State Estimation of a Switched Non-linear System Using an Interacting Multiple Model Estimation Algorithm

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Abstract — **In this paper, the authors have designed and implemented a state estimation scheme, using an interacting multiple model based derivative free Kalman filter algorithm for a stochastic nonlinear hybrid system. The switched non-linear system considered for the simulation study is a non-isothermal continuous stirred tank reactor which can be operated in one of the three modes. It should be noted that the mode transition is triggered when a higher yield is desired. Simulation studies have been carried out to assess the efficacy of the proposed state estimation scheme on the simulated model of the chemical reactor.**

I. Introduction

Recursive estimation of state variables of a continuous stirred tank reactor namely reactor concentration and temperature are very important from the view point of process monitoring and advanced process control. It may be noted that Kalman update based filters (UKF and EnKF) and particle filters have been proposed for hybrid systems [7], [10]. The feature of the hybrid system is its multimodal structure which switches between discrete modes with continuous dynamics. Excellent review articles on state and parameter estimation have been reported recently in the literature [11], [14].

Recently, a fault detection and monitoring scheme for non-isothermal chemical reactor with uncertain mode transitions using deterministic observer for each mode have been proposed [1]. In the above problem, the uncertainty in the mode transition arises due to the lack of a prior knowledge of either the timing or the sequence of transitions between the constituent modes [1]. Modeling, analysis and control of the hybrid system have gained much importance among the research community [2], [3], [4], [5], [9]. The use of moving horizon based state estimation for hybrid system has been reported in [12]. Design and implementation of a Continuum and Non-continuum State Estimator for the Distillation Column have been reported in [10]. Recently state estimation of two-tank hybrid system using an interacting multiple-model algorithm has been proposed in [6]. A novel derivative free estimator based nonlinear model predictive control schemes for an optimal control of autonomous hybrid system has been proposed in [7]. With the exception of few references, to the best of the authors' knowledge formulation of state estimation scheme for stochastic hybrid process control system using an interacting multiple-model based derivative free Kalman filter algorithm has hardly received any attention in the process control literature.

In this work, we develop a state estimation scheme for non-isothermal continuous stirred tank reactor which is subjected to stochastic state disturbances and measurement noise using an UKF based interacting multiple-model algorithm.The organization of the paper is as follows: Section II describes the process description and section III deals with interacting multiple-model algorithm. Simulation studies have been reported in section IV and concluding remarks in section V.

II. Process Description

The schematic diagram of the hybrid non-isothermal chemical reactor is shown in Fig.1 [1]. The reactor can be operated in one of the three modes (r=1, 2, 3). Irreversible exothermic chemical reaction has been taking place inside the reactor with A being the reactant species and B being the desired product. The governing mass and energy balance equations of the reactor for various modes are shown as follows:

MODE – 1

In mode 1, the reactor is provided with feed inflow rate F_1, molar concentration C_{A1} and temperature T_{A1} of the reactant species A.

$$\dot{C}_A = \frac{F_1}{V}(C_{A1} - C_A) - k_0 \exp\left(\frac{-E}{RT}\right) C_A \qquad (1)$$

$$\dot{T} = \frac{F_1}{V}(T_{A1} - T) + \frac{-\Delta H_r}{\rho c_p} k_0 \exp\left(\frac{-E}{RT}\right) C_A + \frac{Q_1}{\rho c_p V}$$

MODE – 2

In mode 2, the reactor is supplied with another feed with inflow rate as F_2, molar concentration C_{A2} and temperature T_{A2} as shown in Fig.1.

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$$\dot{C}_A = \frac{F_1}{V}(C_{A1} - C_A) + \frac{F_2}{V}(C_{A2} - C_A) - k_0 \exp\left(\frac{-E}{RT}\right) C_A$$

$$\dot{T} = \frac{F_1}{V}(T_{A1} - T) + \frac{F_2}{V}(T_{A2} - T) + \frac{-\Delta H_r}{\rho c_p} k_0 \exp\left(\frac{-E}{RT}\right) C_A + \frac{Q_2}{\rho c_p V} \quad (2)$$

MODE – 3

Third feed with reactant species 'A' having inflow rate as F_3, molar concentration C_{A3} and temperature T_{A3} has been added to the reactor in mode 3, as shown in Fig.1.

$$\dot{C}_A = \frac{F_1}{V}(C_{A1} - C_A) + \frac{F_2}{V}(C_{A2} - C_A) + \frac{F_3}{V}(C_{A3} - C_A) - k_0 \exp\left(\frac{-E}{RT}\right) C_A \quad (3)$$

$$\dot{T} = \frac{F_1}{V}(T_{A1} - T) + \frac{F_2}{V}(T_{A2} - T) + \frac{F_3}{V}(T_{A3} - T) + \frac{-\Delta H_r}{\rho c_p} k_0 \exp\left(\frac{-E}{RT}\right) C_A + \frac{Q_3}{\rho c_p V}$$

Based on the desired requirement of the yield, the mode transition has been initiated and the reactor switches between these modes. V is the volume of the reactor, k_0 is a constant, E and ΔH_r are activation energy and the enthalpy of the chemical reaction respectively. R is the gas constant, heat capacity c_p , ρ is the density of the fluid inside the reactor and Q is the rate of heat input provided to the reactor.

TABLE I: PROCESS PARAMETERS

Parameter	Value
F_1	4.998 m^3/h
F_2	12.998 m^3/h
F_3	16.998 m^3/h
C_{A1}	4.0 $kmol/m^3$
C_{A2}	4.5 $kmol/m^3$
C_{A3}	5.0 $kmol/m^3$
T_{A1}	295.0 K
T_{A2}	320.0 K
T_{A3}	340.0 K
T_{A1}^{nom}	300.0 K
Q_1^{nom}	0 kJ/h
Q_2^{nom}	187,768 kJ/h
Q_3^{nom}	367,978 kJ/h
V	1.0 m^3
R	8.314 kJ/kmol. K
ΔH_r^{nom}	-5.0×10^4 kJ/kmol
k_0	3.0×10^6 h^{-1}
E	5.0×10^4 kJ/kmol
P	1000.0 kg/m^3
c_p	0.231 kJ/kg. K
C^s_{A1}	3.59 $kmol/m^3$
C^s_{A2}	4.23 $kmol/m^3$
C^s_{A3}	4.60 $kmol/m^3$
T^s	388.57 K

Unscented Kalman filter has been designed for each mode, r=3 using standard Unscented Kalman filter algorithm as reported in the Appendix-A [8]. The parameters associated with the chemical reactor are reported in Table I.The parameters associated with the UKF are reported in Table II.

III. THE INTERACTING MULTIPLE MODEL ESTIMATOR: IMM-UKF [13, 15, 6]

In this subsection, we describe the steps involved in obtaining state estimates of switched non-linear system using the IMM approach. The IMM algorithm consists of 'r' interacting derivative free Kalman filters operating in parallel as shown in Fig.2. The IMM-UKF based state estimation scheme is shown in Fig.1. At discrete time 'k' the state estimate is computed using 'r' Unscented Kalman filters, with each UKF using a different combination of the previous model-conditioned estimates (mixed initial condition).The steps involved in the design and implementation of IMM based state estimation scheme are as follows:

A. Mixing probability

The probability that the mode M_i was in effect at instant k-1 given that M_j is in effect at k conditioned on Y^{k-1} is

$$\lambda_{i|j}(k-1|k-1) = P[M_i(k-1)|M_j(k), Y^{k-1}]$$

$$\lambda_{i|j}(k-1|k-1) = \frac{P_{ij}\ \mu_i(k-1)}{\sum_{i=1}^{r} P_{ij}\ \mu_i(k-1)} \quad i,j=1,2,...r \quad (4)$$

Where $\lambda_{i|j}(k-1|k-1)$ is mixing probability, P_{ij} is the assumed transition probability for the Markov chain according to which the system model switches from model i to model j, $\mu_i(k-1)$ is the model probability. The input to the filter matched to model j is obtained from an interaction of the 'r' derivative free Kalman filters, which consists of the mixing of estimates $\hat{x}^{(i)}(k-1|k-1)$ with the weights $\lambda_{i|j}(k-1|k-1)$, called the mixing probabilities.

B. Interaction and Mixing

$$\hat{x}^{0j}(k-1|k-1) = \sum_{j=1}^{r} \hat{x}^{i}(k-1|k-1)\lambda_{i|j}(k-1|k-1) \ ; i=1...r \quad (5)$$

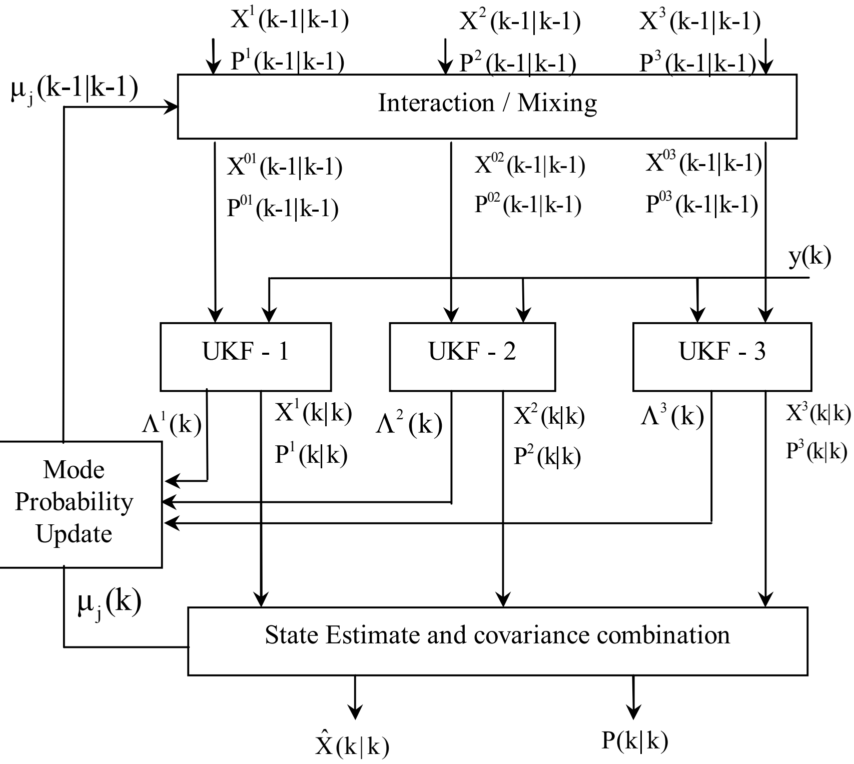


Fig.2. Interacting Multiple Model Filter (Three Mode)

The covariance is computed as

$$P^{0j}(k\text{-}1|k\text{-}1)=\sum_{j=1}^{r}\lambda_{i|j}(k\text{-}1|k\text{-}1)[P^i(k\text{-}1|k\text{-}1) + [\hat{x}^i(k\text{-}1|k\text{-}1)\text{-}\hat{x}^{0j}(k\text{-}1|k\text{-}1)] [\hat{x}^i(k\text{-}1|k\text{-}1)\text{-}\hat{x}^{0j}(k\text{-}1|k\text{-}1)]^T] \quad (6)$$

The likelihood functions corresponding to all derivative free Kalman filters are computed according to

$$\Lambda^j(k)=\frac{\exp\left[-0.5\left[\gamma^j(k)\left[P^j_{yy}(k)\right]^{-1}\gamma^j(k)^T\right]\right]}{\sqrt{(2\pi)^r|P^j_{yy}(k)|}} \quad (7)$$

In the above equation, $\gamma^j(k)$ $P^j_{yy}(k)$ are the innovation and innovation covariance matrix of j^{th} UKF.

C. Mode Probability update

Mode probability update is computed as

$$\mu_j(k)=\frac{\Lambda^j(k)\left[\sum_{i=1}^{r}P_{ij}\,\mu_i(k\text{-}1)\right]}{\sum_{j=1}^{r}\Lambda^j(k)\left[\sum_{i=1}^{r}P_{ij}\,\mu_i(k\text{-}1)\right]} \quad j=1,2,...r \quad (8)$$

D. State estimate and covariance combination

$$\hat{x}(k|k)=\sum_{j=1}^{r}\hat{x}^j(k|k)\mu_j(k)$$

$$P(k|k)=\sum_{j=1}^{r}\mu_j(k)\left[\begin{array}{l}P^j(k|k)\\ +\left[\hat{x}^j(k|k)-\hat{x}\ (k|k)\right]\left[\hat{x}^j(k|k)-\hat{x}(k|k)\right]^T\end{array}\right] \quad (9)$$

IV. SIMULATION STUDY

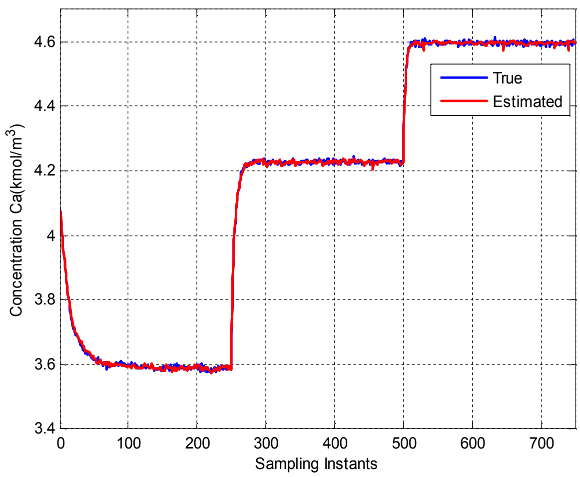
The efficacy of the proposed state estimation scheme has been analyzed on the switched non-linear system subjected to mode transitions. The reactor is operated at the unstable operating point in each mode by maintaining the temperature (T) at 388.57 deg. K using a PI controller.It should be noted that the mode transition is triggered when a higher yield is desired [1].

TABLE II. PARAMETER ASSOCIATED WITH UKF

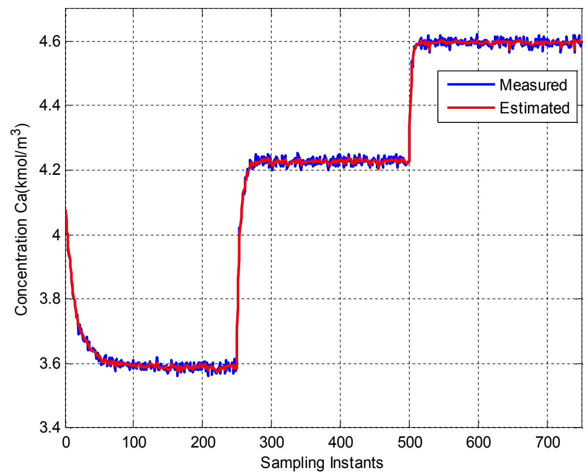
Parameter	Value
Measurement noise covariance Matrix R	$\begin{bmatrix}1.0e^{-4} & 0\\ 0 & 1\end{bmatrix}$

Process noise covariance Matrix Q^j	$\begin{bmatrix} 2.5e^{-5} & 0 \\ 0 & 2.5e^{-3} \end{bmatrix}$ $j = 1, 2, 3$
Markov chain Transition Matrix P_{ij}	$\begin{bmatrix} 0.90 & 0.05 & 0.05 \\ 0.05 & 0.90 & 0.05 \\ 0.05 & 0.05 & 0.90 \end{bmatrix}$
α, β and κ	1, 0 and 0
Initial error covariance $P^j(0 \mid 0)$	$\begin{bmatrix} 2.5e^{-5} & 0 \\ 0 & 2.5e^{-3} \end{bmatrix}$ $j = 1, 2, 3$
Initial state vector $\hat{X}^j(0 \mid 0)$	$\begin{bmatrix} 3.59 & 388.57 \end{bmatrix}^T$ $j = 1$ $\begin{bmatrix} 4.23 & 388.57 \end{bmatrix}^T$ $j = 2$ $\begin{bmatrix} 4.60 & 388.57 \end{bmatrix}^T$ $j = 3$
Mode probability $\mu(0 \mid 0)$	$\begin{bmatrix} 1/3 & 1/3 & 1/3 \end{bmatrix}^T$

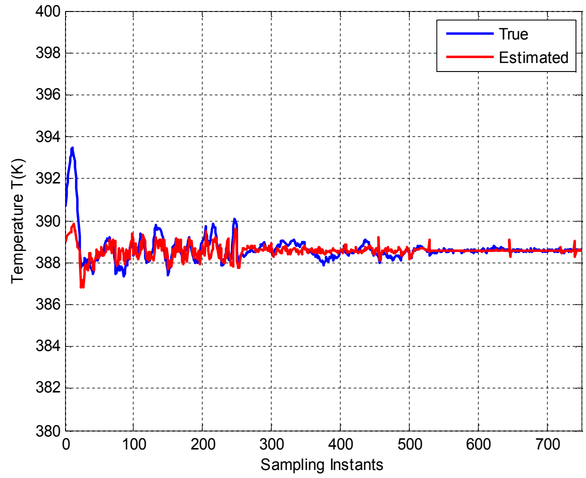
The evolution of true and estimated state variables using an IMM-UKF algorithm is reported in Fig.3 From the Fig.3b and Fig.3d it can be inferred that the IMM-UKF based state estimation scheme is able to generate fairly accurate filtered estimates of state variables of non-isothermal reactor namely reactor concentration and reactor temperature. The mode probability update is reported in Fig.4.



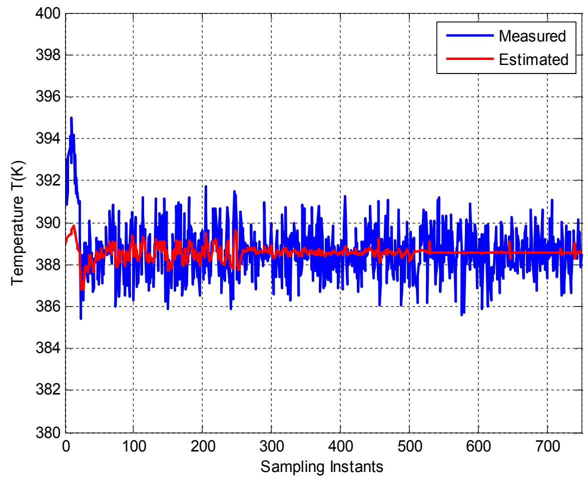
(a)



(b)



(c)



(d)

Fig.3. a) Evolution of true and estimated value of concentration b) Evolution of measured and estimated value of concentration c) Evolution of true and estimated value of temperature d) Evolution of measured and estimated value of temperature

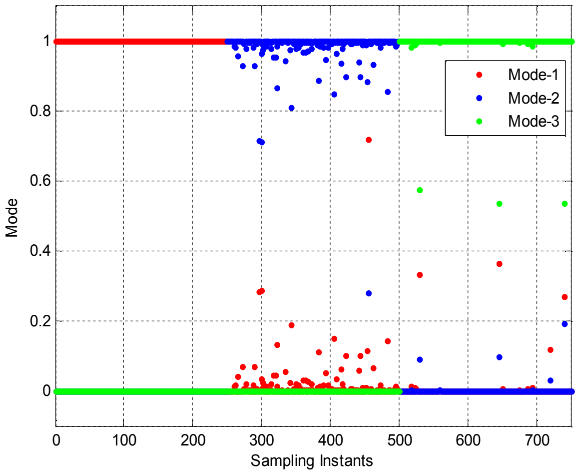


Fig.4. Mode probability update of IMM-UKF based estimation scheme

V. CONCLUDING REMARKS

IMM-UKF based state estimation scheme has been designed and implemented on the simulated model of the nonisothermal chemical reactor exhibiting mode transition. From the simulation studies, it is observed that the IMM-UKF based state estimation scheme is able to generate accurate state estimates of reactor concentration and reactor temperature.

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APPENDIX - A

UNSCENTED KALMAN FILTER ALGORITHM

Generation of sigma points is as follows:

A set of 2L+1 sigma points, $\chi(k-1|k-1,i)$ with the associated weights, $W(i)$ are chosen symmetrically about $\hat{x}(k-1|k-1)$ as given below.

$$\chi(k-1|k-1,0)=\hat{x}(k-1|k-1);$$

$$\chi(k-1|k-1,i)=\hat{x}(k-1|k-1)+\left(\sqrt{(L+\lambda)P(k-1|k-1)}\right)_i \quad i=1,\ldots,L$$

$$\chi(k-1|k-1,i)=\hat{x}(k-1|k-1)-\left(\sqrt{(L+\lambda)P(k-1|k-1)}\right)_{i-L} \quad i=L+1,\ldots,2L$$

$$W^m(0)=\frac{\lambda}{L+\lambda};$$

$$W^c(0)=\frac{\lambda}{L+\lambda}+(1-\alpha^2+\beta);\ \lambda=\alpha^2(L+\kappa)-L$$

$$W^c(i)=W^m(i)=\frac{1}{2(L+\lambda)};\ i=1,\ldots,2L$$

Where κ is a secondary scaling parameter, α is a factor determining the spread of sigma points around $\hat{x}(k-1|k-1)$ and is usually set between 1e-4 to 1. The parameter β is used to incorporate prior knowledge of distribution of x and for Gaussian distribution its optimum value is 2. The 2L+1 sigma points have been derived from the state $\hat{x}(k-|k-1)$ and covariance of the state vector $P(k-1|k-1)$, where L is the dimension of the state vector.

Implemenatation of UKF algorithm is as follows:

In the prediction step, the sigma points are propagated through the nonlinear process model to obtain the predicted set of sigma points as

$$\chi(k|k-1,i)=\chi(k-1|k-1,i)+\int_{(k-1)\Delta t}^{k\Delta t}F[\chi(\tau,i)]d\tau; \quad i=0,\ldots.,2L \qquad (A.1)$$

Predicted Mean is given by

$$\hat{x}(k|k-1) = \sum_{i=0}^{2L} W^m(i)\chi(k|k-1,i) \tag{A.2}$$

Predicted covariance matrix is computed as follows

$$P(k|k-1) = \sum_{i=0}^{2L} W^c(i)\{\chi(k|k-1,i) - \hat{x}(k|k-1)\} * \{\chi(k|k-1,i) - \hat{x}(k|k-1)\}^T + Q \tag{A.3}$$

Sigma points are redrawn using the predicted mean as given below

$$\chi^*(k|k-1,0) = \hat{x}(k|k-1);$$

$$\chi^*(k|k-1,i) = \hat{x}(k|k-1) + \left(\sqrt{(L+\lambda)P(k|k-1)}\right)_i \quad i = 1,...,L$$

$$\chi^*(k|k-1,i) = \hat{x}(k|k-1) - \left(\sqrt{(L+\lambda)P(k|k-1)}\right)_{i-L} \quad i = L+1,...,2L$$

The Predicted observation is given by

$$\hat{y}(k|k-1) = \sum_{i=0}^{2L} W^m(i) * C\left[\chi^*(k|k-1,i)\right] \tag{A.4}$$

The computation of Innovation covariance and cross covariance is as follows:

$$P_{yy}(k) = \sum_{i=0}^{2L} [W^c(i)\{H[\chi^*(k|k-1,i)] - \hat{y}(k|k-1)\} * \{C[\chi^*(k|k-1,i)] - \hat{y}(k|k-1)\}^T] + R \tag{A.5}$$

$$P_{xy}(k) = \sum_{i=0}^{2L} W^c(i)\{\chi^*(k|k-1,i) - \hat{x}(k|k-1)\} * \{C[\chi^*(k|k-1,i)] - \hat{y}(k|k-1)\}^T \tag{A.6}$$

The innovation is computed as follows:

$\gamma(k) = y(k) - \hat{y}(k|k-1)$.

The Kalman gain matrix $K(k)$ can be determined as follows

$$K(k) = P_{xy}(k)P_{yy}^{-1}(k) \tag{A.7}$$

The updated State and Covariance matrix are computed using the following equations

$$\hat{x}(k|k) = \hat{x}(k|k-1) + K(k) * \gamma(k) \tag{A.8}$$

$$P(k|k) = P(k|k-1) - K(k) * P_{yy}(k)K^T(k) \tag{A.9}$$

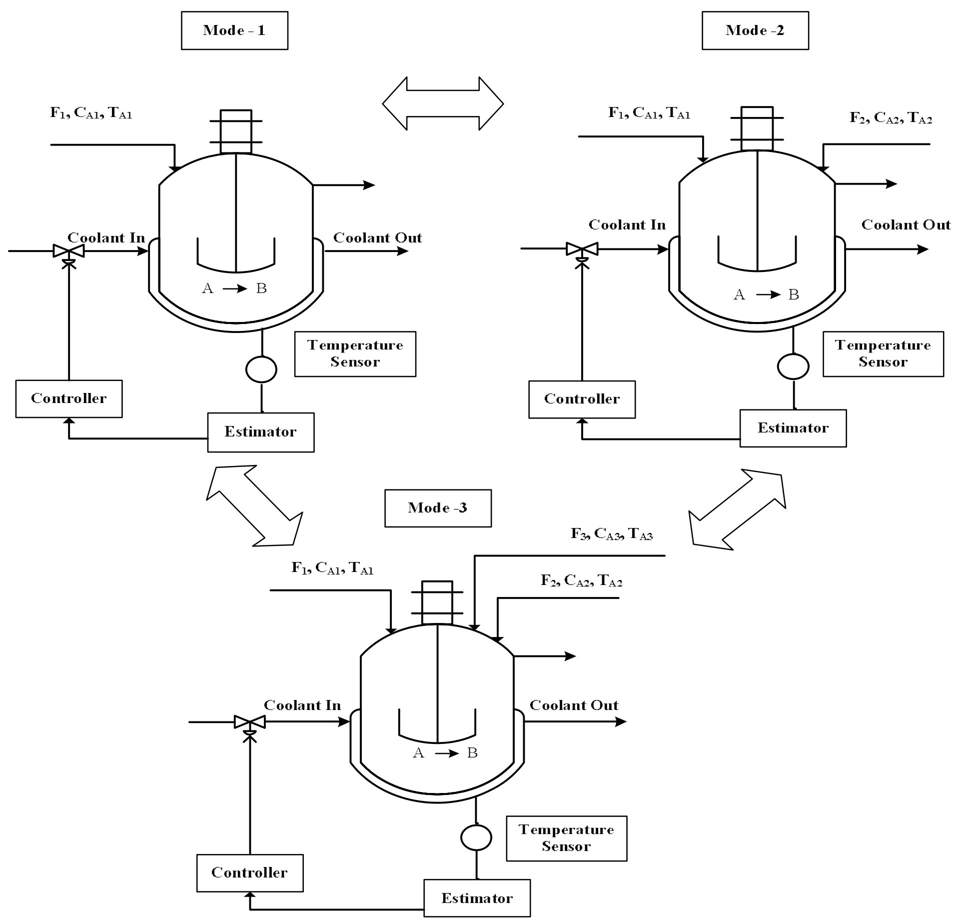

Fig.4. Switched Non-isothermal Continuous Stirred Tank Reactor