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A review on modeling and control of olefin polymerization in fluidized-bed reactors

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Abstract: This is a detailed review on olefin polymerization models, and the most recent process control approaches used to control these nonlinear systems are presented. Great focus has been given to the various approaches of fluidized-bed reactor (FBR) modeling. Currently, there has yet to be a single model that blends these modeling aspects together into one single formulation. In this article, the classification of models works by looking at their assumption in considering the phases inside the system. Researchers have been unraveling vast information to narrate in detail the relations between various variables that can be found in FBRs. Although it is not difficult to understand about the basics of modeling polymer properties, a gap exists for future researchers to justify in detail the phenomena and reduce the gap between model predictions and the actual data. The various controlling approaches to control these FBRs have also been reviewed and categorized depending on the method they used to control significant parameters of this nonlinear system. The progress that can be expected in this field leads to the creation of more efficient reactors and minimizing waste.

Keywords: fluidization; fluidized-bed reactors; olefin polymerization; process control; process modeling.

1 Introduction

Olefin polymerization in gas-phase fluidized-bed reactors (FBRs) is known to be one of the most economic methods of manufacturing commodity polymers including polyethylene (PE), polypropylene (PP) and ethylene-propylene rubber (EPR). FBRs are extensively used in operations that involve solid catalysts. These catalysts are mainly heterogeneous Ziegler-Natta or metallocene in the case of polyolefins production. Unlike other processes that produce PE, polymerizing monomers in a gas-phase FBR has shown to have better heat removal and work at much lower temperatures and pressures and being needless of solvents, which contribute to its very broad use in industries (Alizadeh et al. 2004). Figure 1 sheds light on a typical fluidized-bed PE reactor process flow diagram. Under normal circumstances, FBRs for PE production are available in the industry work at a temperature between 75°C and 111°C and pressure range between 20 and 40 bar (Xie et al. 1994). The amount of superficial gas velocity (U_0) can be between 3 to 8 times of the minimum fluidization velocity. Various models have been recommended; hence, one can understand how a gas-phase ethylene polymerization works in real-life applications. Researchers have modeled these FBRs in the form of single-, two- or three-phase reactors (Choi and Harmon Ray 1985, McAuley et al. 1994, Fernandes and Lona 1999).

Several researchers have reviewed modeling or control of FBRs. Kiparissides (1996) classified the various polymers according to their molecular structure and briefly reviewed the various polymerization mechanisms and main mathematical approaches available at the time and presented a method for developing polymer reactor models. They also discussed the benefits of optimization and control of polymer reactors and future directions related to the development of computer-aided design, monitoring, optimization, and control for polymerization processes. Harmon Ray and Villa (2000) examined the key reaction parameters for a variety of polymers produced using several types of reactors and illustrated the nonlinearity which can arise in industrial reactors. Some of the effects of imperfect mixings were also showed. McKenna and Soares (2001) have reviewed some single

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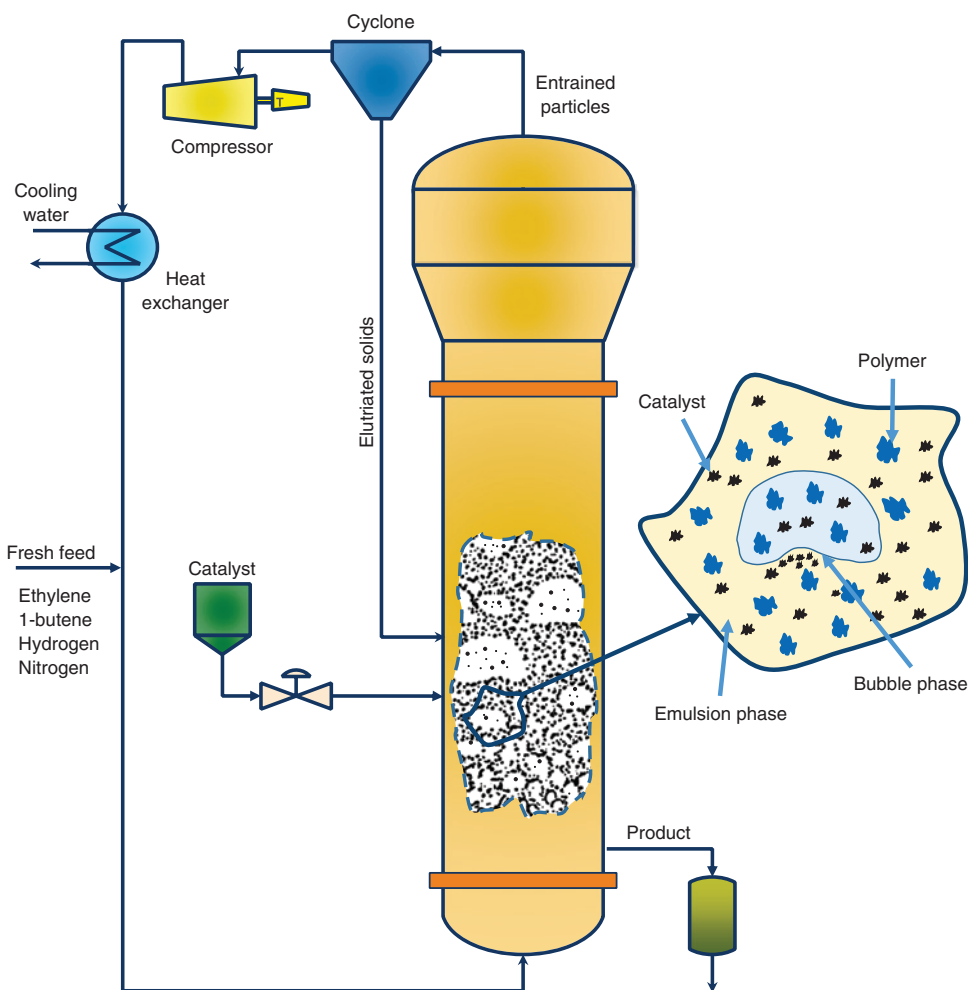


Figure 1: A typical fluidized bed polymerization reactor.

particle models for olefin polymerization that can be used to describe particle growth, polymerization rates, concentration and temperature radial profiles, polymer microstructure, and particle morphology. Mahecha-Botero et al. (2009) presented a comprehensive review of fluidized-bed catalytic reactor models. The authors analyzed and categorized 40 models depending on the characteristics of the conservation equations and their underlying assumptions. Since some approaches consider the reactor as a black box and try to model it using artificial intelligence, Noor et al. (2010) reviewed the use of neural networks in modeling and control of polymerization processes. Computational fluid dynamics (CFD) has also been used extensively in modeling polymerization in FBRs. Khan et al. (2014) reviewed the applications of these approach and the analyzed its capabilities and shortcomings. Recently, Philippssen et al. (2015) presented a general summary of the mathematical models used in modeling FBRs in all its process applications.

Process modeling and control are two fields that are fast-changing, proving that they are useful toward achieving sustainability and green processing. They help forecast the system performance without having to build pilot plants that can be expensive and wasteful. Furthermore, judging the strict environmental constraints we have today, advanced controllers are vital to guarantee that the operation is safe. As new research in modeling and control of FBRs to produce polyolefins came very rapidly, a summary of recent advances would be very timely. What distinguishes this article from other reviews is that it holds the most recent advancements in this area not only in modeling approaches, but in control studies as well. A number of papers have been published in this area during the last decade which need to be reviewed and analyzed. In this article, the basics of modeling and control of olefin polymerization in FBRs are discussed and the latest papers in this field are summarized categorically to give a clearer picture to future researchers.

2 Polymer classification and processes for olefin polymerization

2.1 Classification of polymers

Polymers are made up from many monomers which are connected. These monomers connect in a series of kinetic reactions called polymerization reactions. One way to classify polymers is by their kinetic mechanism and molecular structure. Polymers can be classified into several types by categorizing them based on the number of different structural entities present in a polymer chain:

- Homo-polymers which are the polymer chains that are made of many single repeating units linked together.
- Copolymers are those polymers which are made from two or more types of monomers.

Bi-polymers, ter-polymers, and multi-polymers are the varying types of copolymers made from two, three or more types of monomers, respectively. Polymerizations can be classified into different categories based on their chain growth mechanism:

- Step-growth polymerizations: Typically, step-growth polymerization advances by the reactions among two functional groups that are dissimilar to one another.
- Chain polymerizations: Chain polymerization or addition polymerization occurs when monomer molecules continue to be added to an active chain center in a very brief period until the polymer chains grow to the largest size. Chain polymerization can make its way through free-radical, anionic, cationic, coordination polymerization and group transfer mechanisms, which need a chain initiator that creates the main active sites centers (Kiparissides 1996).

2.2 Processes for olefin polymerization

Polymerization processes can be broken down into homogeneous and heterogeneous. While the reactions of the former occur in one phase only, that of the latter occurs when a different phase is present. In the latter case, chemical reactions, heat transfer, and inter-phase mass transfers are impending. Two scenarios prevail in the heterogeneous system. Polymerization may deal with several phases or insoluble polymer in the monomer phase. This kind of polymerization includes bulk, solution, precipitation, suspension, emulsion, solid-state, inter-facial polycondensation and solid catalyzed polymerization (Kiparissides 1996).

Heterogeneous catalysts are normally used for olefin polymerization processes, but some processes also make use of soluble catalysts. There are three types of catalysts used for olefin polymerization processes: Ziegler-Natta, Phillips, and Metallocene. Most Ziegler-Natta polymerization reactions depend on titanium catalyst systems. Ziegler-Natta catalysts consisting of a transition metal compound and an activator are, in general, variations that have the same theme, integrated with a wide range of electron donors and co-catalysts. The most popular catalysts are the Ziegler-Natta catalysts, used for PE and PP production. Phillips catalysts are made up of a chromium oxide supported on an amorphous material such as silica or silica/alumina (Soares 2001). Metallocene catalysts are based on the metallocene of group 4 transition metals with methylaluminoxane, and they show that olefin polymerization has high activity.

In solid catalyzed polymerization, the main methods adopted to produce polyolefin are: slurry-phase process, liquid solution process and gas-phase process, while continuous-stirred tank and loop reactors are the main reactors for slurry-phase olefin polymerization, and FBRs or vertical or horizontal stirred-bed reactors (VSBR and HSBR, respectively) for gas-phase processes. The existing processes for olefins polymerizations are normally different in the reactor media's physical state and the process unit's operating condition. The catalyst, desired range of products to be produced, economics and feedstock availability are the main parameters or, loosely speaking, determinants of the olefin polymerization process method. Olefin monomers can be polymerized to make up polyolefin. Ethylene or propylene may be homo-polymerized to create PE and PP, or co-polymerized together or with higher 1-olefins such as 1-butene, 1-pentene, 4-methyl-1-pentene, 1-hexene and others using one or more catalytic metal compounds, usually transition metals, together with a co-catalyst and/or a support for example, with alumina or silica. Olefin polymerization processes and their characteristics that are most common are summarized in Table 1 (Ray 1991).

2.2.1 Slurry-phase and solution processes

The two primary reactors for slurry-phase olefin polymerization are the loop reactor and continuous-stirred tanks. In a typical manner, slurry polymerization processes are carried out in a high-pressure continuous reactor. In the process, components such as one or more monomers, a diluent, and a catalyst system and other reactants are introduced to the polymerization reactor to create a reaction mixture, the solid olefin polymer particles and catalyst

Table 1: Most common olefin polymerization processes.

Process	Solution	Liquid slurry	Gas phase
Particle size (μm)	–	10–10 ⁴	10–10 ⁴
Commercial reactor type	CSTR	Batch, CSTR, loop	Fluidized bed, stirred bed
Kinetic mechanism	Coordination	Coordination	Coordination
Examples (including copolymers)	LDPE	HDPE, PP, EP	HDPE, LLDPE, PP, EP

particles are suspended and mixed well in a liquid diluent. Meanwhile, for solution polymerization processes, a monomer is dissolved in a nonreactive solvent having a catalyst where the solvent temperature is high enough for the dissolution of the polymer material. The heat freed by the reaction is absorbed by the solvent, thereby reducing the reaction rate. In both processes, concentrations of the monomers are high, and the liquid can well remove the polymerization heat from the polymer particles which is what is the most attractive about these processes. However, separation of the polymer from in the solution process is often an expensive operation (Zacca et al. 1996).

2.2.2 Gas-phase processes

Gas-phase olefin polymerization processes prepare an environment that is conducive for olefin polymerization. The remarkable characteristics of gas-phase olefin polymerization lie in the fact that as the system does not involve any liquid phase in the polymerization zone; the gas phase plays a role in the provision of monomers, the integration of polymer particles and removal of the heat of reaction. In this system, polymerization reaction occurs at the interface between the solid catalyst and the polymer matrix, and as can be seen, it is swollen with monomers throughout the polymerization stage. This process includes the VSBR, HSBR and FBR. In the gas-phase polymerization process, reactors must work closely to the dew point of the monomer mixture to achieve high monomer concentrations and high yields and the catalyst morphology must be very tightly controlled so that particle melting and agglomeration due to the heat transfer limitation of the gas can be prevented.

3 Modeling of fluidized-bed polymerization reactors

3.1 Introduction

The ability to justify how the reaction mechanism, transport phenomena, reactor type and reactor operating

conditions give the polymer quality of the final product is the major aim of polymerization processes (Kiparissides 1996). The polymer quality concerns with all the molecular structure properties and the polymer product's macroscopic morphological properties. Thus, it is only practical to classify these various phenomena that take place into the following models:

- chemical kinetics;
- reaction engineering;
- hydrodynamics;
- particle population balance.

The kinetics model is concerned with the reaction chemistry and reaction rate laws. The particle size with specific hydrodynamic correlations is given through the hydrodynamics model. The reaction engineering model defines the transient mass and energy balance equations, whereas the population balance model offers a steady-state particle population balance. All the chemical and physical phenomena seen in polymerization can be classified into these modeling levels (Ray 1991, Kiparissides 1996, McKenna and Soares 2001):

- kinetics modeling in microscale;
- physical modeling in mesoscale;
- dynamic modeling in macroscale.

In fact, multi-scale models are needed to fully discuss the nature of this process. To illustrate, Table 2 shows the set of reactions which takes place in copolymerization reactions. The reactions constants are available from various sources within literature based on the number of active sites that we want to consider in modeling the system. These sets of equations normally are solved using the method of moments. The resulting moments equations are given in Table 3.

3.2 Review of fluidization basics

In such reactors, gas or liquid is passed through solid particles at some velocities considered high enough to suspend the solid and makes it act like fluid. Fluidization has an expansive use in industries and the applications

Table 2: Reactions occurring in a copolymerization reaction (McAuley et al. 1990).

Description	Reaction
Formation reaction	$N^*(j) \xrightarrow{k_f(j)} N(0, j)$
Initiation reaction	$N(0, j) + M_i \xrightarrow{k_i(j)} N_i(1, j) \quad i = 1, 2, \dots$
Propagation	$N_i(r, j) + M_k \xrightarrow{k_{pk}(j)} N_k(r+1, j) \quad i = k = 1, 2, \dots$
Transfer to monomer	$N_i(r, j) + M_k \xrightarrow{k_{fm_k}(j)} N_k(1, j) + Q(r, j) \quad i = k = 1, 2, \dots$
Transfer to hydrogen	$N_i(r, j) + H_2 \xrightarrow{k_{fh}(j)} N_H(0, j) + Q(r, j) \quad i = 1, 2, \dots$
	$N_H(0, j) + M_i \xrightarrow{k_{hi}(j)} N_i(1, j) \quad i = 1, 2, \dots$
	$N_H(0, j) + AlEt_3 \xrightarrow{k_{h}(j)} N_i(1, j)$
Transfer to co-catalyst	$N_i(r, j) + AlEt_3 \xrightarrow{k_{fr}(j)} N_i(1, j) + Q(r, j) \quad i = 1, 2, \dots$
Spontaneous transfer	$N_i(r, j) \xrightarrow{k_{fs}(j)} N_H(0, j) + Q(r, j) \quad i = 1, 2, \dots$
Deactivation reactions	$N_i(r, j) \xrightarrow{k_{ds}(j)} N_d(0, j) + Q(r, j) \quad i = 1, 2, \dots$
	$N(0, j) \xrightarrow{k_{ds}(j)} N_d(j)$
	$N_H(0, j) \xrightarrow{k_{ds}(j)} N_d(j)$
Reactions with poisons	$N_i(r, j) + I_m \xrightarrow{k_{dl}(j)} N_{diH}(0, j) + Q(r, j) \quad i = 1, 2, \dots$
	$N_H(0, j) + I_m \xrightarrow{k_{dl}(j)} N_{diH}(0, j)$
	$N(0, j) + I_m \xrightarrow{k_{dl}(j)} N_{di}(0, j)$

of fluidization can be divided into physical and chemical operations. The FBR functions in diverse industrial applications because of the high contacting methods, uniform particle mixing, uniform temperature gradients and the ability to run reactor continuously. Various processes have successfully adopted this technology. This includes olefin polymerization, reforming and cracking of hydrocarbons, coal gasification and carbonization, and many others.

3.2.1 Flow regimes in fluidization

There are different behaviors noted for the fluidized beds in which the solid particles are fluidized because of the variety in the gas, solid and velocity properties. With a growth in the gas velocity in the minimum fluidization regime, the bed voidage will escalate marginally and the drag force conveyed by the rising gas equals the weight of the particles. Next, the bed will go into the gas fluidization state. Higher levels of gas velocity mean that bubbles will set in and a bubbling fluidized bed would be seen. The bubbles in a bubbling fluidized bed will propagate and coalesce when it rises while the velocity intensifies. In

Table 3: Moment equations that resulted from the equations in Table 2.

$$\begin{aligned} \frac{dY(0, j)}{dt} &= [M_T] \{ k_t(j)N(0, j) + k_{ht}(j)N_H(0, j) \} + k_{ht}(j)N_H(0, j)[AlEt_3] \\ &\quad - Y(0, j) \left\{ k_{fr}(j)[H_2] + k_{fs}(j) + k_{ds}(j) + k_{di}(j)[I_m] + \frac{R_v}{V_p} \right\} \\ \frac{dY(1, j)}{dt} &= [M_T] \{ k_t(j)N(0, j) + k_{ht}(j)N_H(0, j) \} \\ &\quad + k_{ht}(j)N_H(0, j)[AlEt_3] + [M_T]k_{prt}(j)Y(0, j) \\ &\quad + \{ Y(0, j) - Y(1, j) \} \{ k_{fm}(j)[M_T] + k_{fr}(j)[AlEt_3] \} \\ &\quad - Y(1, j) \left\{ k_{fr}(j)[H_2] + k_{fs}(j) + k_{ds}(j) + k_{di}(j)[I_m] + \frac{R_v}{V_p} \right\} \\ \frac{dY(2, j)}{dt} &= [M_T] \{ k_t(j)N(0, j) + k_{ht}(j)N_H(0, j) \} \\ &\quad + k_{ht}(j)N_H(0, j)[AlEt_3] + [M_T]k_{prt}(j) \{ 2Y(1, j) - Y(0, j) \} \\ &\quad + \{ Y(0, j) - Y(2, j) \} \{ k_{fm}(j)[M_T] + k_{fr}(j)[AlEt_3] \} \\ &\quad - Y(2, j) \left\{ k_{fr}(j)[H_2] + k_{fs}(j) + k_{ds}(j) + k_{di}(j)[I_m] + \frac{R_v}{V_p} \right\} \\ \frac{dX(n, j)}{dt} &= \{ k_{fm}(j)[M_T] + k_{fr}(j)[AlEt_3] + k_{fr}(j)[H_2] + k_{fs}(j) + k_{ds}(j) \\ &\quad + k_{di}(j)[I_m] \} \\ &\quad \{ Y(n, j) - N_r(1, j) \} - X(n, j) \frac{R_v}{V_p} \quad n = 0, 1, 2 \end{aligned}$$

the slugging bed, the height-to-diameter ratio (H/D) of the bed is high enough and the bubble size may become the same as the bed's diameter. The fluidization of particles will occur at a high enough gas flow rate in a turbulent bed, where the velocity will exceed the particles' terminal velocity. Instead of the bubbles, the upper surface of the bed vanishes and a turbulent motion of solid masses and voids of gas with different dimensions are seen. Pneumatic transport of solids occurs with higher amount of gas velocity, and the fluidized bed becomes an entrained bed in which dispersed, lean or dilute phase fluidized bed would be found.

3.2.2 Bubbling fluidized beds

Gas fluidized beds are differentiated by the bubbles formed at superficial gas velocities larger than minimum fluidization velocity. In this state, it appears that the bed is distributed into the emulsion phase and the bubble phase. The bubbles are very analogous to gas bubbles in liquid form, and they act similarly and merge while rising through the bed. The movement of particles in fluidized beds receives most influence from the rising bubbles passing through the bed. As the result, extreme

consideration is given to these bubbles and their properties. To compare the processes occurring inside an FBR, the fluidization bubbles, bubble formation, the way particles are transported and their path through the bed are not to be taken lightly.

3.3 Modeling approaches

The mixing conditions and the number of phases existing in the bed are the focal point of the literature in terms of modeling the operation of a catalytic olefin polymerization in FBRs. The many phases that carry their own chemical reactions and interphase heat and mass transfer exist in various heterogeneous polymerization systems, resulting in a comprehensive and realistic model that will account for all these complex gas and solid flows, mechanisms of mass and heat transfers and polymerization kinetics. Regarding the hydrodynamics, several methods were recommended in the literature to explain in detail the fluidized-bed polyolefin reactors.

McAuley et al. (1994) and Xie et al. (1994) introduced a well-mixed reactor as their attempt to describe fluidized-bed polyolefin reactors. They drew a comparison between this approach and simple two-phase models in steady state and conclusively said that the latter shows very little errors when it predicts the reactor temperature and monomer concentration. Choi and Harmon Ray (1985) considered the reactor to come in two phases of emulsion and bubble and they recommended the simple two-phase model. They rested their conclusion on the solid-free bubbles which shows that polymerization only takes place in the emulsion phase.

Fernandes and Lona (2001) pitched the idea of a three-phase heterogeneous model which considered emulsion, bubble and solid phases and believed that they work as a plug flow. Hatzantonis et al. (2000) broke the reactor further into several solid-free well-mixed compartments in series and considered that the emulsion and bubble phases are altogether mixed. Alizadeh et al. (2004) also embodied the reactor hydrodynamics using a tanks-in-series model. Harshe et al. (2004) further created an inclusive mathematical model based on the mixing cell framework to study the fluidized-bed PP reactors' momentary behavior. The authors also combined this model with a population balance model in steady state. This model could be the answer to multi-site and multi-monomer polymerization kinetics.

Ibrehem et al. (2009) put forth a four-phase model and suggested that an FBR can involve emulsion, bubble, solid and cloud phases, but the authors guessed that the

polymerization reactions only happen in the emulsion and solid phases. They also accounted for the effect of catalyst particle type and porosity on the reaction rate. Kiashemshaki et al. (2006) had reserved four parallel sections for the reactor. Each section has its emulsion phase and the mixed and the bubble phase as plug flow. The authors believed that the polymerization would occur in both phases.

Khare et al. (2004) and Luo et al. (2009) used software like Aspen Dynamic and Polymer Plus together with major basics of chemical engineering for the development of their model. Consideration was given to key issues such as selecting thermodynamic model and physical property, catalyst characterization, to name but a few. Khare et al. (2004) introduced a model for gas-phase PP polymerization in stirred-bed reactors applicable to both steady-state and dynamic gas phase while Luo et al. (2009) built a model for commercial bulk PP polymerization with Hypo Technology. An assumption is made by Khare et al. (2004) with respect to the existence of multiple catalyst active sites in Ziegler-Natta catalyst. Their model that has a set of thermodynamic and kinetic parameters predicts the polymer production rate, polydispersity index, and molecular weight. The authors highlighted the measures for the development and validation of the polymerization model by focusing on the thermodynamic and physical model selections, reactor model, catalyst characterization, and Ziegler-Natta polymerization kinetics.

The very intention of the reactor modeling and control problems is to reach acceptable heat removal and production rate from the reactor. The reactor model behavior is subjected to several process variables like monomer concentration, catalyst feed rate, feed gas temperature, superficial gas velocity and catalyst activity.

3.3.1 Hydrodynamics

FBRs have several issues. They, for starters, are non-ideal and challenging to elaborate due to complicated transport phenomena, flow patterns, and polymerization reactions. A number of studies have focused on several mixing models to model such non-ideality to characterize FBRs' behavior. Non-ideal FBR modeling would need the integration of transport phenomena, kinetics, and hydrodynamics equations. Choi and Harmon Ray (1985) put forth a two-phase model with constant bubble. The authors placed it on a plug-flow bubble phase and a fully mixed emulsion phase to find traits of the FBR dynamic behavior. McAuley et al. (1990) further guessed that there is an unlimited heat and mass transfer between the emulsion

and bubble phases and recommended a much simpler well-mixed model.

The traditional well-mixed and constant-bubble-size models presume solid-free bubbles ($\varepsilon_b = 1$) and that the fluidization of the emulsion phase is at the minimum ($\varepsilon_e = \varepsilon_{mf}$). This concept does not gauge the impact of the dynamic gas-solid distribution on the heat/mass transfer and reaction rate in the fluidized beds and has its restrictions when it comes to describing the low-velocity bubbling fluidization. Cui et al. (2000), nonetheless, have been able to prove theoretically and experimentally the presence of solid particles in the bubbles. They also proved that the emulsion phase may have more gas at higher gas velocities and it does not stay at minimum conditions of fluidization. Increasing the superficial gas velocity contributes to the better mixing of the two phases, making more amounts of gas to enter the emulsion phase and further leading to higher solid particles entering the bubbles.

Readers can refer to various works that have collected different hydrodynamic formulations from the literature (Shamiri et al. 2015, Abbasi et al. 2016).

3.3.2 The well-mixed model

McAuley et al. (1990, 1994) made a proper introduction of the fluidized bed approximated by a single-phase continuous stirred tank reactor (CSTR) in the well-mixed model. This assumption is believed valid for very high mass and heat transfer rates between phases (uniform monomer concentration and temperature throughout the bed) or small-size bubbles. The bubble phase does not function in the model and the bed voidage (ε_{bed}) contemplates on the entire gas volume fraction in the bed. The following is a set of assumptions that would work for the well-mixed model:

- The polymerization reactor is a single-phase (emulsion phase) well-mixed reactor because of high heat and the mass transfer rates between phases or possibly because bubbles are sufficiently small.
- Composition and temperature are the same throughout the bed.
- The emulsion phase stays at minimum fluidization state.

Dynamic mass and energy balances are obtainable for the system based on the above assumptions for hydrogen and monomers. The mole balance is given by:

$$(V\varepsilon_{mf})\frac{d[M_i]}{dt} = U_0A([M_i]_{in} - [M_i]) - R_v\varepsilon_{mf}[M_i] - (1 - \varepsilon_{mf})R_i.$$

The energy balance is expressed by:

$$\begin{aligned} & \left[\sum_{i=1}^m [M_i]C_{pi}V\varepsilon_{mf} + V(1 - \varepsilon_{mf})\rho_{pol}C_{p,pol} \right] \frac{dT}{dt} \\ & = U_0A \sum_{i=1}^m [M_i]C_{pi}(T_{in} - T_{ref}) \\ & - R_v \left[\sum_{i=1}^m [M_i]C_{pi}\varepsilon_{mf} + (1 - \varepsilon_{mf})\rho_{pol}C_{p,pol} \right] (T - T_{ref}) \\ & + (1 - \varepsilon_{mf})\Delta H_R R_p - U_0A \sum_{i=1}^m [M_i]C_{pi}(T - T_{ref}). \end{aligned}$$

In the energy balance equation, the monomer internal energy is considered insignificant. The conditions needed to address the model equation are as follows:

$$\begin{aligned} [M_i]_{t=0} &= [M_i]_{in} \\ T(t=0) &= T_{in}. \end{aligned}$$

For kinetics and hydrodynamics equations, one can take guidance from the literature for added information (McAuley et al. 1990, 1994, Hatzantonis et al. 2000).

3.3.3 The constant bubble size model

In this model, we consider the assumption made by Choi and Harmon Ray (1985) that the fluidized bed comes in two phases depending on the phase where polymerization happens (emulsion or bubble phase). In the constant bubble size model, it is safe to assume that the bubbles, at constant velocity, travel through the bed in plug flow where the spherical size is characterized as fixed and consistent. We also need to consider the fact that the emulsion phase is interchanging heat and mass with the bubble phase and the mixture comes in full mixture. To add, the mass and heat transfer coefficients are constant throughout the bed, and we are led to believe that the heat and mass transfer resistances between the solid polymer particles and the monomer gas in the emulsion phase are trivial (Floyd et al. 1986). The constant bubble size model however does not ignore these assumptions:

- The fluidized bed is made of the emulsion and bubble phases. The former is where the reactions would occur.
- The bubbles are in plug flow and the spherical size is the same among each other. Their velocity is also constant.
- It is believed that the emulsion phase is fixed at the minimum stage of fluidization, and that it the mixture

is perfect, exchanging mass and heat with the bubble phase at constant rates over the bed height.

- The gas and the solid polymer particles in the emulsion phase have negligible inter-phase heat and mass transfer resistances (Floyd et al. 1986).

It is through these assumptions that the steady-state mass and energy balances are derived. The mole balance for monomer and hydrogen can be expressed as

$$\begin{aligned} [\bar{M}_i]_b &= \frac{1}{H} \int_0^H [M_i]_b dh \\ &= [M_i]_e + ([M_i]_{e,(in)} - [M_i]_e) \frac{U_b}{K_{be} H} \left(1 - \exp\left(-\frac{K_{be} H}{U_b}\right) \right). \end{aligned}$$

The bubble-phase energy balance can be written as

$$\sum_{i=1}^m [M_i]_b C_{pi} \frac{dT_b}{dz} = \frac{H_{be}}{U_b} (T_b - T_e).$$

The dynamic molar balance for the i th monomer in the emulsion phase is expressed by

$$\begin{aligned} (V_e \varepsilon_{mf}) \frac{d[M_i]_e}{dt} &= U_e A_e \varepsilon_{mf} ([M_i]_{e,(in)} - [M_i]_e) + \frac{V_e \delta K_{be}}{(1-\delta)} ([\bar{M}_i]_b \\ &- [M_i]_e) - R_v \varepsilon_{mf} [M_i]_e - (1 - \varepsilon_{mf}) R_i. \end{aligned}$$

The dynamic energy balance for emulsion phase can be written as

$$\begin{aligned} &\left[\sum_{i=1}^m V_e \varepsilon_{mf} [M_i]_e C_{pi} + V_e (1 - \varepsilon_{mf}) \rho_{p01} C_{p,p01} \right] \\ &\frac{dT_e}{dt} = - \sum_{i=1}^m V_e \varepsilon_{mf} C_{pi} \frac{d[M_i]_e}{dt} (T_e - T_{ref}) \\ &+ U_e A_e \varepsilon_{mf} \sum_{i=1}^m [M_i]_{e,(in)} C_{pi} (T_{e,(in)} - T_{ref}) \\ &- U_e A_e \varepsilon_{mf} \sum_{i=1}^m [M_i]_e C_{pi} (T_e - T_{ref}) - \frac{V_e \delta H_{be}}{(1-\delta)} (T_e - \bar{T}_b) \\ &+ R_v \left((1 - \varepsilon_{mf}) \rho_{p01} C_{p,p01} + \varepsilon_{mf} \sum_{i=1}^m [M_i]_e C_{pi} \right) (T_e - T_{ref}) \\ &+ (1 - \varepsilon_{mf}) \Delta H_R R_p. \end{aligned}$$

The boundary and initial conditions for solving the model equations are as follows:

$$\begin{aligned} [M_i]_{b,z=0} &= [M_i]_{in} \\ T_b(z=0) &= T_{in} \\ [M_i]_{e,t=0} &= [M_i]_{in} \\ T_{e,t=0} &= T_{in}. \end{aligned}$$

To estimate the gas velocities for bubble phase and emulsion phases, the bubble phase and emulsion phases voidage, the bed bubble volume fraction, and heat and mass transfer coefficients for the constant bubble size mode, the correlations needed for that purpose can be found from diverse sources in the literature (Shamiri et al. 2012, 2015).

3.3.4 The bubble-growth model

In the bubble-growth model, the constant bubble size model was extended to account for the varying bubble size with respect to the bed's height (Hatzantonis et al. 2000). Spurred by the developments of Kato and Wen (1969), in this model, an assumption is that the bubble phase is divided into “ N ” well-mixed sections in series and the emulsion phase is mixed perfectly and at developing fluidization conditions ($\varepsilon_{bed} = \varepsilon_{mf}$). The bubble-phase sections' size is fixed to be equal to the bubble diameter at the equivalent bed height. The local mass and heat transfer coefficients between the emulsion and bubble phases, the bubble rise velocity, and the local bubble volume fraction are found by the bubble diameter and thus the equivalent bed height. This is because the bubble size has its minimum value at the gas distributor and it enlarges to its largest constant size while it moves through the bed.

This model does not weigh the heat and mass transfer restrictions between the solid particles and the surrounding gas in the emulsion phase. Nevertheless, these limitations can become something that should not be taken lightly for high rates of polymerization.

If the bubbles are solid-free (no reaction), we can write the molar balance for the i monomer in the n compartment:

$$\begin{aligned} [M_i]_{b,n} &= [1 + (K_{be,n} d_{b,n} / u_{b,n})^{-1}] \\ &\times \left\{ \frac{\delta_{b,n-1} u_{b,n-1}}{\delta_{b,n} u_{b,n}} [M_i]_{b,n-1} + \frac{K_{be,n} d_{b,n}}{u_{b,n}} [M_i]_e \right\}, \end{aligned}$$

where $d_{b,n}$ is the bubble size corresponding to the n compartment.

In effect, the energy balance for the n compartment can be written as

$$\begin{aligned} T_{b,n} &= \left(\sum_{i=1}^{N_m} [M_i]_{b,n} C_{pM_i} + \frac{H_{be,n} d_{b,n}}{u_{b,n}} \right)^{-1} \\ &\times \left\{ \frac{\delta_{b,n-1} u_{b,n-1}}{\delta_{b,n} u_{b,n}} \sum_{i=1}^{N_m} [M_i]_{b,n-1} C_{pM_i} (T_{b,n-1} - T_{ref}) \right. \\ &\left. + \sum_{i=1}^{N_m} [M_i]_{b,n} C_{pM_i} T_{ref} + \frac{H_{be,n} d_{b,n}}{u_{b,n}} T_e \right\}. \end{aligned}$$

The dynamic mass and energy equations can also be derived and this had been discussed by Hatzantonis et al. (2000).

3.3.5 Other mathematical approaches

Fernandes and Ferrareso Lona (2001) had contemplated on gas in bubble and emulsion phases plus solid polymer particles, all as plug-flow phases, to suggest on their three-phase heterogeneous model. Jafari et al. (2004) brought to comparison the performance of some available models of the time such as simple two-phase model and generalized bubbling/turbulent model. They summed up that the later model gives the most fitted results to experimental data. Luo et al. (2009) had worked further on a method to model the PP process based on Hypol Technology. The authors adopted the Polymer Plus and Aspen Dynamics to foresee process behavior and physical properties in the steady-state and dynamic modes. In something similar, Zheng et al. (2011) developed a steady-state and dynamic method to model the propylene process with the aid of the Spheripol Technology. Their kinetic model leaned on both single and multi-site catalyst and their molecular weight distribution results were fitted with the help of the actual gel permeation chromatography (GPC) data.

In the meantime, some researchers focused on particle size distribution studies in fluidized beds rather than kinetic or property estimation (Khang and Lee 1997, Immanuel et al. 2002, Ashrafi et al. 2008). That said, fluidization regimes have also been studied in vast literature. Different methods that can find the fluidization regimes in gas-solid FBRs have been applied on these reactors to study several hydrodynamic aspects (Makkawi and Wright 2002, Sederman et al. 2007, Tamadondar et al. 2012). Alizadeh et al. (2004) put forth a pseudo-homogeneous tanks-in-series model to guess on the behavior of industrial-scale gas-phase PE production reactor. Kiashemshaki et al. (2006) were inspired by this model and they suggested a two-phase model to describe the fluidized-bed ethylene polymerization reactor. Their model was a dynamic model except in terms of the computation of the temperature and co-monomer concentrations.

Shamiri et al. (2010, 2011, 2013, 2014) analyzed different dynamic and non-dynamic modeling and control approaches for gas phase homopolymerization or copolymerization of olefin in FBRs.

Abbasi et al. (2016) proposed a dynamic two-phase ethylene copolymerization model which considers particle carryover in the model. Their model showed to be a more realistic model where the accuracy was shown by

confirming the results with industrial data. The main equations in the developed model are as follows:

Mass balance for emulsion phase:

$$\frac{d}{dt}(V_e \varepsilon_e [M_i]_e) = [M_i]_{e,(in)} U_e A_e - [M_i]_e U_e A_e - R_v \varepsilon_e [M_i]_e + K_{be} ([M_i]_b - [M_i]_e) V_e \left(\frac{\delta}{1-\delta} \right) - (1-\varepsilon_e) R_{ie} - \frac{K_e V_e \varepsilon_e A_e [M_i]_e}{W_e}$$

Mass balance for bubble phase:

$$\frac{d}{dt}(V_b \varepsilon_b [M_i]_b) = [M_i]_{b,(in)} U_b A_b - [M_i]_b U_b A_b - R_v \varepsilon_b [M_i]_b - K_{be} ([M_i]_b - [M_i]_e) V_b - (1-\varepsilon_b) \frac{A_b}{V_{PFR}} \int R_{ib} dz - \frac{K_e V_e \varepsilon_e A_e [M_i]_e}{W_e}$$

Energy balance for emulsion phase:

$$\begin{aligned} & U_e A_e (T_{e,(in)} - T_{ref}) \sum_{i=1}^m [M_i]_{e,(in)} C_{pi} - U_e A_e (T_e - T_{ref}) \sum_{i=1}^m [M_i]_e C_{pi} \\ & - R_v (T_e - T_{ref}) \left[\sum_{i=1}^m \varepsilon_e C_{pi} [M_i]_e + (1-\varepsilon_b) \rho_{pol} C_{p,pol} \right] \\ & + (1-\varepsilon_e) R_{pe} \Delta H_R - H_{be} V_e \left(\frac{\delta}{1-\delta} \right) (T_e - T_b) \\ & - V_e \varepsilon_e (T_e - T_{ref}) \sum_{i=1}^m C_{pi} \frac{d}{dt} ([M_i]_e) \\ & - \frac{K_e A_e}{W_e} (T_e - T_{ref}) \left(\sum_{i=1}^m \varepsilon_e C_{pi} [M_i]_e + (1-\varepsilon_b) \rho_{pol} C_{p,pol} \right) \\ & = V_e \left(\varepsilon_e \sum_{i=1}^m C_{pi} [M_i]_e + (1-\varepsilon_e) \rho_{pol} C_{p,pol} \right) \frac{d}{dt} (T_e - T_{ref}). \end{aligned}$$

Energy balance for bubble phase:

$$\begin{aligned} & U_b A_b (T_{b,(in)} - T_{ref}) \sum_{i=1}^m [M_i]_{b,(in)} C_{pi} - U_b A_b (T_b - T_{ref}) \sum_{i=1}^m [M_i]_b C_{pi} \\ & - R_v (T_b - T_{ref}) \left(\sum_{i=1}^m \varepsilon_b C_{pi} [M_i]_b + (1-\varepsilon_e) \rho_{pol} C_{p,pol} \right) \\ & + (1-\varepsilon_b) \frac{A_b \Delta H_R}{V_{PFR}} \int R_{pb} dz + H_{be} V_b (T_e - T_b) \\ & - V_b \varepsilon_b (T_b - T_{ref}) \sum_{i=1}^m C_{pi} \frac{d}{dt} ([M_i]_b) \\ & - \frac{K_b A_b}{W_b} (T_b - T_{ref}) \left(\sum_{i=1}^m \varepsilon_b C_{pi} [M_i]_b + (1-\varepsilon_b) \rho_{pol} C_{p,pol} \right) \\ & = \left(V_b \left(\varepsilon_b \sum_{i=1}^m C_{pi} [M_i]_b + (1-\varepsilon_b) \rho_{pol} C_{p,pol} \right) \right) \frac{d}{dt} (T_b - T_{ref}). \end{aligned}$$

Solid elutriation constants gathered from the literature are obtained from Rhodes (2008) and are as follows:

$$K_e = 23.7 \rho_g U_0 \frac{A}{W_e} \exp\left(\frac{-5.4U_t}{U_0}\right)$$

$$K_b = 23.7 \rho_g U_0 \frac{A}{W_b} \exp\left(\frac{-5.4U_t}{U_0}\right)$$

$$W_e = AH(1 - \varepsilon_e) \rho_{pol}$$

$$W_b = AH(1 - \varepsilon_b) \rho_{pol}$$

$$U_t = U_t^* [\mu \rho_g^{-2} (\rho_{pol} - \rho_g) g]^{0.33}$$

$$U_t^* = \left[18(d_p^*)^{-2} + (2.335 - 1.744\phi_s)(d_p^*)^{-0.5} \right]^{-1}$$

$$d_p^* = d_p [\mu^{-2} \rho_g (\rho_{pol} - \rho_g) g]^{0.33} \quad \text{for } 0.5 < \phi_s \leq 1.$$

These equations can be solved using the following initial conditions:

$$\begin{aligned} [M_i]_{b,t=0} &= [M_i]_{in} \\ T_{b,t=0} &= T_{in} \\ [M_i]_{e,t=0} &= [M_i]_{in} \\ T_{e,t=0} &= T_{in}. \end{aligned}$$

3.3.6 Condensed mode cooling modeling

Injection of a quench liquid into the reactor is an accepted heat removal method in olefin polymerization FBRs. Although in PE the “quench” liquid is usually an inert alkane (often referred to as an induced condensing agent, ICA), but it is the liquefied monomer in the case of PP. Introduction of propylene copolymers and heavier monomers such as hexane or butene gives the possibility of condensing these monomers and inserting them in liquid form in a gas-phase process.

To find out the effect of liquefied co-monomer injection on the reaction rate, the influence of these components on solubility, transport, and other “physical” processes on one hand and their impact on the reaction on other hand need to be found. As an example, the instantaneous rate of ethylene polymerization increased in the presence of an ICA in the study which was done by Namkajorn et al. (2014). The authors related this to the enhancement of the local concentration of ethylene due to the heavier hydrocarbon at the catalyst active sites. They also examined different isomers of pentane and hexane. Alizadeh et al. (2015) concluded that the complex effects were the result of the alkane replacement with a similar alkene. Based on thermodynamics, both alkanes and alkenes increase the rate of ethylene polymerization via the cosolubility effect, but considering that the alkenes are also co-monomers, they have a direct influence on the

reaction rate. Moreover, they boost the polymerization rate (called co-monomer effect) at low concentrations; nonetheless, they decrease the reaction rate at higher concentrations despite the cosolubility effect. Nevertheless, the ethylene’s concentration is higher in the existence of a heavier compound rather than ethylene alone.

Although condensed mode cooling is common in industries, only a few studies have focused on modeling this approach to analyze its effect on the hydrodynamics, transport phenomena and polymerization reactions, and there is still a need for models that can accurately account for the entire process considering the condensed mode cooling practice (Jiang et al. 1997, Yang et al. 2002, Mirzaei et al. 2007, Zhou et al. 2013, Alizadeh et al. 2017, Pan et al. 2017).

3.3.7 CFD approaches

CFD is a category of fluid mechanics that uses numerical analysis and data structures to solve and analyze problems that involve flow of fluids (Schneiderbauer et al. 2015). Researchers use computers to do the essential calculations to simulate the fluid and surface interactions defined by boundary conditions. With high-performance computations, better solutions can be completed in less time.

CFD model development is a progressive research area for picturing fundamental phenomena without executing real-time experiments. It can be used to solve momentum and conservation equations in multi-phase flows. For polymerization reactors, an added benefit of CFD is that it can offer information on turbulent zones which is very important because the reactants are mostly inserted within these areas where the reaction yield is superior (Dompazis et al. 2008).

Two methods of CFD models, i.e. Eulerian and Lagrangian, are used to define gas-solid fluidized reactors. Both phases (gas and solid) are counted as continuum (fluid) in the Eulerian model, and momentum and continuity equations are dealt with for both phases. The Lagrangian model, meanwhile, solves Newton’s equations of motion for each particle and particle-particle collisions and applied forces on the particle are considered. The Eulerian-Lagrangian method, which is also known as discrete element method or discrete particle model, studies the fluid as a continuum and considers solids to be dispersed phase (Schneiderbauer et al. 2016). The discrete element method models the continuous phase and particle trajectories using the Eulerian and Lagrangian frameworks, respectively. The continuous phase

can be modeled by averaging its properties over an extensive variety of these paths or trajectories. However, to obtain an average of all quantities in a moment, it is recommended that a plentiful of particle trajectories be simulated. Gas and emulsion phases are presumed to be continuous in the Eulerian-Eulerian approach while they are considered completely interpenetrating in all control volumes.

Particle size distribution is a key factor in CFD studies of this system. To define the particle size distribution in a multi-phase flow, the population balance equation (PBE), continuity, momentum, and energy equations need to be solved simultaneously. Researchers have used a combination of PBE solving methods with CFD to discuss particle size distributions and flow patterns within polymerization FBRs (Yan et al. 2012, Akbari et al. 2015a,c, Che et al. 2015a, 2016).

Several researchers also performed advanced investigations on the influence of operating conditions and geometry of the reactor, such as distributor type, size of solid particles, gas velocity and operating pressure on the hydrodynamics of the reactor, for accurate scale-up and design of reactors (Akbari et al. 2014, 2015b; Che et al. 2015b) and some used the results of CFD for further analysis using signal or image processing to study fluid structures during the process (Aramesh et al. 2016).

For more details on CFD modeling of olefin polymerization in FBRs, readers may refer to a comprehensive review by Khan et al. (2014).

4 Control of olefin polymerization in FBRs

Modeling and controlling polyolefins polymerization in FBRs are difficult to perform because of its highly nonlinear behavior. This is the direct impact of having complex flow characteristics of gas and solids, various mass and heat transfer mechanisms, very complex reaction mechanisms and the interaction that takes place between process control loops. Bequette (1991) reviewed the nonlinear control system techniques extensively. He regarded the techniques promising since they can address common problems associated with chemical processes. While the progress in nonlinear control is encouraging, several goals for future research in nonlinear control of chemical processes were explained thoroughly. Several research articles were published in the past years on the control of olefin polymerization processes. This literature

using various algorithm types as control strategy is shown in a summary in Table 4. Figure 2 illustrates some of the control loop structures which are used to control different polymer and reactor properties such as temperature, production rate and MFI.

4.1 Conventional control

Despite many sophisticated control theories and techniques that have been devised in the last decades, conventional controllers especially proportional integral (PI) controllers are still the most implemented in real-world cases. In fact, due to their simple structure, PI controllers are easy to tune, and their use is well understood by a clear majority of industrial practitioners and automatic control designers.

Choi and Harmon Ray (1985) used PI controller to control the reactor temperature in an olefin homopolymerization FBR by manipulating feed gas temperature. The authors concluded that reactor temperature can be controlled if there is sufficient heat removal capacity in the system. The authors later studied the PID control of temperature, bed level, and pressure in a solid catalyzed gas phase CSTR (Choi and Ray 1988).

The closed-loop simulations by Ali and Abasaeed (1998) using a PI controller on an industrial model of gas-phase ethylene polymerization reactor showed that a single control loop with the feed temperature as the manipulated variable is not sufficient to stabilize the reactor temperature against external disturbances. Another disadvantage of the PI controller was the need to retune the controller parameters from case to case. The authors found that a multi-loop control scheme must be used to improve the feedback response and they did so using an NLMPC controller. The authors, in another study, tried to overcome the PI shortcomings in SISO and MIMO cases by on-line adaptive tuning and finding proper control structures (Ali and Abasaeed 1999).

Ghasem (2000) also studied the dynamics of a UNIPOL[®] process using their model a PI controller. In the same year, Sato et al. (2000) developed a model based on the work of McAuley et al. (1990) and applied a two-by-two MIMO PI control structure to control MFI and density by changing feed hydrogen and butene flow rates.

Salau et al. (2008) studied the dynamic behavior of this process using their proposed model and utilized PID controller designed via optimization in the frequency domain to control the reactor temperature by manipulating the cold-water valve position.

Table 4: Summary of control studies in olefin polymerization.

Reactor type	Model	Controller	Control variables	References
FBR-PE and PP	Two-phase	PI	Temperature	(Choi and Harmon Ray 1985)
CSTR-PP	Well mixed	PID	Temperature, bed level, pressure	(Choi and Ray 1988)
FBR-PE	Well mixed	IMC	MFI, density	(McAuley and Macgregor 1993)
FBR-PE	Well mixed	ETC	Temperature	(Dadebo et al. 1997)
FBR-PE	Two-phase	PI, NMPC	Temperature, monomer concentration	(Ali and Abasaheed 1998)
FBR-PE	Two-phase	PI	Temperature, monomer concentration	(Ali and Abasaheed 1999)
slurry-PE	Well mixed	NMPC	Amount of unreacted monomer, MFI	(Bolsoni et al. 2000)
FBR-PE	Two-phase	PI	Temperature	(Ghasem 2000)
FBR-PE	Well mixed	PID, Optimal servo system	Density and MFI	(Sato et al. 2000)
FBR-PE	Two-phase	MPC	Temperature, MFI, production rate and density	(Brempt et al. 2001)
CSTR-PE	Well mixed	NNMPC	Production rate, partial pressures of the gas phase compositions	(Seki et al. 2001)
FBR-PE	Well mixed	LMPC, NMPC, PI	Bleed flow and pressure, feed flow rates, temperature	(Ali et al. 2003)
FBR-PE	Well mixed	PI	Bed level, production rate, temperature, MFI, pressure, density	(Chatzidoukas et al. 2003)
FBR-PE	Well mixed	fuzzy logic	Temperature	(Ghasem 2006)
HSR-PP	Well mixed	GMC	MFI, monomer conversion	(Ali et al. 2007)
FBR-PE	Four-phase	NNMPC	Molecular weight, temperature	(Ibrehem et al. 2008)
FBR-PE	Two-phase	PID	Temperature, bed level, feed concentration, pressure	(Vahidi and Shahrokhi 2008)
FBR-PE	Two-phase and well mixed	PID	Temperature, pressure, bed level	(Sarvaramini et al. 2008)
FBR-PE	Well mixed	PID	Temperature	(Salau et al. 2008)
FBR-PE	Two-phase	PID	Bed level	(Hassimi et al. 2009)
FBR-PE	Well mixed	NMPC	Molecular weight distribution	(Ali and Ali 2010)
Batch-PS	Kinetics based NN	NN-MPC	Temperature	(Anwar et al. 2011)
FBR-PP	Two-phase	APMBC	Temperature, production rate	(Ho et al. 2012)
jCSTR-PS	Well mixed	Adaptive back stepping	Temperature, monomer concentration	(Biswas and Samanta 2013)
FBR-PP	Two-phase	MPC	Temperature, production rate	(Shamiri et al. 2013)

4.2 AI-based control

Conventional controllers such as PID controllers are popular in industrial applications since their design is easy, the structure is straightforward, and the cost is reasonable. However, their performance is abysmal when they are vulnerable to unknown disturbances. An effective way of handling such nonlinearity is to adopt fuzzy logic, characterizing an enhancement in the transient characteristic of the control performance (Rashid et al. 2011). By contrast, setting up a systematic design method for fuzzy control is not easy to do, since it is nonlinear in nature and, as a result, has no mathematical design method as its support. The excellent performance of fuzzy control in transient state combined with the high accuracy of PI control in the steady state would give us a solution that could be very workable. Alexandridis et al. (2002), based on fuzzy systems, had set

up a systematic method to the nonlinear system identification problem. This fresh method had led to a linguistic and an analytic system model. The method was tested in a CSTR to diagnose fixed operating states. The model could display several types of nonlinear manners successfully.

Mollov et al. (2002) offered the synthesis of a TS fuzzy-based predictive controller for a nonlinear process which led to a robust control system. The success of this method was proven via both simulation and laboratory setups for on-line control of a cascaded-tanks setup. A predictive control technique which takes its guidance from the dynamic TS fuzzy model was put forth by Sarimveis and Bafas (2003). This model was employed to forecast the upcoming performance of the control variable in a SISO control loop. Aided by a genetic algorithm, the controller's objective function was solved on line. The suggested method was put on an arbitrary process in a non-isothermal

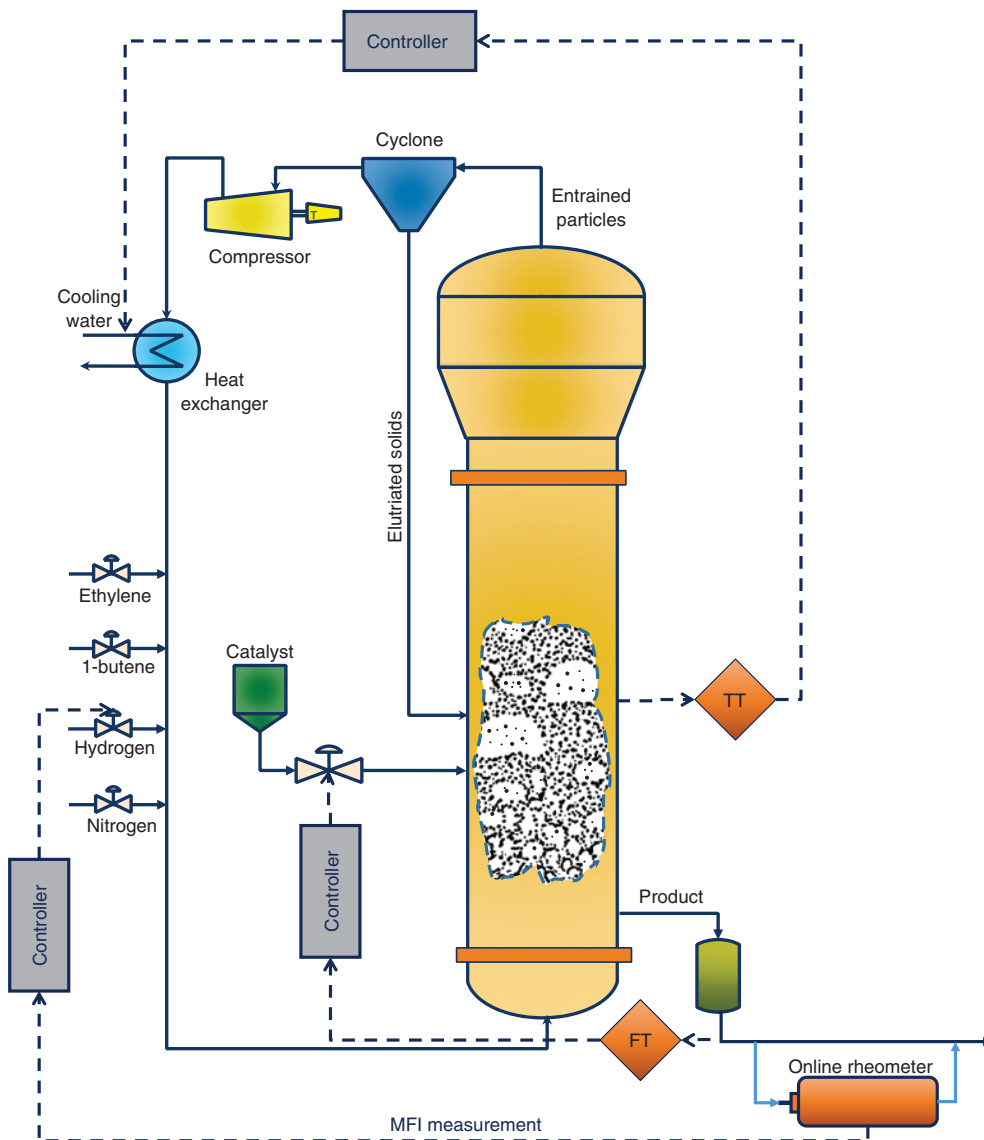


Figure 2: Some of the control loop structures applied on fluidized bed reactors.

CSTR and the authors claimed that it can be applied to all types of fuzzy models, being primarily beneficial in cases where a fuzzy controller cannot be constructed directly as the system is found to be a complicated one.

Habbi et al. (2003) studied a natural circulation drum-boiler-turbine and suggested a nonlinear dynamic fuzzy model. The authors showed that the dynamic fuzzy model brings proper and precise universal nonlinear estimates, and at the same time, the proposed local models are near estimates to the local linearization of the nonlinear dynamic system.

Cerrada et al. (2005) introduced a method for adaptive dynamic fuzzy modeling. Their method combines the historical performance of the system variables with membership functions of fuzzy systems. The authors illustrated

tolerable identification errors by giving some descriptive examples of system identification which can unravel the effectiveness of the fuzzy models suggested. Despite the abrupt fluctuations in the input variables, these models adhere to the real output which is vital in an acceptable identification model in experimental practices. The focus of this tactic rests on cases that cause an identification model.

The usage of fuzzy logic in modeling of the systems and their control studies needs to be stressed, as they may propel a more straightforward execution of algorithms for integration. They are interesting since they boast off execution simplicity, time, ability to swiftly model complex systems, and its moderately low cost.

Ghasem (2006) used the fuzzy logic controllers based on the TS inference method to regulate the reaction

temperature of the industrial ethylene polymerization FBRs. The simulation results suggest that the conventional fuzzy logic controller will oscillate in the process response. For a better performance of the conventional scheme, the authors proposed that a hybrid control scheme needs to be adopted. Some striking improvements in the controller performance could be achieved by bringing together these approaches. The hybrid control scheme mitigates the severe oscillations of the common method and contributes toward better control precision. The comparison between Mamdani fuzzy logic and Takagi-Sugeno-type fuzzy controller has been investigated. Results have shown that Mamdani fuzzy logic is not difficult to build, that it is too simple to control the process quickly and that it only works with the long delay system. Takagi-Sugeno controller is ideal to play its role as multiple linear controllers to run dynamic nonlinear systems. This says that it can control the process that changes swiftly and has high frequent input signals.

4.3 Model-based control

4.3.1 Model predictive control

Polymerization plants must function under different grade transition scenarios. This is to fully cater for the many types of product qualities needed for various applications. The best answer for this situation depends on a suitable objective function defined for a minimization problem. This optimization problem depends on time needed to change product quality specifications, process safety limitations and the quantity of off-spec polymer. Since choosing the best control scheme has significant impacts on process quality and process operability

optimization, the time optimal transition problem needs to be considered together with this control strategy simultaneously.

It should be said that many conventional control algorithms are not enough in dealing with the strict limitations enforced in a few industrial processes, specifically once a first-rate commodity is needed. This is particularly valid for polymerization processes wherein definite properties like MFI or average molecular weight with the effect on plastic quality should be fulfilled. At this point, a proper way is to adopt a model predictive control (MPC), that makes use of a process tailored dynamic model as an essential part for the process control structure.

The MPC is an optimization-based control strategy which is very suitable for constrained, multi-variable processes. The MPC predicts the actual system's future behavior over a time interval defined by the prediction horizon. The implication made by the simpler diagram of the MPC algorithm shown in Figure 3 is that a parallel process model to the controller is used in MPC to predict the controlled variable.

MPC works by minimizing a cost function given by Seborg et al. (2004):

$$V(k) = \sum_{i=1}^P \sum_{j=1}^{n_y} (w_j^y [y_i(k+i) - r_j(k+i)])^2 + \sum_{i=1}^M \sum_{j=1}^{n_{mv}} \{w_j^{\Delta u} [\Delta u_j(k+i-1)]\}^2,$$

where P is the prediction horizon, n_y is the number of plant outputs, w_j^y is the weight for output j , k is the current sampling interval, $k+i$ is a future sampling interval (within the prediction horizon), $[y_i(k+i) - r_j(k+i)]$ is the predicted deviation at future instant $k+i$, n_{mv} is the

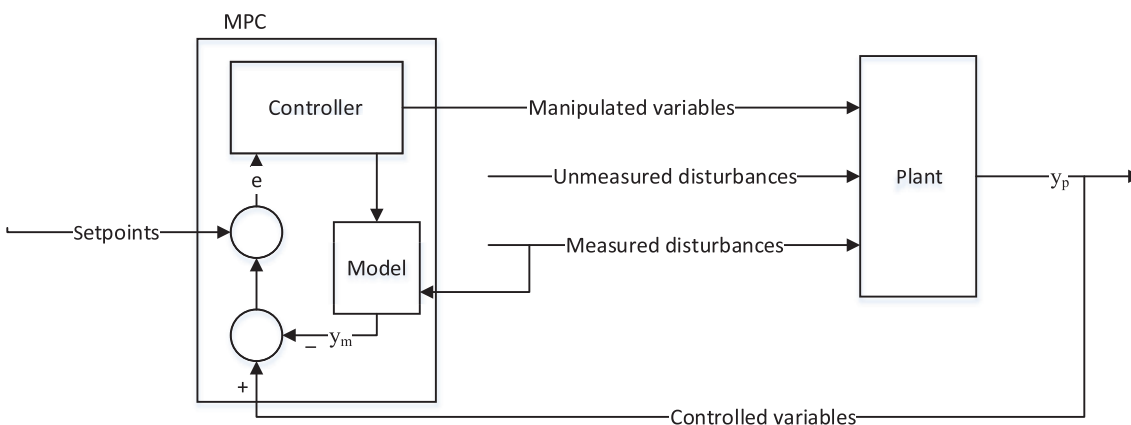


Figure 3: Model predictive control system (Shamiri et al. 2013).

number of manipulate variables (inputs), M is the control horizon, $w_j^{\Delta u}$ is the weight for input j and $\Delta u_j(k+i-1)$ is the predicted adjustment (i.e. move) in manipulated variable j at future (or current) sampling interval $k+i$.

The unequal constraints of the manipulated and control variables also restrict the cost function as follows:

Manipulated variable constraint:

$$u_{\max}(k) \geq u(k+i-1) \geq u_{\min}(k)$$

Manipulated variable rate constraint:

$$\Delta u_{\max}(k) \geq u(k+i-1) \geq \Delta u_{\min}(k)$$

Output variable constraint:

$$y_{\max}(k) \geq u(k+i-1) \geq y_{\min}(k).$$

The problem formulation would decide if several parameters such as the control horizon, prediction horizon and weighting matrices in the optimization formulation should be completed so that the predicted output can perform better.

As mentioned by Campello et al. (2003), MPC algorithms have been used for chemical process control for their usage simplicity and capability to deal with limitations that involve the input and output variables in procedures. Schnelle and Rollins (1997) adopted a continuous polymerization (CP) process design and applied an MPC. They illustrated that MPC technology proved to be a promising substitute for this type of process. Santos et al. (2001) made the effort to control the temperature and liquid level in a pilot plant CSTR reactor and they implemented an on-line nonlinear MPC algorithm. The authors also established several sources of unmeasured disturbances and model mismatch. They leave an impact on the model quality in representing the reactor dynamics. While there are mismatches and disturbances, the closed loop system performed credibly in terms of disturbance rejection and set-point tracking. The application of a nonlinear MPC based on extended Kalman filter to control polymer properties had been analyzed by Park and Rhee (2003), for a semi-batch methyl methacrylate/methacrylate copolymerization reactor. The authors drew a comparison between the experimental results and other techniques to show the superior performance of this control strategy.

Ramaswamy et al. (2005) had sought to control an unsteady-state CSTR bioreactor with the help of an MPC. A vital MPC parameter for its tuning is prediction horizon which was analyzed in this work by concentrating on the variation effects.

The DMC (dynamic matrix control) strategy has the utmost applications in industry between MPC control

techniques. It is because of its design and application straightforwardness together with its ability to soundly handle cases where manipulated variable is restricted within a range.

Within chemical industries, MPC has stood out to become the principal method of advanced multi-variable. In another approach, Dougherty and Cooper (2003) had given a multiple model adaptive control approach for multi-variable DMC. This technique blends the output of multiple linear DMCs without adding extra computational intricacy contrasting to the non-adaptive DMC. Adaptive linear DMC (ALDMC) algorithm was developed and employed by Guiamba and Mulholland (2004) in a MIMO pump-tank setup. Where the plant/model mismatch is concerned, ALDMC presented better performance in comparison to the non-adaptive linear DMC (LDMC). Haeri and Beik (2005) considered the handling of MIMO systems within specified circumstances and recommended an approach which extended the nonlinear DMC procedure. The authors have illustrated that the method usefulness is clear by presenting the simulated control results of a MIMO stirred reactor nonlinear model and another MIMO power unit nonlinear model.

Carlos et al. (1989) highlighted critical issues whereby any control system should discuss and review MPC techniques in the light of those issues to highlight their advantages in terms of the design and implementation. Several design techniques such as internal model control and inferential control emanate from MPC; they were put in perspective with respect to one another and the similarity with more traditional methods like linear quadratic control were investigated. The malleable constraint management capabilities of MPC were a prominent asset in the framework of the global operating goals of the process industries and the 1-, 2-, and ∞ -norm formulations of the performance goal. The application of MPC to nonlinear systems was examined and its attractions were also studied. The authors also suggested that, although the MPC is not any stronger than classical feedback, its robustness can be adjusted more easily.

The nonlinear model based control was applied by Özkan et al. (2001) to the styrene solution polymerization in a jacketed batch reactor and checked its effectiveness to reach the required molecular weight and monomer conversion. The authors used Hamiltonian optimization to assess the optimal temperature profiles for the properties of polymer quality. Analytical and experimental nonlinear model based control were analyzed to keep tab of the temperature at the trajectory which was believed to be optimal. Two types of parametric and nonparametric models were assessed to control temperature optimally.

Nonlinear auto regressive moving average exogenous (NARMAX) gives an association among reactor temperature and heat input to depict the system dynamics. It should also be added that this model served to define the control system as a parametric model. Simulation results were brought for comparison with experimental control data. Authors summed up that the control simulation program is the representative of the behavior of the controlled reactor temperature with some good prediction capabilities. Moreover, nonlinear model based control keeps the reactor temperature stable within the optimal trajectory.

Qin and Badgwell (2003) did a survey on commercially available MPC technology, both linear and nonlinear, based primarily on data provided by MPC vendors and described approaches taken by each vendor for the various aspects of the calculation. A review of the identification technology was needed to enable a list of similarities and differences to be found between the approaches. MPC applications performed by each vendor were summarized following the application area.

Ibrehem et al. (2008) implemented adaptive predictive model-based control to control the system and compared with the conventional PID controller, giving acceptable results.

Mjalli et al. (2009) considered a multi-model adaptive control strategy to handle the variation of operational process parameters and the effect of process disturbances in a biodiesel transesterification reactor.

Ho et al. (2012) had concentrated on the control of a gas phase propylene polymerization model in an FBR, where a two-phase dynamic model was used, and since the process is nonlinear, an advanced control scheme was adopted to ensure an efficient regulation of the process variables. Adaptive predictive model-based control (APMBC) strategy (an integration of the recursive least squares algorithm, RLS and the generalized predictive control algorithm, GPC) have the function to control the emulsion phase temperature and PP production rate by manipulating the reactor cooling water flow rate and catalyst feed rate again. The APMBC in set point tracking was reported to be superior, as compared to the conventional PI controller and the ability of APMBC to capture the effects of monomer concentration, hydrogen concentration and superficial gas velocity on the process variables as efficiently as possible. It is common for the polymerization processes to have a highly nonlinear dynamic behavior leading to an abysmal performance of controllers based on conventional internal models to be poor or for it to need a considerable amount of effort in controller tuning.

Shamiri et al. (2013) took advantage of a two-phase model to delve into the dynamic behavior and process control of a fluidized-bed PP production reactor production rate and temperature. To control the reactor temperature and the PP production rate, a centralized MPC technique was used by making use of the catalyst feed rate and cooling water flow rate, respectively. They reached a conclusion that the MPC could yield some controller moves which not only were subjected to the specified input constraints for both control variables, but also that they are characteristically non-aggressive and sufficiently smooth for practical use.

Broadly speaking, the challenge is to organize the sophisticated chemical processes due to their volatile nature of parameters and structural mismatch. Adaptive linear or nonlinear algorithm is a very important tool to control these kinds of processes. In normal circumstances, the stability of Lyapunov functions serves to design nonlinear adaptive controllers. This algorithm can also deal with other parametric uncertainties throughout the input saturation. Biswas and Samanta (2013) considered the controlling polymerization process with input saturation and parametric uncertainty and worked on an adaptive back stepping methodology. The controller is showed to be robust in modeling uncertainties in a polymerization process and it also showed powerful disturbance rejection ability. The adaptive controller could take both matched and unmatched uncertainties. In addition, to get better results, the authors made use of several parameters in which the controller gave a sturdy performance even around high parametric uncertainty.

4.3.2 Fuzzy-based MPC

Nascimento Lima et al. (2009) built a predictive control system based on type Takagi-Sugeno fuzzy models for polymerization, where they had a close look into the copolymerization of methyl methacrylate with vinyl acetate to test the ability of the recommended control system. They adopted a nonlinear mathematical model to justify the reaction plant that can generate data and probe deeper into the controller performance. The fuzzy approach adopted in their work suggested that it can predict outputs as a function of dynamic data input. The authors drew a comparison with this fuzzy approach with conventional predictive control in regulatory and servo issues, and as the result, the fuzzy controller was easy to implement, and its response is much more reliable.

Bringing together the capability of fuzzy logic predictive approaches and system characterization is appealing

for designing controllers. Roubos et al. (1999) integrated the MPC algorithms with Takagi-Sugeno fuzzy models. In this approach, what happens first is that the model identification using fuzzy logic is given for MIMO architectures. With the establishment of the fuzzy model, it was brought together with MPC. The authors ran a test on this method for a two input-four output MIMO liquid level control case.

With the help of fuzzy-Hammerstein (FH) models, the nonlinear system was identified and controlled and this was described by Abonyi et al. (2000). This model carries a static fuzzy model linked with a series of a linear dynamic model. This model was integrated in a MPC control structure and a new method was introduced to handle constraints. To elaborate further, a simulated water-heater process was adopted. Simulation results have shown not only good dynamic modeling performance but also a well-captured steady-state behavior of the system. The application of fuzzy decision making (FDM) in MPC was studied by da Costa Sousa and Kaymak (2001), and there is a conformity of the results with those obtained from the usual MPC. Experiments with nonlinear dynamics were run on three states, namely an air conditioning system, unstable linear system, and a non-minimum phase. Results have suggested that the MPC performance can be made better using fuzzy criteria in the framework of fuzzy decision making.

To address the many optimization problems that are non-convex which come from the application of MPCs to nonlinear processes, Mendonça et al. (2004) gave the simplified version of fuzzy predictive filters to multi-variable processes. The introduced structure was implemented on a portal crane control. The benefits of the method were presented following the simulation results. The TS fuzzy design for a hybrid fuzzy modeling methodology was an idea proposed by Karer et al. (2007). The authors analyzed an MPC algorithm which was fit for systems with discrete inputs and the results have given a clue on the advantages of the MPC algorithm using the proposed fusion fuzzy model on a batch-reactor simulation example. The hybrid fuzzy predictive control design that is leaning on a genetic algorithm was suggested by Causa et al. (2008). Using two on/off input valves and a discrete-position mixing valve, the batch reactor temperature was controlled. The strategy revealed to be a proper technique to control hybrid systems, delivering the same performance in comparison with conventional hybrid predictive controllers plus large reductions in computation time. To add, the authors also formulated a problem with hybrid predictive adaptive control structure, and the results were believed highly potential.

4.3.3 Generic model controller

Generic model control (GMC) is a type of control scheme which directly uses the nonlinear process model. The dynamic mass, momentum, and energy balances are used to get first-principle models. If the process was still ambiguous, black-box models can be used to represent the unknown parts. Being a process model based control algorithm, the GMC incorporates a process model within the control structure directly. It has been illustrated to show excellent control, despite reasonable modeling errors. Abonyi et al. (2002) looked into these hybrid GMC models. They concluded that the first principles part of these models focuses on the main structure of the controller, while the black-box section plays its role as state/disturbance estimators.

Signal and Lee (1992) had built an algorithm within a GMC framework which seeks to mitigate larger modeling errors by updating the model parameters occasionally. Authors made a strong claim that this adaptive algorithm had the capability of adapting model parameters in a nonlinear model, where the parameters manifest themselves nonlinearly. Several examples were presented to highlight the technique principles.

Ali et al. (2007) had worked on a modified GMC and simulated it to analyze the results. It entails a model-based control of a propylene polymerization reactor in which the melt index and monomer conversion of the polymer are controlled by manipulating the inlet hydrogen concentration and the reactor cooling water flow. Nonlinear control is made, using a simplified nonlinear model, to show the strength of the control strategy. Two model variables are updated on-line to make sure that the outputs of the controlled process and their estimated values are followed carefully. The controller is the static inverse of the process model with set points of the measured process outputs changed to set points for several state variables. The simulation study illustrated that the suggested controller has good set point tracking and disturbance rejection properties and is the best, compared to the conventional GMC and Smith predictor control approaches.

4.4 On-line monitoring of polymerization processes

As the need to produce polymers with pre-specified properties intensifies, great emphasis is laid on the progress of precise, strong instruments developments that can be used for on-line monitoring of polymerization reactions. The viscous and complex nature of polymerization systems

makes on-line measurements difficult. Poor reliability and long measurement delays are two prevalent issues which lead to these difficulties. Even the off-line measurement of several polymer properties cannot be considered an easy task, as they need sophisticated and time-consuming analytical techniques. The manufacturing of on-line polymer sensors needs an interdisciplinary struggle, improved process knowledge and understanding, reactor design, and instrumentation engineering to name but a few.

Kammona et al. (1999) reviewed the progress that has been made in developing on-line hardware sensors to oversee polymerization reactions, in addition to analyzing the accuracy and robustness of the on-line techniques used to gauge the molecular weight, monomer conversion, molecular weight distribution (MWD), copolymer composition, and particle size distribution (PSD) in a continuous manner in polymer reaction operations.

Automatic Continuous On-line Monitoring of Polymerization Reactions (ACOMP) is a name given to a technique that was developed at Tulane University by Reed (2004). The ACOMP technique oversees the polymerization reactions in real-time. In this method, small quantities of polymer are withdrawn from the reactor continuously and diluted. After this step, the diluted polymer sample will undergo several detectors to calculate standard parameters such as intrinsic viscosity, light scattering, and refractive index. Subsequently, the polymer is continuously characterized as the reaction is running. ACOMP can be used for reaction optimization or feedback control of reactors. The method is independent from any model and it can perform an analysis on the polymer properties on-line. It is a direct measurement rather than a theoretical understanding of the reaction (Alb and Reed 2008).

Different reaction parameters can be fine-tuned based on which ACOMP is used in real-time. This method would be helpful for the reaction efficiency and product consistency maximization and waste minimization (Alb and Reed 2010).

5 Conclusions

This article goes through the basics and latest advances in modeling and control of FBRs. Different modeling approaches have been elaborated, and the most recent papers have been analyzed. In addition, the latest papers on controlling fluidized-bed polymerization reactors are also covered in this article. It has been shown that although a lot of progress has been made recently, there is a call to further improve the accuracy of mathematical

models and introduce control algorithms that can control the variables linked with this highly nonlinear system in an optimal manner. Moreover, current models still fall short on explaining the whole polymerization phenomena within fluidized-bed polymerization reactors especially industrial ones. Future models need to fully consider hydrodynamics, kinetics and transport phenomena in industrial reactors and account for custom processes such as condensed mode polymerization and the effect of additives. Controlling polymer parameters is another area which has still plenty of advancement space. Controlling properties such as MWD accurately, needs innovation in all fields of chemistry, catalysis, multi-scale modeling and advanced process control. New innovative MIMO controllers can be designed to control multiple variables of FBR process at once. Lastly, an integrated dynamic model that considers all the scenarios which could happen within an FBR would be the future goal of this research field and it will have many applications for designing, scale-up, optimization and controller designs of FBRs to come up with much greener, cost-effective and efficient processes. That would only be possible with advancement in all related research fields such as first-principle modeling, accurate empirical models, advanced control methods, CFD modeling, computer science and progress in high-performance computing.

Nomenclature

A	Cross-sectional area of the reactor (m^2)
ALDMC	Adaptive linear DMC
$AlEt_3$	Triethyl aluminum co-catalyst
APMBC	Adaptive predictive model-based control
Ar	Archimedes number
B_i	Moles of reacted monomer bound in the polymer in the reactor
CFD	Computational fluid dynamics
$C_{p,pol}$	Specific heat capacity of solid product ($J/kg \cdot K$)
C_{pg}	Specific heat capacity of gaseous stream ($J/kg \cdot K$)
C_{pi}	Specific heat capacity of component i ($J/kg \cdot K$)
CSTR	Continuous stirred tank reactor
d_b	Bubble diameter (m)
d_{b0}	Initiate bubble diameter (m)
D_g	Gas diffusion coefficient (m^2/s)
DMC	Dynamic matrix control
d_p	Particle diameter (m)
D_r	Reactor diameter (m)
FBR	Fluidized-bed reactor
F_{cat}	Catalyst feed rate (kg/s)
FDM	Fuzzy decision making
f_i	Fraction of total monomer in the reactant gas which is monomer M_i
FH	Fuzzy Hammerstein

G	Gravitational acceleration (m/s^2)	N_{H}	uninitiated site of type j produced by transfer to hydro- gen reaction
GPC	Gel permeation chromatography	$N_j(r, j)$	living polymer molecule of length r , growing at an active site of type j , with terminal monomer M
H	Height of the reactor (m)	P	pressure (Pa)
H_2	Hydrogen	PBE	population balance equation
H_{bc}	Bubble-to-cloud heat transfer coefficient ($\text{W/m}^3 \cdot \text{K}$)	PID	proportional-integral-differential
H_{be}	Bubble-to-emulsion heat transfer coefficient ($\text{W/m}^3 \cdot \text{K}$)	PDI	polydispersity index
H_{ce}	Cloud-to-emulsion heat transfer coefficient ($\text{W/m}^3 \cdot \text{K}$)	$Q(r, j)$	dead polymer molecule of length r produced at a site of type j
HDPE	High-density polyethylene	r	number of units in polymer chain
ICA	Induced condensing agent	Re_{mf}	Reynolds number of particles at minimum fluidization condition
i	Monomer type	R_i	Instantaneous consumption rate of monomer (kmol/s)
I_{m}	Impurity such as carbon monoxide (kmol/m^3)	R_p	Production rate (kg/s)
j	Active site type	R_v	Volumetric polymer outflow from the reactor (m^3/s)
K_b	Elutriation constant in bubble phase ($\text{kg} \cdot \text{m}^2/\text{s}$)	SISO	Single input-single output
K_{bc}	Bubble-to-cloud mass transfer coefficient (1/s)	T	Temperature (K)
K_{be}	Bubble-to-emulsion mass transfer coefficient (1/s)	t	Time (s)
K_{ce}	Cloud-to-emulsion mass transfer coefficient (1/s)	T_{in}	Temperature of the inlet gaseous stream (K)
$k_{\text{di}}(j)$	Deactivation by impurities rate constant for a site of type j	TS	Takagi-Sugeno fuzzy inference system
$k_{\text{ds}}(j)$	Spontaneous deactivation rate constant for a site of type j	T_{ref}	Reference temperature (K)
K_e	Elutriation constant in emulsion phase ($\text{kg} \cdot \text{m}^2/\text{s}$)	U_t^*	Dimensionless terminal falling velocity coefficient
$k_f(j)$	Formation rate constant for a site of type j	U_o	Superficial gas velocity (m/s)
$k_{\text{fhi}}(j)$	Transfer rate constant for a site of type j with terminal monomer M_i reacting with hydrogen	U_b	Bubble velocity (m/s)
$k_{\text{fmi}}(j)$	Transfer rate constant for a site of type j with terminal monomer M_i reacting with monomer M_k	U_{br}	Bubble rise velocity (m/s)
$k_{\text{fii}}(j)$	Transfer rate constant for a site of type j with terminal monomer M_i reacting with AlEt_3	U_{mf}	Minimum fluidization velocity (m/s)
$k_{\text{fsi}}(j)$	Spontaneous transfer rate constant for a site of type j with terminal monomer M_i	U_t	Terminal velocity of falling particles (m/s)
k_g	Gas thermal conductivity ($\text{W/m} \cdot \text{K}$)	V	Reactor volume (m^3)
$k_{\text{hi}}(j)$	Rate constant for reinitiating of a site of type j by mono- mer M_i	V_p	Volume of polymer phase in the reactor (m^3)
$k_{\text{hr}}(j)$	Rate constant for reinitiating of a site of type j by cocatalyst	W_b	Weight of solids in the bubble phase (kg)
$k_i(j)$	Rate constant for initiation of a site of type j by monomer M_i	W_e	Weight of solids in the emulsion phase (kg)
$k_{\text{pik}}(j)$	Propagation rate constant for a site of type j with termi- nal monomer M_i reacting with monomer M_k	$X(n, j)$	n th moment of chain length distribution for dead poly- mer produced at a site of type j
k_{pti}	Propagation rate constant ($\text{m}^3/\text{kmol} \cdot \text{s}$)	$Y(n, j)$	n th moment of chain length distribution for living polymer produced at a site of type j
LDMC	Linear DMC	Z-N	Ziegler-Natta catalyst
LDPE	Low-density polyethylene		
LLDPE	Linear low-density polyethylene		
MFI	Melt flow index (g/10 min)		
$[M_i]$	Concentration of component i in the reactor (kmol/m^3)		
$[M_i]_{\text{in}}$	Concentration of component i in the inlet gaseous stream		
MIMO	Multi-input-multi-output	ΔH_{R}	Heat of reaction (J/kg)
Mn	Number average molecular weight of polymer (kg/kmol)	δ	Volume fraction of bubbles in the bed
MPC	Model predictive controller	ε_b	Void fraction of bubble for Geldart B particles
Mw	Weight average molecular weight of polymer (kg/kmol)	ε_e	Void fraction of emulsion for Geldart B particles
MWD	Molecular weight distribution	ε_{mf}	Void fraction of the bed at minimum fluidization
mw_i	Molecular weight of monomer i (g/mol)	μ	Gas viscosity ($\text{Pa} \cdot \text{s}$)
$N(0, j)$	Uninitiated site of type j produced by formation reaction	ρ_g	Gas density (kg/m^3)
NARMAX	Nonlinear Auto Regressive Moving Average with eXog- enous input	ρ_{pol}	Polymer density (kg/m^3)
$N^*(j)$	potential active site of type j	ϕ_s	Sphericity for sphere particles
$N_d(j)$	spontaneously deactivated site of type j		
$N_{\text{dih}}(0, j)$	impurity killed sites of type j		

Greek letters

ΔH_{R}	Heat of reaction (J/kg)
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
μ	Gas viscosity ($\text{Pa} \cdot \text{s}$)
ρ_g	Gas density (kg/m^3)
ρ_{pol}	Polymer density (kg/m^3)
ϕ_s	Sphericity for sphere particles

Subscripts and superscripts

1	Ethylene
2	1-Butene
b	Bubble phase

e	Emulsion phase
i	Component-type number
j	Active site-type number
mf	Minimum fluidization
pol	Polymer
ref	Reference condition
T,TT	Pseudo-kinetic rate constants

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References

- Abbasi MR, Shamiri A, Hussain MA. Dynamic modeling and molecular weight distribution of ethylene copolymerization in an industrial gas-phase fluidized-bed reactor. *Adv Powder Technol* 2016; 27: 1526–38.
- Abonyi J, Babuška R, Szeifert F, Nagy L. Identification and control of nonlinear systems using fuzzy Hammerstein models. *Ind Eng Chem Res* 2000; 39: 4302–14.
- Abonyi J, Madar J, Szeifert F. Combining first principles models and neural networks for generic model control. In: Roy R, Köppen M, Ovaska S, Furuhashi T, Hoffmann F, editors. *Soft computing and industry*. London: Springer London, 2002: 111–22.
- Akbari V, Borhani TNG, Godini HR, Hamid MKA. Model-based analysis of the impact of the distributor on the hydrodynamic performance of industrial polydisperse gas phase fluidized bed polymerization reactors. *Powder Technol* 2014; 267: 398–411.
- Akbari V, Borhani TNG, Shamiri A, Aramesh R, Hussain MA, Hamid MKA. 2D CFD-PBM simulation of hydrodynamic and particle growth in an industrial gas phase fluidized bed polymerization reactor. *Chem Eng Res Des* 2015a; 104: 53–67.
- Akbari V, Nejad Ghaffar Borhani T, Aramesh R, Hamid MKA, Shamiri A, Hussain MA. Evaluation of hydrodynamic behavior of the perforated gas distributor of industrial gas phase polymerization reactor using CFD-PBM coupled model. *Comput Chem Eng* 2015b; 82: 344–61.
- Akbari V, Nejad Ghaffar Borhani T, Shamiri A, Hamid MKA. A CFD-PBM coupled model of hydrodynamics and mixing/segregation in an industrial gas-phase polymerization reactor. *Chem Eng Res Des* 2015c; 96: 103–20.
- Alb AM, Reed WF. Recent advances in automatic continuous online monitoring of polymerization reactions (ACOMP). *Macromol Symp* 2008; 271: 15–25.
- Alb AM, Reed WF. Fundamental measurements in online polymerization reaction monitoring and control with a focus on ACOMP. *Macromol React Eng* 2010; 4: 470–85.
- Alexandridis AP, Siettos CI, Sarimveis HK, Boudouvis AG, Bafas G V. Modelling of nonlinear process dynamics using Kohonen's neural networks, fuzzy systems and Chebyshev series. *Comput Chem Eng* 2002; 26: 479–86.
- Ali E, Al-Humaizi K, Ajbar A. Multivariable control of a simulated industrial gas-phase polyethylene reactor. *Ind Eng Chem Res* 2003; 42: 2349–64.
- Ali EM, Abasaheed AE. Optimization and control of industrial gas-phase ethylene polymerization reactors. *Ind Eng Chem Res* 1998; 37: 3414–23.
- Ali EM, Abasaheed AE. Improved regulatory control of industrial gas-phase ethylene polymerization reactors. *Ind Eng Chem Res* 1999; 38: 2383–90.
- Ali EM, Ali MA. Broadening the polyethylene molecular weight distribution by controlling the hydrogen concentration and catalyst feed rates. *ISA Trans* 2010; 49: 177–87.
- Ali MA-H, Betlem B, Weickert G, Roffel B. Non-linear model based control of a propylene polymerization reactor. *Chem Eng Process Process Intensif* 2007; 46: 554–64.
- Alizadeh A, Chmelař J, Sharif F, Ebrahimi M, Kosek J, McKenna TFL. Modeling condensed mode operation for ethylene polymerization: part I. Thermodynamics of sorption. *Ind Eng Chem Res* 2017; 56: 1168–85.
- Alizadeh A, Namkajorn M, Somsook E, McKenna TFL. Condensed mode cooling for ethylene polymerization: part II. The effect of different condensable comonomers and hydrogen on polymerization rate. *Macromol Chem Phys* 2015; 216: 985–95.
- Alizadeh M, Mostoufi N, Pourmahdian S, Sotudeh-Gharebagh R. Modeling of fluidized bed reactor of ethylene polymerization. *Chem Eng J* 2004; 97: 27–35.
- Anwar M, Azlan M, Mjalli FS, Hosen MA, Hussain MA, Mjalli FS. Control of polystyrene batch reactors using neural network based model predictive control (NNMPC): an experimental investigation. *Control Eng Pract* 2011; 19: 454–67.
- Aramesh R, Akbari V, Shamiri A, Hussain MA, Aghamohammadi N. Hydrodynamics and particle mixing/segregation measurements in an industrial gas phase olefin polymerization reactor using image processing technique and CFD-PBM model. *Measurement* 2016; 83: 106–22.
- Ashrafi O, Nazari-pouya H, Mostoufi N. Particle size distribution in gas-phase polyethylene reactors. *Adv Powder Technol* 2008; 19: 321–34.
- Bequette BW. Nonlinear control of chemical processes: a review. *Ind Eng Chem Res* 1991; 30: 1391–413.
- Biswas P, Samanta AN. Backstepping control of polymerization reactor. In: 2013 9th Asian Control Conference (ASCC). IEEE; 2013:1–5.
- Bolsoni A, Lima EL, Pinto JC. Advanced control of propylene polymerizations in slurry reactors. *Brazilian J Chem Eng* 2000; 17: 565–74.
- Brempt W Van, Backx T, Ludlage J, Overschee P Van, Moor B De. A high performance model predictive controller: application on a polyethylene gas phase reactor. *Control Eng Pract* 2001; 9: 829–35.
- Campello RJGB, Von Zuben FJ, Amaral WC, Meleiro LAC, Maciel Filho R. Hierarchical fuzzy models within the framework of orthonormal basis functions and their application to bioprocess control. *Chem Eng Sci* 2003; 58: 4259–70.
- Carlos EG, David MP, Manfred M. Model predictive control: theory and practice a survey. *Automatica* 1989; 25: 335–8.
- Causa J, Karer G, Núñez A, Sáez D, Škrjanc I, Zupančič B. Hybrid fuzzy predictive control based on genetic algorithms for the temperature control of a batch reactor. *Comput Chem Eng* 2008; 32: 3254–63.
- Cerrada M, Aguilar J, Colina E, Titli A. Dynamical membership functions: an approach for adaptive fuzzy modelling. *Fuzzy Sets Syst* 2005; 152: 513–33.

- Chatzidoukas C, Perkins JD, Pistikopoulos EN, Kiparissides C. Optimal grade transition and selection of closed-loop controllers in a gas-phase olefin polymerization fluidized bed reactor. *Chem Eng Sci* 2003; 58: 3643–58.
- Che Y, Tian Z, Liu Z, Zhang R, Gao Y, Zou E, Wang S, Liu B. A CFD-PBM model considering ethylene polymerization for the flow behaviors and particle size distribution of polyethylene in a pilot-plant fluidized bed reactor. *Powder Technol* 2015a; 286: 107–23.
- Che Y, Tian Z, Liu Z, Zhang R, Gao Y, Zou E, Wang S, Liu B. CFD prediction of scale-up effect on the hydrodynamic behaviors of a pilot-plant fluidized bed reactor and preliminary exploration of its application for non-pelletizing polyethylene process. *Powder Technol* 2015b; 278: 94–110.
- Che Y, Tian Z, Liu Z, Zhang R, Gao Y, Zou E, Wang S, Liu B. An insight into the temperature field and particle flow patterns in a fluidized bed reactor for nonpelletizing polyethylene process using a 3d CFD-PBM model. *Ind Eng Chem Res* 2016; 55: 8258–70.
- Choi K-Y, Harmon Ray W. The dynamic behaviour of fluidized bed reactors for solid catalysed gas phase olefin polymerization. *Chem Eng Sci* 1985; 40: 2261–79.
- Choi KY, Ray WH. The dynamic behavior of continuous stirred-bed reactors for the solid catalyzed gas phase polymerization of propylene. *Chem Eng Sci* 1988; 43: 2587–604.
- Cui H, Mostoufi N, Chaouki J. Characterization of dynamic gas-solid distribution in fluidized beds. *Chem Eng J* 2000; 79: 133–43.
- da Costa Sousa JM, Kaymak U. Model predictive control using fuzzy decision functions. *IEEE Trans Syst Man, Cybern Part B* 2001; 31: 54–65.
- Dadebo SA, Bell ML, McLellan PJ, McAuley KB. Temperature control of industrial gas phase polyethylene reactors. *J Process Control* 1997; 7: 83–95.
- Dompazis G, Kanellopoulos V, Touloupides V, Kiparissides C. Development of a multi-scale, multi-phase, multi-zone dynamic model for the prediction of particle segregation in catalytic olefin polymerization FBRS. *Chem Eng Sci* 2008; 63: 4735–53.
- Dougherty D, Cooper D. A practical multiple model adaptive strategy for multivariable model predictive control. *Control Eng Pract* 2003; 11: 649–64.
- Fernandes FAN, Ferrareso Lona LM. Fluidized-bed reactor modeling for polyethylene production. *J Appl Polym Sci* 2001; 81: 321–32.
- Fernandes FAN, Lona LMF. Fluidized-bed reactor and physical-chemical properties modeling for polyethylene production. *Comput Chem Eng* 1999; 23: S803–6.
- Fernandes FAN, Lona LMF. Heterogeneous modeling for fluidized-bed polymerization reactor. *Chem Eng Sci* 2001; 56: 963–9.
- Floyd S, Hutchinson RA, Ray WH. Polymerization of olefins through heterogeneous catalysis – V. Gas-liquid mass transfer limitations in liquid slurry reactors. *J Appl Polym Sci* 1986; 32: 5451–79.
- Ghasem NM. Dynamic behavior of industrial gas phase fluidized bed polyethylene reactors under PI control. *Chem Eng Technol* 2000; 23: 133–40.
- Ghasem NM. Design of a fuzzy logic controller for regulating the temperature in industrial polyethylene fluidized bed reactor. *Chem Eng Res Des* 2006; 84: 97–106.
- Guiamba IRF, Mulholland M. Adaptive linear dynamic matrix control applied to an integrating process. *Comput Chem Eng* 2004; 28: 2621–33.
- Habbi H, Zemat M, Ould Bouamama B. A dynamic fuzzy model for a drum-boiler-turbine system. *Automatica* 2003; 39: 1213–9.
- Haeri M, Beik HZ. Application of extended DMC for nonlinear MIMO systems. *Comput Chem Eng* 2005; 29: 1867–74.
- Harmon Ray W, Villa CM. Nonlinear dynamics found in polymerization processes – a review. *Chem Eng Sci* 2000; 55: 275–90.
- Harshe YM, Utikar RP, Ranade V V. A computational model for predicting particle size distribution and performance of fluidized bed polypropylene reactor. *Chem Eng Sci* 2004; 59: 5145–56.
- Hassimi A, Mostoufi N, Sotudeh-Gharebagh R. Unsteady-state modeling of the fluidized bed polyethylene reactor. *Iran J Chem Eng* 2009; 6: 23–39.
- Hatzantonis H, Yiannoulakis H, Yiagopoulos A, Kiparissides C. Recent developments in modeling gas-phase catalyzed olefin polymerization fluidized-bed reactors: the effect of bubble size variation on the reactor's performance. *Chem Eng Sci* 2000; 55: 3237–59.
- Ho YK, Shamiri A, Mjalli FS, Hussain MA. Control of industrial gas phase propylene polymerization in fluidized bed reactors. *J Process Control* 2012; 22: 947–58.
- Ibrehem AS, Hussain MA, Ghasem NM. Mathematical model and advanced control for gas-phase olefin polymerization in fluidized-bed catalytic reactors. *Chinese J Chem Eng* 2008; 16: 84–9.
- Ibrehem AS, Hussain MA, Ghasem NM. Modified mathematical model for gas phase olefin polymerization in fluidized-bed catalytic reactor. *Chem Eng J* 2009; 149: 353–62.
- Immanuel CD, Cordeiro CF, Sundaram SS, Meadows ES, Crowley TJ, Doyle FJ. Modeling of particle size distribution in emulsion co-polymerization: comparison with experimental data and parametric sensitivity studies. *Comput Chem Eng* 2002; 26: 1133–52.
- Jafari R, Sotudeh-Gharebagh R, Mostoufi N. Modular simulation of fluidized bed reactors. *Chem Eng Technol* 2004; 27: 123–9.
- Jiang Y, McAuley KB, Hsu JCC. Nonequilibrium modeling of condensed mode cooling of polyethylene reactors. *AIChE J* 1997; 43: 13–24.
- Kammona O, Chatzi EG, Kiparissides C. Recent developments in hardware sensors for the on-line monitoring of polymerization reactions. *J Macromol Sci Part C Polym Rev* 1999; 39: 57–134.
- Karer G, Mušič G, Škrjanc I, Zupančič B. Hybrid fuzzy model-based predictive control of temperature in a batch reactor. *Comput Chem Eng* 2007; 31: 1552–64.
- Kato K, Wen CY. Bubble assemblage model for fluidized bed catalytic reactors. *Chem Eng Sci* 1969; 24: 1351–69.
- Khan MJH, Hussain MA, Mansourpour Z, Mostoufi N, Ghasem NM, Abdullah EC. CFD simulation of fluidized bed reactors for polyolefin production – a review. *J Ind Eng Chem* 2014; 20: 3919–46.
- Khang DY, Lee HH. Particle size distribution in fluidized beds for catalytic polymerization. *Chem Eng Sci* 1997; 52: 421–31.
- Khare NP, Lucas B, Seavey KC, Liu YA, Sirohi A, Ramanathan S, Lingard S, Song Y, Chen CY. Steady-state and dynamic modeling

- of gas-phase polypropylene processes using stirred-bed reactors. *Ind Eng Chem Res* 2004; 43: 884–900.
- Kiashemshaki A, Mostoufi N, Sotudeh-Gharebagh R. Two-phase modeling of a gas phase polyethylene fluidized bed reactor. *Chem Eng Sci* 2006; 61: 3997–4006.
- Kiparissides C. Polymerization reactor modeling: a review of recent developments and future directions. *Chem Eng Sci* 1996; 51: 1637–59.
- Luo Z-H, Su P-L, Shi D-P, Zheng Z-W. Steady-state and dynamic modeling of commercial bulk polypropylene process of Hypol Technology. *Chem Eng J* 2009; 149: 370–82.
- Mahecha-Botero A, Grace JR, Elnashaie SSEH, Lim CJ. Advances in modeling of fluidized-bed catalytic reactors: a comprehensive review. *Chem Eng Commun* 2009; 196: 1375–405.
- Makkawi Y., Wright P. Fluidization regimes in a conventional fluidized bed characterized by means of electrical capacitance tomography. *Chem Eng Sci* 2002; 57: 2411–37.
- McAuley KB, Macgregor JF. Nonlinear product property control in industrial gas-phase polyethylene reactors. *AIChE J* 1993; 39: 855–66.
- McAuley KB, MacGregor JF, Hamielec AE. A kinetic model for industrial gas-phase ethylene copolymerization. *AIChE J* 1990; 36: 837–50.
- McAuley KB, Talbot JP, Harris TJ. A comparison of two-phase and well-mixed models for fluidized-bed polyethylene reactors. *Chem Eng Sci* 1994; 49: 2035–45.
- McKenna TFL, Soares JBP. Single particle modelling for olefin polymerization on supported catalysts: a review and proposals for future developments. *Chem Eng Sci* 2001; 56: 3931–49.
- Mendonça LF, Sousa JM, Sá da Costa JMG. Optimization problems in multivariable fuzzy predictive control. *Int J Approx Reason* 2004; 36: 199–221.
- Mirzaei A, Kiashemshaki A, Emami M. Fluidized bed polyethylene reactor modeling in condensed mode operation. *Macromol Symp* 2007; 259: 135–44.
- Mjalli FS, Kim San L, Chai Yin K, Azlan Hussain M. Dynamics and control of a biodiesel transesterification reactor. *Chem Eng Technol* 2009; 32: 13–26.
- Mollov S, van den Boom T, Cuesta F, Ollero A, Babuska R. Robust stability constraints for fuzzy model predictive control. *IEEE Trans Fuzzy Syst* 2002; 10: 50–64.
- Namkajorn M, Alizadeh A, Somsook E, McKenna TFL. Condensed-mode cooling for ethylene polymerization: the influence of inert condensing agent on the polymerization rate. *Macromol Chem Phys* 2014; 215: 873–8.
- Nascimento Lima NM, Manenti F, Filho RM, Embirucu M, Wolf Maciel RM. Fuzzy model-based predictive hybrid control of polymerization processes. *Ind Eng Chem Res*. 2009; 48: 8542–50.
- Noor R a. M, Ahmad Z, Don MM, Uzir MH. Modelling and control of different types of polymerization processes using neural networks technique: a review. *Can J Chem Eng* 2010; 88: 1065–84.
- Özkan G, Özen Ş, Erdoğan S, Hapoğlu H, Alpbaz M. Nonlinear control of polymerization reactor. *Comput Chem Eng* 2001; 25: 757–63.
- Pan H, Liang X-F, Zhu L-T, Luo Z-H. Importance analysis of liquid vaporization modeling scheme in CFD modeling of gas-liquid-solid polyethylene FBR. *Ind Eng Chem Res* 2017; acs.iecr.7b02912.
- Park M-J, Rhee H-K. Property evaluation and control in a semibatch MMA/MA solution copolymerization reactor. *Chem Eng Sci* 2003; 58: 603–11.
- Philippssen CG, Vilela ACF, Zen LD. Fluidized bed modeling applied to the analysis of processes: review and state of the art. *J Mater Res Technol* 2015; 4: 208–16.
- Qin SJ, Badgwell TA. A survey of industrial model predictive control technology. *Control Eng Pract* 2003; 11: 733–64.
- Ramaswamy S, Cutright TJ, Qammar HK. Control of a continuous bioreactor using model predictive control. *Process Biochem* 2005; 40: 2763–70.
- Rashid MM, Rahim NA, Hussain MA, Rahman MA. Analysis and experimental study of magnetorheological-based damper for semiactive suspension system using fuzzy hybrids. *IEEE Trans Ind Appl* 2011; 47: 1051–9.
- Ray WH. Modelling of addition polymerization processes – free radical, ionic, group transfer, and Ziegler-Natta kinetics. *Can J Chem Eng* 1991; 69: 626–9.
- Reed W. Feature article: automatic continuous online monitoring of polymerization reactions (ACOMP). *Polym News* 2004; 29: 271–9.
- Rhodes M. Introduction to particle technology. West Sussex, England: John Wiley and Sons Ltd, 2008.
- Roubos JA, Mollov S, Babuška R, Verbruggen HB. Fuzzy model-based predictive control using Takagi-Sugeno models. *Int J Approx Reason* 1999; 22: 3–30.
- Salau NPG, Neumann GA, Trierweiler JO, Secchi AR. Dynamic behavior and control in an industrial fluidized-bed polymerization reactor. *Ind Eng Chem Res* 2008; 47: 6058–69.
- Santos LO, Afonso PAFNA, Castro JAAM, Oliveira NMC, Biegler LT. On-line implementation of nonlinear MPC: an experimental case study. *Control Eng Pract* 2001; 9: 847–57.
- Sarimveis H, Bafas G. Fuzzy model predictive control of non-linear processes using genetic algorithms. *Fuzzy Sets Syst* 2003; 139: 59–80.
- Sarvaramini A, Mostoufi N, Sotudeh-Gharebagh R. Influence of hydrodynamic models on dynamic response of the fluidized bed polyethylene reactor. *Int J Chem React Eng* 2008; 6. DOI: <https://doi.org/10.2202/1542-6580.1708>.
- Sato C, Ohtani T, Nishitani H. Modeling, simulation and nonlinear control of a gas-phase polymerization process. *Comput Chem Eng* 2000; 24: 945–51.
- Schneiderbauer S, Haider MF, Hauenberger F, Pirker S. A Lagrangian-Eulerian hybrid model for the simulation of industrial-scale gas-solid cyclones. *Powder Technol* 2016; 304: 229–40.
- Schneiderbauer S, Puttinger S, Pirker S, Aguayo P, Kanellopoulos V. CFD modeling and simulation of industrial scale olefin polymerization fluidized bed reactors. *Chem Eng J* 2015; 264: 99–112.
- Schnelle PD, Rollins DL. Industrial model predictive control technology as applied to continuous polymerization processes. *ISA Trans* 1997; 36: 281–92.
- Seborg DE, Edgar TF, Mellichamp DA. Process dynamics and control, 2nd, ed., New Jersey, USA: John Wiley and Sons, Inc., 2004.
- Sederman AJ, Gladden LF, Mantle MD. Application of magnetic resonance imaging techniques to particulate systems. *Adv Powder Technol* 2007; 18: 23–38.

- Seki H, Ogawa M, Ooyama S, Akamatsu K, Ohshima M, Yang W. Industrial application of a nonlinear model predictive control to polymerization reactors. *Control Eng Pract* 2001; 9: 819–28.
- Shamiri A, Azlan Hussain M, Sabri Mjalli F, Mostoufi N, Saleh Shafeeyan M. Dynamic modeling of gas phase propylene homopolymerization in fluidized bed reactors. *Chem Eng Sci* 2011; 66: 1189–99.
- Shamiri A, Hussain MA, Mjalli FS, Mostoufi N, Hajimolana S. Dynamics and predictive control of gas phase propylene polymerization in fluidized bed reactors. *Chinese J Chem Eng* 2013; 21: 1015–29.
- Shamiri A, Hussain MA, Mjalli FS, Mostoufi N. Kinetic modeling of propylene homopolymerization in a gas-phase fluidized-bed reactor. *Chem Eng J* 2010; 161: 240–9.
- Shamiri A, Hussain MA, Mjalli FS, Mostoufi N. Improved single phase modeling of propylene polymerization in a fluidized bed reactor. *Comput Chem Eng* 2012; 36: 35–47.
- Shamiri A, Hussain MA, Mjalli FS, Shafeeyan MS, Mostoufi N. Experimental and modeling analysis of propylene polymerization in a pilot-scale fluidized bed reactor. *Ind Eng Chem Res* 2014; 53: 8694–705.
- Shamiri A, Wei S, Fauzi M, Hussain MA, Mostoufi N. Modified two-phase model with hybrid control for gas phase propylene copolymerization in fluidized bed reactors. *Chem Eng J* 2015; 264: 706–19.
- Signal PD, Lee PL. Generic model adaptive control. *Chem Eng Commun* 1992; 115: 35–52.
- Soares JBP. Mathematical modelling of the microstructure of polyolefins made by coordination polymerization: a review. *Chem Eng Sci* 2001; 56: 4131–53.
- Tamadondar MR, Azizpour H, Zarghami R, Mostoufi N, Chaouki J. Using particle trajectory for determining the fluidization regime in gas-solid fluidized beds. *Adv Powder Technol* 2012; 23: 349–51.
- Vahidi O, Shahrokhi M. Control of a fluidized bed polyethylene reactor. *Iran J Chem Chem Eng* 2008; 27: 87–101.
- Xie T, McAuley KB, Hsu JCC, Bacon DW. Gas phase ethylene polymerization: production processes, polymer properties, and reactor modeling. *Ind Eng Chem Res* 1994; 33: 449–79.
- Yan W-C, Luo Z-H, Lu Y-H, Chen X-D. A CFD-PBM-PMLM integrated model for the gas-solid flow fields in fluidized bed polymerization reactors. *AIChE J* 2012; 58: 1717–32.
- Yang YR, Yang JQ, Chen W, Rong SX. Instability analysis of the fluidized bed for ethylene polymerization with condensed mode operation. *Ind Eng Chem Res* 2002; 41: 2579–84.
- Zacca JJ, Debling JA, Ray WH. Reactor residence time distribution effects on the multistage polymerization of olefins – I. Basic principles and illustrative examples, polypropylene. *Chem Eng Sci* 1996; 51: 4859–86.
- Zheng Z-W, Shi D-P, Su P-L, Luo Z-H, Li X-J. Steady-state and dynamic modeling of the Basell multireactor olefin polymerization process. *Ind Eng Chem Res* 2011; 50: 322–31.
- Zhou Y, Wang J, Yang Y, Wu W. Modeling of the temperature profile in an ethylene polymerization fluidized-bed reactor in condensed-mode operation. *Ind Eng Chem Res* 2013; 52: 4455–64.

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