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Temperature Control of Industrial Gas Phase Propylene Polymerization in Fluidized Bed Reactors Using Model Predictive Control

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Abstract. A two-phase dynamic model describing gas phase propylene polymerization in a fluidized bed reactor which considers the polymerization reaction in both phases was used to explore the control of the reactor temperature by manipulating the heat exchanger cooling water flow rate. A model predictive control (MPC) technique is implemented to control of the nonlinear process and compared its performance with conventional PI controllers tuned using the Internal Model Control (IMC) method as well as the standard Ziegler-Nichols (Z-N) method. The closed-loop simulations revealed that the Z-N PI controller produced oscillatory responses and the MPC and the IMC-Based PI controllers were able to track the changes in the set point. However the quality of the MPC set point tracking was superior to that of the IMC-Based PI controller.

Keywords: Temperature Control, Propylene Polymerization, Model Predictive Control.

1. Introduction

Modeling and control of the polymerization process in fluidized bed reactors such as polypropylene production are challenging issues in process and control engineering. This is mainly because of the high non-linearity of the process dynamics due to complicated reaction mechanisms, complex flow characteristics of gas and solids, various heat and mass transfer mechanisms and the interaction between the control loops. Many studies were reported for the modeling and control of olefin polymerization processes using various types of algorithms [1-2].

A process schematic of an industrial gas-phase fluidized bed polypropylene reactor is shown in Figure 1. To maintain acceptable polymer production rate which is an important goal for industry it is necessary to keep the reactor bed temperature above the dew point of the reactants to avoid gas condensation and below the melting point of the polymer to prevent particle melting and agglomeration and consequently reactor shut down.

Choi and Ray [1] used a dynamic model considering bubble and emulsion phases in the bed in the first attempt to describe the dynamics of polypropylene production. They showed that a PI feedback control scheme can be used to control the process transients, but it is limited by the recycle gas cooling capacity.

Dadebo et al. [2] showed that for the temperature control of industrial gas phase polyethylene reactors the nonlinear error trajectory controller (ETC) exhibits significantly superior responses in terms of speed, damping and robustness compared with an optimally-tuned PID controller over a wide range of operating conditions.

Due to the high nonlinearities and difficulties involved in the dynamics and control of the gas phase propylene polymerization fluidized bed reactor, an efficient process control scheme need to be implemented. However, it is beyond the capability of the conventional controller with fixed controller settings to achieve excellent control of the reactor variables. In order to achieve good control of the reactor variables, a more intelligent and efficient process control scheme is needed where the controller is able to automatically re-design itself in real time according to the changing process dynamics.

In the present study, a two-phase model with comprehensive kinetics for propylene homo-polymerization in a fluidized bed reactor that considers the presence of particles in the bubbles and the excess gas in the emulsion phase with polymerization reaction in both phases is considered [3-4]. A Model Predictive Control (MPC) algorithm is used for controlling the reactor temperature by manipulating the coolant flow rate.

2. Mathematical Modeling of Propylene Polymerization

In the present study, the kinetic model of propylene homo-polymerization over a Ziegler-Natta catalyst based on the kinetic model developed by Shamiri et al. [3-5] and the dynamic two-phase flow structure were combined and implemented to provide a more realistic understanding of the phenomena encountered in the bed hydrodynamics.

For details of the kinetic scheme, definitions of pseudo-kinetic rate constants and the correlations required for estimating the bubble volume fraction in the bed, the voidage of the emulsion phase and bubble phases, the emulsion phase and bubble phases gas velocities and mass and heat transfer coefficients for two-phase model, the reader is referred to a paper by Shamiri et al. [3].

The following dynamic material balances were written for all of the components in the bed.

For bubbles:

$$[M_i]_{b,(in)}U_bA_b - [M_i]_bU_bA_b - R_v\varepsilon_b[M_i]_b - K_{be}([M_i]_b - [M_i]_e)V_b - (1-\varepsilon_b)\frac{A_b}{V_{PFR}}\int R_{i_b}dz$$
$$= \frac{d}{dt}\left(V_b\varepsilon_b[M_i]_b\right) \tag{1}$$

For emulsion:

$$[M_i]_{e,(in)}U_eA_e - [M_i]_eU_eA_e - R_v\varepsilon_e[M_i]_e + K_{be}([M_i]_b - [M_i]_e)V_e\left(\frac{\delta}{1-\delta}\right) - (1-\varepsilon_e)R_{i_e}$$
$$= \frac{d}{dt}\left(V_e\varepsilon_e[M_i]_e\right) \tag{2}$$

The direction of mass transfer was assumed to be from bubble to emulsion phase. Furthermore, the energy balances can be expressed as:

For bubbles:

$$U_bA_b(T_{b,(in)} - T_{ref})\sum_{i=1}^{m}[M_i]_{b,(in)}C_{pi} - U_bA_b(T_b - T_{ref})\sum_{i=1}^{m}[M_i]_bC_{pi}$$
$$-R_v(T_b - T_{ref})\left(\sum_{i=1}^{m}\varepsilon_bC_{pi}[M_i]_b + (1-\varepsilon_b)\rho_{pol}C_{p,pol}\right) + (1-\varepsilon_b)\frac{A_b\Delta H_R}{V_{PFR}}\int R_{pb}dz$$
$$+H_{be}(T_e - T_b)V_b - V_b\varepsilon_b(T_b - T_{ref})\sum_{i=1}^{m}C_{pi}\frac{d}{dt}([M_i]_b)$$
$$= \left(V_b(\varepsilon_b\sum_{i=1}^{m}C_{pi}[M_i]_b + (1-\varepsilon_b)\rho_{pol}C_{p,pol})\right)\frac{d}{dt}(T_b - T_{ref}) \tag{3}$$

For emulsion:

$$U_eA_e(T_{e,(in)} - T_{ref})\sum_{i=1}^{m}[M_i]_{e,(in)}C_{pi} - U_eA_e(T_e - T_{ref})\sum_{i=1}^{m}[M_i]_eC_{pi}$$
$$-R_v(T_e - T_{ref})\left(\sum_{i=1}^{m}\varepsilon_eC_{pi}[M_i]_e + (1-\varepsilon_e)\rho_{pol}C_{p,pol}\right) - (1-\varepsilon_e)R_{pe}\Delta H_R$$
$$-H_{be}V_e\left(\frac{\delta}{1-\delta}\right)(T_e - T_b) - V_e\varepsilon_e(T_e - T_{ref})\sum_{i=1}^{m}C_{pi}\frac{d}{dt}([M_i]_e) =$$
$$\left(V_e(\varepsilon_e\sum_{i=1}^{m}C_{pi}([M_i]_e) + (1-\varepsilon_e)\rho_{pol}C_{p,pol})\right)\frac{d}{dt}(T_e - T_{ref}) \tag{4}$$

3. Results and Discussion

The process was simulated at the operating conditions shown in Table 1.

The presented mathematical model for the gas phase propylene polymerization fluidized bed reactor consists of cooling water flow rate (F_{cw}) as a manipulated variable and emulsion phase temperature (Te) as a controlled variable.

A model-predictive controller was designed using the MPC toolbox GUI and implemented in simulink using the MPC simulink block.

The closed loop performance of the MPC scheme in tracking series of setpoint changes for the emulsion phase temperature in the polymerization reactor is evaluated. For this purpose, series of setpoint changes in opposite directions were introduced. The magnitude of the setpoints introduced for this loop was typical of the respective nominal operating range. For comparison purposes, conventional PI controllers tuned using the IMC [6] method and the standard Z-N [7] method, were included in this simulation. Both the IMC and Z-N PI controller tuning parameters were calculated based on analyses of the open loop process reaction curve for a particular operational region of the process.

To ensure good performance of the MPC controller, the tuning parameters must be appropriately tuned. Although Shridhar and Cooper [8] suggestion were good starting values for tuning the controller parameter but the exact values used in this work were the result of further fine tuning based on actual control performance. In addition to the selection of controller tuning parameters, the values were chosen for the constraints and imposed on loop are based on practical considerations acquired through real operational experience of the authors.

The resulting controller had a sampling time of 10 sec, a prediction horizon of 17, a control horizon of 1, an output variables weight of 0.09, and a manipulated variables weight of 0.008.

Figs. 2 and 3 show the performance of the MPC as compared to the IMC and Z-N PI controllers in tracking series of setpoint changes for the temperature loop as well as the corresponding controller moves. From Fig. 2, the failure of the Z-N PI controller to track the changes in the setpoints for the temperature loop was obvious. The Z-N PI controller produced oscillatory responses. Furthermore, as shown in Fig. 3, the controller moves observed were vigorous. However the shortcomings exhibited by the Z-N PI controller were not observed for the cases of MPC and the IMC-Based PI controllers. In general, both the MPC and the IMC-Based PI controllers were able to track the changes in the set point. However, the quality of the set point tracking as demonstrated by the MPC was superior to the IMC-Based PI controller in terms of their ability to attain minimal overshoot. Moreover, the MPC was able to not only produce controller moves which were well within the specified input constraints, but also the controller moves produced were non-aggressive and smooth for practical implementations. These were attributed to the ability of the MPC to handle constraints in the inputs, of which the conventional PI controller was unable to achieve. To summarize, Table 2 shows the Integral Absolute Error (IAE) for the three controllers in tracking the series of set point changes. The values of the IAE calculated were consistent with the previous discussions, where the performance of the MPC was superior to the conventional PI controllers.

4. Conclusions

The closed-loop simulations revealed that the Z-N PI controller produced an oscillatory response while the MPC and the IMC-Based PI controller were able to track the changes in the setpoint. However, the quality of the setpoint tracking as demonstrated by the MPC was superior to that of the IMC-Based PI controller in terms of the ability to attain minimal overshoot. Moreover, the MPC was able to not only produce controller moves which were well within the specified input constraints, but also the controller moves produced were non-aggressive and smooth for practical implementations. The values of the IAE calculated for the temperature loop indicate that the performance of the MPC was superior to the conventional PI controllers.

Tab. 1: Operating conditions considered for modeling fluidized bed polypropylene reactors.

Operating conditions	Physical parameters
$V\ (m^3)$=50	$\mu\ (Pa.s)$=1.14×10^{-4}
$T_{ref}\ (K)$=353.15	$\rho_g\ (kg/m^3)$=23.45

T_{in} *(K)*=317.15	ρ_s *(kg/m^3)*=910
P (bar)=25	*dp (m)* =500×10^{-6}
Propylene concentration *(kmol/m^3)*=0.9	ε_{mf}=0.45
Hydrogen concentration *(kmol/m^3)*= 0.015	
Catalyst feed rate *(kg/s)*= 0.0003	

Tab. 2: Integral absolute error (IAE) for the MPC, IMC-Based PI controller, and the Z-N PI controller in tracking series of setpoint changes for the emulsion phase temperature.

Controller	IAE
MPC	2527
IMC-Based PI Controller	2712
Z-N PI Controller	4655

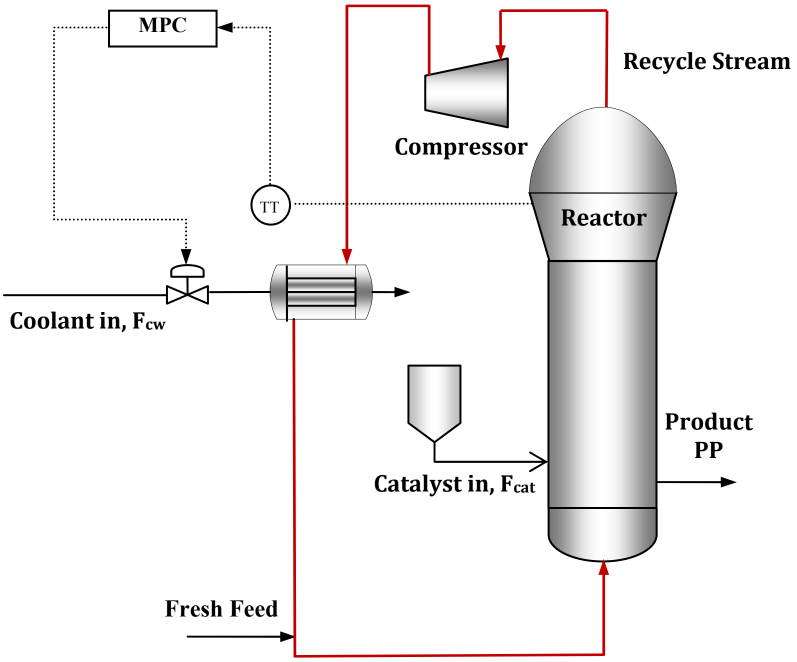

Fig. 1: Simplified schematic of the MPC design on the gas phase propylene polymerization fluidized bed reactor.

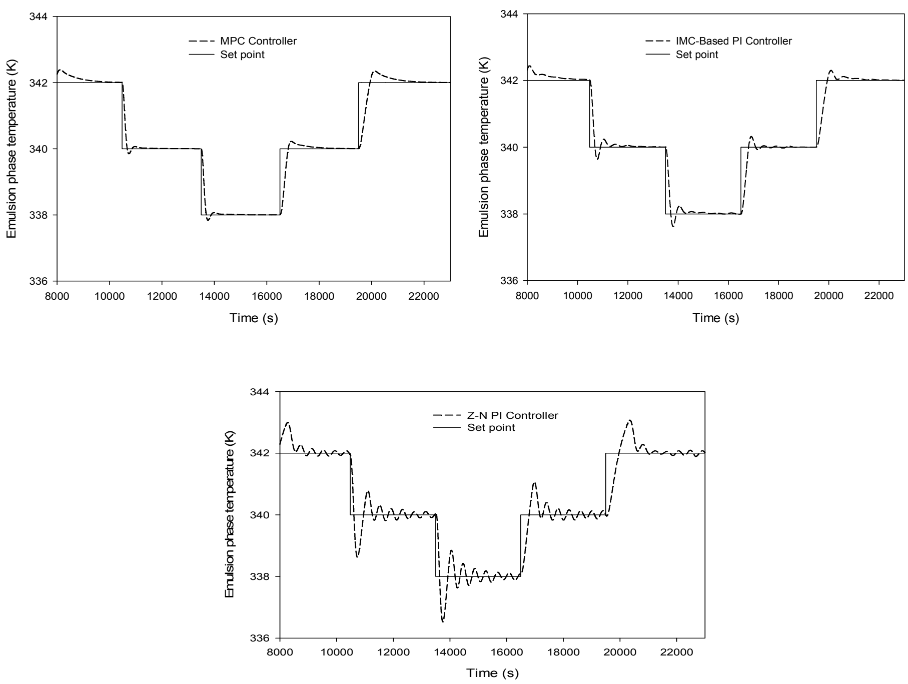

Fig. 2: Comparison of the performance between the MPC, IMC-Based PI controller (K_c = -18.5345, τ_I = 858.0787, τ_D = 0), and the Z-N PI controller (K_c = -33.3620, τ_I = 266.4696, τ_D = 0) in tracking series of setpoint changes in the emulsion phase temperature (T_e) (U_0=0.45m/s, F_{cat}=0.0003kg/s).

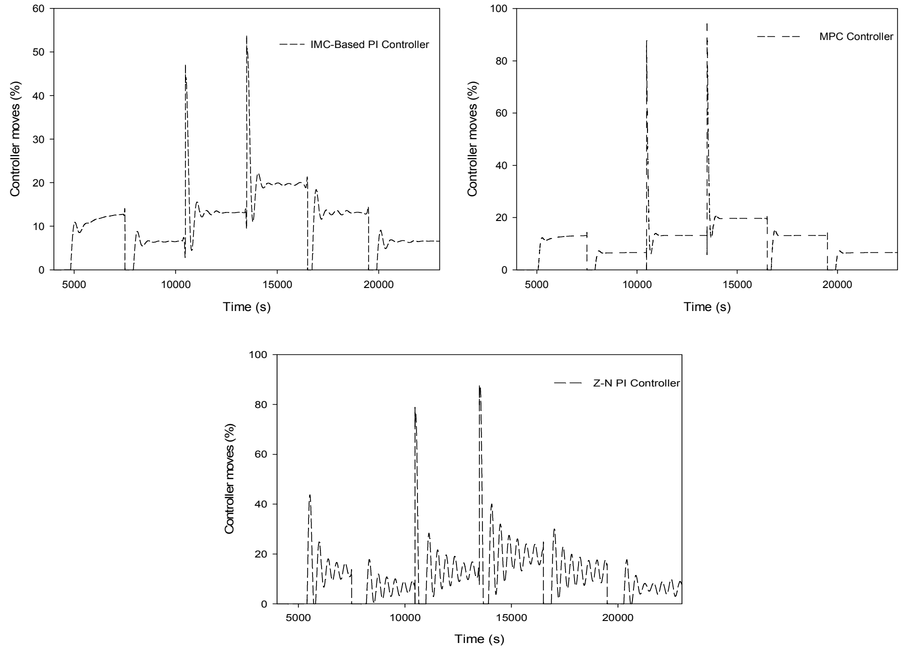

Fig. 3: Comparison of the corresponding controller moves between the MPC, IMC-Based PI controller, and the Z-N PI controller for the emulsion phase temperature.

Nomenclature

H_{be}	bubble to emulsion heat transfer coefficient, (W/m^3.K)
K_{be}	bubble to emulsion mass transfer coefficient, (s^{-1})
$[M_i]$	concentration of component *i* in the reactor (kmol/m^3)
R_p	production rate (kg/s)
R_i	instantaneous rate of reaction for monomer *i* (kmol/s)
R_v	volumetric polymer phase outflow rate from the reactor (m^3/s)
U_0	superficial gas velocity (m/s)
U_b	bubble velocity (m/s)
U_e	emulsion gas velocity (m/s)
V_b	volume of the bubble phase
V_e	volume of the emulsion phase
V_{PFR}	volume of PFR
δ	volume fraction of bubbles in the bed
ε_b	void fraction of bubble for Geldart B particles
ε_e	void fraction of emulsion for Geldart B particles
ε_{mf}	void fraction of the bed at minimum fluidization

5. References

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