Modeling of a Fluidized Bed Reactor for Ethylene Polymerization

by J. Mazák
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Abstract

Fluidized bed reactors are widely used in petrochemical and mining industries to transform a variety of different feedstocks into useful products. One of the applications is to produce ethylene from heavy oil which can then be polymerized to make polyethylene plastic. Modern control techniques are mainly model based oriented designs and availability of a good model of the process is essential.

In this report we developed a rigorous mathematical dynamical model of a fluidized bed low pressure polymerization reactor and discussed its dynamic behavior through model simulations. The modeling is based on physical laws for material and energy balances in the reactor from which a set of ordinary differential equations used in simulations is derived. The mathematical model includes also a counter-current heat exchanger mathematical model and a primary bed temperature PID controller. A computation of the steady state of the reactor for the choice of some parameters is also shown.

This model appears to be applicable for studying and testing of different control strategies to optimize the production quality and quantity.

Keywords: fluidized beds; modeling / reactor kinetics.

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1 Introduction

Fluidized bed reactors remain as one of the most important challenges for process modeling. The equations which represent the heat and mass exchange between the different phases as well as the treatment of these phases depend strongly on the approach and background of the different authors. Based on previous studies [10, 4], a detailed description of the modeling procedure will be presented. Knowledge on fundamentals of fluidization and polymerization in fluidized bed reactors is assumed from now on [6, 5, 3].

After a brief overview of the process in Section 2, operating conditions of the reactor are commented in Section 3. Section 4 presents general assumptions and simplifications made in the fluidized bed model and Section 5 presents the computation of physical parameters. Section 6 is devoted to the equations which model the mass and energy exchange as well as the catalyst activity in the fluidized bed. Sections 7 and 8 present models for the gascap and heat exchanger, respectively. The corresponding steady state computations are presented in Section 9. Section 10 presents the results of staircase experiments on this model. Appendix A contains a summary of all symbols used in previous sections, appendix B presents the implemented SIMULINK model and appendix C contains the required initialization file with the steady state computations for given process conditions.

2 Process Description

An schematic representation of the process is shown in Fig. 1. It consists of

1. A fluidized bed of solid catalyst-polymer particles and an interstitial gas. They will be considered together as the emulsion phase through which large bubbles rise in plug flow.

2. A gascap, which is a free space above the fluidized bed with about half of its volume. Its function is to prevent the solid particles to go into the gas recycle loop.

3. A gas recycle loop which takes the un-converted gas-phase reactants and the inert gas back to the fluidized bed, mixing them with the input flows. The delay time from the top of the gascap via the heat exchanger to the bottom of the bed is set to 1 minute.

4. A counter-current heat exchanger where the recycled gas is cooled with water at a certain (controlled) temperature.

5. Composition analyzers (not shown): The monomer partial pressure $P_{C2}$ in the gascap, the ratio $P_{C2}/P_{C}$ of partial pressure comonomer $P_{C2}$ to partial pressure monomer in the gascap and the production rate $Q_0$ are sampled once every five minutes and values are given with a delay of five minutes.
Figure 1: Schematic description of the process

6. Sensors (not shown) for the emulsion temperature $T_e$, and for total pressure $P_t$ in the gascap. These measurements are available every five seconds.

7. A PID controller for bed temperature. It must be always in operation for safety reasons, because even very small perturbations say in temperature are known to cause a slow drift away of the reactor.
2.1 Process conditions

The reactor has a diameter \( D \) and the effective height of the fluidized bed will be \( H \). The total pressure in the gascap is \( P \), and the steady-state values for \( P_{C_2}, (C_x/C_2), T_{bed} \) \((\equiv T)\), production and partial pressure of hydrogen \( P_{H_2} \) are given. From these values and assuming ideal gas behavior in the gascap, we obtain for concentrations of monomer and comonomer in the gascap the following formulas

\[
C_{2g} = \frac{P_{C_2}M_{C_2}}{R_gT} \quad (1a)
\]
\[
C_{xg} = \frac{P_{C_2}M_{C_x}}{R_gT} \quad (1b)
\]

where \( P_{C_x} = P_{C_2}(C_x/C_2) \), \( M_{C_2} \) is the molecular weight of monomer and \( M_{C_x} \) is the molecular weight of comonomer. The gas constant is denoted by \( R_g \). With these results, the partial pressure of nitrogen in the gascap is

\[
P_{N_2} = P - P_{C_2} - P_{C_x} - P_{H_2} \quad (2)
\]

And the density of the gas in the gascap can be estimated then as

\[
\rho_g = \frac{P_{H_2}M_{H_2}}{R_gT} + \frac{P_{N_2}M_{N_2}}{R_gT} + C_{2g} + C_{xg} \quad (3)
\]

In the model we will assume constant density \( \rho_g \) for the gas mixture circulating in the fluidized bed and recycle loop. From real process measurements this density is known to be \( \rho_a \) and the measured flow rate is \( \psi_a \). In order to keep the mass flow rate in the model equal to the process value \( \rho_a \psi_a \), the flow rate \( \psi \) in the model must then verify

\[
\rho_a \psi_a = \rho_g \psi = \text{const} \quad (4)
\]

And then

\[
\psi = \psi_a \frac{\rho_a}{\rho_g} \quad (5)
\]

From this, we can estimate the inlet gas velocity as

\[
U_0 = \frac{\psi}{A} = \frac{\psi}{\frac{1}{4}\pi D^2} \quad (6)
\]

From now on we will assume that this is the value for the superficial gas velocity in our model. However, the effect on \( U_0 \) of internals such as the distributor plate should be considered when necessary. Values for the minimum fluidization velocity \( U_{mf} \) and the voidage of emulsion phase at minimum fluidizing conditions \( \varepsilon_{mf} \) will be also considered as data for this reactor. The values of \( C_{pg}, C_{ps} \) specific heat of gas resp. solid in emulsion and \( \rho_s \), the density of solid are assumed to be known constants during process operation. Input mass flows of monomer \( \phi_{z_{in}} \) and comonomer \( \phi_{z_{in}} \) in steady state are related by

\[
\phi_{z_{in}} = \phi_{z_{in}}(C_x/C_2)_{set} \left( \frac{k_{p0,C_x}}{k_{p0,C_2}} \right) \left( \frac{M_{C_x}}{M_{C_2}} \right) \quad (7)
\]
On the other hand, the total input mass flow that holds this steady state is given by

\[ \phi_{\text{flow}} = \phi_{2_{\text{in}}} + \left( \frac{k_{p_0,C_2}}{k_{p_0,C_x}} \right) \left( \frac{M_{C_2}}{M_{C_x}} \right) \phi_{x_{\text{in}}} \]  \hspace{1cm} (8)

where \( k_{p_0,C_2} \) and \( k_{p_0,C_x} \) are reaction constants. From these two equations it is possible to compute the requested input flows given the total input flow and the desired comonomer to monomer ratio:

\[ \phi_{2_{\text{in}}} = \frac{\phi_{\text{flow}}}{1 + (C_x/C_2)_{\text{set}}} \]  \hspace{1cm} (9a)

\[ \phi_{x_{\text{in}}} = \phi_{\text{flow}} \frac{(C_x/C_2)_{\text{set}}}{1 + (C_x/C_2)_{\text{set}}} \left( \frac{k_{p_0,C_2}}{k_{p_0,C_x}} \right) \left( \frac{M_{C_x}}{M_{C_2}} \right) \]  \hspace{1cm} (9b)

Mixing of recycle flow and input flow can be described considering separate balances for monomer and comonomer concentrations:

\[ \rho_g C_{2g} \psi + \rho_g C_{2_{\text{in}}} \psi_{\text{in}} = \rho_g C_{20} \psi \]  \hspace{1cm} (10a)

\[ \rho_g C_{xg} \psi + \rho_g C_{x_{\text{in}}} \psi_{\text{in}} = \rho_g C_{x0} \psi \]  \hspace{1cm} (10b)

where

\[ C_{2_{\text{in}}} \psi_{\text{in}} = \phi_{2_{\text{in}}} \]  \hspace{1cm} (11a)

\[ C_{x_{\text{in}}} \psi_{\text{in}} = \phi_{x_{\text{in}}} \]  \hspace{1cm} (11b)

and \( \psi_{\text{in}} \) is the input gas flow. Concentrations of monomer and comonomer in the mixed flow are the given by

\[ C_{20} = C_{2g} + \frac{\phi_{2_{\text{in}}}}{\psi} \]  \hspace{1cm} (12a)

\[ C_{x0} = C_{xg} + \frac{\phi_{x_{\text{in}}}}{\psi} \]  \hspace{1cm} (12b)

### 2.2 Fluidized bed assumptions

In order to develop a first principle model which can be useful for control purposes, a number of simplifications and assumptions will be needed. However, it must be noticed that these assumptions are quite common in fluidization theory and they do not represent a serious deficiency in the final model.

1. Behavior in the vicinity of a single bubble. In the vicinity of any of the many rising bubbles in a bubbling fluidized bed let us assume that the gas flow is given by the Davidson model with its spherical bubble surrounded with a spherical cloud. The velocity of rise of a single bubble of diameter \( d_B \), hence the velocity relative to solids far from the bubble is

\[ U_{br} = 0.711 (gd_B)^{1/2} \]  \hspace{1cm} (13)

where \( g \) is the gravity acceleration.
2. Bubble size. The importance of this parameter is critical for the mass and heat transfer coefficients. Therefore, it is very convenient to have an accurate estimation as well as information about reactor internals. In [4] and previous model [9] to estimate the bubble diameter $d_B$ is chosen:

$$d_{BO} = 0.00376 (U_o - U_{mf})^2$$
$$d_{BM} = 0.652 \left( \frac{A}{U_o - U_{mf}} \right)^{2/5}$$

where $d_{BO}$ is the initial bubble diameter at the surface of the perforated plate and $d_{BM}$ is the bubble diameter if there were a single train of bubbles. Then

$$d_B(z^*) = d_{BM} - (d_{BM} - d_{BO})e^{-0.3z^*/D}$$

where $z^*$ is the position (height) in the bed, $U_{mf}$ is the minimum fluidization velocity and $U_o$ is the inlet gas velocity. All $d$'s must be in cm and all $U$'s in cm/s, because they are experimental correlations. However, this model requires four conditions:

$$30 < D < 130 \text{ cm}$$
$$0.5 < U_{mf} < 20 \text{ cm/s}$$
$$0.006 < d_p < 0.045 \text{ cm}$$
$$U_o - U_{mf} < 48 \text{ cm/s}$$

and $d_p$ is a mean diameter of the particles. It must be carefully checked that the design characteristics of the reactor meet these requirements; otherwise this model could not be valid.

3. Bubble velocity. Let us relate the velocity of rise of a crowd of bubbles to the velocity of rise of a single bubble by

$$U_b = U_o - U_{mf} + U_{br} = U_o - U_{mf} + 0.711 (gd_B)^{1/2}$$

4. Voidage of bubbles and emulsion. Although experimental evidence [7] indicates that rising bubbles contain small amounts of solids, we can with negligible error ignore this and take the bubble void fraction $\varepsilon_b = 1$. In addition, let us assume the emulsion voidage to be that of the bed at minimum fluidizing conditions.

5. The bubble phase will be always at quasi-steady state.

6. Polymerization occurs only in the emulsion phase and no reaction occurs in the bubble phase.

7. Mass and heat transfer between the bubble and emulsion phases occurs at uniform rate over the bed height $H$. Therefore, an average value of bubble equivalent diameter $d_B$ and hence average values of the mass and heat exchange parameters will be used.
8. There is negligible mass and heat transfer resistance between the solid polymer-catalyst particles and the interstitial gas in the emulsion phase. This assumption can be seen as an excellent approximation to the real process and is very useful for transient computations. The resulting equations are presented in [3, 2] and in all cases appear terms which take into account the presence of solid particles in the emulsion with a certain residence time in the reactor. A model which completely ignores the presence of particles might represent an over-simplification. Although the terms related to mass transfer between emulsion gas and solid particles can be neglected in practise, the conditions that enable us neglecting the corresponding heat transfer term must be carefully analyzed and depend greatly on the kind of reaction. Following [4], we will also assume that this term is negligible although it will be convenient to further investigate its validity for these concrete reactor and catalyst.

9. No elutriation of solids occurs.

10. Catalyst injection is continuous.

11. The product withdrawal rate $Q_0$ is always adjusted to maintain the bed height $H$ constant.

12. There is catalyst de-activation and the catalyst activity is only a function of time. In general this assumption has a direct effect on modeling heat and mass transfer, in our case, however, an ad hoc treatment of de-activation will be followed.

13. Hydrogen and nitrogen are used as inert gases. They are neither fed nor withdrawn from the reactor.

14. The reactor is adiabatic.

15. Gas recycle flow $\psi$ is constant.

16. Ideal mixing is assumed in the gascap for heat and mass transfer.

17. Gas density is constant in reactor bed and in top.

18. The polymerization rate constants $k_{p_0,C_1}, k_{p_0,C_2}$ are depending on temperature and follow the Arrhenius form.

2.3 Physical parameters

In view of the complexity of the process and the lack of a reliable model for the bubble equivalent diameter $d_B$, a value must be carefully chosen according to real process measurements, if available, and design characteristics of the reactor. With this value we obtain
1. Relative fraction of bubble phase to total volume in bed. With the assumptions presented in [7] is the fraction of bubble phase volume in fluidized bed \( \delta^* \) given as

\[
\delta^* \approx \frac{U_0 - U_{mf}}{U_b}
\]  

(18)

2. Velocity of emulsion gas. In [1], and under the assumption that conditions in the emulsion phase at any flow rate are the same as at minimum fluidizing conditions, the following expression for the velocity of emulsion gas \( U_e \) is derived

\[
U_e = \frac{U_{mf}}{\varepsilon_{mf}(1 - \delta^*)}
\]  

(19)

3. Mass transfer coefficient bubble phase – emulsion. For this coefficient the Kunii-Levenspiel model [8] will be followed:

\[
K_{bc} = 4.5 \frac{U_{mf}}{d_B} + 5.85 \left( \frac{D^{1/2} g^{1/4}}{d_B^{5/4}} \right)
\]  

(20a)

\[
K_{ee} \approx 6.78 \left( \frac{\varepsilon_{mf} D_e U_b}{d_B^3} \right)^{1/2}
\]  

(20b)

where \( K_{bc} \) is the mass transfer coefficient bubble-cloud per unit bubble volume, \( K_{ee} \) is the mass transfer coefficient cloud-emulsion per unit bubble volume and \( D, D_e \) are the diffusion and effective diffusion coefficients of the gas in emulsion. Then the mass transfer coefficient bubble-emulsion per unit bubble volume \( K_{be} \) is determined from

\[
\frac{1}{K_{bc}} \approx \frac{1}{K_{bc}} + \frac{1}{K_{ee}}
\]  

(21)

We will assume [7] that \( D_e \approx D \).

4. Heat transfer coefficient bubble phase – emulsion. In [4] and [1, 2], the model proposed in [6] is followed; that is

\[
H_{bc} = 4.5 \frac{U_{mf} \rho g C_{pg}}{d_B} + 5.85 \left( \frac{(\rho g C_{pg})^{1/2} g^{1/4}}{d_B^{5/4}} \right)
\]  

(22a)

\[
H_{ce} = 6.78 (\rho g C_{pg} k_g)^{1/2} \left( \frac{\varepsilon_{mf} U_b}{d_B^3} \right)^{1/2}
\]  

(22b)

where \( H_{bc} \) is the heat transfer coefficient bubble-cloud per unit bubble volume, \( H_{ce} \) is the heat transfer coefficient cloud-emulsion per unit bubble volume and \( k_g \) is the heat conductivity of gas. Then the heat transfer coefficient bubble-emulsion per unit bubble volume \( H_{be} \) is determined by

\[
\frac{1}{H_{bc}} \approx \frac{1}{H_{bc}} + \frac{1}{H_{ce}}
\]  

(23)
It was found that, when the process conditions above presented were used, this heat exchange coefficients underestimated the real values. In [3] the value

$$H_{bc} \approx H_{bc}$$

is finally accepted as a better option for the overall $H_{bc}$. In our model, this choice also gave reasonable values for the steady-state temperatures of feed flow and bubble phase. It is obvious that this difference is due to the fact that $H_{bc} \gg H_{ce}$. Again, it would be necessary a deeper study on the characteristics of this specific reaction in order to model appropriately the heat transfers: The importance of this coefficients must not be underestimated and rough or "typical" values would lead only to a wrong description of the dynamics.

### 3 Model of the Fluidized Bed

Except for the catalyst activity, the equations here presented are similar to those in [4] and the changes proposed by [10] to include the comonomer have been also followed.

In the bubble phase the material balances are described by these equations for monomer and comonomer, respectively

$$\frac{z}{C_0} \frac{dC_{2b}}{dz^*} = \frac{K_{be}z}{U_b} \left( \frac{C_{2e}}{C_0} - \frac{C_{2b}}{C_0} \right)$$

$$\frac{z}{C_0} \frac{dC_{xb}}{dz^*} = \frac{K_{be}z}{U_b} \left( \frac{C_{xe}}{C_0} - \frac{C_{xb}}{C_0} \right)$$

where $z = \frac{h}{h}$ is the relative height in the bed and $C_0$ is a chosen concentration reference value.

The material balance equation for the monomer in the emulsion phase takes the form

$$\frac{t_0}{C_0} \frac{dC_{2e}}{dt'} = \frac{U_{e}t_0}{H} \left( \frac{C_{20}}{C_0} - \frac{C_{2e}}{C_0} \right) + \frac{K_{be}t_0 \delta^*}{\varepsilon_{mf}(1-\delta^*)} \left( \frac{C_{2b}}{C_0} - \frac{C_{2e}}{C_0} \right)$$

$$- \frac{t_0}{\varepsilon_{mf}} k_{p0,ce} e^{-E_c/(RT_c)} \rho_{a}(1 - \varepsilon_{mf}) X_{cat} \frac{C_{2e}}{C_0}$$

$$+ \frac{C_{2e}}{C_0} \frac{t_0 Q_o}{AH(1-\delta^*)}$$

where $t' = t/t_0$ is a relative time with respect to a reference time value $t_0$. $X_{cat}$ is a mass fraction of the catalyst in the solid phase and $E_a$ is an activation energy.

A similar equation to (27) is used also for the comonomer

$$\frac{t_0}{C_0} \frac{dC_{xe}}{dt'} = \frac{U_{e}t_0}{H} \left( \frac{C_{xe}}{C_0} - \frac{C_{xe}}{C_0} \right) + \frac{K_{be}t_0 \delta^*}{\varepsilon_{mf}(1-\delta^*)} \left( \frac{C_{xe}}{C_0} - \frac{C_{xe}}{C_0} \right)$$
The energy balance in the bubble phase is modeled by the following equation

\[- \frac{t_0}{\varepsilon_{mf}} k_{p0_c} C_{e} e^{-E_a/(R_T)} \rho_b (1 - \varepsilon_{mf}) X_{cat} \frac{C_{xe}}{C_0} \]

\[- \frac{C_{xe}}{C_0} \frac{t_0 Q_0}{AH (1 - \delta^*)} \] (28)

while neglecting the changes in \(C_{2b}\) and \(C_{zb}\) with respect to much faster bubbles rise.

In the emulsion phase is the energy balance described as follows

\[ \frac{dT_b}{dz^*} = \frac{H_{be}}{U_b C_{pg}(C_{2b} + C_{xb})} (T_e - T_b) \] (29)

where \(-\Delta H_r\) is the heat of the reaction and \(\bar{T}_b\) is a mean value of the bed temperature along its height.

Initial and boundary conditions for (27), (28) and (30) are as follows:

at \(t' = 0\), \(C_{2e} = C_{20}\), \(C_{xe} = C_{x0}\), \(T_e = T_e(0)\), \(X_{cat} = X_{cat}(0)\).

at \(z^* = 0\), \(C_{2b} = C_{2b0}\), \(C_{zb} = C_{zb0}\), \(T_b = T_b(0)\).

By defining a notation according to Table 1 we make all the state variables dimensionless.

With respect to the operating conditions of the reactor we can assume:

1. Concentration of monomer in inlet gas \(C_{20}\) equals concentration of monomer in the bubble phase for \(z = 0\), therefore \(C_{20} = C_{2b0}\) and \(A_{11} = A_{21}\).

2. For the same reason \(C_{x0} = C_{xb0}\) and \(A_{16} = A_{26}\).

3. Feed temperature of inlet gas \(T_f\) equals temperature of the bubble phase \(T_{b0}\) at \(z = 0\), therefore \(B_1 = B_2\).

Constant bed height implies that the mass rate of product removal \(Q_0\) – also called production rate – is approximately equal to the rate of increase in bed mass due to
\[
t = \frac{t}{t_0} \quad z = \frac{z'}{H} \quad x_2 = X_{\text{Cat}}
\]

\[
x_1 = \frac{C_{p0}}{C_0} \quad x_3 = \frac{T_1}{T_{ref}} \quad x_6 = \frac{C_{p6}}{C_0}
\]

\[
x_4 = \frac{C_{p4}}{C_0} \quad x_5 = \frac{T_4}{T_{ref}} \quad x_7 = \frac{C_{p7}}{C_0}
\]

\[
\bar{x}_4 = \frac{\bar{C}_{p4}}{C_0} \quad \bar{x}_5 = \frac{\bar{T}_4}{T_{ref}} \quad \bar{x}_7 = \frac{\bar{C}_{p7}}{C_0}
\]

\[
K_B = \frac{K_B H}{U_0} \quad K_H = \frac{H_{B2} H}{U_0 C_0 C_y}
\]

\[
A_{11} = \frac{C_{p0}}{C_0} \quad A_{21} = \frac{C_{p2}}{C_0} \quad A_{31} = \frac{C_{p3(0)}}{C_0}
\]

\[
A_{15} = \frac{C_{p5}}{C_0} \quad A_{26} = \frac{C_{p6}}{C_0} \quad A_{36} = \frac{C_{p7(0)}}{C_0}
\]

\[
B_1 = \frac{T_1}{T_{ref}} \quad B_2 = \frac{T_{p2}}{T_{ref}} \quad B_3 = \frac{T_{p3(0)}}{T_{ref}}
\]

\[
\alpha = \frac{t_0 \beta}{H} \quad \beta = \frac{t_0 \beta}{H_{m_f}} \quad \gamma = \frac{-\Delta H}{C_{p0} T_{ref}}
\]

\[
\delta = \frac{E_p}{R_{g} T_{ref}} \quad \theta = \frac{\rho_s(1-\epsilon_{m_f})}{\epsilon_{m_f} C_0} \quad \Gamma = \frac{\delta^*}{1-\delta}
\]

\[
\rho = \frac{(1-\epsilon_{m_f}) \rho_s C_{p4}}{C_0 C_{y}} \quad \xi_1 = \frac{\rho_s k_{p0} C_{p2}(1-\epsilon_{m_f})}{\epsilon_{m_f}} \quad \xi_6 = \frac{\rho_s k_{p0} C_{p6}(1-\epsilon_{m_f})}{\epsilon_{m_f}}
\]

---

Table 1: Dimensionless variables and parameters definitions.

polymerization. Thus

\[
Q_0 = AH(1 - \delta^*) (1 - \epsilon_{m_f}) \rho_s (k_{p0} C_{p2} C_{2e} + k_{p0} C_{p6} C_{ze}) e^{\frac{E_p}{RT_{ref}}} X_{\text{Cat}}
\]

Using the substitutions in (31), equations (27) (28) and (30) become

\[
\frac{dx_1}{dt} = \alpha (A_{21} - x_1) + K_B \beta \Gamma (\bar{x}_4 - x_1)
\]

\[
-\xi_1 e^{-\delta/\epsilon_{m_f}} x_2 x_1 - \frac{(\xi_1 x_1 + \xi_6 x_6) x_1 x_2 e^{-\delta/\epsilon_{m_f}}}{\theta + x_1 + x_6}
\]

\[
\frac{dx_6}{dt} = \alpha (A_{26} - x_6) + K_B \beta \Gamma (\bar{x}_7 - x_6)
\]

\[
-\xi_6 e^{-\delta/\epsilon_{m_f}} x_2 x_6 - \frac{(\xi_1 x_1 + \xi_6 x_6) x_5 x_6 e^{-\delta/\epsilon_{m_f}}}{\theta + x_1 + x_6}
\]

\[
\frac{dx_3}{dt} = -\frac{x_3 - 1}{\rho + x_1 + x_6} \left( \frac{dx_1}{dt} + \frac{dx_6}{dt} \right) - \alpha \frac{(x_1 + x_6)(x_3 - B_1)}{\rho + x_1 + x_6} + \Gamma K_B \beta (\bar{x}_5 - x_3)
\]

\[
+ \gamma (\xi_1 x_1 + \xi_6 x_6) e^{-\delta/\epsilon_{m_f}} \frac{\bar{x}_2}{\theta + x_1 + x_6} - \frac{(\xi_1 x_1 + \xi_6 x_6) e^{-\delta/\epsilon_{m_f}}}{\theta + x_1 + x_6} x_2 (x_3 - 1)
\]
And (25), (26) and (29) become

\[
\frac{dx_4}{dz} = KB(x_1 - x_4) \\
\frac{dx_7}{dz} = KB(x_6 - x_7) \\
\frac{dx_5}{dz} = \frac{KH}{x_4 + x_7}(x_3 - x_5)
\] (36) (37) (38)

Finally (32) becomes

\[
Q_0 = \frac{\left(\xi x_1 + \xi_6 x_5\right)e^{-\delta x_3}AH C_0(1 - \delta^*\epsilon_{m} x_2)}{t_0}
\] (39)

Because we suppose that the bubble phase is always at a quasi-steady state the equations (36), (37) and (38) can be easily solved and give the following solution

\[
x_4 = x_1 + (A_{11} - x_1)e^{-KBz} \\
x_7 = x_6 + (A_{16} - x_6)e^{-KBz} \\
x_5 = x_3 + (B_2 - x_3)e^{-KHz/(x_4 + x_7)}
\] (40) (41) (42)

where the average values of \(x_4, x_5\) and \(x_7\) along the normalized bed height are given by

\[
\bar{x}_4 = \int_0^1 x_4dz = x_1 + (A_{11} - x_1)(1 - e^{-KB})/KB \\
\bar{x}_7 = \int_0^1 x_7dz = x_6 + (A_{16} - x_6)(1 - e^{-KB})/KB \\
\bar{x}_5 = \int_0^1 x_5dz = x_3 + (B_2 - x_3)(1 - e^{-KH/(x_4 + x_7)})/KH
\] (43) (44) (45)

The dimensionless initial conditions at \(t = 0\) are

\[
x_1 = A_{31}, \quad x_6 = A_{36}, \quad x_2 = X_{col}(0), \quad x_3 = B_3
\]

and the dimensionless boundary conditions at \(z^* = 0\) are

\[
x_4 = A_{11}, \quad x_7 = A_{16}, \quad x_5 = B_2
\]

For later use we define a notation

\[
\begin{align*}
r_{x_1} &= \xi_1 e^{-\delta x_3} x_2 x_1 \\
r_{x_6} &= \xi_6 e^{-\delta x_3} x_2 x_6 \\
R &= \frac{\left(\xi_1 x_1 + \xi_6 x_6\right)x_2 e^{-\delta x_3}}{\theta + x_1 + x_6}
\end{align*}
\] (46a) (46b) (46c)

where \(r_{x_1}, r_{x_6}\) and \(R\) are symbols for right hand side expressions.
3.1 Catalyst activity model

The activity of the catalyst in the reactor can be empirically described by a FIR transfer function in discrete time domain, assuming a sampling time of 5 minutes as follows

\[ x_2(k) = q^{-d}B(q^{-1})qc(k) \] (47)

\( qc \) is the catalyst feed into the bed and \( x_2 \) stands for the catalyst activity. The polynomial \( B(q^{-1}) \) is defined as

\[ B = b_0 + b_1q^{-1} + b_2q^{-2} \ldots + b_nq^{-n} \quad n = 23 \] (48)

The constant \( d \) stands for a one hour delay observed in the catalyst activity and \( q^{-1} \) is the usual shift operator.

To implement this model in SIMULINK we rewrite the model (47) into a state-space form in discrete time as follows

\[ x_{ca}(k + 1) = \Phi_{ca}x_{ca}(k) + \Gamma_{ca}qc(k - d) \] (49a)

\[ x_2(k) = \Psi_{ca}x_{ca}(k) + \Delta_{ca}qc(k - d) \] (49b)

where \( x_{ca} \in \mathbb{R}^{24} \) and

\[ \Phi_{ca} = \begin{bmatrix} \Omega^T & 0 \\ I & \Omega \end{bmatrix} \quad \Gamma_{ca} = \begin{bmatrix} 1 \\ \Omega \end{bmatrix} \]

\[ \Psi_{ca} = [b_1 \ b_2 \ \ldots \ b_{23}] \quad \Delta_{ca} = b_0 \]

Then we compute a balanced realization of this model, reducing the state-space dimension to 2. After that the discrete-time model is converted into a second order continuous-time model using a zero-order hold at the input resulting in

\[ \dot{x}_{ca}(t) = A_{ca}x_{ca}(t) + B_{ca}qc(t - \tau) \] (50a)

\[ x_2(t) = C_{ca}x_{ca}(t) + D_{ca}qc(t - \tau) \] (50b)

The final continuous time approximation of the empirical catalyst activity function is shown in Fig. 3.1.

3.2 Model of the gascap

The dynamics of the gascap are modeled by a system of first order differential equations given by

\[ \frac{t_0}{C_0} \frac{dC_{Zg}}{dt'} = \frac{t_0\phi_g}{V} \left( \frac{C_{Zb}}{C_0} - \frac{C_{Zg}}{C_0} \right) \] (51a)

\[ \frac{t_0}{C_0} \frac{dC_{Zb}}{dt'} = \frac{t_0\phi_g}{V} \left( \frac{C_{Zb}}{C_0} - \frac{C_{Zg}}{C_0} \right) \] (51b)

\[ \frac{t_0}{T_{ref}} \frac{dT_g}{dt'} = \frac{t_0\phi_g}{V} \left( \frac{T_b}{T_{ref}} - \frac{T_g}{T_{ref}} \right) \] (51c)
For simulation purposes it is convenient to rewrite the above equations into a state-space form given by matrices

\[
A_{gc} = \begin{bmatrix} -f & 0 & 0 \\ 0 & -f & 0 \\ 0 & 0 & -f \end{bmatrix}, \quad B_{gc} = \begin{bmatrix} f & 0 & 0 \\ 0 & f & 0 \\ 0 & 0 & f \end{bmatrix}, \quad C_{gc} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\]

where \( f = \frac{60\phi_4}{V^2} \). If we take as states

\[
x_{gc} = \begin{bmatrix} C_{2g} \\ C_{2g} \\ \frac{T_g}{T_{ref}} \end{bmatrix}
\]

and as inputs \( u_{gc} = [x_4 \ x_7 \ x_5]^T \) then we obtain

\[
\begin{aligned}
\dot{x}_{gc} &= A_{gc} x_{gc} + B_{gc} u_{gc} \\
y_{gc} &= C_{gc} x_{gc}
\end{aligned}
\]

### 3.3 Model of the heat exchanger

The output gas from the gascap enters a counter-current heat exchanger where the gas is cooled with water. The corresponding partial differential equations are

\[
\begin{align*}
m_g C_{pg} \frac{\partial T_{gh}}{\partial t'} &= -\phi_g C_{pg} \frac{\partial T_{gh}}{\partial z} - h_f A_f (T_{gh} - T_{wh}) \\
m_w C_{pw} \frac{\partial T_{wh}}{\partial t'} &= -\phi_w C_{pw} \frac{\partial T_{wh}}{\partial z} + h_f A_f (T_{gh} - T_{wh})
\end{align*}
\]
As proposed in [11], the heat exchanger will be divided in four equally sized compartments where an ideal mixing of gas and water is assumed. The following set of linear differential equations is then obtained

\[
\begin{align*}
C_g \frac{dT_{gh,i}}{dt'} &= -\phi_g C_{pg} \frac{T_{gh,i} - T_{gh,i-1}}{\Delta Z} - h_f A_f (T_{gh,i} - T_{wh,i}) \\
m_{g,i} \frac{dT_{wh,i}}{dt'} &= -\phi_w C_{pw} \frac{T_{wh,i} - T_{wh,i+1}}{\Delta Z} + h_f A_f (T_{gh,i} - T_{wh,i})
\end{align*}
\]

where \( i = 1, 2, 3, 4 \). This is in fact a state space model where the inputs are the water feed temperature \( T_w = T_{wh,5} \) and the temperature of the gas coming from the gas cap \( T_g = T_{gh,0} \). The output is the temperature of the gas coming out of the last segment \( T_f = T_{gh,4} \). Noting that

\[
\begin{align*}
m_{g,i} &= \rho_g V_{g,i} = \rho_g A_g \Delta Z \\
m_{w,i} &= \rho_w V_{w,i} = \rho_w A_w \Delta Z
\end{align*}
\]

And also that

\[
\phi_g = \rho_g \nu_g \quad \phi_w = \rho_w \nu_w
\]

We can rewrite (56a) and (56b) as

\[
\begin{align*}
\frac{1}{t_0} \frac{dT_{gh,i}}{dt} &= -\frac{v_g}{A_g} \frac{(T_{gh,i} - T_{gh,i-1})}{\Delta Z^2} - \frac{h_f A_f}{\rho_g A_g \Delta Z C_{pg}} (T_{gh,i} - T_{wh,i}) - \frac{h_f A_f}{\rho_g A_g \Delta Z C_{pg}} (T_{gh,i} - T_{wh,i}) \\
\frac{1}{t_0} \frac{dT_{wh,i}}{dt} &= -\frac{v_w}{A_w} \frac{(T_{wh,i} - T_{wh,i+1})}{\Delta Z^2} + \frac{h_f A_f}{\rho_w A_w \Delta Z C_{pw}} (T_{gh,i} - T_{wh,i}) + \frac{h_f A_f}{\rho_w A_w \Delta Z C_{pw}} (T_{gh,i} - T_{wh,i})
\end{align*}
\]

If we define

\[
\begin{align*}
F_g &= \frac{v_g}{A_g \Delta Z} \frac{1}{t_0} \\
F_w &= \frac{v_w}{A_w \Delta Z} \frac{1}{t_0} \\
gg &= \frac{h_f A_f}{\rho_g A_g \Delta Z C_{pg}} \frac{1}{t_0} \\
gw &= \frac{h_f A_f}{\rho_w A_w \Delta Z C_{pw}} \frac{1}{t_0}
\end{align*}
\]

then a state space representation can be presented as a state vector \( \mathbf{x}_{he} \)

\[ \mathbf{x}_{he} = [T_{gh1}, T_{wh1}, T_{gh2}, T_{wh2}, T_{gh3}, T_{wh3}, T_{gh4}, T_{wh4}]^T \]

an input vector \( \mathbf{u}_{he} \)

\[ \mathbf{u}_{he} = [T_g, T_w]^T \]

and the matrices

\[
A_{he} = \begin{bmatrix}
-F_g \frac{\Delta Z}{\Delta Z} - gg & gg & 0 & 0 & \ldots \\
gw & -F_w \frac{\Delta Z}{\Delta Z} - gw & 0 & 0 & \ldots \\
F_g \frac{\Delta Z}{\Delta Z} & 0 & -F_g \frac{\Delta Z}{\Delta Z} - gg & gg & \ldots \\
0 & 0 & gw & -F_w \frac{\Delta Z}{\Delta Z} - gw & \ldots \\
0 & 0 & 0 & 0 & \ldots \\
0 & 0 & 0 & 0 & \ldots \\
0 & 0 & 0 & 0 & \ldots
\end{bmatrix}
\]
With these definitions, the heat exchanger is modeled by

\[
\begin{align*}
\dot{x}_{he} &= A_{he} x_{he} + B_{he} u_{he} \\
y_{he} &= C_{he} x_{he}
\end{align*}
\]  

(60a)  

(60b)

4 Steady State Computations

In this section we describe, how a steady state operating point of the model can be computed. We take the following degrees of freedom to fix the operating point:

1. Temperature of emulsion \( T \)
2. Total pressure in gascap \( P_3 \)
3. Partial pressure of monomer in gascap \( P_{C2} \)
4. Ratio partial pressure of comonomer to partial pressure monomer \((C_x/C_2)_{set}\)
5. Production rate \( Q_0 \)

With these values and using (1a) and (1b) we obtain \( C_{2g} \) and \( C_{xg} \) for steady state. As it can be seen from (53), the steady state for the gascap gives

\[
\begin{align*}
C_{2g} \big|_{ss} &= C_{2b} \big|_{ss} \quad \text{at } z = 1 \\
C_{xg} \big|_{ss} &= C_{xb} \big|_{ss} \quad \text{at } z = 1
\end{align*}
\]
where by \( x_{ss} \) we denote a steady state value. Therefore, concentration of monomer and comonomer in bubble phase are also known for steady state. Or equivalently

\[
x_4|_{ss} = \frac{C_{2b}}{C_o} \bigg|_{ss} \quad \text{at } z = 1 \tag{61a}
\]
\[
x_7|_{ss} = \frac{C_{2b}}{C_o} \bigg|_{ss} \quad \text{at } z = 1 \tag{61b}
\]

With \( x_4 \) and \( x_7 \) known and using equations (40) (41), we can write \( A_{11} \) and \( A_{16} \) as functions of \( x_1 \) and \( x_6 \), respectively

\[
A_{11} = (x_4 - x_1)e^{KB} + x_1 \tag{62a}
\]
\[
A_{16} = (x_7 - x_6)e^{KB} + x_6 \tag{62b}
\]

And also, from (43) and (44)

\[
\bar{x}_4 = x_1 + (x_4 - x_1)e^{KB}\left(\frac{1 - e^{KB}}{KB}\right) \tag{63a}
\]
\[
\bar{x}_7 = x_6 + (x_7 - x_6)e^{KB}\left(\frac{1 - e^{KB}}{KB}\right) \tag{63b}
\]

From equation (39) we can obtain \( x_2 \) as a function of \( x_1 \) and \( x_6 \) for a given \( Q_0 \)

\[
x_2 = \frac{Q_0t_0}{(\xi_1x_1 + \xi_6x_6)e^{-\delta/2}AH\epsilon_{m}(1 - \delta^*)\epsilon_{mf}} \tag{64}
\]

With this, we can substitute (62a), (63a), (64) in (33) making \( \frac{dx_1}{dt} = 0 \) and (62b), (63b), (64) in (34) making \( \frac{dx_6}{dt} = 0 \), obtaining

\[
0 = \alpha(x_4 - x_1)e^{KB} + KB\beta\Gamma(x_4 - x_1)e^{KB}\left(\frac{1 - e^{KB}}{KB}\right) - \\
\frac{Q_0t_0}{AH(1 - \delta^*)\epsilon_{mf}C_o\xi_1x_1} - \frac{Q_0t_0}{AH(1 - \delta^*)\epsilon_{mf}C_o\theta + x_1 + x_6} \tag{65}
\]
\[
0 = \alpha(x_7 - x_6)e^{KB} + KB\beta\Gamma(x_7 - x_6)e^{KB}\left(\frac{1 - e^{KB}}{KB}\right) - \\
\frac{Q_0t_0}{AH(1 - \delta^*)\epsilon_{mf}C_o\xi_6x_6} - \frac{Q_0t_0}{AH(1 - \delta^*)\epsilon_{mf}C_o\theta + x_1 + x_6} \tag{66}
\]

If we add these two expressions, and we define a new variable \( r = x_1 + x_6 \), the following equation results:

\[
0 = \left(\epsilon e^{KB} + KB\beta\Gamma e^{KB}\left(\frac{1 - e^{KB}}{KB}\right)\right)(x_4 + x_7 - r) - \\
\frac{Q_0t_0}{AH(1 - \delta^*)\epsilon_{mf}C_o} - \frac{Q_0t_0}{AH(1 - \delta^*)\epsilon_{mf}C_o\theta + r} \tag{67}
\]
which is readily solved for $r$. Substituting $x_6 = r - x_1$ with $r$ known in (65), we can solve then this equation for $x_1$. To obtain $B_1$, substituting (45) in (35) and making \( \frac{dx_6}{dt} = 0 \), we obtain a linear equation in $B_1$. Solving for this value, the steady state computations for bed and gascap are completed. From these steady state values it is also possible to obtain the required $\phi_{2in|ss}$ and $\phi_{xin|ss}$ from (12) as

\[
\begin{align*}
\phi_{2in|ss} &= \psi(C_{20} - C_{2g})|_{ss} \\
\phi_{xin|ss} &= \psi(C_{x0} - C_{xg})|_{ss}
\end{align*}
\]

Substituting these values in (8), we obtain $\phi_{flow|ss}$.

As $x_5$ was obtained from the previous computations, we must now determine $T_w$ and the temperatures of gas and water in each segment of the exchanger that will hold the steady state. From (60a)

\[ x_{he|ss} = -A^{-1}_{he}B_{he}u_{he|ss} \quad (68) \]

The value of $y_{he|ss}$ is known: It is $B_1$ because the feed temperature of inlet gas in the fluidized bed equals the temperature of the gas coming out of the heat exchanger (in equilibrium)

\[ y_{he|ss} = C_{he}x_{he|ss} = -C_{he}A^{-1}_{he}B_{he}u_{he|ss} \quad (69) \]

And this can be solved for $T_w$ obtaining then $x_{he|ss}$ from (68). In a similar way, it is possible to obtain from (50a) and (50b) the required steady state value for the catalyst flow $qc$ as

\[ x_{2|ss} = \left(-C_{ca}A^{-1}_{ca}B_{ca} + D_{ca}\right)qc|_{ss} \quad (70) \]

where we must solve for the unknown $qc|_{ss}$ using $x_{2|ss}$ obtained in (64).

The contribution of the different terms to mass exchange in steady-state is (normalized to the biggest term)

<table>
<thead>
<tr>
<th>Term</th>
<th>$C_2$</th>
<th>$C_x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mix with incoming gas flow</td>
<td>+229.9</td>
<td>+23.3</td>
</tr>
<tr>
<td>Exchange with bubble phase</td>
<td>+773.7</td>
<td>+78.6</td>
</tr>
<tr>
<td>Disappeared by reaction</td>
<td>-1000.0</td>
<td>-99.6</td>
</tr>
<tr>
<td>Product removal</td>
<td>-3.6</td>
<td>-2.3</td>
</tr>
</tbody>
</table>

Table 2: Contribution of successive terms in mass balance

Results for which the relative importance between the two first mechanisms depends on the value of $K_{he}$. It is also illustrative to present the contributions to the energy balance These results are in accordance with those presented by [4]: For a ratio $\frac{V_{mf}}{U_{mf}} > 10$ the heat transfer from emulsion to bubble is expected to absorb around 85% of the heat of reaction, while the cooling of incoming (emulsion) gas represents less than a 10%.
<table>
<thead>
<tr>
<th>Term</th>
<th>Contribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Warm up of incoming gas</td>
<td>-7.7</td>
</tr>
<tr>
<td>Exchange with bubble phase</td>
<td>-87.8</td>
</tr>
<tr>
<td>Heat of reaction</td>
<td>+100.0</td>
</tr>
<tr>
<td>Heat removed with products</td>
<td>-4.5</td>
</tr>
</tbody>
</table>

Table 3: Contribution of successive terms in heat balance

5 Non-Linearities Analysis

Following [10], staircase experiments on the inputs will be performed in order to evaluate the importance of non-linear behaviors. However, the outcome of these experiments differs from [10] because our model reproduces also the mass and heat exchange between bubble and emulsion phase, leading to a higher degree of non linearity.

5.1 Steps in reference emulsion temperature

The input reference $T_{set}$ for the PID temperature controller is changed as shown in Fig.3. The PID controller was tuned manually and the proportional gain was chosen 3 and the integration constant was chosen 200 seconds. It can be seen that the response of total pressure $P$ and partial monomer $P_{C2}$ and comonomer pressures $P_{C_2}$ is clearly affected by the exponential character of the temperature dependence in (33), (34). It is also seen that the production rate $Q$ and the ratio $C_{\pi}/C_{\tau}$ responses show a strongly non-linear behavior.

5.2 Steps in input ratio

The input ratio is changed as shown in Fig.4. The same kind of asymmetry can be observed, although the non linear behavior is now much less significant.

5.3 Steps in total input flow

The transfer in this case could be considered with linear dynamics followed by some nonlinear gain, as it can be seen from Fig.5.
As it can be seen from Fig 6, this transfer is highly non linear for all pressures and ratio.
Figure 4: Staircase experiment on input ratio
Figure 5: Staircase experiment on total input flow
Figure 6: Staircase experiment on catalyst feed
6 Conclusions

In this report we presented a theoretical model of a fluidized bed polymerization process and its implementation in a SIMULINK program. Our intention was to develop a nonlinear process model, which we could use to test our ideas concerning nonlinear identification, filtering and control. This model can be as well used for the controller design of a real process. Interesting feature of this process from the controller design point of view is its complex nonlinear behavior with unstable dynamics. Therefore a design of a nonlinear controller is here of particular interest. The process is multivariable, that means it is possible to specify a couple of manipulated inputs and a couple of controlled outputs for a control problem. Also a number of disturbance inputs can be easily introduced, which might be interesting from the practical point of view.
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A
Summary of Symbols

$A$ cross-sectional area of the fluidized bed, $A = (1/4)\pi D^2 \ m^2$

$A_f$ heat exchange area in heat exchanger, $m^2$

$A_g$ cross section for gas in heat exchanger, $m^2$

$A_w$ cross section for water in heat exchanger, $m^2$

$A_{ca}$ state space $A$ matrix for catalyst activity

$A_{gc}$ state space $A$ matrix for gascap

$A_{he}$ state space $A$ matrix for heat exchanger

$A_{11}$ dimensionless group defined in (31)

$A_{21}$ dimensionless group defined in (31)

$A_{31}$ dimensionless group defined in (31)

$A_{16}$ dimensionless group defined in (31)

$A_{26}$ dimensionless group defined in (31)

$A_{36}$ dimensionless group defined in (31)

$B(q^{-1})$ polynomial defined in (48)

$B_{ca}$ state space $B$ matrix for catalyst activity

$B_{gc}$ state space $B$ matrix for gascap

$B_{he}$ state space $B$ matrix for heat exchanger

$B_1$ dimensionless group defined in (31)

$B_2$ dimensionless group defined in (31)

$B_3$ dimensionless group defined in (31)

$C_{ca}$ state space $C$ matrix for catalyst activity

$C_{gc}$ state space $C$ matrix for gascap

$C_{he}$ state space $C$ matrix for heat exchanger

$C_{pg}$ specific heat of gas, J/(kg K)

$C_{ps}$ specific heat of solid in emulsion, J/(kg K)

$C_{pw}$ specific heat of water, J/(kg K)

$C_0$ reference concentration, kg/m$^3$

$C_{2e}$ concentration of monomer in emulsion phase, kg/m$^3$

$C_{2e}$ concentration of comonomer in emulsion phase, kg/m$^3$

$C_{2b}$ concentration of monomer in bubble phase at $z = 1$, kg/m$^3$

$C_{2b}$ concentration of comonomer in bubble phase at $z = 1$, kg/m$^3$

$C_{2g}$ concentration of monomer in gascap, kg/m$^3$

$C_{2g}$ concentration of comonomer in gascap, kg/m$^3$

$C_{2in}$ concentration of monomer in input flow, kg/m$^3$

$C_{2in}$ concentration of comonomer in input flow, kg/m$^3$

$C_{20}$ concentration of monomer in mixed inlet flow, kg/m$^3$

$C_{20}$ concentration of comonomer in mixed flow, kg/m$^3$

$C_{260}$ concentration of monomer in bubble phase at $z = 0$, kg/m$^3$

$C_{260}$ concentration of comonomer in bubble phase at $z = 0$, kg/m$^3$

$C_e/C_2$ ratio monomer to comonomer concentration in gascap

$(C_e/C_2)_{set}$ desired (steady state) ratio of monomer to comonomer concentration in gascap
\( d \) discrete time delay in catalyst activity
\( D \) diffusion coefficient of gas in emulsion, \( m^2/s \)
\( D_e \) effective diffusion coefficient of gas in emulsion, \( m^2/s \)
\( D \) bed diameter, m
\( D_{ca} \) state space \( D \) matrix for catalyst activity
\( d_B \) mean equivalent bubble diameter, m
\( d_{BO} \) initial bubble diameter at the surface of the perforated plate, m
\( d_{BM} \) bubble diameter if there were a single train of bubbles rising along the centerline of the bed, m
\( d_p \) mean diameter of the particles, m
\( E_a \) activation energy, J/mol
\( F_g \) group defined in (58), m
\( F_w \) group defined in (58), m
\( g \) acceleration of gravity, m/s\(^2\)
\( g_g \) dimensionless group defined in (59)
\( g_w \) dimensionless group defined in (59)
\( h_f \) heat exchange coefficient in heat exchanger, J/(m\(^3\)sK)
\( H \) bed height, m
\( H_{bc} \) heat transfer coefficient bubble-cloud per unit bubble volume, J/(m\(^3\)sK)
\( H_{be} \) heat transfer coefficient bubble-emulsion per unit bubble volume, J/(m\(^3\)sK)
\( H_{ce} \) heat transfer coefficient cloud-emulsion per unit bubble volume, J/(m\(^3\)sK)
\( I \) identity matrix of order 22
\( -\Delta H_r \) heat of reaction, J/kg
\( K_B \) dimensionless group defined in (31)
\( K_H \) dimensionless group defined in (31)
\( K_{bc} \) mass transfer coefficient bubble-cloud per unit bubble volume, 1/s
\( K_{bc} \) mass transfer coefficient bubble-emulsion per unit bubble volume, 1/s
\( K_{ce} \) mass transfer coefficient cloud-emulsion per unit bubble volume, 1/s
\( k_g \) heat conductivity of gas J/(m s K)
\( k_{p0,C_1} \) reaction rate constant for monomer, m\(^3\)/kgcat s
\( k_{p0,C_2} \) reaction rate constant for comonomer, m\(^3\)/kgcat s
\( m_g \) mass of gas in heat exchanger, kg
\( m_{g,i} \) mass of gas in segment \( i \) of heat exchanger, kg
\( m_w \) mass of water in heat exchanger, kg
\( m_{w,i} \) mass of water in segment \( i \) of heat exchanger, kg
\( M_{C_2} \) molecular weight of monomer, kg/mol
\( M_{C_x} \) molecular weight of comonomer, kg/mol
\( M_{H_2} \) molecular weight of hydrogen, kg/mol
\( M_{N_2} \) molecular weight of nitrogen, kg/mol
\( P \) total pressure in the reactor, Pa
\( P_{C_2} \) partial pressure of the monomer, Pa
\( P_{C_x} \) partial pressure of the comonomer, Pa
$P_{H_2}$ partial pressure of hydrogen, Pa
$P_{N_2}$ partial pressure of nitrogen, Pa
$Q_o$ mass production rate, kg/s
$q_c$ catalyst feed, kg/s
$q^{-1}$ unit delay operator
$R$ dimensionless group defined in (46c)
$r_{x_1}$ dimensionless group defined in (46c)
$r_{x_6}$ dimensionless group defined in (46c)
$R_g$ gas constant, J/(mol K)
$T_e$ temperature of emulsion, K
$T$ temperature of emulsion, K
$T_b$ temperature of bubble phase at $z = 1$, K
$T_{b_0}$ temperature of bubble phase at $z = 0$, K
$T_f$ inlet gas feed temperature, K
$T_g$ temperature in the gas cap, K
$T_{wh}$ water temperature in heat exchanger, K
$T_{wh,i}$ water temperature in segment $i$ of the heat exchanger, K
$T_{gh}$ gas temperature in heat exchanger, K
$T_{gh,i}$ gas temperature in segment $i$ of the heat exchanger, K
$T_{ed}$ temperature of emulsion in steady state, K
$T_{ref}$ reference temperature, K
$t_o$ reference time, s
$t$ dimensionless variable defined in (31)
$t'$ time, s
$U_b$ absolute velocity of the bubble phase gas, m/s
$U_{br}$ velocity of rise of a single bubble, m/s
$U_{mf}$ minimum fluidization velocity, m/s
$U_o$ inlet gas velocity, m/s
$U_e$ velocity of emulsion gas, m/s
$V$ volume of the gas cap, m$^3$
$V_g$ volume of gas in heat exchanger, m$^3$
$V_{gh,i}$ volume of gas in segment $i$ of the heat exchanger, m$^3$
$V_w$ volume of water in heat exchanger, m$^3$
$V_{w,i}$ volume of water in segment $i$ of the heat exchanger, m$^3$
$v_g$ gas flow rate in heat exchanger, m$^3$/s
$v_w$ water flow rate in heat exchanger, m$^3$/s
$X_{cat}$ mass fraction of catalyst in solid phase
$x_1$ dimensionless variable defined in (31)
$x_2$ dimensionless variable defined in (31)
$x_3$ dimensionless variable defined in (31)
$x_4$ dimensionless variable defined in (31)
$x_5$ dimensionless variable defined in (31)
$x_6$ dimensionless variable defined in (31)
$x_7$ dimensionless variable defined in (31)
\( \mathbf{x}_{ca} \) state vector for catalyst activity
\( \mathbf{x}_{he} \) state vector for heat exchanger
\( \mathbf{x}_{gc} \) state vector for gascap
\( y_{he} \) output for heat exchanger
\( y_{gc} \) output for gascap
\( z \) dimensionless variable defined in (31)
\( z^* \) position (height) in the bed, m

Greek letters

\( \alpha \) dimensionless group defined in (31)
\( \beta \) dimensionless group defined in (31)
\( \gamma \) dimensionless group defined in (31)
\( \Gamma \) dimensionless group defined in (31)
\( \Gamma_{ca} \) discrete time state space \( B \) matrix for catalyst activity
\( \delta \) dimensionless group defined in (31)
\( \delta^* \) fraction of bubble phase volume in fluidized bed
\( \Delta Z \) length of one segment of the heat exchanger, m
\( \Delta_{ca} \) discrete time state space \( D \) matrix for catalyst activity
\( \varepsilon \) voidage of the emulsion phase
\( \varepsilon_{mf} \) value of \( \varepsilon \) at minimum fluidizing conditions
\( \theta \) dimensionless group defined in (31)
\( \xi_1 \) dimensionless group defined in (31)
\( \xi_2 \) dimensionless group defined in (31)
\( \rho \) dimensionless group defined in (31)
\( \Psi_{ca} \) discrete time state space \( C \) matrix for catalyst activity
\( \psi \) gas flow circulating in the model, m\(^3\)/s
\( \psi_m \) measured gas flow m\(^3\)/s
\( \psi_{in} \) input gas flow, m\(^3\)/s
\( \rho_g \) measured density of gas flow kg/m\(^3\)
\( \rho_s \) density of gas circulating in the model, kg/m\(^3\)
\( \rho_s \) density of solid, kg/m\(^3\)
\( \rho_w \) density of water, kg/m\(^3\)
\( \Phi_{ca} \) discrete time state space \( A \) matrix for catalyst activity
\( \phi_{i,n} \) monomer input mass flow, kg/s
\( \phi_{c,n} \) comonomer input mass flow, kg/s
\( \phi_{flow} \) total input mass flow, kg/s
\( \phi_{g} \) gas mass flow in heat exchanger, kg/s
\( \phi_{w} \) water mass flow in heat exchanger, kg/s
\( \tau \) continuous time delay for catalyst activity, s
B Simulink Model

In this section we show the SIMULINK model of the process as it was used to generate the non-linearity tests of section 5.

Figure 7: Simulink model of the process

Figure 8: Simulink model of the PID controller and heat exchanger
THEORETICAL MODEL OF THE POLYMERIZATION REACTOR

Figure 9: Simulink model of the reactor
C Initialization File

%clear
%fixed values:
Rg=8.31;
Ea=9000*4.19;
D=3.5;
Mc2=28.05e-3;
Mcx=56.11e-3;
Wh=2e-3;
Mn=28.01e-3;
rhoa=21;
rhox=0.95*1e3;
cps=0.456*4.19*1e3;
cpg=0.518*4.19*1e3;
kg=7.6e-5*4.19*1e2;
A=0.25*pi*D^2;
m1=1.16e-4*1e-1;
dp=0.05*1e-2;
g=9.81;
Unf=0.06;
emf=0.38;
Tref=300;
to=30*3600;
Pp0=8.6;
P=20.9e5;
delta=Ea/(Rg*Tref);
%the following 3 variables are determined from measured process data by fixing the mass and heatbalances.
xi1=1.5640e+12;
xi6=2.3696e+11;
gamma=3.593e091086489;
km=xi6/xi1*Mcx/Mc2;
%input values:
Ps=20.99e5;
Pc20=5.9948e5;
CxC20=0.3;
Tb=82+273;
psia=350/60;
H=12.2;
H2=3.57e5;
Tin=Tb/Tref;
%calculated values:
C2b=Pc20*Mc2/(Rg*Tb);
Pcx0=Pc0*CxC20;
Cxb=Pcx0*Mcx/(Rg*Tb);
N2=Ps-Pc0-Pcx0-H2;
Pinert=(H2+N2);
%gasconstant [j/mol K]
%Activation energy [j/mol]
%Diameter reactor
%mole masses several components
%density recycle flow [kg/m3]
%density solid [kg/m3]
%Heat capacity solid [j/kg K]
%Heat capacity gas [j/kg K]
%thermal conductivity [j/m s K]
%cross area reactor
%Viscosity of fluid [kg/m s]
%diameter particle size
%gravity constant [m/s2]
%minimum fluidizing velocity [m/s]
%void fraction in the bed at minimum fluidizing conditions
%reference value temperature
%reference value time
%reference production rate
%reference pressure
%Activation energy
%dimensionless reaction constant for monomer
%dimensionless reaction constant for comonomer
%dimensionless heat of reaction
%xpressure [Pa]
%xpartial pressure monomer [Pa]
%xratio comonomer/monomer [mol/mol] in gasphase
%Tbed K
%actual gas flow [m3/s]
%bed height [m]
%inert mol fractions
%concentration monomer in bubble phase [kg/m3]
%xpartial pressure comonomer [Pa]
%concentration comonomer in bubble phase [kg/m3]
%xpartial pressure nitrogen [Pa]
%xpartial pressure inert gas [Pa]
\( \rho g = H_2 \cdot M_{H_2} / (R_g \cdot T_b) + N_2 \cdot M_{N_2} / (R_g \cdot T_b) + C_{2b} \cdot C_{xb} \):

\( \psi = \rho_{ta} / \rho g ; \)

\( U_{nul} = \psi / A_j \)

\( C_0 = 6.0231 ; \)

\( x_4 = C_{2b} / C_0 ; \)

\( x_7 = C_{xb} / C_0 ; \)

% Diffusion:

\( D_f = 2e-5 ; \)

\( d_b = 0.5 ; \)

\( U_b = U_{nul} - U_{mf} + 0.711 \cdot (g \cdot d_b)^{-0.5} ; \)

\( \text{deltaster} = (U_{nul} - U_{mf}) / U_b ; \)

\( \Gamma = \text{deltaster} / (1 - \text{deltaster}) ; \)

\( U_e = U_{mf} / (\text{emf} \cdot \Gamma) ; \)

\( K_c = 6.78 \cdot (\text{emf} \cdot D_f / d_b)^{-0.5} ; \)

\( K_b = 4.5 \cdot U_{mf} / d_b \cdot 5.85 \cdot (D_f \cdot 0.5 \cdot g^{-0.25} \cdot d_b^{-1.25}) ; \)

\( \text{Kbc} = 1 / (K_b \cdot C_{co}) ; \)

\( H_b = 4.5 \cdot U_{mf} \cdot \rho g \cdot \rho_{s} / (d_b \cdot 5.85 \cdot (D_f \cdot 0.5 \cdot g^{-0.25} \cdot d_b^{-1.25})) ; \)

\( \text{hbe} = \text{Kbc} ; \)

% Dimensionless parameters:

\( \text{Kb} = K_b / U_b ; \)

\( \text{Kb} = H_b / (U_b \cdot \text{Co} \cdot \rho_{s}) ; \)

\( \text{alpha} = U_e / (3.6 \cdot \text{emf}) ; \)

\( \text{theta} = \rho_{s} \cdot (1 - \text{emf}) / (\text{emf}) ; \)

\( \rho_{s} = (1 - \text{emf}) \cdot \rho_{s} \cdot (1 - \text{emf}) / (\text{emf} \cdot \text{Co} \cdot \rho_{s}^2) ; \)

\( \text{x3} = T_b / \text{Tref} ; \)

% Catalytic activity:

\( \text{fca} = \alpha^2 \cdot \exp(K_b) \cdot K_b \cdot \exp(K_b) / (1 - \exp(-K_b)) ; \)

\( \text{Cc} = \text{PpO} / (\alpha \cdot \text{H} \cdot 3.6 \cdot (1 - \text{deltaster}) \cdot \text{emf} \cdot \text{Co}) ; \)

\( \text{xc} = \text{fsolve}'x1\cdot x6'([0.5, .5], [0.1e-8, 1e-8], [], \text{Ac}, \text{Cc}, \text{x1}, \text{x1}, \text{x1}, \text{x1}, \text{theta}) ; \)

\( \text{x1} = \text{Xc}(1) ; \)

\( \text{x6} = \text{Xc}(2) ; \)

\( \text{A1x1} = (x4 - x1) \cdot \exp(K_b) + x1 ; \)

\( \text{A1x6} = (x7 - x6) \cdot \exp(K_b) + x6 ; \)

\( \text{C2in} = \psi \cdot (\text{A1x1} - x4) ; \)

\( \text{C2in} = \psi \cdot (\text{A1x6} - x7) ; \)

\( \text{x4m} = x1 + (x4 - x1) \cdot \exp(K_b) \cdot (1 - \exp(-K_b)) / K_b ; \)

\( \text{x7m} = x6 + (x7 - x6) \cdot \exp(K_b) \cdot (1 - \exp(-K_b)) / K_b ; \)

\( \text{cax} = \text{PpO} / (3.6 \cdot \text{A} \cdot \text{H} \cdot (1 - \text{deltaster}) \cdot \text{emf}) ; \)

\( \text{Cc} = \text{PpO} / (\alpha \cdot \text{H} \cdot 3.6 \cdot (1 - \text{deltaster}) \cdot \text{emf}) ; \)

\( \text{Hc} = (\alpha \cdot \text{x1} \cdot \text{x6} \cdot \text{x7} \cdot \text{x8} \cdot \text{x9} \cdot \text{x10} \cdot \text{x11} \cdot \text{x12}) \cdot \exp(-\text{delta} / \text{x3}) \cdot \text{A} \cdot \text{H} \cdot \text{Co} \cdot (1 - \text{deltaster}) \cdot \text{emf} ; \)

\( \text{Gc} = \alpha^2 \cdot (\text{x1} \cdot \text{x6} \cdot (\text{rho} \cdot \text{x1} \cdot \text{x6})) \cdot \text{GAMMA} \cdot \text{beta} / (\text{rho} \cdot \text{x1} \cdot \text{x6}) \cdot \text{...} \)

\( \text{x4m} = x1 + (x4 - x1) \cdot \exp(K_b) \cdot (1 - \exp(-K_b)) / K_b ; \)

\( \text{x7m} = x6 + (x7 - x6) \cdot \exp(K_b) \cdot (1 - \exp(-K_b)) / K_b ; \)

\( \text{cax} = \text{PpO} / (3.6 \cdot \text{A} \cdot \text{H} \cdot (1 - \text{deltaster}) \cdot \text{emf}) ; \)

\( \text{Cc} = \text{PpO} / (\alpha \cdot \text{H} \cdot 3.6 \cdot (1 - \text{deltaster}) \cdot \text{emf}) ; \)

\( \text{Hc} = (\alpha \cdot \text{x1} \cdot \text{x6} \cdot \text{x7} \cdot \text{x8} \cdot \text{x9} \cdot \text{x10} \cdot \text{x11} \cdot \text{x12}) \cdot \exp(-\text{delta} / \text{x3}) \cdot \text{A} \cdot \text{H} \cdot \text{Co} \cdot (1 - \text{deltaster}) \cdot \text{emf} ; \)

\( \text{Gc} = \alpha^2 \cdot (\text{x1} \cdot \text{x6} \cdot (\text{rho} \cdot \text{x1} \cdot \text{x6})) \cdot \text{GAMMA} \cdot \text{beta} / (\text{rho} \cdot \text{x1} \cdot \text{x6}) \cdot \text{...} \)

\( \text{x4m} = x1 + (x4 - x1) \cdot \exp(K_b) \cdot (1 - \exp(-K_b)) / K_b ; \)

\( \text{x7m} = x6 + (x7 - x6) \cdot \exp(K_b) \cdot (1 - \exp(-K_b)) / K_b ; \)

\( \text{cax} = \text{PpO} / (3.6 \cdot \text{A} \cdot \text{H} \cdot (1 - \text{deltaster}) \cdot \text{emf}) ; \)

\( \text{Cc} = \text{PpO} / (\alpha \cdot \text{H} \cdot 3.6 \cdot (1 - \text{deltaster}) \cdot \text{emf}) ; \)

\( \text{Hc} = (\alpha \cdot \text{x1} \cdot \text{x6} \cdot \text{x7} \cdot \text{x8} \cdot \text{x9} \cdot \text{x10} \cdot \text{x11} \cdot \text{x12}) \cdot \exp(-\text{delta} / \text{x3}) \cdot \text{A} \cdot \text{H} \cdot \text{Co} \cdot (1 - \text{deltaster}) \cdot \text{emf} ; \)

\( \text{Gc} = \alpha^2 \cdot (\text{x1} \cdot \text{x6} \cdot (\text{rho} \cdot \text{x1} \cdot \text{x6})) \cdot \text{GAMMA} \cdot \text{beta} / (\text{rho} \cdot \text{x1} \cdot \text{x6}) \cdot \text{...} \)

% Catalyst activity:

\( \text{fca} \cdot \exp(K_b) \cdot (1 - \text{deltaster}) \cdot (1 - \text{emf}) \cdot \text{rho} \cdot \text{s} \cdot \text{12} ; \)
activf=[zeros(1,12) 0.5 0.95 1;-0.0470]*5.4932/fcc;
Aq=[zeros(1,23);eye(23),zeros(23,1)];
Bq=[1;zeros(23,1)];
Cq=activf(13:36);
Dq=0;
[Ab,Bb,Cb]=dbalreal(Aq,Bq,Cq);
Db=Dq;
[Ar,Br,Cr,Dr]=dmodred(Ab,Bb,Cb,Db,[3;24]);
[Aqc,Bqc]=d2c(Ar,Br,300/to);
Cq=Cr;
Dq=0;
dc_val=-Cqc*inv(Aqc)*Sqc;
qc=x2/dc_val;

"needed catalyst flow [kg/h]"

%calculations gascap
Vg=0.5*A*(12.2-A*(12.2-H));
f=to/psi/(Vg);
etau2=Ag*ref/Co/(Mc2*P);
etau=Ag*ref/Co/(Mw2*P);
etu=-Pinert/(xS*P);
Ag=-f*eye(3);
Bg=-Ag;
Cg=eye(3);
Dg=zeros(3,3);
xOg=[x4;x7;x5];

% Heat exchanger
Hg=480*to/O.05;
Agg=0.2*S*pi*(O.5)-2;
Aw=Agg;
Fg=to*psi/(Agg*3600);
gg=Hg/(Agg*rhog*cpg);
rhog=1.3;  
cpg=4.1*10^3;  
gg=Hg/(Aw*rhog*cpw);  
dz=2;

Fg=Fg/600/4;
Fw=Fw/20/4;
gg=gg/600/4;
gw=gw/600/4;
% The state-space form of the heat exchanger
Ah=(diag(-gg gw gg gw gg gw gg gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw gw
B2=Ch*x0h;
aux=dcgain(Ah,Bh,Ch,Dh);
k1=aux(1);
k2=aux(2);
clear aux;
%
% some more constants
Kb=exp(-Kb);
eKb=(1-exp(-Kb))/Kb;
KbbG=Kb*beta*GAMMA;
KhbG=Kh*beta*GAMMA;
alphap=alpha*KbbG*eKb;
%
% parameters for the water temperature PI controller
Pval=3;
Ival=200;
% x0val=Tw/Ival;
%
% parameters for the pressure controller
Ppval=0.45;
Ipval=120;
%
Cflow=C2in+Cxin*(33/5.59/2);
% equilibria input flow
%
% save initval;

An auxiliary function to solve (65) and (66) for $x_1$ and $x_6$

function f=f1x6(x,Ac,Bc,x11,x16,x4,x7,theta)
% parameters Ac Bc x11 x16 x4 x7 theta
x1=x(1);x6=x(2);
f(1)=Ac*(x4-x1)-x11*x1*Bc/(x11*x1+x16*x6)-Bc*x1/(theta+x1+x6);
f(2)=Ac*(x7-x6)-x16*x6*Bc/(x11*x1+x16*x6)-Bc*x6/(theta+x1+x6);
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