

Closed Loop Regulatory Control Strategies for a Fluidized Bed Reactor: An Industrial Case Study

Arjun Shenoy*, Chetan Bhat*, Madhukar Gundappa**, Gudi Ravindra***

*National Institute of Technology Karnataka, Surathkal - 575025, India.

Honeywell Technologies, Bangalore - 560226, India (e-mail: Madhukar.Gundappa@honeywell.com), *Dept. of Chemical Engineering, IIT Bombay, Mumbai - 400076, India.

Abstract: Polyethylene is a thermoplastic commodity heavily used in consumer products. Today's gas phase LLDPE (Linear Low Density Poly Ethylene) process employs a Fluidized Bed Reactor (FBR). Modeling, Control and Optimization of FBR has received renewed interests from both industry and academia in the last two decades. The FBR model exhibits complex non-linear dynamic behavior and multiple time scales that pose challenges to control and optimization studies. In this paper we discuss various potential control strategies to regulate the reactor conditions at their set-points. Simulation results are presented to highlight the advantages and disadvantages of different controller pairing along with the possible control strategies to operate the FBR at grade conditions and also during grade transitions. This preliminary study is a gateway to more rigorous analysis and plant validation to identify the best control strategy and to provide guidelines to the operator to operate the plant at optimal conditions.

1. INTRODUCTION

The first industrially practical polyethylene synthesis was discovered in 1933 by Fawcett and Gibson. Subsequent landmarks in polyethylene synthesis have revolved around the development of highly active and selective catalysts, and various processes that promote ethylene polymerization at relatively mild temperatures and pressures, resulting in significant reduction of the plant capital expenditure and energy consumption. Over sixty million tons of polyethylene is produced world wide every year.

Researchers have developed various models describing the polyolefin gas phase process (Chatzidoukas et al., 2003; Hatzantonis et al., 2000; McAuley et al., 1994 and Choi & Ray, 1985) taking into account the complex flow characteristics of gas and solids, the kinetics of heterogeneous polymerization and the various heat and mass transfer mechanisms. In recent years, control and optimization of these processes have gained importance and optimal control methods have been developed to satisfy the diverse product quality specifications required by the broad range of polyolefin applications.

Fluidized bed reactor exhibits highly complex nonlinear dynamics and interactions between the control loops. For process safety and operability, the reactor temperature (T) and pressure (P) as well as bed height (h) need to be maintained at specified operating points through regulatory PID control loops. The reactor temperature is controlled by directly removing heat from the reactor. The polymer product which is continuously discharged from the reactor is used as a manipulated variable (MV) to control bed height. Reactor pressure is controlled by manipulating either ethylene flow rate or nitrogen flow rate or purge flow rate.

As mentioned earlier, the MVs and the CVs for the FBR result in a strongly nonlinear system that exhibits a fairly high amount of interaction. There are also some degrees of freedom for the control of the MVs. Also, some of the MVs and CVs are also tightly coupled with the quality variables, viz. melt index and polymer density. Although there are fairly well established guidelines for the MV-CV pairing that are based both on the steady state characteristics as well as the dynamics, such measures generally tend to ignore the effect on the quality variables, especially if it is not directly measurable.

This paper seeks to analyze the above issues for the complex fluidized bed reactor that exhibits some of these characteristics. The fluidized bed reactor is mandated by frequent grade transitions and is also affected by disturbances while operating at a grade. In the presence of such external inputs, we examine the dynamic effects of the MVs on the quality variables and recommend pairings that promote the optimal operation of the reactor. Using a multi-loop control scheme, we demonstrate that a co-ordinated, dynamic pairing during different regions of operation is able to provide productivity-oriented closed loop control.

This paper is organized as follows: First the gas phase catalytic copolymerization process is described in section-2. In section-3 the kinetic mechanisms are briefly described, followed by mass, energy and energy balance descriptions in section-4. The MV-CV pairing results are presented through closed loop studies in section-5. Conclusions are drawn based on the results obtained in section-6. The appendix in section-7 contains the gain and time constant matrix for melt index and polymer density with respect to H₂C₂ ratio, nitrogen flow and purge flow.

2. PROCESS DESCRIPTION – GAS PHASE CATALYTIC COPOLYMERIZATION PROCESS

The gas-phase solid catalyzed polymerization process has long been recognized as one of the most efficient processes for producing polyolefins. The advantages of this gas phase process include moderate operating conditions, the absence of solvents, as well as the high catalyst activity. In the fluidized bed reactor (FBR), catalyst particles are continuously fed into the reactor and react with the incoming fluidizing reaction medium to produce a broad distribution of polymer particles. The incoming fluidizing medium includes monomers (ethylene and butene), hydrogen, nitrogen and various other components based on the type of olefin being produced. The polyolefin product is removed from the reactor at a point close to the bottom of the reactor. The recycle stream includes a heat exchanger for the removal of heat of polymerization. Industrial polyolefin FBR typically operate at temperatures of 75-110°C and pressures of 20-40 bar (Xie, McAuley, Hsu, & Bacon, 1994). The above described catalytic gas-phase olefin polymerization using a FBR has been modified and simulated in MATLAB. Instead of recycling the gas outlet, it is continuously purged. The heat removal mechanism is modelled as a single term that denotes the enthalpy removal from the reactor, instead of describing the same using a heat exchanger.

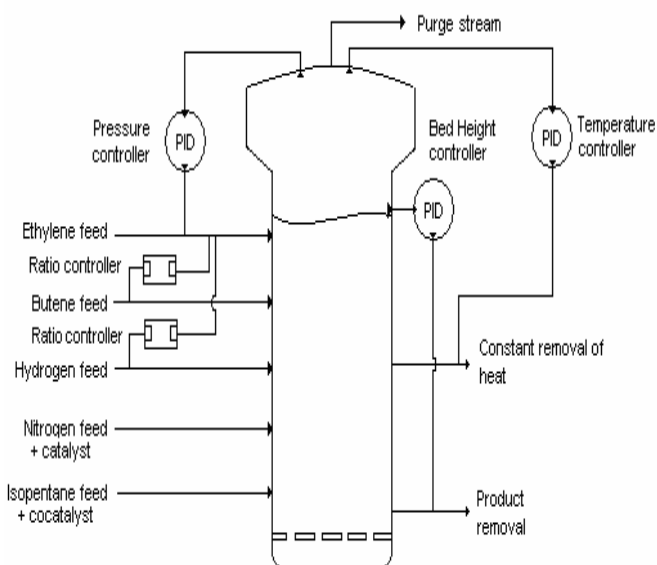
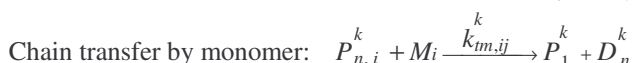
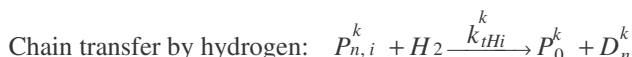
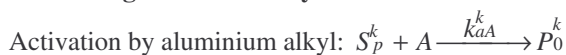


Fig.1. Model of fluidized bed reactor where ethylene flow rate is used to control reactor pressure

3. KINETICS

The kinetic mechanism comprises of a series of elementary reactions which include site activation, initiation, propagation, site deactivation and chain transfer reactions as shown below.

Kinetic mechanism of ethylene-1-butene copolymerization over a Ziegler-Natta catalyst



Net production-consumption rates of the various molecular species

Potential catalyst sites pf type 'k':

$$R_{Sp}^k = -k_{aA}^k [A][S_p^k]$$

Vacant catalyst sites pf type 'k':

$$R_{P_0}^k = -k_{dsp}^k [P_0^k] - \sum_{i=1}^{Nm} k_{0,i}^k [P_0^k][M_i] - R_{Sp}^k + (k_{tsp,T}^k + k_{tH,T}^k [H_2]) \lambda_0^k$$

Pseudo-kinetic rate constant for chain transfer reactions:

$$r_{i,T}^k = k_{tsp,T}^k + k_{tH,T}^k [H] + k_{tm,TT}^k [M_T]$$

Zero-order moment rate of 'live' polymer chains:

$$R_{\lambda_0}^k = \lambda_0^k [-k_{dsp}^k - r_{i,T}^k + [M_T] k_{tm,TT}^k] + k_{0,T}^k [P_0^k][M_T]$$

First-order moment rate of 'live' polymer chains:

$$R_{\lambda_1}^k = \lambda_1^k [-k_{dsp}^k - r_{i,T}^k] + \lambda_0^k [M_T] (k_{tm,TT}^k + k_{p,TT}^k) + k_{0,Y}^k [P_0^k][M_T]$$

Second-order moment rate of 'live' polymer chains:

$$R_{\lambda_2}^k = \lambda_2^k [-k_{dsp}^k - r_{i,T}^k] + k_{tm,TT}^k \lambda_0^k [M_T] + k_{p,TT}^k [M_T] (\lambda_0^k + 2\lambda_1^k) + k_{0,T}^k P_0^k [M_T]$$

Zero-order moment rate of 'dead' polymer chains:

$$R_{\mu_0}^k = \lambda_0^k [k_{dsp}^k + r_{i,T}^k]$$

First-order moment rate of 'dead' polymer chains:

$$R_{\mu_1}^k = \lambda_1^k [k_{dsp}^k + r_{i,T}^k]$$

Second-order moment rate of 'dead' polymer chains:

$$R_{\mu_2}^k = \lambda_2^k [k_{dsp}^k + r_{i,T}^k]$$

Monomer consumption rate:

$$R_{M_i}^k = [M_i] [k_{0,i}^k [P_0^k] + (k_{tm,Ti}^k + k_{p,Ti}^k) \lambda_0^k]$$

Hydrogen consumption rate:

$$R_{H_2}^k = k_{iH,T}^k \lambda_0^k [H_2]$$

Overall copolymerization rate:

$$R_P = \sum_{i=1}^{Nm} \sum_{k=1}^{Ns} (R_{M_i}^k MW_i)$$

4. BALANCE EQUATIONS

The FBR system is governed by a set of differential algebraic equations (DAE's). The pressure dynamics is relatively fast compared to other variables like temperature. Thus the pressure equation is represented by an algebraic equation whereas differential equations are used to represent the dynamics of the other variables. The mass balances of the components in the reactor are of the following general form:

In – Out + Generation = Accumulation

Where Generation = (-Consumption)

Ethylene

$$\begin{aligned} & F_{C_2} * MassFrnC_2 - F_{Poly} * MassFrnC_2_{Poly} \\ & - F_{Purge} * MassFrnC_2_{Purge} + RC2_{gen} * AmPolyVol \\ & = \frac{d(holdupMass_{C_2})}{dt} \end{aligned}$$

$$\begin{aligned} holdupMass_{C_2} = & TotLiqHoldupMass * MassFrnC_2_{Poly} \\ & + TotVapHoldupMass * MassFrnC_2_{Purge} \end{aligned}$$

Butene

$$\begin{aligned} & F_{C_4} * MassFrnC_4 - F_{Poly} * MassFrnC_4_{Poly} \\ & - F_{Purge} * MassFrnC_4_{Purge} + RC4_{gen} * AmPolyVol \\ & = \frac{d(holdupMass_{C_4})}{dt} \end{aligned}$$

$$\begin{aligned} holdupMass_{C_4} = & TotLiqHoldupMass * MassFrnC_4_{Poly} \\ & + TotVapHoldupMass * MassFrnC_4_{Purge} \end{aligned}$$

Hydrogen

$$\begin{aligned} & F_{H_2} * MassFrnH_2 - F_{Poly} * MassFrnH_2_{Poly} \\ & - F_{Purge} * MassFrnH_2_{Purge} + RH2_{gen} * AmPolyVol \\ & = \frac{d(holdupMass_{H_2})}{dt} \end{aligned}$$

$$\begin{aligned} holdupMass_{H_2} = & TotLiqHoldupMass * MassFrnH_2_{Poly} \\ & + TotVapHoldupMass * MassFrnH_2_{Purge} \end{aligned}$$

Poly-ethylene

$$\begin{aligned} & RPoly_{gen} * AmPolyVol - F_{Poly} * MassFrnPoly_{Poly} \\ & = \frac{d(holdupMass_{Poly})}{dt} \end{aligned}$$

$$\begin{aligned} holdupMass_{Poly} = & TotLiqHoldupMass * MassFrnPoly_{Poly} \\ & + TotVapHoldupMass * MassFrnPoly_{Purge} \end{aligned}$$

Nitrogen

$$\begin{aligned} & F_{N_2} * MassFrnN_2 - F_{Poly} * MassFrnN_2_{Poly} \\ & - F_{Purge} * MassFrnN_2_{Purge} = \frac{d(holdupMass_{N_2})}{dt} \end{aligned}$$

$$\begin{aligned} holdupMass_{N_2} = & TotLiqHoldupMass * MassFrnN_2_{Poly} \\ & + TotVapHoldupMass * MassFrnN_2_{Purge} \end{aligned}$$

Iso-pentane (IC5)

$$\begin{aligned} & F_{IC5} * MassFrnIC5 - F_{Poly} * MassFrnIC5_{Poly} \\ & - F_{Purge} * MassFrnIC5_{Purge} = \frac{d(holdupMass_{IC5})}{dt} \end{aligned}$$

$$\begin{aligned} holdupMass_{IC5} = & TotLiqHoldupMass * MassFrnIC5_{Poly} \\ & + TotVapHoldupMass * MassFrnIC5_{Purge} \end{aligned}$$

Energy Balance

$$\begin{aligned} & F_{IC5} * MassSpeEnthalpy_{IC5} + F_{C_2} * MassSpeEnthalpy_{C_2} \\ & + F_{C_4} * MassSpeEnthalpy_{C_4} + F_{H_2} * MassSpeEnthalpy_{H_2} \\ & + F_{N_2} * MassSpeEnthalpy_{N_2} - F_{Poly} * MassSpeEnthalpy_{Poly} \\ & - F_{Purge} * MassSpeEnthalpy_{Purge} - Rt_{22} * AmPolyVol \\ & + InputEnergyRate = \frac{d(holdupEnergy)}{dt} \end{aligned}$$

$$\begin{aligned} holdupEnergy = & TotLiqHoldupMass * MassSpeEnthalpy_{Poly} \\ & + TotVapHoldupMass * MassSpeEnthalpy_{Purge} \end{aligned}$$

PI Controllers implemented in State-Space form

Pressure Controller Equation

$$\Delta U_1 = K_{C_{Pr ess}} * \epsilon_{Pr ess} + \frac{K_{C_{Pr ess}}}{\tau_{i_{Pr ess}}} * \int \epsilon_{Pr ess}$$

$$F_{C_2} = U_1 = U_{1,ss} + \Delta U_1$$

Level Controller Equation

$$\Delta U_4 = K_{C_{Level}} * \epsilon_{Level} + \frac{K_{C_{Level}}}{\tau_{i_{Level}}} * \int \epsilon_{Level}$$

$$F_{Poly} = U_4 = U_{4,SS} + \Delta U_4$$

Temperature Controller Equation

$$\Delta U_{10} = Kc_{Temp} * \varepsilon_{Temp} + \frac{Kc_{Temp}}{\tau_{Temp}} * \int \varepsilon_{Temp}$$

$$InputEnergyRate = U_{10} = U_{10,SS} + \Delta U_{10}$$

Entity Balance

There are totally 18 pseudo entities defined for this system for which the mass balance equation has been written in the form: In – Out + Generation = Accumulation.

The first 16 Entities corresponds to Potential Catalyst Active sites, Vacant Catalyst Active sites, Live Polymer Moments and Dead Polymer Moments of various orders (0th, 1st & 2nd) based on statistics.

For each of the pseudo entity “i” (i = 1:16)

$$Rt_i * AmPolyVol - F_{Poly} * MassSpeVol_{poly} * EntityConc_i = \frac{d(holdupEntity_i)}{dt}$$

where, $holdupEntity_i = AmPolyVol * x_i$

The last 2 Entities are defined for cumulative co-polymer composition.

The balance equation for Phi1 - cumulative co-polymer composition with respect to Monomer -1 (i = 17)

$$Rt_{23} * AmPolyVol - F_{Poly} * MassFrnPoly_{poly} * EntityConc_{17} = \frac{d(holdupEntity_{17})}{dt}$$

where,

$$holdupEntity_{17} = \frac{holdupMass_4 * EntityConc_{17} * AmPolyVol}{TotalVol}$$

The balance equation for Phi2 - cumulative co-polymer composition with respect to Monomer -2 (i = 18)

$$Rt_{24} * AmPolyVol - F_{Poly} * MassFrnPol_{y_{poly}} * EntityConc_{18} = \frac{d(holdupEntity_{18})}{dt}$$

where,

$$holdupEntity_{18} = \frac{holdupMass_4 * EntityConc_{18} * AmPolyVol}{TotalVol}$$

$$EntityConc_{17} = 1 - EntityConc_{18}$$

Quality Variables

The Melt Index is governed by the following correlation,

$$MI = aM_w^b$$

Similarly for Polymer density the correlation is,
 $\rho = C_0 + C_1 \exp(-\phi_2 / C_2)$

Number average molecular weight and Weight average molecular weight are given by these correlations,

$$M_n = \frac{MW \sum_{k=1}^{N_s} (\lambda_1^k + \mu_1^k)}{\sum_{k=1}^{N_s} (\lambda_0^k + \mu_0^k)} \quad \& \quad M_w = \frac{MW \sum_{k=1}^{N_s} (\lambda_2^k + \mu_2^k)}{\sum_{k=1}^{N_s} (\lambda_1^k + \mu_1^k)}$$

The average molecular weight of the copolymer chain is,

$$\overline{MW} = \sum_{i=1}^{Nm} (\phi_i MW_i)$$

Polymer Dispersivity index is given by

$$PD = M_w / M_n$$

5. CASE STUDY

The following case study highlights the various benefits achieved by choosing a particular scheme to control pressure. Fig.1 represents a fluidized bed reactor along with input feeds and ratio controllers. The three PID control loops are – The temperature in the reactor is controlled using a single term to remove heat from the reactor, the bed height is controlled by the polymer withdrawal rate of the reactor and the pressure in the reactor is controlled by ethylene flow rate. Fig.2 also represents a FBR, but with a different control strategy for pressure. The reactor pressure is controlled using nitrogen flow rate and for bed height and temperature the control configuration remains same.

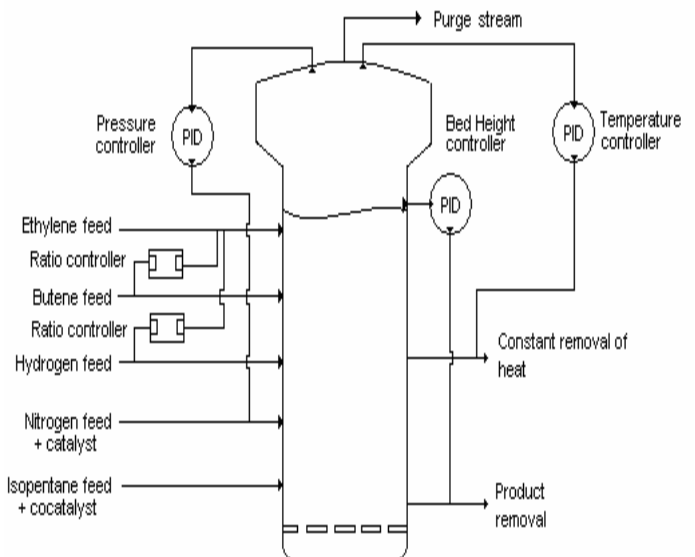


Fig.2. Model of fluidized bed reactor where nitrogen flow rate is used to control reactor pressure

Operation at a Grade:

As described in Fig.1 and Fig.2 the FBR employs two ratio controllers apart from the 3 regulatory PID control loops. The first ratio controller maintains the ratio of hydrogen flow to ethylene flow (H2C2 ratio). The second ratio controller fixes the ratio of butene flow to ethylene flow (C4C2 ratio). Towards the evaluation of the 2 control strategies, we first analyze the effect of a positive step change of 10% in the H2C2 ratio.

This step change increases the hydrogen flow rate and hence causes an increase in reactor pressure. In the case where ethylene flow rate is the pressure control related MV, the ethylene flow rate is decreased to bring pressure back to its set point. In order to maintain the H2C2 ratio, this action in the ethylene flow rate necessitates a decrease in the hydrogen flow rate; also, to maintain C4C2 ratio, the butene flow rate is also decreased. Until equilibrium is reached and the pressure is brought to its set-point the various flows (hydrogen, ethylene and butene) keep changing. Due to the coupling of ethylene flow rate with PID controller as well as ratio controller, pressure deviates more from its set-point and takes longer time (30000s ~ 8hrs) to return to the set-point.

On the other hand when nitrogen flow rate is the pressure control variable and a 10% step change is introduced in the H2C2 ratio. The same step change increases the hydrogen flow rate which in turn increases reactor pressure. Nitrogen flow rate is manipulated to minimize the pressure deviation from the set-point. The ethylene flow rate is not altered and hence the butene and hydrogen flow rates remain unaffected. In this case the equilibrium is attained faster and the pressure is brought back to the set-point very quickly.

Fig. 3a indicates the effect of 10% step change in H2C2 ratio on reactor temperature, pressure and height for the above discussed 2 control strategies. Fig. 3b shows the response of quality variables for the same 10% step change in H2C2 ratio for the 2 control strategies. Fig. 4 contains the responses of (quality variables) melt index, polymer density, production rate and poly dispersivity for a 10% step change introduced in purge flow rate. Both in Fig. 3b and Fig. 4 the solid line represents ethylene (C₂ Control) flow rate as MV and the dashed line represents nitrogen (N₂ Control) flow rate as MV. It is clearly evident that in both these figures the dashed line is not perturbed much from the step change in H2C2 ratio.

A tabulation of the gains and time constants for the above discussed cases has been shown in section-7, at the end of the paper. In the case where pressure is controlled by nitrogen flow rate, the table indicate low values of gain, i.e. little or no influence on the grade of the polymer (melt index, polymer density etc) for step changes in H2C2 ratio, C4C2 ratio and purge flow rate.

Thus employing nitrogen flow rate to control pressure provides a better and efficient way of regulating reactor conditions to their set points and help to operate the FBR optimally at a particular grade.

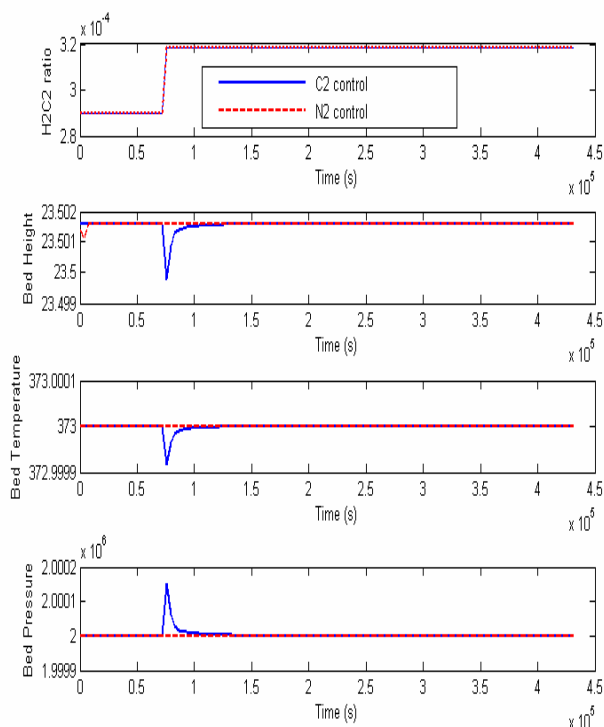


Fig.3a. Plot of Height, Temperature and Pressure for 10% positive step in H2C2 ratio

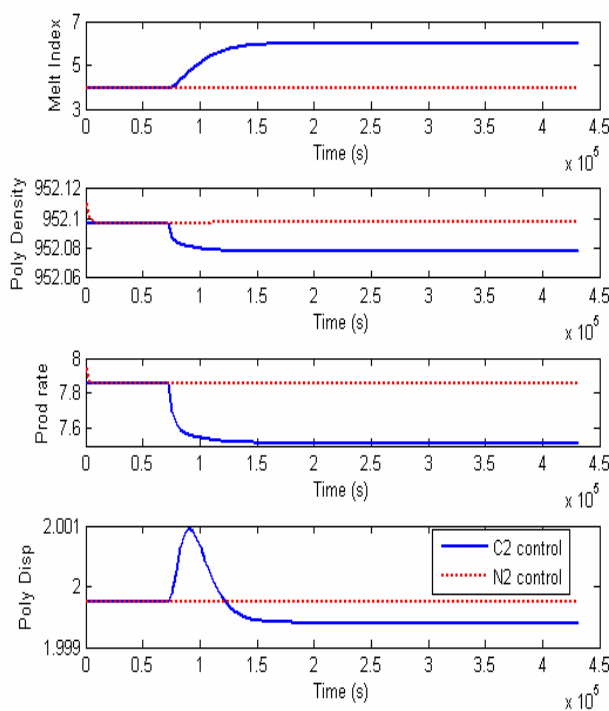


Fig.3b. Plot of Quality variables for 10% positive step in H2C2 ratio

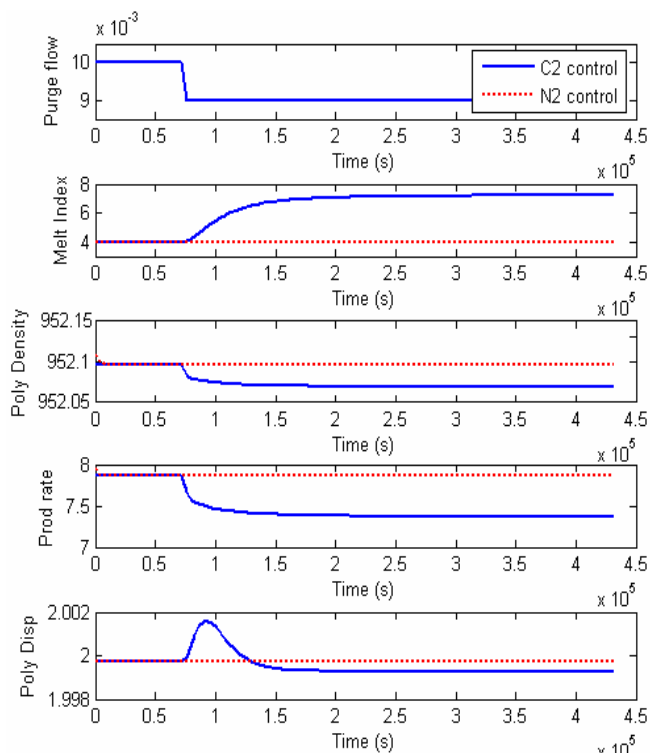


Fig.4. Plot of Quality variables for 10% negative step in purge flow rate

During Grade Transitions:

Controlling pressure with ethylene flow rate however does bring an important advantage, viz. a small step change in H2C2 ratio, C4C2 ratio, purge flow rate, nitrogen flow rate and iso-pentane flow rate causes significant changes in polymer quality variables like melt index and polymer density. Fig. 4 contains plots of quality variables for a 10% step change in purge flow rate for both control strategies. The solid line represents ethylene (C₂ Control) flow rate as MV and the dashed line represents nitrogen (N₂ Control) flow rate as MV. Similarly Fig. 5 shows responses of quality variables for a 10% step change in nitrogen flow rate when ethylene (C₂ Control) flow rate is used as a MV to control pressure.

In both these plots the change in quality variables are significant and represents a different grade of polymer produced. Thus effective grade transitions can be carried out by making relatively small step changes in any of these variables (H₂C₂ ratio, C₄C₂ ratio, purge flow rate, nitrogen flow rate and iso-pentane flow rate), when pressure is regulated by ethylene flow rate.

When nitrogen flow rate is manipulated to control reactor pressure except ethylene flow rate all other variables (H₂C₂ ratio, C₄C₂ ratio, purge flow rate, nitrogen flow rate and iso-pentane flow rate) have little influence on the quality variables. A plot of quality variables for 10% negative step change in ethylene flow rate for nitrogen flow rate as pressure control handle is shown in Fig. 6 where one can observe reasonable changes in quality variables. In the gain matrix tabulated in section-7, a relatively lower gain values can be observed for reactor pressure controlled by nitrogen

flow rate instead of ethylene flow rate. This substantiates the observation mentioned in the earlier paragraph.

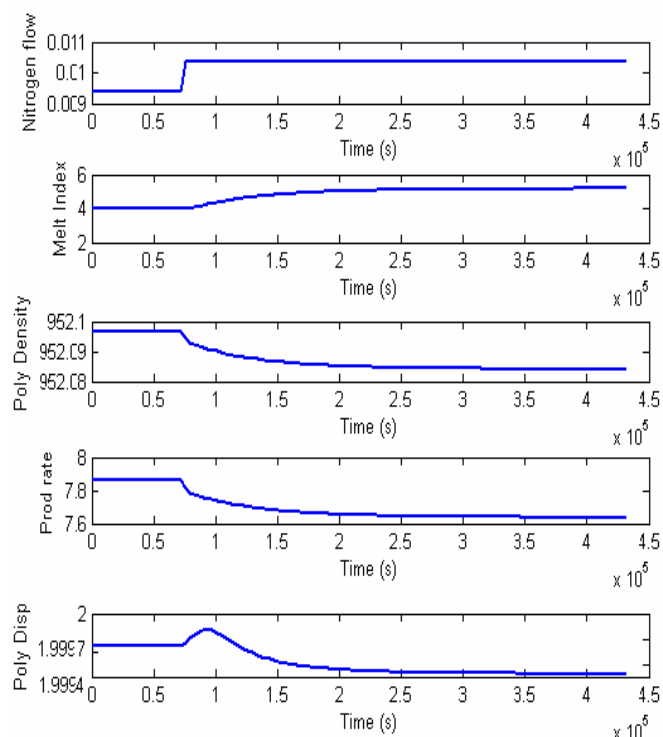


Fig.5. Plot of Quality variables for 10% positive step in nitrogen flow rate with ethylene flow rate as the pressure controlling manipulated variable

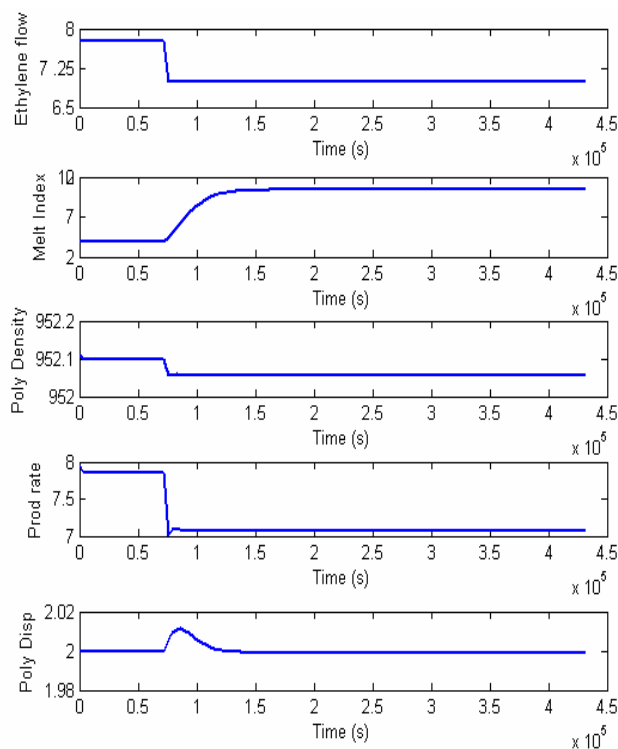


Fig.6. Plot of Quality variables for 10% negative step in ethylene flow rate with nitrogen flow as pressure controlling manipulated variable.

6. CONCLUSIONS

The paper discusses different control strategies for polymer industry to operate at a grade as well as during grade transition. The proposed control strategies were validated using a dynamic FBR model which exhibits complex non-linear dynamics posing a challenge for control and optimization studies. In most industries, monomer flow rate is used to control pressure. However, nitrogen flow rate too has been employed for the same purpose by some polymer plants. Each scenario offers its own set of advantages and disadvantages as presented earlier. This study highlight that use of nitrogen flow rate to control pressure is favourable for operating the plant at a grade. If one intends to use nitrogen flow rate to control reactor pressure then large changes in input flow rates are required to bring about significant changes in the quality variables, to achieve the necessary grade transition. During grade transition, pressure control by ethylene flow rate proves to be a good option. Similarly, at grade conditions, if one intends to use ethylene flow rate to control pressure then small changes in ratios or disturbances in flow rate can alter the quality variables significantly. As a result, dynamically adapting these control strategies in plant would help the operator to operate the plant at optimal conditions and reap maximum benefits.

7. TABULATION

Gain and time constant matrix for melt index and polymer density

Pressure controlled by ethylene flow rate		Melt Index	
		Gain	Time constant
+10% step	H2C2 ratio	69060	38000
+10% step	Nitrogen flow	1063.8	58000
-10% step	Purge flow	-3000	38000
		Polymer Density	
+10% step	H2C2 ratio	-690.6	18000
+10% step	Nitrogen flow	-13.829	43000
-10% step	Purge flow	30	8000

Pressure controlled by nitrogen flow rate		Melt Index	
		Gain	Time constant
+10% step	H2C2 ratio	276.24	48000
-10% step	Ethylene flow	-7.575	28000
-10% step	Purge flow	11	53000
		Polymer Density	
+10% step	H2C2 ratio	-86.32	38000
-10% step	Ethylene flow	0.057	3000
-10% step	Purge flow	2	48000

Nomenclature

F	Mass flow rate
MassFrn	Mass fraction of component
R	Rate
AmPolyVol	Amorphous polymer volume
MassSpeEnthalpy	Mass Specific enthalpy of the streams
Hc	Henry's Constant
RhoPoly	Polymer density
Kc	Controller gain
E	Error with respect to set-point
τ_i	Integral time constant
MassSpecVol _{Polv}	Polymer Mass specific Volume
Rt _i	Production Rate of components
ΔU	Deviation Variable of the manipulated variable
EntityConc	Concentration of the entities
TotalVol	Total volume of the reactor
holdupentity	Hold up of various entities
a = 1.0	Melt index coefficient
b = -3.5	Melt index coefficient
c ₀ = 900.01	Polymer density coefficient
c ₁ = 70	Polymer density coefficient
c ₂ = -0.04	Polymer density coefficient
λ	Live copolymer moment
μ	Dead copolymer moment
MW	Molecular weight
ϕ	Cumulative copolymer composition

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