

Modeling of Bisphenol A Condensation Reaction based on UKF Algorithm

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Abstract: The Bisphenol A concentration at the reactor outlet is a direct response to the production quality index, and online soft measurement of Bisphenol A concentration is very necessary. Based on the mechanism of Bisphenol A condensation process, the mechanism equations describing the dynamic behavior of reactor are established, and the state equation and observation equation of Bisphenol A are derived through simplification and derivation of the soft measurement model, and then an Unscented Kalman Filtering is adopted to estimate the Bisphenol A concentration. Simulation results confirm that the method is feasible and effective.

Keywords: Unscented Kalman Filtering; Condensation Reaction; Soft Sensor; Mechanism Model; Bisphenol A

1. INTRODUCTION

Bisphenol A (BPA), an important common monomer for production of many polymers such as polycarbonate and epoxy resins, is manufactured by acid catalyzed condensation of acetone and phenol. Industrial processes for BPA production usually use fixed-bed reactors filled with strong acid ion exchange resins as catalysts [1]. BPA synthesis kinetics has been widely studied and reported in recent years. Various BPA synthesis kinetics models have differences because of the complexities of BPA synthesis. For example, Chen Liangcheng [2] et al. proposed reaction kinetics of BPA synthesis with strong acid conditions. Rahimi [3] studied kinetics of BPA synthesis by condensation reaction. Bao-he Wang [4] proposed reaction kinetics of BPA synthesis with cyst amine modified resin catalyst. This paper focuses on soft sensor development for online prediction of the BPA concentration, which has important practical significance.

In a BPA reaction process, the BPA concentration at the reactor outlet is the most important index, which directly determines the production efficiency. However, the real-time BPA concentration cannot be measured online in majority of industrial fields. In order to solve this problem, this paper establishes a nonlinear state-space model for the estimation of BPA concentration by taking the temperature distribution in the reactor and the acetone concentration at the reactor inlet as the observation variables. Hence, the BPA synthesis can be described by a nonlinear distributed parameter model.

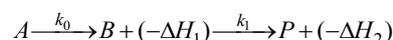
As a nonlinear estimation method, the extended Kalman filter (EKF) is widely used in state estimation. But the EKF has some deficiencies, including the requirement of differentiability of the state dynamics as well as susceptibility to bias and divergence in the state estimates. On the contrary, the unscented Kalman filter (UKF) can improve the effect of

nonlinear system filtering by approximating the probability distribution of the nonlinear functions and the posterior probability density of state based on a series of deterministic samples [5-9], and the UKF can use nonlinear model directly instead of linearizing. In this paper, UKF is employed in state estimation and the simulation results are provided to demonstrate the effectiveness of the proposed method.

2. DYNAMIC MODEL OF BPA SYNTHESIS

2.1 Observation Equation of BPA Concentration

In industrial production, acetone and phenol are continuously fed from the top of the reactor. The phenol is excessive in order to improve the conversion rate of acetone and reduce side reaction. The main reaction formula is [10]:



where A , B , P denote acetone, BPA and by-product 2-4'BPA, respectively. The dynamic characteristics of the reaction process can be written as [11]:

Material balance equation:

$$-u \frac{\partial C_A(t, z)}{\partial z} = R_1 \quad (1)$$

$$-u \frac{\partial C_B(t, z)}{\partial z} = R_2 - R_2' \quad (2)$$

Energy balance equation:

$$\rho_S C_{PS} \frac{\partial T(t, z)}{\partial t} = -C_p \rho u \frac{\partial T(t, z)}{\partial z} + \sum_{i=1}^2 \Delta H_i R_i - \rho_c C_{pc} u_c \frac{\partial T_c}{\partial z} \quad (3)$$

where $R_1 = k_0 e^{-E/RT} C_A$, $R_2 = k_0 e^{-E/RT} C_A$, $R_2' = k_1 e^{-E/RT} C_B$. z is the axial length of the reactor and $z = L$. In the industrial

production process, the radial temperature grade is much smaller to the axial one, and eqn. (3) can be simplified as:

$$C_p \rho u \frac{\partial T(t, z)}{\partial z} = \sum_{i=1}^2 \Delta H_i R_{i-1} - \rho_c C_{pc} u_c \frac{\partial T_c}{\partial z} \quad (4)$$

In order to solve nonlinear partial differential eqn. (1), (2) and (4), the reactor is divided into two sections according to the distribution of temperature measurement points and the height of each section is $\Delta z = 1m$, then disperse eqn. (1), (2) and (4) to:

$$\begin{cases} -u \frac{C_{A1}(t) - C_{A0}(t)}{\Delta z} = k_0 e^{-E/RT_1(t)} C_{A1}(t) \\ -u \frac{C_{A2}(t) - C_{A1}(t)}{\Delta z} = k_0 e^{-E/RT_2(t)} C_{A2}(t) \end{cases} \quad (5)$$

$$\begin{cases} -u \frac{C_{B1}(t) - C_{B0}(t)}{\Delta z} = k_0 e^{-E/RT_1(t)} C_{A1}(t) - k_1 e^{-E/RT_1(t)} C_{B1}(t) \\ -u \frac{C_{B2}(t) - C_{B1}(t)}{\Delta z} = k_0 e^{-E/RT_2(t)} C_{A2}(t) - k_1 e^{-E/RT_1(t)} C_{B2}(t) \end{cases} \quad (6)$$

$$\begin{cases} C_p \rho u \frac{T_1(t) - T_0(t)}{\Delta z} = \Delta H_1 k_0 e^{-E/RT_1(t)} C_{A1}(t) + \Delta H_2 k_1 e^{-E/RT_1(t)} C_{B1}(t) \\ \quad - \rho_c C_{pc} u_c \frac{T_{c1}(t) - T_{c0}(t)}{\Delta z} \\ C_p \rho u \frac{T_2(t) - T_1(t)}{\Delta z} = \Delta H_1 k_0 e^{-E/RT_2(t)} C_{A2}(t) + \Delta H_2 k_1 e^{-E/RT_2(t)} C_{B2}(t) \\ \quad - \rho_c C_{pc} u_c \frac{T_{c2}(t) - T_{c1}(t)}{\Delta z} \end{cases} \quad (7)$$

When eqn. (5) is introduced into eqn. (6), the latter becomes:

$$C_{A2}(t) = \frac{u^2}{(k_0 e^{-E/RT_1(t)} + u)(k_0 e^{-E/RT_2(t)} + u)} C_{A0}(t) \quad (8)$$

Take $T_0(t)$, $T_1(t)$, $T_2(t)$ and $C_{A0}(t)$ as the measurement variables, the observation equation of BPA concentration can be expressed as:

$$C_p \rho u \frac{T_2(t) - T_1(t)}{\Delta z} = \Delta H_1 k_0 e^{-E/RT_2(t)} \frac{u^2}{(k_0 e^{-E/RT_1(t)} + u)(k_0 e^{-E/RT_2(t)} + u)} \times C_{A0}(t) \\ + \Delta H_2 k_1 e^{-E/RT_2(t)} C_{B2}(t) - \rho_c C_{pc} u_c \frac{T_{c2}(t) - T_{c1}(t)}{\Delta z} \quad (9)$$

Unfortunately, the real-time temperature of cooling water cannot be measured in the actual production. This paper assumes that the thermal performance of the heat exchanger is good and the temperature difference of cooling water in the axial direction can be approximated as:

$$\begin{cases} T_{c1}(t) - T_{c0}(t) = T_0(t) - T_1(t) \\ T_{c2}(t) - T_{c1}(t) = T_1(t) - T_2(t) \end{cases} \quad (10)$$

Eqn. (9) can be written in a standard form:

$$y(t) = g(C_{B2}(t)) + v(k) \quad (11)$$

where $y(t) = e^{-E/RT_1(t)}$,

$$g(C_{B2}(t)) = -\frac{u}{k_0} + \frac{\Delta H_1 k_0 e^{-E/RT_2(t)} u^2 C_{A0}(t)}{k_0 e^{-E/RT_2(t)} + u} \times \\ \frac{1}{k_0 \left[(\rho C_p u - \rho_c C_{pc} u_c)(T_2(t) - T_1(t)) - \Delta H_2 k_1 e^{-E/RT_2(t)} C_{B2}(t) \right]}$$

2.2 State Equation of BPA Concentration

The simplest concentration equation is independent of temperature:

$$C_{B2}(k+1) = KC_{B2}(k) + w(k) \quad (12)$$

where K is the state transfer coefficient of BPA concentration, $w(k)$ represent the process noise. The state space expression of BPA concentration can be obtained by combining eqn. (11) and (12):

$$\begin{cases} C_{B2}(k+1) = KC_{B2}(k) + w(k) \\ y(k) = g(C_{B2}(k)) + v(k) \end{cases} \quad (13)$$

where $w(k)$ and $v(k)$ are the uncorrelated Gaussian white noise and their variance are $q_k = 0.1$ and $r_k = 0.05$, respectively.

3. UNSCEBTED KALMAN FILTERING

Consider the general discrete nonlinear system:

$$\begin{cases} a(k+1) = f(a(k)) + w(k) \\ y(k) = g(a(k)) + v(k) \end{cases} \quad (14)$$

where $a(k) \in R^n$ is the state vector, $y(k) \in R^m$ is the output vector. According to the additive noise model shown as Eq. (14), the UKF procedure is given as follows.

(1) Initialization

$$\begin{cases} a_0 = E(a_0) \\ P_0 = Var(a_0) = E[(a_0 - a_0)(a_0 - a_0)^T] \end{cases} \quad (15)$$

(2) Sigma points calculation

Sigma points sequence is

$$\chi_i(k|k-1) = \begin{cases} \bar{a}, i=0 \\ \bar{a} - \left[\sqrt{(n+\lambda) \cdot P_a} \right]_i, i=1, 2, \dots, n \\ \bar{a} + \left[\sqrt{(n+\lambda) \cdot P_a} \right]_i, i=n+1, \dots, 2n \end{cases} \quad (16)$$

The weights of Sigma points sequence accordingly are

$$\begin{cases} \omega_0^m = \lambda / (n + \lambda) \\ \omega_0^c = \lambda / (n + \lambda) + (1 - \alpha^2 + \beta) \\ \omega_i^m = \omega_i^c = 1 / 2(n + \lambda), i=1, 2, \dots, 2n \\ \lambda = n(\alpha^2 - 1) \end{cases} \quad (17)$$

where ω^m is the weight of the first-order statistical property, and ω^c is the weight of the second-order statistical property, \bar{a} is the average of a , λ is a free parameter, n is state vector dimension. The constant α is usually set to $10^{-4} \leq \alpha \leq 1$ and $\beta = 2$ is optimal for Gaussian distributions.

(3) Time update

$$\gamma_i(k|k-1) = f(\chi_i(k|k-1)) + w_k, i=0, 1, \dots, 2n \quad (18)$$

$$a(k|k-1) = \sum_{i=0}^{2n} \omega_i^m \gamma_i(k|k-1) \quad (19)$$

$$P(k|k-1) = \sum_{i=0}^{2n} \omega_i^c \left[\gamma_i(k|k-1) - a(k|k-1) \right] \times \left[\gamma_i(k|k-1) - a(k|k-1) \right]^T \quad (20)$$

$$\varepsilon_i(k|k-1) = g(\chi_i(k|k-1)) + v_k, i=0, 1, \dots, 2n \quad (21)$$

$$y(k|k-1) = \sum_{i=0}^{2n} \omega_i^m \varepsilon_i(k|k-1) \quad (22)$$

(4) Measurement update

$$P_{yy} = \sum_{i=0}^{2n} \omega_i^c \left[\varepsilon_i(k|k-1) - y(k|k-1) \right] \times \left[\varepsilon_i(k|k-1) - y(k|k-1) \right]^T \quad (23)$$

$$P_{ay} = \sum_{i=0}^{2n} \omega_i^c \left[\gamma_i(k|k-1) - a(k|k-1) \right] \times \left[\varepsilon_i(k|k-1) - y(k|k-1) \right]^T \quad (24)$$

$$a(k|k) = a(k|k-1) + K(k) \cdot [y(k) - y(k|k-1)] \quad (25)$$

$$P(k) = P(k|k-1) - K(k) \cdot P_{yy} \cdot K^T(k) \quad (26)$$

$$K(k) = P_{ay} \cdot P_{yy}^{-1} \quad (27)$$

4. INDUSTRIAL CASE STUDY

The state estimation of the BPA concentration is based on the dynamic model described by eqn. (13). However, $\Delta H_2 \cdot k_1$ and K are both unknown parameters in eqn. (13). In order to determine the values of $\Delta H_2 \cdot k_1$ and K , we recorded 178 historical data from industry site, and the total of 178 cases was split into 3 parts: one set of 50 samples for reverse calculation of $\Delta H_2 \cdot k_1$, the other set of 70 samples for fitting K , and the last set of 58 samples for model testing.

According to chemical principle, heat of reaction ΔH_2 and pre-exponential factor k_1 are constants for the known side reaction, and it is obvious that $(\Delta H_2 \cdot k_1)$ can be approximated by a constant and $(\Delta H_2 \cdot k_1)$ is set to $(\Delta H_2 \cdot k_1) = 2.9 \times 10^4$ by nonlinear regression. In order to calculate K , the least squares fitting is adopted and K is set to $K = 0.972$.

In order to verify the effectiveness of the proposed method, UKF algorithm is adopted to estimate BPA concentration. The BPA concentration estimation results of 58 group data are shown in Fig. 1. Parameters in eqn. (13) are specified in Tab. 1.

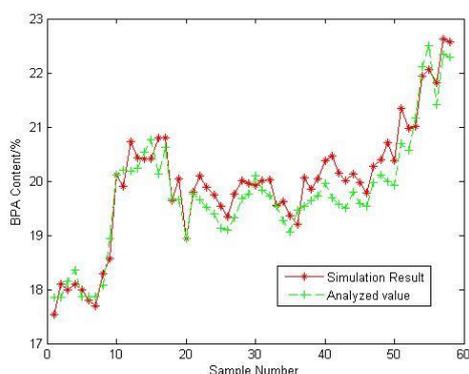


Figure. 1 BPA concentration estimation results.

The MaxRE (Maximum Relative Error) and MeanRE (Mean Relative Error) are used to quantify the prediction errors and they are shown in Tab. 2.

Table 1. Model parameters

Symbols	Values
ΔH	410.228
k_0	371.7125
C_{pc}	4.2
C_p	0.541
K	0.972
$\Delta H_2 \times k_1$	29000
u	2
u_c	0.27

Tab.2 Estimation errors of the model

Estimation method	MaxRE/%	MeanRE/%
UKF	3.9248	1.5572

5. CONCLUSIONS

In this paper we have established the state-space model for the estimation of BPA concentration by taking the temperature distribution and the acetone concentration as the observation variables, and then UKF is adopted in the state estimation. The simulation results show that the state-space model is able to track the trends of BPA concentration accurately, and the accuracy of the model is satisfactory. This method can be used for online estimation of the BPA concentration, which has guiding significance for the industrial production of BPA.

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NOMENCLATURE

C_A	acetone concentration, wt%
C_B	BPA concentration, wt%
C_p	specific heat of reactant, $kJ \cdot (mol \cdot K)^{-1}$
C_{pc}	specific heat of cooling water, $kJ \cdot (mol \cdot K)^{-1}$
C_{PS}	specific heat of catalyst, $kJ \cdot (mol \cdot K)^{-1}$
E	reaction activation energy, kJ
ΔH_1	heat of main reaction, $kJ \cdot kg^{-1}$
ΔH_2	heat of side reaction, $kJ \cdot kg^{-1}$
k_0	reaction rate constant of main reaction
k_1	reaction rate constant of side reaction
L	axial length of reactor, m
T	reaction temperature, K
T_c	cooling water temperature, K
u	feed velocity, m/s
u_c	cooling water velocity, m/s
ρ	average density of reactant, kg/m^3
ρ_c	density of cooling water, kg/m^3
ρ_s	density of catalyst, kg/m^3