1-\Sigma\theta)$$

2. The hydrogen breaks into free atom.
3. The product dose not be adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = 1/(1+K_{activity}\Sigma Ac)$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = (K_{H2}C_{H2})^{0.5}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}K_{H2}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{4}$$

$$-r_{Ac} = K1C_{Ac}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^{4}$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^4$$

$$-r_{MA} = K4C_{MA}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^4$$

$$-r_{PD} = K5C_{PD}C_{H2}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^4$$

B.20 The simulation result of the MODEL XI

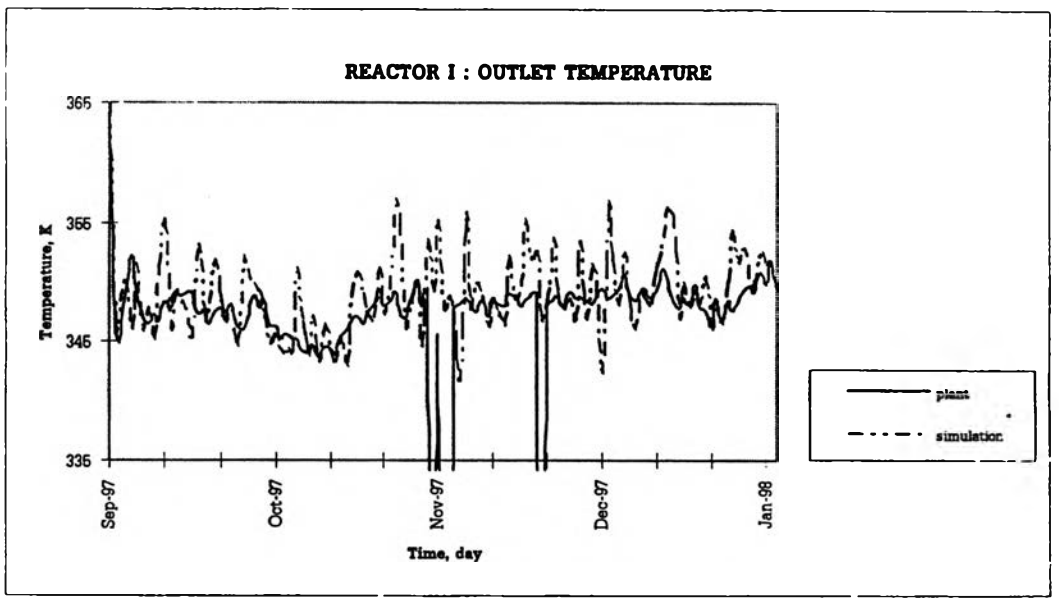

Figure B.82 MODEL XI : Outlet temperature of reactor I with error 0.63%

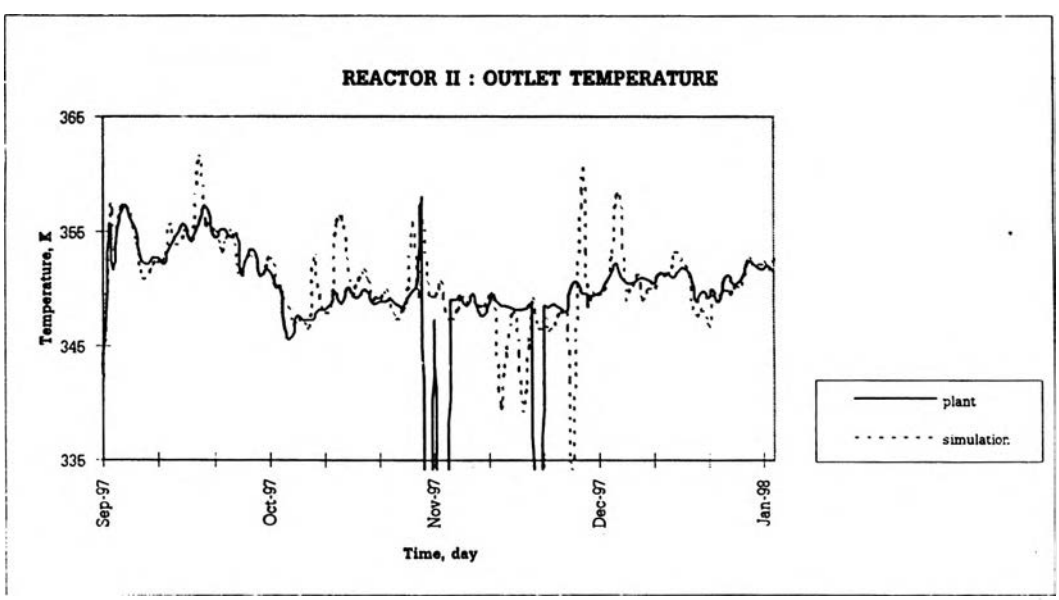

Figure B.83 MODEL XI : Outlet temperature of reactor II with error 0.43%

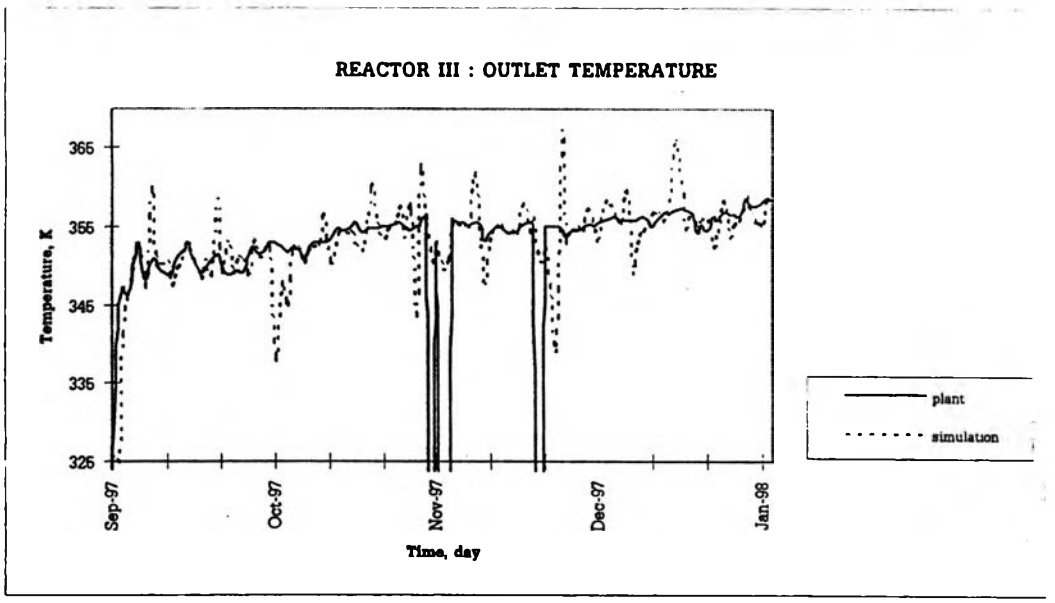

Figure B.84 MODEL XI : Outlet temperature of reactor III with error 0.63%

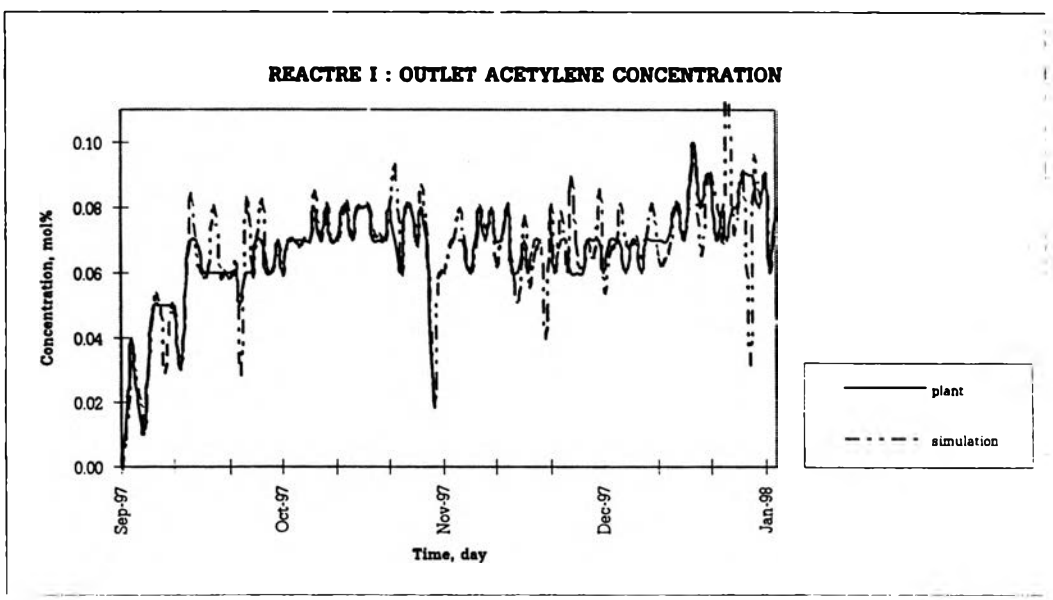

Figure B.85 MODEL XI : Outlet acetylene concentration of reactor I with error 8.44%

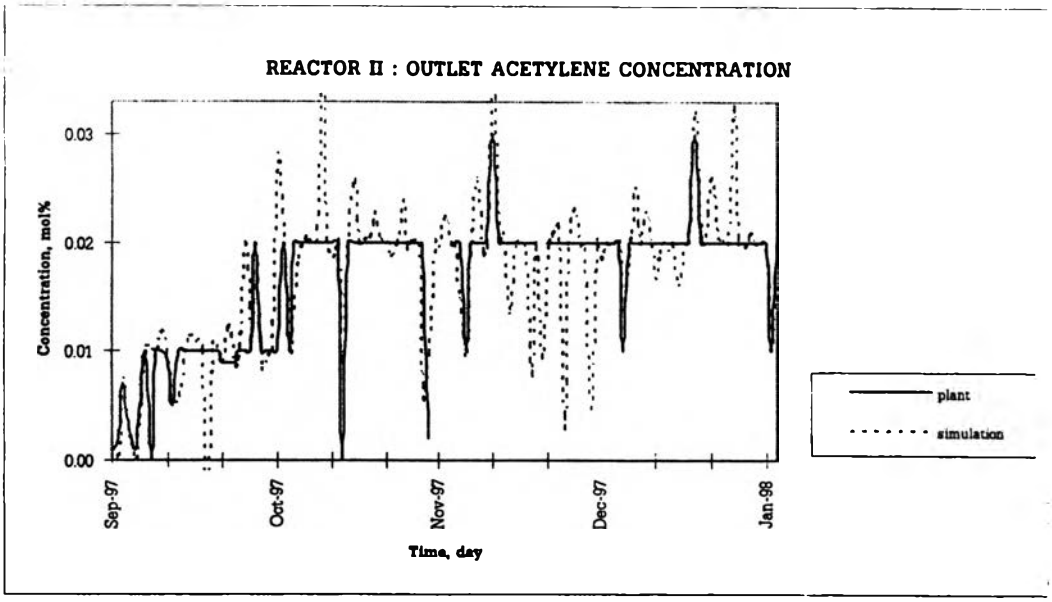

Figure B.86 MODEL XI : Outlet acetylene concentration of reactor II with error 13.67%

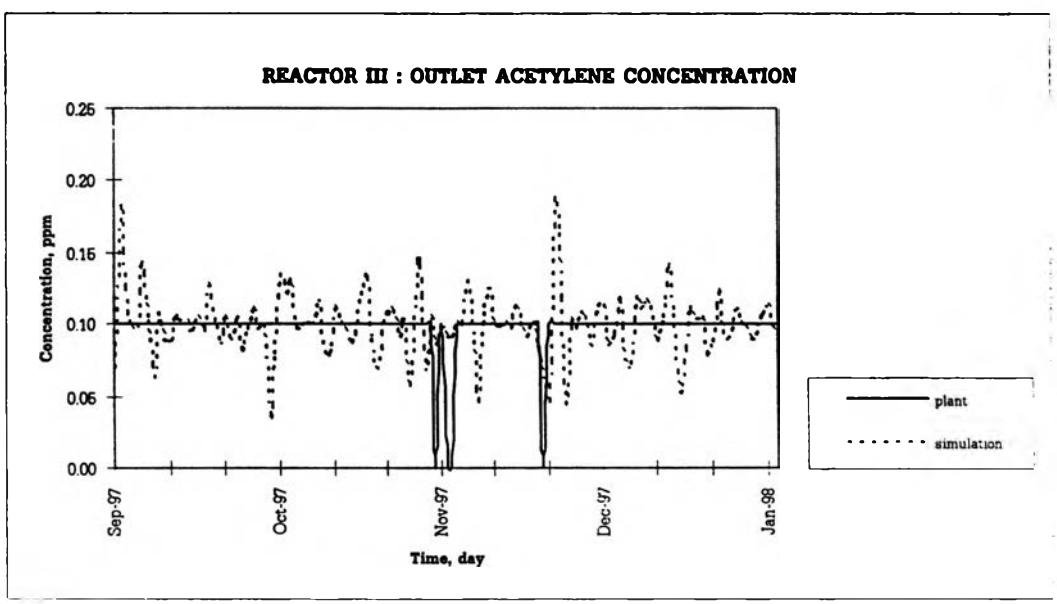

Figure B.87 MODEL XI : Outlet acetylene concentration of reactor III with error 15.46%

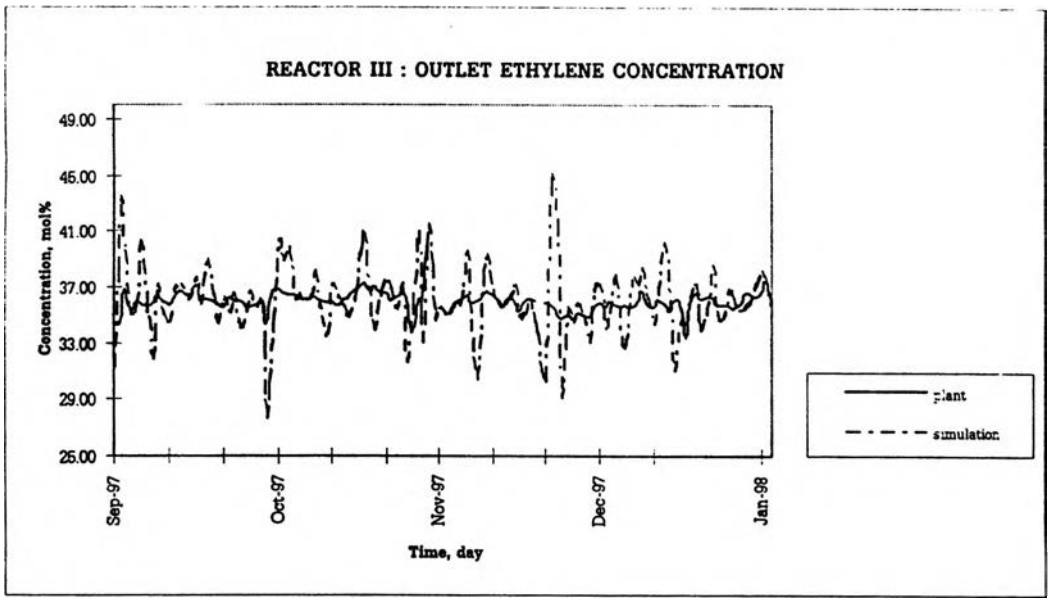

Figure B.88 MODEL XI : Outlet ethylene concentration of reactor III with error 4.49%

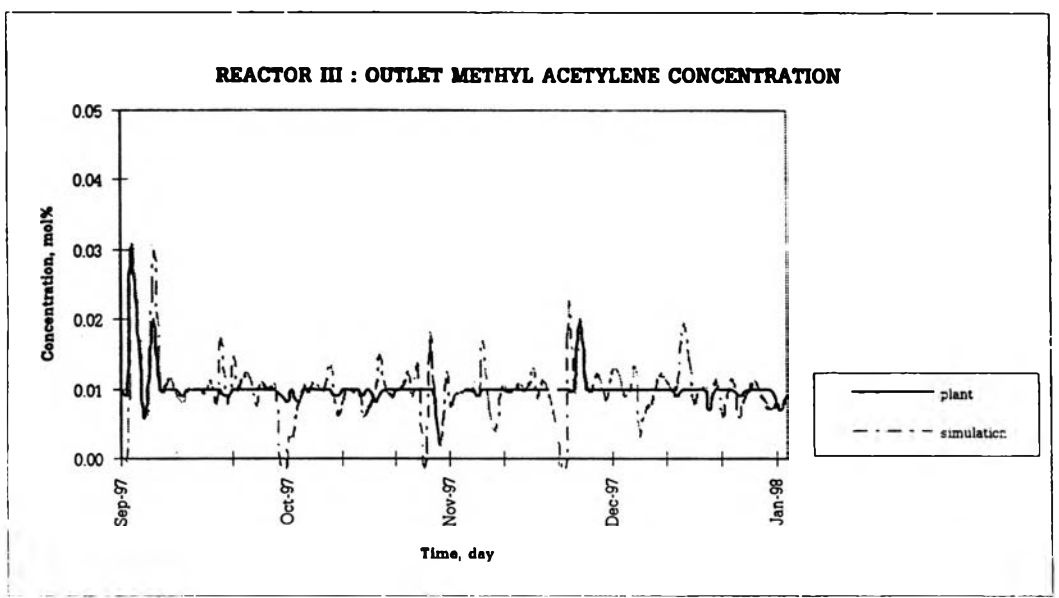

Figure B.89 MODEL XI : Outlet methyl acetylene concentration of reactor III with error 23.1%

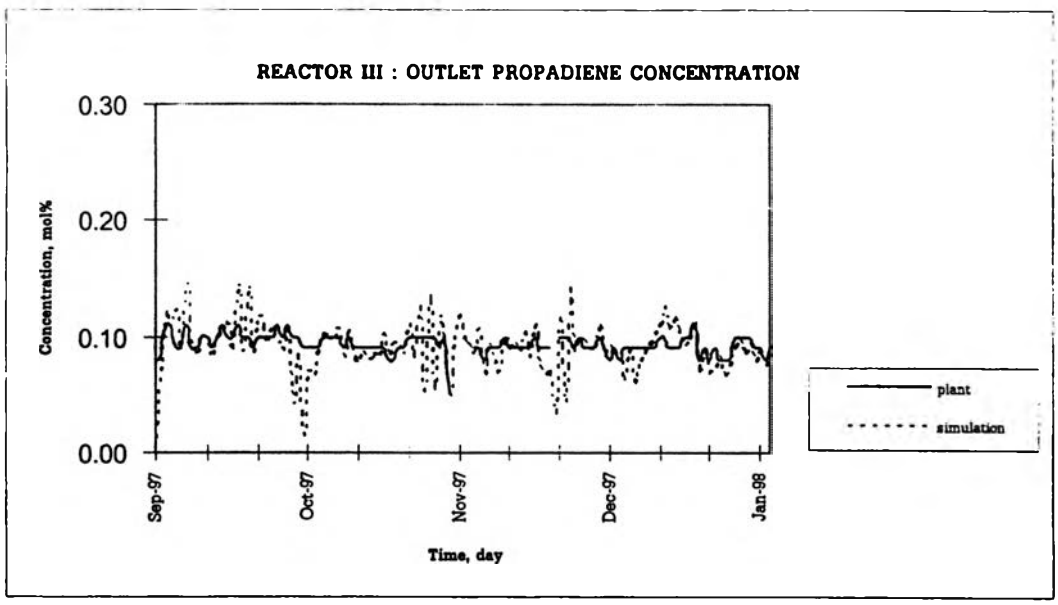

Figure B.90 MODEL XI : Outlet propadiene concentration of reactor III with error 13.45%

B.21 Kinetic model for MODEL XII

The assumption :

1. The rate limiting step is a surface rate of reaction.

   The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}^{2}(1-\Sigma\theta)$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}^{2}(1-\Sigma\theta)$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}^{2}(1-\Sigma\theta)$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}^{2}(1-\Sigma\theta)$$

2. The hydrogen breaks into free atom.
3. The product dose not be adsorbed on the catalytic surface.
4. The catalyst activity equation is

$$activity = K_{activity}EXP(E_{activity}/RT)C_{Ac}$$

Use the Langmuir-Hinshelwood kinetics concept will obtain

$$\theta_{Ac} = K_{Ac}C_{Ac}(1-\Sigma\theta)$$

$$\theta_{Eth} = K_{Eth}C_{Eth}(1-\Sigma\theta)$$

$$\theta_{H2} = (K_{H2}C_{H2})^{0.5}(1-\Sigma\theta)$$

$$\theta_{MA} = K_{MA}C_{MA}(1-\Sigma\theta)$$

$$\theta_{PD} = K_{PD}C_{PD}(1-\Sigma\theta)$$

$$\theta_{CO} = K_{CO}C_{CO}(1-\Sigma\theta)$$

$$\Sigma\theta = \theta_{Ac}+\theta_{Eth}+\theta_{H2}+\theta_{MA}+\theta_{PD}+\theta_{CO}$$

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{MA}C_{MA}+K_{PD}C_{PD}+K_{CO}C_{CO})$$

To comparison with others $K_{MA}C_{MA}$ and $K_{PD}C_{PD}$ is very small, thus can ignore (Schbib *et. al.*, 1996)

$$\Sigma\theta = (1-\Sigma\theta)(K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

$$(1-\Sigma\theta) = 1/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})$$

Replacing θ_{Ac}, θ_{Eth}, θ_{H2}, θ_{MA}, and θ_{PD} in the rate equations. Obtain :

$$-r_{Ac} = k_{Ac}K_{Ac}C_{Ac}K_{H2}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^4$$

$$-r_{Ac} = K1C_{Ac}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^4$$

and

$$-r_{Eth} = K2C_{Eth}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^4$$

$$-r_{MA} = K4C_{MA}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^4$$

$$-r_{PD} = K5C_{PD}C_{H2}/(1+K_{Ac}C_{Ac}+K_{Eth}C_{Eth}+(K_{H2}C_{H2})^{0.5}+K_{CO}C_{CO})^4$$

B.22 The simulation result of the MODEL XII

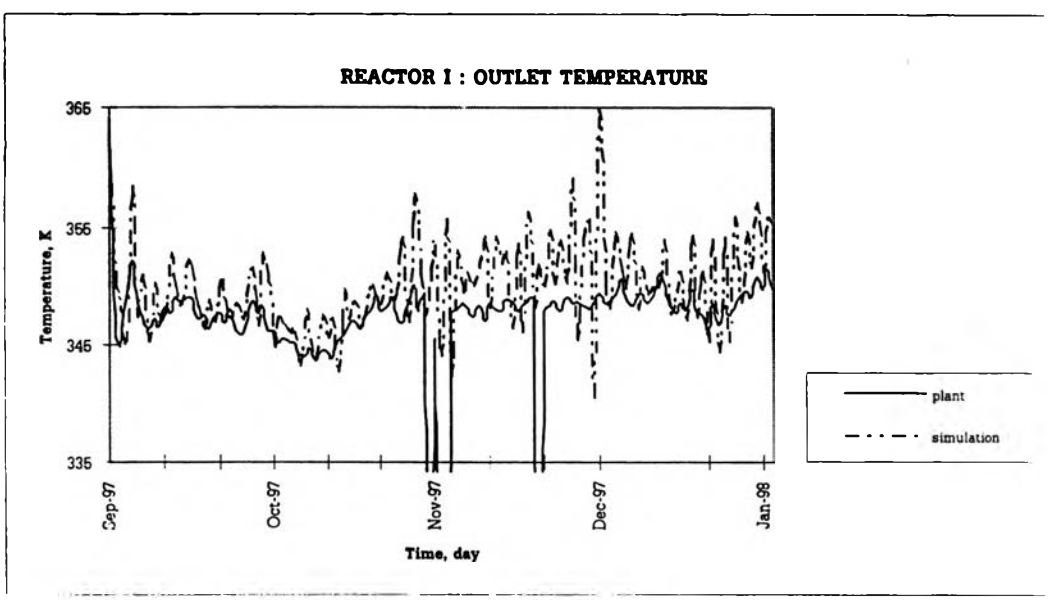

Figure B.91 MODEL XII : Outlet temperature of reactor I with error 0.86%

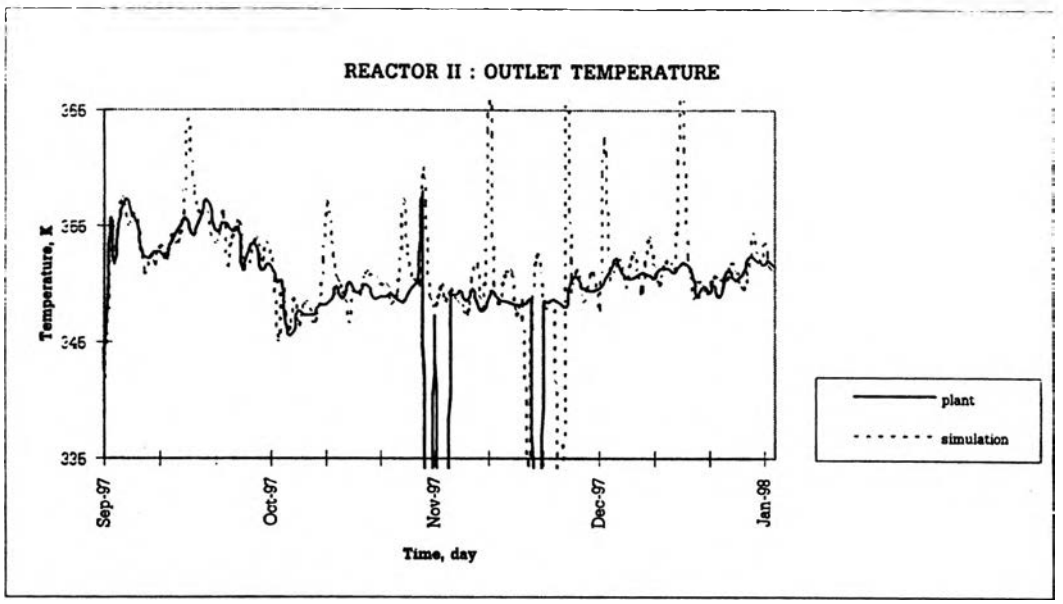

Figure B.92 MODEL XII : Outlet temperature of reactor II with error 68%

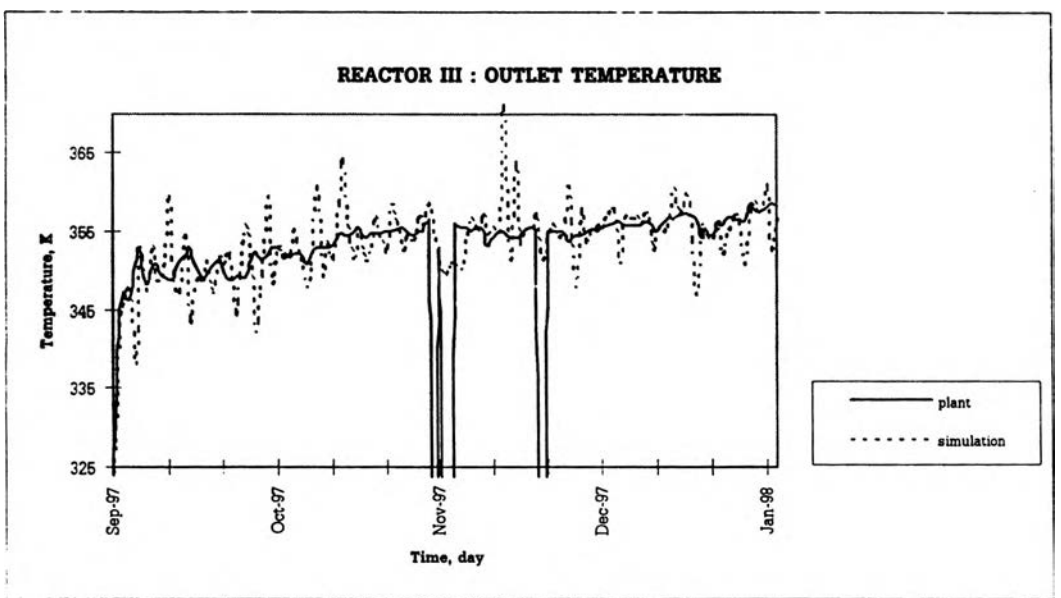

Figure B.93 MODEL XII : Outlet temperature of reactor III with error 0.71%

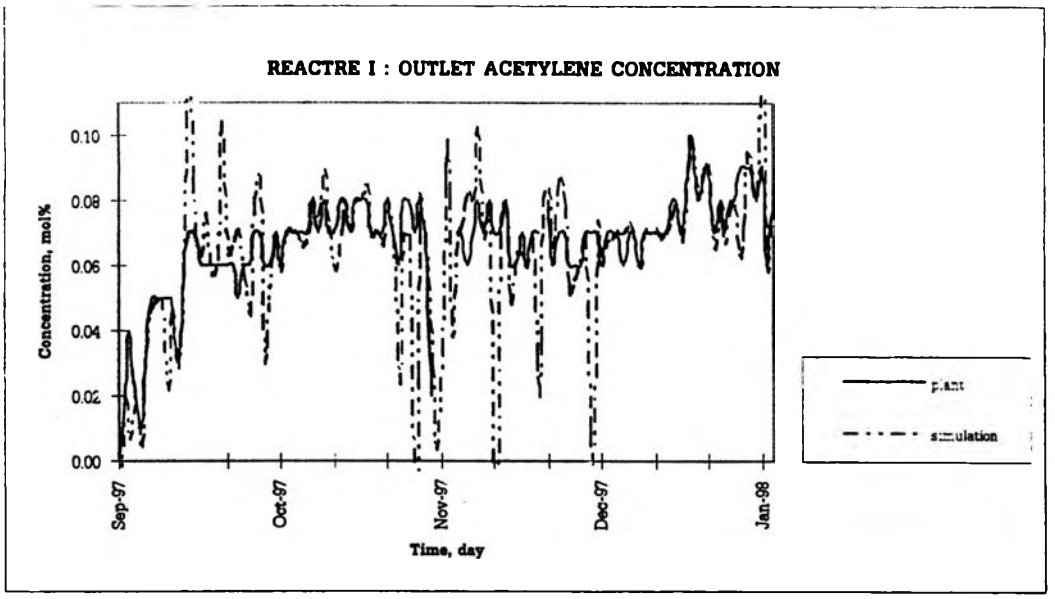

Figure B.94 MODEL XII : Outlet acetylene concentration of reactor I with error 22.65%

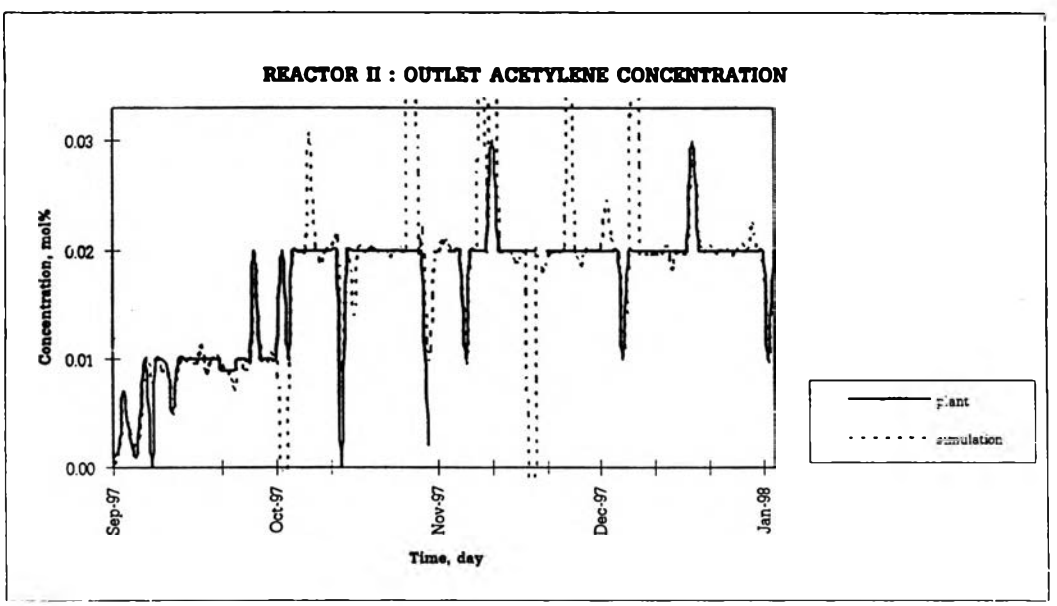

Figure B.95 MODEL XII : Outlet acetylene concentration of reactor II with error 18.76%

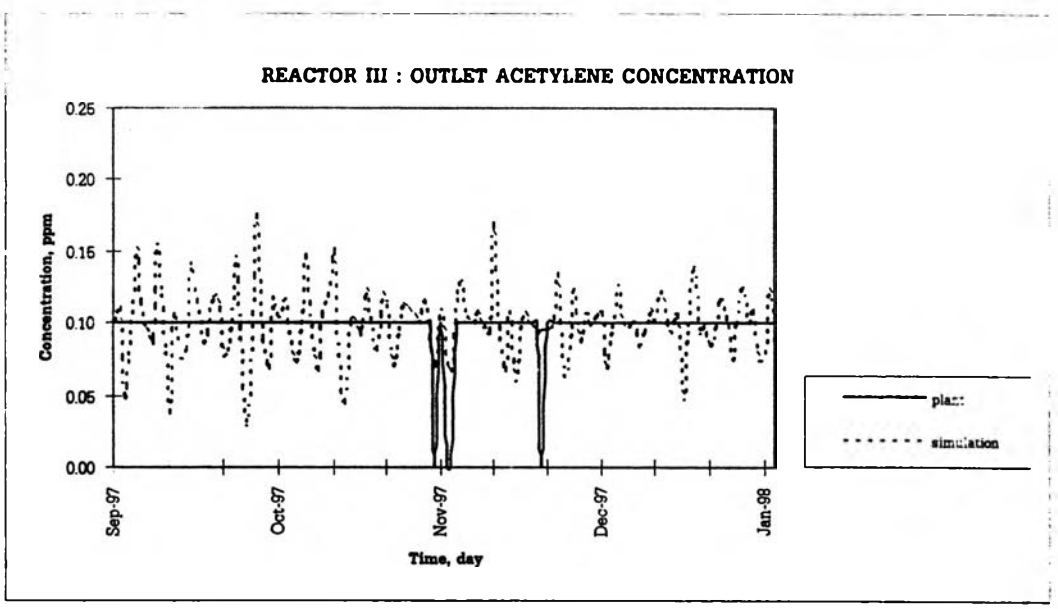

Figure B.96 MODEL XII : Outlet acetylene concentration of reactor III with error 17.09%

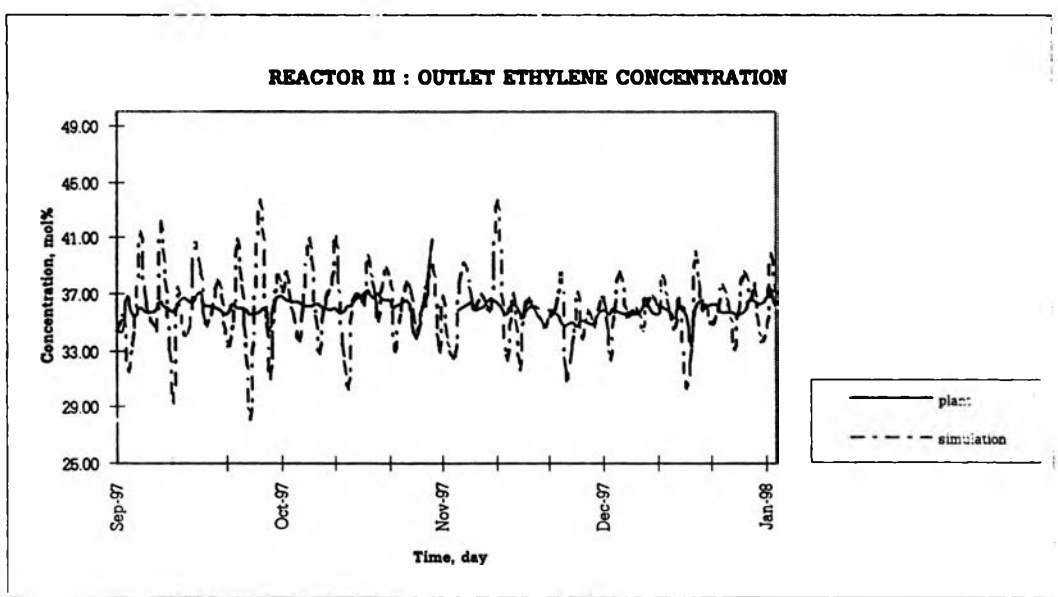

Figure B.97 MODEL XII : Outlet ethylene concentration of reactor III with error 4.94%

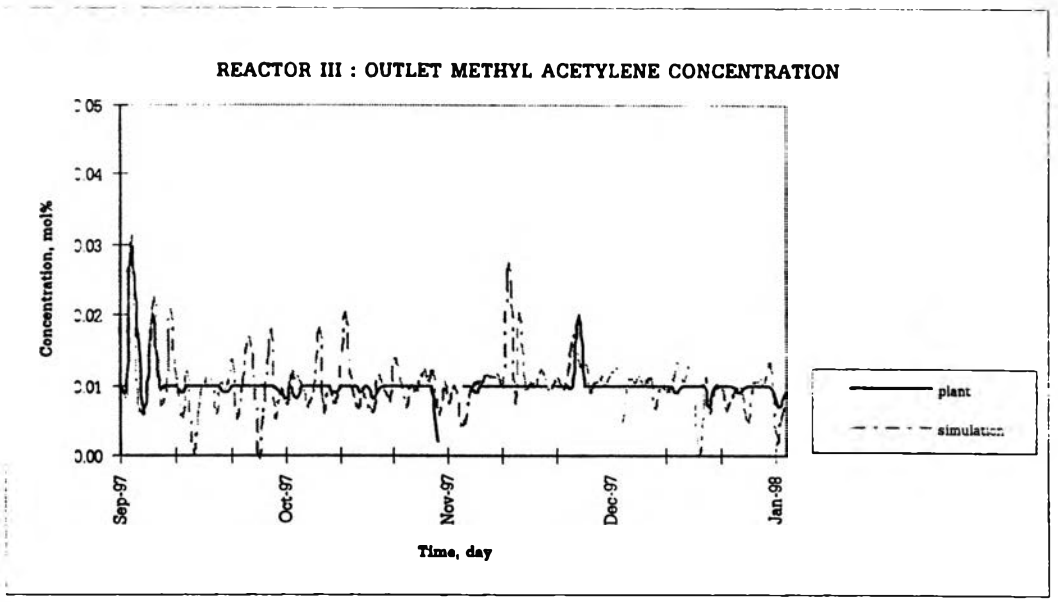

Figure B.98 MODEL XII : Outlet methyl acetylene concentration of reactor III with error 25.91%

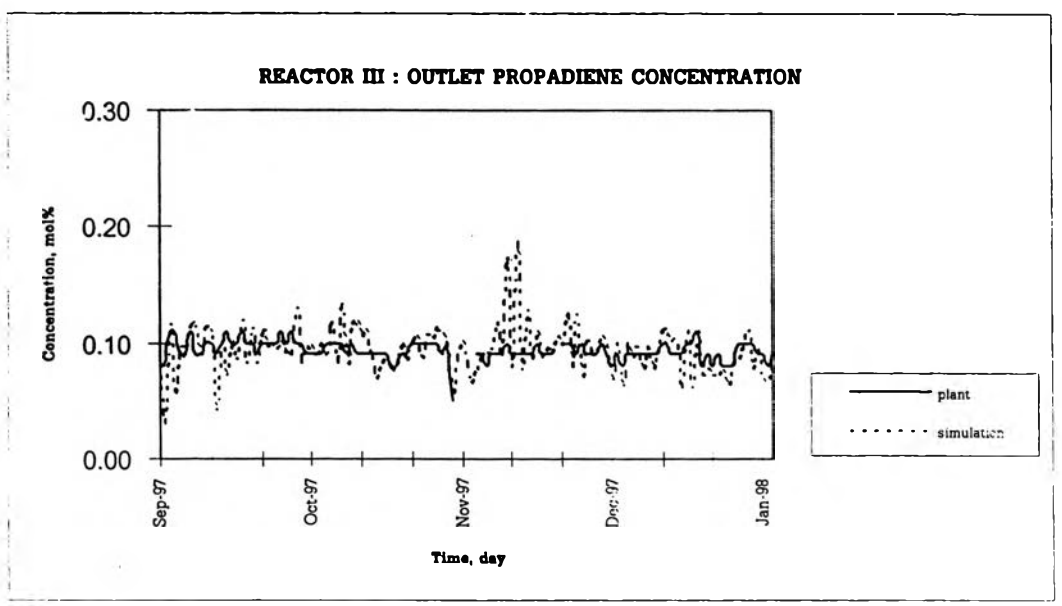

Figure B.99 MODEL XII : Outlet propadiene concentration of reactor III with error 14.11%

APPENDIX C

SPEEDUP PROGRAM

SPEEDUP is a comprehensive plant modeling package designed to model processes as they occur in chemical or process engineering environments—as a series of unit operations interconnected by process streams. SPEEDUP can easily make new models form the set of equations(both algebraic and ordinary differential equations) that define the model because SPEEDUP is an equation-based flowsheeting package. When SPEEDUP solve for solution, the problems are viewed as set of equations rather than sets of unit operations

A problem that SPEEDUP is to solve must be written all description in SPEEDUP input language. A problem description is composed of a number of input section, each problem description is unlikely to use all type of sections. The sections used will depend upon each problem description. Ana the sections which may be used are :

- Flowsheet and Unit sections

  These sections describing the topology of the flowsheet being modelled. The Flowsheet section defines all of the interconnections between the UNITS within a problem. The interconnections are either process flows which are known as 'streams', or information connections which are known as 'connections'.The Unit section defines the occurrence of a unit within the flowsheet. Each Unit section specifies the MODEL or MACRO to be use for UNIT, and gives values for the Unit parameter (that required by the MODEL or MACRO being used)

- Model, Macro, Procedure and Function sections

  These sections are used in modelling items of equipment. MODELs are the central part of any problem definition. One Model section is required to

define each MODEL used in a problem. The Macro section used as a device for tresting a group of MODELs as a single uint. One Macro section is required to define each MACRO. For Procedure and Function section, both are devices for using FORTRAN. But they have a major difference as follows : The Procedure uses a FORTRAN subroutine then may return any number of values and can only be used in the Procedure subsection of a MODEL.Unlike Procedure, the Function uses a FORTRAN function that can only return a single output value and the Function may be used in a simple assignment statement within a Model, Operation, Report, Conditions or Global section.

- Global section

  This section is used to define optimization problems and flowsheet-wide equations. The Global section allows you to write equations involving variables from more than one UNIT.

- Conditions section

  This section is used to specify the conditions under which a SPEEDUP dynamic simulation should stop or print a message.

- Estimation section

  This section used to define both parameter estimation and data reconciliation problems.

- Operation and Options sections

  These sections providing specification and simulation options data for a particular run. The operation section is to specify operating data for the process being modelled. The Option section is used to define the problem description such as various translation and run time options. If the valve for an option is not specified the default value is used.

- Report and Profiles sections

  These sections are used to define the presentation of output. The Profiles section is used to define one or more composite variables for use within the

axial profile plotting facility. The Report section is used to define customized reports for displaying result of any variable in the problem.

The complete problem description that include the only six sections(as list: Flowsheet, Model, Unit, Declare, Operation, and Option sections) is allowed to run for the solution.

C.1 Flowsheet section

The Flowsheet section defines all of the interconnections between the Units within a problem. This section is as same as the process flow diagram.

Syntax for Flowsheet section

```
FLOWSHEET
        STREAM stream_name  connectivity_statement TYPE stream_type
```

Where connectivity_statement is of the form:

```
| FEED    name                | IS | FEED    name                |
| PRODUCT name                |    | PRODUCT name                |
| INPUT   name OF unit_name   |    | INPUT   name OF unit_name   |
| OUTPUT  name OF unit_name   |    | OUTPUT  name OF unit_name   |
```

or

```
CONNECTION name OF unit_name IS CONNECTION name OF unit_name
```

Example C.1 Mixing process

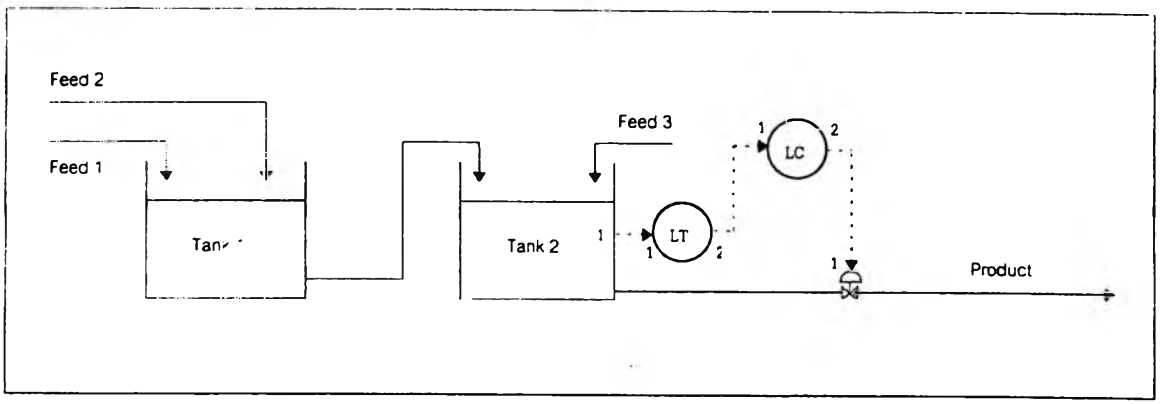

Figure C.1 Mixing process flowshart

****

Flowsheet

Feed 1	is	Input 1 of Tank 1
Feed 2	is	Input 2 of Tank 1
Output of Tank 1	is	Input 1 of Tank 2
Feed 3	is	Input 2 of Tank 2
Output of Tank 2	is	Input of Valve
Output of Valve	is	Product

#----------#

connectivity

#----------#

Connection 1 of Tank2	is Connection 1 of LT
Connection 2 of LT	is Connection 1 of LC
Connection 2 of LC	is Connection 1 of Valve

****

C.2 MODEL section

Models are the central part of any problem definition. One Model section is required to define each Model used in a problem. A model may contain up to 6 different subsections, each of which deals with part of the model definition:

HELP	Contains help text that can be viewed using the EXPLAIN command. Optional.
SET	Defines any constants or parameters used. Optional.

TYPE	Assigns variable types to all of the variables. Also defines the size of vector variables. Compulsory.
STREAM	Defines the interconnections that can be made to the model Compulsory.
EQUATION	Contains all of the equations used to define the Model Compulsory.
PROCEDURE	Contains all of the procedure calls used in defining the Model. Optional.

Syntax for Model section

```
MODEL modelname
        HELP
                help_text
        $ENDHELP
        SET
                parameter1, parameter2, ...
                constant1 = {*}value1, constant2 = {*}value2, ...
        TYPE
                variable1, variable2, ... AS  | variable_type                    |
                                              | ARRAY(size) OF variable_type     |

        STREAM
                | INPUT          | name  variable1, variable2, ...
                | OUTPUT         |
                | CONNECTION     |
                        :
        EQUATION
                expression1 = expression2 ;
                        :
        PROCEDURE
                (output_arg_list) procedure_name (input_arg_list) {| INPUT  | name}{,TEAR}
                                                                  |OUTPUT|
                                        :
```

Example C.1 Mixing process (continue)

```
****
Model CSTR
Set
        Area
Type
        FLOWIN1,FLOWIN2,FLOWOUT          as flowrate
        Dens1, Dens2, Dens_out           as density
        Cp1,Cp2,Cp_out                   as heat_capacity
        TIN1,TIN2,TOUT                   as temperature
        h,H                              as hieght
Stream
        Input 1          is  FLOWIN1,Dens1,Cp1,TIN1
        Input 2          is  FLOWIN2, Dens2,Cp2,TIN2
        Output           is  FLOWOUT, Dens_out,Cp_out,TOUT
        Connection 1     is  H
Equation
        Area*dh/dt   =  FLOWIN1+FLOWIN2-FLOWOUT
        Dens_out     =  ((FLOWIN1*Dens1)+(FLOWIN2*Dens2))/(Area*h)
        Cp_out       =  ((Cp1*FLOWIN1*Dens1)+(Cp2*FLOWIN2*Dens2))/(Dens_out*Area*h);
        TOUT* Dens_out*Area*h*Cp_out = TIN1*Cp1*FLOWIN1*Dens1+TIN2*Cp2*FLOWIN2*Dens2;
        H            =  h;
****
Model SENSOR
Set
        bias
Type
        sigin            as  control_signal
        sigout           as  control_signal
Stream
        Connection 1     is  sigin
        Connection 2     is  sigout
Equation
        sigout       =  sigin+bias;
****
```

```
Model PI
Set
        gain,
        integral_time,
        bias
Type
        error           as  control_signal
        I_error         as  control_signal
        set_point       as  control_signal
Stream

Equation
        error           =   set_point- h_measured;
        $I_error        =   error;
        control_action  =   bias+gain*(error+I_error/ integral_time);
****
```

C.3 UNIT section

A Unit section must be included for each of the process units in the FLOWSHEET. Each Unit section specifies the Model or Macro to be used for the Unit, and gives values for the Unit parameters (if required by the Model or Macro being used).

It is not necessary to use all Unit sections during a run Units may be stored on the database then used when required. Only Units that appear in the FLOWSHEET will be included in the run.

Syntax for Unit section

```
UNIT   unit_name  IS  A   | model_name |
                          | macro_name |
       { Routines         |EULER       |}
                          |IMPEULER    |

       SET        parameter1 = value1,
                  parameter2 = value2,
                             :
```

Example C.1 Mixing process (continue)

```
****
Unit Tank 1   is  a CSRT
Set
        Area = 10
****
Unit Tank 2   is  a CSRT
Set
        Area = 8
****
Unit LT       is  a SENSOR
Set
        Bias = 0.5
****
Unit LC       is  a PI
Set
        gain          =  1,
        integral_time =  1,
        bias          =  1.5
****
```

C.4 DECLARE section

The Declare section is used to declare the characteristics of the different variables and stream types used in the problem. If a physical properties package is interfaced, you may also use the Declare section to alter component data, or to define new components.

Syntax for Declare section

```
DECLARE
        TYPE  variable_type_statements
        STREAM  stream_name
                SET             parameter = value, etc.
                TYPE            type_list
                                * COMPONENTS  component_list
                                * OPTIONS     pp_options_list
```

```
                    * THERMO    stream_name
        CODE
                    user_text
        $ENDCODE
```

Keywords marked with a * apply only to installations which have a physical property interface in which these features are used.

Example C.1 Mixing process (continue)

```
****
Declare
#-------------------------------------------------------------------------------------#
# Variable type  = initial value : lower limit : upper limit  Unit  =  Header text #
#-------------------------------------------------------------------------------------#
  flowrate      = 5          : 0          : 15          Unit  =  "m3/hr"
  density       = 2          : 0          : 5           Unit  =  "mol/m3"
  heat_capacity = 10         : 0          : 15          Unit  =  "cal/mol*K"
  temperature   = 340        : 330        : 400         Unit  =  "K"
  hiegth        = 1.5        : 0.5        : 1.7         Unit  =  "m"
  control_signal = 0         : -1E10      : 1E10        Unit  =  " "
#-------------------------------------------------------------------------------------#
Stream MAINSTREAM
        Type    flowrate, density, heat_capacity, temperature
****
```

C.5 OPERATION section

The Operation section is used to specify operating data for the process being modelled. The Operation section may contain up to four subsections. These are:

SET — Used to SET variables within the problem to known, fixed values. The Set subsection is always required.

PRESET — Used to enter estimates of solution values, and bounds for individual variables. The Preset subsection is optional. An optional scale factor may also be entered to scale individual

variables.

INITIAL — Used to provide INITIAL values of variables, that is, those at time equals zero, for dynamic simulations. The initial subsection is only required for dynamic simulations. It may be omitted if INITIAL values from a saved RESULT are to be used.

FREE — Used to specify which variables are to be FREEd (i.e varied to achieve the optimum) during optimizations. The Free subsection is only required for optimizations.

Syntax for Operation section

```
OPERATION
        SET
                WITHIN unit1
                        variable = expression { : low_bound : up_bound }
                                :
                WITHIN unit2
                        variable = expression { : low_bound : up_bound }
                                :
        PRESET
                WITHIN unit1
                        variable = value { : low_bound : up_bound : scale }
                                :
                WITHIN unit2
                        variable = value { : low_bound : up_bound : scale }
                                :
        INITIAL
                WITHIN unit1
                        variable = value { : low_bound : up_bound }
                                :
                WITHIN unit2
                        variable = value { : low_bound : up_bound }
        FREE
                unit.variable { : scale }
```

Example C.1 Mixing process (continue)

```
****
Operations
Set
        Within Tank1
                FLOWIN1   = 8
                FLOWIN2   = 6
                Dens1     = 4.2
                Dens2     = 4.5
                Cp1       = 10.3
                Cp2       = 9.7
                TIN1      = 356
                TIN2      = 364
        Within Tank2
                FLOWIN2   = 7
                Dens2     = 3.21
                Cp2       = 10.7
                TIN2      = 335
Initial
        Within LC
                error     = 0
****
```

C.6 OPTIONS Section

The Options section of the problem description allows you to specify values for various translation and run time options. These options are

The numerical routines to be used

Options to be used during translation

The level of translator output for each input section

Parameters (output levels, tolerances, etc) for the execution phase

If a value for an option is not specified the default value is used. The only options which do not have defaults are the reporting time step (TIME_STEP) and

number of intervals (INTERVALS). For dynamic runs, these must be specified. For other run modes, they need not be specified.

Example C.1 Mixing process (continue)

```
****
Options
Execution
        TARGET          = TERMINAL
        PRINTLEVEL      = 1
        INTERVAL        = 100
****
```

VITA

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