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Modeling of the PE3 Plant at Borealis AB

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Contents

1. Plant Overview

The polyethylene producing plant PE3 at Borealis AB in Stenungsund, Sweden, consists of three reactors and three distillation columns, see Figure 1. The three reactors, that are of Borealis Borstar® technology, are

1. Pre-polymerization reactor
2. Loop reactor
3. Gas-phase reactor,

while the three distillation columns are

1. Propane column
2. Heavies column
3. Lights column.

To the first reactor there are inflows of catalyst, ethylene, hydrogen and propane and the polymerization conditions are mild such that the catalyst will not break. The polymer slurry is transferred to the loop reactor by transfer legs. Compared to the pre-polymerization reactor, the temperature and pressure are higher in the loop reactor, yielding a super-critical state of the polymer slurry. The loop reactor is considerably larger than the pre-polymerization reactor and additional ethylene, hydrogen and propane is inserted, yielding about half of all polymer at the plant is produced in the loop reactor. From the loop reactor, the polymer slurry is transferred using settling legs and continuous outtake to a flash tank where the raw material and diluent are flashed and transferred to the heavies column in the recycle area, while the polymer is transferred towards the gas phase reactor (GPR). A constant feed of propane helps the transfer of polymer to the GPR and also assures that no leakage of GPR gas mixture is transferred to the loop area. Apart from the same type of

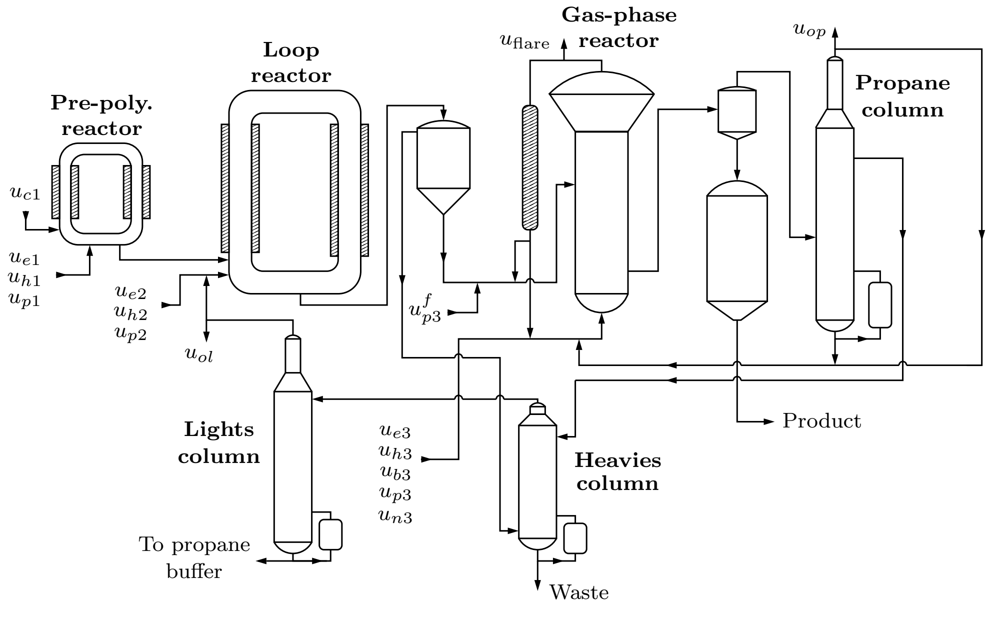

Figure 1 Schematic diagram of the plant PE3 at Borealis AB with the three cascaded Borealis Borstar® reactors and a recycle area with three distillation columns.

fresh feed to the loop reactor, the GPR also has inflows of butene and nitrogen. Approximately half of all polymer is produced in the GPR, which has an internal recycle system for the gas that reaches the top section of the reactor. At the top section outflow, a flare is present that may be used to reduce the recycle flow of raw material and diluents. The polymer and gas mixture is withdrawn from the reactor bottom to a separator, from where the polymer is transferred to packaging (not part of the model) and the gas is transferred to the propane column in the recycle area.

The propane columns main task is to remove propane from the gas mixture from the GPR, and transfer all other components back to the GPR via the column top and bottom outtakes. It has an off-gas on the top stream that may be used to control how much of the top stream is transferred back to the GPR. The column side outtake is mainly composed of propane, and is transferred together with the gas mixture from the flash tank to the heavies column. At the heavies column, heavier components than propane is removed and considered waste, while all other components are transferred to the lights column. From the bottom of the lights column, essentially pure propane is removed and transferred to a propane buffer to be used as fresh feeds to the reactors again. The top flow of the lights column are directly inserted into the loop reactor, i.e., recycled, except for an off-gas stream.

The reactor models described in this report have been developed by Borealis AB, while the distillation column models have been developed in a collaboration between Borealis AB and Lund University.

2. Notation

The notation used in the plant model is described briefly in Table 1. Each type of component flow or off-gas/flare flow has an abbreviation that is used in subscripts. The different subsystems of the plant, i.e., reactors and column, are numbered 1–6 and also used in subscripts.

3. Reactor Models

The two loop reactors are both assumed to have perfect temperature control, constant pressures and well mixed contents. Control systems in regulatory mode are incorporated in the models for holding reactor content volumes constant using outflows as control variables. As the polymer slurry is taken out from the pre-polymerization reactor using transfer legs, the outflow has the same concentrations as the reactor content and the reactor may be modeled as an ideal continuously stirred tank reactor (CSTR). However, since the loop reactor uses both continuous outtake and settling legs, the outflow has a higher concentration of polymer than the reactor content, see [4]. Therefore, using a modeling approach of a non-ideal CSTR where the settling legs are modeled using a discharge factor is thus suitable, see [4, 5]. The subsequent flash tank is assumed to have negligible hold-up time compared to the reactors and recycle area and is excluded from the model.

The temperature in the GPR is assumed to be controlled to a constant value and the regulatory system for the bed volume is incorporated in the model using the outflow as control variable. The polymer and gas in the bed

Table 1 Flow, reactor and distillation column notations.

Flow	Subscript	Subsystem	Subscript
Ethylene	e	Pre-poly. reactor	1
Hydrogen	h	Loop reactor	2
Butene	b	Gas-phase reactor	3
Propane	p	Propane column	4
Nitrogen	n	Heavies column	5
Polyethylene	pe	Lights column	6
Incorp. butene	pb		
Catalyst	c		
Off-gas propane column	op		
Off-gas lights column	ol		
Flare gas GPR	flare		

are assumed well mixed and the conversion per pass-through is low. The gas composition in and above the bed is therefore assumed equal and uniform, see [3, 7]. It is also assumed that the time delay associated with gas recycling through the cooler is negligible. With these assumptions, the GPR may be modeled with outflow and reactor bed concentrations equal. The subsequent separator between the GPR and the propane column has negligible hold-up time for the gas mixture and is excluded from the model together with the degassing tank.

The reactor models, derived by Borealis AB and used today in an on-line non-linear model predictive controller (NMPC) of the plant, include both first principles, semi-empirical, and empirical relations. For optimization, there are 12 control inflows of raw material, diluents and catalyst to the reactors and one flare flow from the GPR.

3.1 Pre-Polymerization Reactor

For the pre-polymerization reactor, which has no direct inflows from the recycle area, the mass balances for fluids, polymer and catalyst are

$$\dot{m}_{e1} = u_{e1} - w_{e1} - r_{e1} \tag{1}$$

$$\dot{m}_{h1} = u_{h1} - w_{h1} - r_{h1} \tag{2}$$

$$\dot{m}_{p1} = u_{p1} - w_{p1} \tag{3}$$

$$\dot{m}_{pe1} = r_{pe1} - w_{pe11} \tag{4}$$

$$\dot{m}_{c1} = u_{c1} - w_{c1} \tag{5}$$

$$m_{f1} = m_{e1} + m_{h1} + m_{p1} \tag{6}$$

$$m_{s1} = m_{pe1} + m_{c1}, \tag{7}$$

where u_{i1} are inflows, $w_{i1(1)}$ and r_{i1} are outflows and reaction rates, respectively, and m_{f1} and m_{s1} are total masses of fluids and solids. The reaction rates are extended non-linear Arrhenius expressions with pre-factors $R_{i1}(\cdot)$

depending on reactor condition, i.e.,

$$r_{e1} = R_{e1}(m_{c1}, a_1, X_{e1}, X_{h1}, P_1) \exp\left(\frac{k_{e11}}{T_1} + k_{e12}\right) \tag{8}$$

$$r_{h1} = R_{h1}(m_{c1}, a_1, X_{h1}, P_1) \exp\left(\frac{k_{h11}}{T_1} + k_{h12}\right) \tag{9}$$

$$r_{pe1} = r_{e1} + r_{h1}, \tag{10}$$

where P_1 and T_1 are the reactor pressure and temperature, respectively, k_{e11}, k_{e12}, k_{h11} and k_{h12} are reaction kinetics parameters and r_{pe1} is the total reaction rate in the pre-polymerization reactor. The molar concentrations X_{i1} of the fluids are defined as

$$X_{i1} = \frac{m_{i1}/M_i}{\sum\limits_{j\in\{e,h,p\}} m_{j1}/M_j}, \qquad i \in \{e, h, p\}, \tag{11}$$

where M_i and M_j are the molar weights of the different components.

The plant model use a Ziegler-Natta catalyst activity profile along the cascaded reactors, modeled with mean activity and deactivated sites. For the pre-polymerization reactor, the catalyst states are

$$\dot{a}_1 = f_{a1}(u_{c1}, m_{c1}, a_1, d_1, a_0, d_0, r_{pe1}) \tag{12}$$

$$\dot{d}_1 = f_{d1}(u_{c1}, m_{c1}, a_1, d_1, a_0, d_0), \tag{13}$$

where $f_{a1}(\cdot)$ and $f_{d1}(\cdot)$ are non-linear functions and a_0 and d_0 are initial values of mean activity and deactivated sites for unused catalyst.

Polymer properties such as melt index and density will be used for defining a polymer grade in the loop reactor and the GPR. However, reliable models of these quantities could not be found for the pre-polymerization reactor due to lack of data. Since production in the prepolymerization reactor compared to in the loop reactor and in the GPR is small and that it has similar reactor conditions as the loop reactor, its end effect on the product quality variables is negligible. Instead, for further calculations, polymer density is set to an average value ρ_{s1} of pre-polymerization reactor polymer produced at the plant for different grades, while melt index is not calculated. To define the polymer grade in the pre-polymerization reactor, the bed average of the molar ratio of hydrogen and ethylene will be used, which is calculated from the instantaneous ratio defined as

$$X_{he1} = \frac{X_{h1}}{X_{e1}}. \tag{14}$$

Using the solid-phase residence time, which is the ratio between mass of solids m_{s1} and solids outflow w_{s1}, the bed average ratio is found as

$$\dot{\overline{X}}_{he1} \frac{m_{s1}}{w_{s1}} = -\overline{X}_{he1} + X_{he1}. \tag{15}$$

Fluid density ρ_{f1} in the pre-polymerization reactor is calculated using an empirical relation depending on pressure, temperature and fluid molar concentrations, utilized when calculating reactor content volume V_1 as,

$$\rho_{f1} = \varrho_1(P_1, T_1, X_{e1}, X_{h1}, X_{p1}) \tag{16}$$

$$V_1 = \frac{m_{f1}}{\rho_{f1}} + \frac{m_{s1}}{\rho_{s1}}. \tag{17}$$

Assuming the reactor is always full of fluids and solids and that the fluid is incompressible, the total volumetric outflow q_1 is set by

$$q_1 = \frac{u_{p1} + u_{e1} + u_{h1}}{\rho_{f1}} + \frac{u_{c1}}{\rho_c} - r_{pe1}\left(\frac{1}{\rho_{f1}} - \frac{1}{\rho_{s1}}\right) + K_1\left(V_1 - V_1^{\text{ref}}\right), \tag{18}$$

where ρ_c is the catalyst density. The two first terms are the total inflow to the pre-polymerization reactor, while the third term compensate for volume contraction due to polymerization. At stationarity, due to the incompressibility assumptions on the fluids and the mass balances, the volumetric flow constituted of the three first terms is equal to the volumetric outflow. An additional volumetric outflow is added to obtain correct volume of reactor content at stationarity, i.e., a proportional controller with gain K_1 and set-point V_1^{ref}. At stationarity, the contribution of this terms is zero and there will be no stationary error of V_1.

The volumetric outflow from the pre-polymerization reactor is the sum of solid and fluid volumetric outflows, i.e.,

$$q_1 = \frac{w_{s1}}{\rho_{s1}} + \frac{w_{f1}}{\rho_{f1}}. \tag{19}$$

Since transfer legs are used, the ratio of solid and fluid outflows and the ratio of solid and fluid masses in the reactor are equal. Using this relation and solving for the two mass flows yields,

$$w_{s1} = \frac{m_{s1}}{\frac{m_{s1}}{\rho_{s1}} + \frac{m_{f1}}{\rho_{f1}}} q_1 \tag{20}$$

$$w_{f1} = \frac{m_{f1}}{\frac{m_{s1}}{\rho_{s1}} + \frac{m_{f1}}{\rho_{f1}}} q_1. \tag{21}$$

The component-wise fluid and solid outflows are found using mass fractions as

$$w_{i1} = \frac{m_{i1}}{m_{f1}} w_{f1}, \qquad i \in \{e, h, p\} \tag{22}$$

$$w_{j1} = \frac{m_{j1}}{m_{s1}} w_{s1}, \qquad j \in \{pe, c\}. \tag{23}$$

3.2 Loop Reactor

The loop reactor has the same model structure as the pre-polymerization reactor. However, it has both fresh inflows, inflows from recycle area, and also inflows from the pre-polymerization reactor. The mass balances for fluids, polymer and catalyst and the total mass of fluids and solids are written as,

$$\dot{m}_{e2} = u_{e2} + w_{e2}^{\text{rec}} + w_{e1} - w_{e2} - r_{e2} \tag{24}$$

$$\dot{m}_{h2} = u_{h2} + w_{h2}^{\text{rec}} + w_{h1} - w_{h2} - r_{h2} \tag{25}$$

$$\dot{m}_{p2} = u_{p2} + w_{p2}^{\text{rec}} + w_{p1} - w_{p2} \tag{26}$$

$$\dot{m}_{pe21} = w_{pe11} - w_{pe21} \tag{27}$$

$$\dot{m}_{pe2} = r_{pe2} - w_{pe22} \tag{28}$$

$$\dot{m}_{c2} = w_{c1} - w_{c2} \tag{29}$$

$$m_{f2} = m_{e2} + m_{h2} + m_{p2} \tag{30}$$

$$m_{s2} = m_{pe21} + m_{pe2} + m_{c2}, \tag{31}$$

where superscript rec indicates that a flow is coming from the recycle area. The outflows are controlled by a volume controller and a settling factor models the settling leg effect. To be able to calculate the grade defining split factors, the polymer mass in the loop reactor is divided into two states. First, m_{pe21} is the mass of polyethylene formed in the pre-polymerization reactor and second, m_{pe2} is the mass polyethylene formed in the loop reactor.

Similar to the pre-polymerization reactor, the reaction rates are extended non-linear Arrhenius expressions as

$$r_{e2} = R_{e2}(m_{c2}, a_2, X_{e2}, X_{h2}, P_2) \exp\left(\frac{k_{e21}}{T_2} + k_{e22}\right) \tag{32}$$

$$r_{h2} = R_{h2}(m_{c2}, a_2, X_{h2}, P_2) \exp\left(\frac{k_{h21}}{T_2} + k_{h22}\right) \tag{33}$$

$$r_{pe2} = r_{e2} + r_{h2}, \tag{34}$$

where P_2 and T_2 are the reactor pressure and temperature, respectively, k_{e21}, k_{e22}, k_{h21} and k_{h22} are reaction kinetics parameters and r_{pe2} is the total reaction rate in the loop reactor. The molar concentrations X_{i2} of fluids are found as,

$$X_{i2} = \frac{m_{i2}/M_i}{\sum\limits_{j\in\{e,h,p\}} m_{j2}/M_j}, \qquad i \in \{e, h, p\}, \tag{35}$$

where M_i and M_j are the molar weights of the different components.

The catalyst properties have non-linear dependencies on catalyst inflow and mass and total reaction rate, similar to the catalyst property models in the pre-polymerization reactor model, i.e.,

$$\dot{a}_2 = f_{a2}(w_{c1}, m_{c2}, a_2, d_2, a_1, d_1, r_{pe2}) \tag{36}$$

$$\dot{d}_2 = f_{d2}(w_{c1}, m_{c2}, a_2, d_2, a_1, d_1). \tag{37}$$

Modeling of the polymer density in the loop reactor could not be performed reliably due to lack of plant data. Therefore, the density was set to an average value ρ_{s2} of the loop polymer produced at the plant for different grades, yielding the instantaneous and bed average densities equal. As the polymer in the loop reactor is produced without any co-monomer, no branching of the polymer is present which results in a polymer density with only minor variations due to raw material concentrations. Thus, a constant value is justified. Fluid density may, as in the previous reactor, be calculated using an empirical relation and is used when calculating reactor content volume V_2 as

$$\rho_{f2} = \varrho_2(P_2, T_2, X_{e2}, X_{h2}, X_{p2}) \tag{38}$$

$$V_2 = \frac{m_{f2}}{\rho_{f2}} + \frac{m_{s2}}{\rho_{s2}}, \tag{39}$$

where m_{f2} and m_{s2} are total masses of fluids and solids, respectively.

As for the pre-polymerization reactor, the volumetric outflow is set by the total volumetric inflow, a volume contraction term due to polymerization, and a proportional controller with gain K_2 and set-point V_2^{ref} for obtaining correct stationary volume, i.e.,

$$
\begin{aligned}
q_2 = {} & \frac{u_{p2} + u_{e2} + u_{h2}}{\rho_{f2}} + \frac{w_{p2}^{\text{rec}} + w_{e2}^{\text{rec}} + w_{h2}^{\text{rec}}}{\rho_{f2}} \\
& + \frac{w_{s1}}{\rho_{s2}} + \frac{w_{f1}}{\rho_{f2}} - r_{pe2}\left(\frac{1}{\rho_{f2}} - \frac{1}{\rho_{s2}}\right) + K_2\left(V_2 - V_2^{\text{ref}}\right). \qquad (40)
\end{aligned}
$$

The volumetric outflow is composed of solid and fluid flows as

$$q_2 = \frac{w_{s2}}{\rho_{s2}} + \frac{w_{f2}}{\rho_{f2}}. \qquad (41)$$

As the loop reactor uses settling legs, the concentration of solids is higher in the outflow than in the reactor. The ratio of solid and fluid outflows is not equal to the ratio of solid and fluid masses in the reactor and is instead modeled using a settling factor $s_2 > 1$ and the mass fraction z_{s2} of solids in the reactor as,

$$
\begin{aligned}
w_{f2} &= w_{s2} g_2 && (42) \\
g_2 &= \frac{1 - s_2 z_{s2}}{s_2 z_{s2}}, && (43)
\end{aligned}
$$

where the mass fraction of solids is

$$z_{s2} = \frac{m_{s2}}{m_{s2} + m_{f2}}. \qquad (44)$$

Solving for solid and fluid flows in Eq. (41) and using Eq. (42) yields

$$
\begin{aligned}
w_{s2} &= \frac{1}{\dfrac{1}{\rho_{s2}} + \dfrac{g_2}{\rho_{f2}}} q_2 && (45) \\
w_{f2} &= \frac{g_2}{\dfrac{1}{\rho_{s2}} + \dfrac{g_2}{\rho_{f2}}} q_2. && (46)
\end{aligned}
$$

For a settling factor $s_2 = 1$, no settling of the polymer is present and the above equations degenerate to equations similar to the pre-polymerization reactor case. However, for the loop reactor, a settling factor of $s_2 > 1$ is used due to the settling legs.

The component-wise fluid and solid outflows used in the mass balances are found by the mass ratios of the reactor content and the fluid and solid outflows, i.e.,

$$
\begin{aligned}
w_{i2} &= \frac{m_{i2}}{m_{f2}} w_{f2}, \qquad i \in \{e, h, p\} && (47) \\
w_{j2} &= \frac{m_{j2}}{m_{s2}} w_{s2}, \qquad j \in \{pe, c\} && (48) \\
w_{pe21} &= \frac{m_{pe21}}{m_{s2}} w_{s2}. && (49)
\end{aligned}
$$

A model for the instantaneous melt index MI_2 of the loop reactor produced polymer, based on the work in [2], is used. The model has the structure

$$\ln MI_2 = l_{21} + \beta \ln\left(l_{22} + l_{23}\frac{X_{h2}}{X_{e2}}\right), \qquad (50)$$

where X_{h2} and X_{e2} are molar concentrations of hydrogen and ethylene, respectively, β is a constant approximately equal to 3.5, see [6] and l_{21}, l_{22} and l_{23} are model parameters. Following [2], the dynamics of the bed average melt index is found by mixing the current bed average with the melt index of the currently produced polymer as

$$\frac{d}{dt}\left(\overline{MI}_2^{-\frac{1}{\beta}}\right)\frac{m_{s2}}{w_{s2}} = -\overline{MI}_2^{-\frac{1}{\beta}} + MI_2^{-\frac{1}{\beta}}, \tag{51}$$

where the quotient m_{s2}/w_{s2} is the solid-phase residence time of the loop reactor.

Note that there is no modeling of the mixing of pre-polymerization reactor polymer and loop reactor polymer with regards to quality variables, motivated by the low production of polymer in the pre-polymerization reactor and similar reactor conditions. It is thus assumed that the polymer transferred out from the loop reactor have density and melt index equal to the density and melt index of the polymer produced in the loop reactor.

3.3 Gas-Phase Reactor

Except for the fluid components in the two previous reactors, the co-monomer butene and the diluent nitrogen are used in the GPR. The mass balances for the gases, polymer produced in either pre-polymerization reactor, loop reactor or GPR and catalyst and total masses of gas and polymer are given by

$$\begin{aligned}
\dot{m}_{e3} &= u_{e3} + w_{e3}^{\text{rec}} - w_{e3}^{\text{flare}} - w_{e3} - r_{e3} && (52)\\
\dot{m}_{h3} &= u_{h3} + w_{h3}^{\text{rec}} - w_{h3}^{\text{flare}} - w_{h3} - r_{h3} && (53)\\
\dot{m}_{b3} &= u_{b3} + w_{b3}^{\text{rec}} - w_{b3}^{\text{flare}} - w_{b3} - r_{b3} && (54)\\
\dot{m}_{p3} &= u_{p3} + w_{p3}^{\text{rec}} - w_{p3}^{\text{flare}} - w_{p3} + u_{p3}^{f} && (55)\\
\dot{m}_{n3} &= u_{n3} + w_{n3}^{\text{rec}} - w_{n3}^{\text{flare}} - w_{n3} && (56)\\
\dot{m}_{pe31} &= w_{pe21} - w_{pe31} && (57)\\
\dot{m}_{pe32} &= w_{pe22} - w_{pe32} && (58)\\
\dot{m}_{pe3} &= r_{pe3} - w_{pe33} && (59)\\
\dot{m}_{pb3} &= r_{pb3} - w_{pb33} && (60)\\
\dot{m}_{c3} &= w_{c2} - w_{c3} && (61)\\
m_{f3} &= m_{e3} + m_{h3} + m_{b3} + m_{p3} + m_{n3} && (62)\\
m_{s3} &= m_{pe31} + m_{pe32} + m_{pe3} + m_{pb3} + m_{c3}, && (63)
\end{aligned}$$

where w_{i3}^{flare} is the flare flow of component i, u_{p3}^{f} is the fixed propane flow assuring no leakage of GPR gas mixture to the flash tank and m_{pb3} is the mass of polyethylene with incorporated butene. The total solids outflow from the GPR is the production rate of the plant, i.e.,

$$w_{s3} = w_{pe31} + w_{pe32} + w_{pe33} + w_{pb33} + w_{c3}. \tag{64}$$

The reaction rates are analogous to the reaction rates in the two previous reactors, i.e.,

$$r_{e3} = R_{e3}(m_{c3}, a_3, X_{e3}, X_{h3}, X_{b3}, P_3) \exp\left(\frac{k_{e31}}{T_3} + k_{e32}\right) \tag{65}$$

$$r_{h3} = R_{h3}(m_{c3}, a_3, X_{h3}, P_3) \exp\left(\frac{k_{h31}}{T_3} + k_{h32}\right) \tag{66}$$

$$r_{b3} = R_{b3}(m_{c3}, a_3, X_{b3}, P_3) \exp\left(\frac{k_{b31}}{T_3} + k_{b32}\right) \tag{67}$$

$$r_{pe3} = r_{e3} + r_{h3} \tag{68}$$

$$r_3 = r_{pe3} + r_{b3}, \tag{69}$$

where P_3 and T_3 are the pressure and temperature, respectively, k_{e31}, k_{e32}, k_{h31}, k_{h32}, k_{b31} and k_{b32} are reaction kinetics parameters and r_3 is the total reaction rate in the GPR. The reaction rate of hydrogen is several magnitudes smaller than for ethylene and butene and it is assumed that all reacted hydrogen gives polyethylene without incorporated butene.

The catalyst property models are similar to the analogous in the prepolymerization and loop reactor models, i.e.,

$$\dot{a}_3 = f_{a3}(w_{c2}, m_{c3}, a_3, d_3, a_2, d_2, r_3) \tag{70}$$

$$\dot{d}_3 = f_{d3}(w_{c2}, m_{c3}, a_3, d_3, a_2, d_2), \tag{71}$$

and so is also the fluid molar concentrations X_{i3},

$$X_{i3} = \frac{m_{i3}/M_i}{\sum\limits_{j \in \{e,h,b,p,n\}} m_{j3}/M_j}, \qquad i \in \{e, h, b, p, n\}, \tag{72}$$

where M_i and M_j are molar weights of the different components.

The instantaneous split factors for the polymer in the GPR may be calculated directly from the different polymer masses as

$$S_1 = \frac{m_{pe31}}{m_{pe31} + m_{pe32} + m_{pe3} + m_{pb3}} \tag{73}$$

$$S_2 = \frac{m_{pe32}}{m_{pe31} + m_{pe32} + m_{pe3} + m_{pb3}} \tag{74}$$

$$S_3 = \frac{m_{pe3} + m_{pb3}}{m_{pe31} + m_{pe32} + m_{pe3} + m_{pb3}}, \tag{75}$$

and using the GPR solids residence time m_{s3}/w_{s3}, the bed average bi-modality measures are given by

$$\dot{\overline{S}}_1 \frac{m_{s3}}{w_{s3}} = -\overline{S}_1 + S_1 \tag{76}$$

$$\dot{\overline{S}}_2 \frac{m_{s3}}{w_{s3}} = -\overline{S}_2 + S_2 \tag{77}$$

$$\dot{\overline{S}}_3 \frac{m_{s3}}{w_{s3}} = -\overline{S}_3 + S_3. \tag{78}$$

The polymer in the GPR is essentially a mixture of loop produced polymer and polymer being produced in the GPR. Several mixing rules for polymers with different melt indices and densities exist and the most commonly used in literature are presented in [2] and will also be used here.

The instantaneous melt index of the mixed polymer is calculated from the bed average melt index $\overline{MI}_2$ of the incoming loop reactor polymer and the instantaneous melt index MI_3 of the polymer produced in the GPR as

$$MI_{\mathrm{mix}}^{-\frac{1}{\beta}} = (1 - S_3)\overline{MI}_2^{-\frac{1}{\beta}} + S_3 MI_3^{-\frac{1}{\beta}}. \tag{79}$$

MI_3 is modeled by following the structure in [2] as

$$\ln MI_3 = l_{31} + \beta \ln \left(l_{32} + l_{33} \frac{X_{h3}}{X_{e3}} + l_{34} \frac{X_{b3}}{X_{e3}} \right), \tag{80}$$

where l_{31}, l_{32}, l_{33} and l_{34} are model parameters. The bed average melt index $\overline{MI}_{\mathrm{mix}}$ of the mixed polymer in the GPR, i.e., the melt index of the final product, is found by mixing bed average melt index and instantaneous melt index of polymer added to the bed as

$$\frac{d}{dt}\left(\overline{MI}_{\mathrm{mix}}^{-\frac{1}{\beta}}\right)\frac{m_{s3}}{w_{s3}} = -\overline{MI}_{\mathrm{mix}}^{-\frac{1}{\beta}} + MI_{\mathrm{mix}}^{-\frac{1}{\beta}}. \tag{81}$$

The instantaneous density ρ_{mix} of the mixed polymer in the GPR is calculated as

$$\frac{1}{\rho_{\mathrm{mix}}} = \frac{1 - S_3}{\rho_{s2}} + \frac{S_3}{\rho_{s3}}, \tag{82}$$

where ρ_{s2} is the density of the polymer from the loop reactor and ρ_{s3} is the instantaneous density of polymer produced in the GPR. Again, using the model structure in [2], ρ_{s3} may be calculated as

$$\rho_{s3} = p_{31} + p_{32} \ln MI_3 - p_{33} \left(\frac{X_{b3}}{X_{e3}}\right)^{p_{34}}, \tag{83}$$

where p_{31}, p_{32}, p_{33} and p_{34} are model parameters. The bed average density $\overline{\rho}_{\mathrm{mix}}$ of the mixed polymer in the GPR is found from

$$\frac{d}{dt}\left(\frac{1}{\overline{\rho}_{\mathrm{mix}}}\right)\frac{m_{s3}}{w_{s3}} = -\frac{1}{\overline{\rho}_{\mathrm{mix}}} + \frac{1}{\rho_{\mathrm{mix}}}. \tag{84}$$

The gas density ρ_{f3} in the reactor is found by using the total reactor volume V_3 as

$$\rho_{f3} = \frac{m_{f3}}{V_3 - V_{s3}}, \tag{85}$$

where V_{s3} is the solids volume, i.e.,

$$V_{s3} = \frac{m_{s3}}{\overline{\rho}_{\mathrm{mix}}}, \tag{86}$$

and m_{f3} is the total mass of gas in the GPR. The reactor pressure is subsequently given by the ideal gas law as

$$P_3 = \frac{\rho_{f3} R T_3}{\overline{M}_3}, \tag{87}$$

where $\overline{M}_3$ is the mean molar weight of the gases, i.e.,

$$\overline{M}_3 = \frac{\sum\limits_{i \in \{e,h,b,p,n\}} m_{i3}}{\sum\limits_{j \in \{e,h,b,p,n\}} m_{j3}/M_j}, \tag{88}$$

and M_j is the molar weight of component j.

The partial pressures in the reactor are found by the reactor pressure and the molar concentrations as

$$P_{i3} = P_3 X_{i3}, \qquad i \in \{e, h, b, p, n\}. \tag{89}$$

The fluidized bed in the GPR is composed of both polymer and gas and its density depends on the gas velocity through the reactor. As the velocity is close to constant, and both ρ_{f3} and $\overline{\rho}_{\text{mix}}$ only have minor variations, the bed density ρ_{b3} is assumed constant in the model. The total bed volume V_{b3}, used for bed volume control in the model, is the sum of gas volume V_{fb3} in the bed and polymer volume V_{s3}, i.e.,

$$V_{b3} = V_{fb3} + V_{s3}. \tag{90}$$

The total mass of the fluidized bed, i.e., both polymer and gases, is

$$V_{b3}\rho_{b3} = V_{fb3}\rho_{f3} + V_{s3}\overline{\rho}_{\text{mix}} \tag{91}$$

and solving for gas volume in the bed yields

$$V_{fb3} = \frac{\overline{\rho}_{\text{mix}} - \rho_{b3}}{\rho_{b3} - \rho_{f3}} V_{s3}, \tag{92}$$

which may be used when calculating total bed volume.

The outflow from the GPR is at the bottom of the bed, and the ratio of solids and gas in the bed and the ratio of solids and gas in the outflow are thus equal. The volumetric outflow is set by a PI bed volume controller with set-point V_{b3}^{ref}, i.e.,

$$q_3 = K_3 \left(V_{b3} - V_{b3}^{\text{ref}}\right) + K_4 \int\limits_{-\infty}^{t} \left(V_{b3} - V_{b3}^{\text{ref}}\right) d\tau, \tag{93}$$

with proportional and integral gain K_3 and K_4, respectively. The mass outflows of solids and gas are found by using the volumetric outflow and the bed density as

$$w_{s3} = \frac{m_{s3}}{m_{s3} + V_{fb3}\rho_{f3}} \rho_{b3} q_3 \tag{94}$$

$$w_{f3} = \frac{V_{fb}\rho_{f3}}{m_{s3} + V_{fb}\rho_{f3}} \rho_{b3} q_3. \tag{95}$$

The component-wise bottom outflows are given by the mass ratios and the gas and solids outflows, i.e.,

$$w_{i3} = \frac{m_{i3}}{m_{f3}} w_{f3}, \qquad i \in \{e, h, b, p, n\} \tag{96}$$

$$w_{j3} = \frac{m_{j3}}{m_{s3}} w_{s3}, \qquad j \in \{pe, pb, c\} \tag{97}$$

$$w_{pe31} = \frac{m_{pe31}}{m_{s3}} w_{s3} \tag{98}$$

$$w_{pe32} = \frac{m_{pe32}}{m_{s3}} w_{s3}. \tag{99}$$

Similarly, the component-wise outflows in the flare flow u_{flare} of the top stream of the GPR are

$$w_{i3}^{\text{flare}} = \frac{m_{i3}}{m_{f3}} u_{\text{flare}}, \qquad i \in \{e, h, b, p, n\}. \tag{100}$$

4. Distillation Column Models

Modeling of distillation columns may be made very detailed. However, even these detailed models will not describe the recycle area completely since there is also an extensive overlaying control system of the columns and also e.g., pre-condensers and different transport systems for the gas needed to be modeled. The columns also have 3–5 inflow components and the propane column has a side flow, which comprise an even greater modeling task. Additionally, similar to the reactors, a high level of detailed modeling of the distillation columns are not feasible if the models are to be used for optimization.

Two of the most important aspects of recycle area modeling are to estimate how much of the total inflow of components to the reactors are recycle flows and how the recycle flows change when the plant operating point is changed. For instance, approximately half of all hydrogen to the loop reactor is recycled hydrogen and even more for the GPR. Additionally, the recycled part of total butene inflow to the GPR is comparable in size to the fresh feed.

The structure chosen for the recycle area model is similar to the one used in the off-line planning and optimization models currently in use by Borealis AB cracker plant, see [1]. It is assumed that pressures and temperatures in the columns are perfectly controlled, which thus gives constant split factors for the components. Every distillation column together with its control system and supporting components such as pre-condensers, are lumped together to one system where the dominating time constant for each component flow into the system is estimated from measurement data. However, the measurement data could not give a complete mass balance over each system due to lack of sensors and insufficient data quality, and could therefore not support modeling of different time constants for e.g. top, side, and bottom flows of the columns. A crude approximation was made by setting these equal.

Two control flows are present in the recycle area, i.e., the off-gas flows u_{op} and u_{ol} on the propane and lights column, respectively.

4.1 Propane Column

The overall propane column system is modeled as described above, and each component has an associated time constant T_{i4} as,

$$\dot{w}_{i4} T_{i4} = -w_{i4} + w_{i3}, \quad i \in \{e, h, b, p, n\}, \tag{101}$$

Table 2 Propane and lights column split factors.

	i	e	h	b	p	n
Propane Column	Top, S_{i4}^t	0.88	1	0.13	0.35	1
	Side, S_{i4}^s	0.09	0	0	0.44	0
	Bottom, S_{i4}^b	0.03	0	0.87	0.21	0
Lights Column	Top, S_{i6}^t	1	1	-	0.1	-
	Bottom, S_{i6}^b	0	0	-	0.9	-

where w_{i3} is the component flow from the GPR. The resulting flows are then divided into the different outtake flows of the system, i.e., top, side and bottom flow, as

$$w_{i4}^t = S_{i4}^t w_{i4} \tag{102}$$

$$w_{i4}^s = S_{i4}^s w_{i4} \tag{103}$$

$$w_{i4}^b = S_{i4}^b w_{i4}, \tag{104}$$

where S_{i4}^t, S_{i4}^s and S_{i4}^b are the component split factors for top, side and bottom, respectively, and are found in Table 2. It is assumed that the light components hydrogen and nitrogen are only present at column top. The heaviest component, i.e., butene, is present at both top and bottom, but not side. Some butene is condensed together with light components in the pre-condenser and added to the top flow back to the GPR, while the column itself is assumed to distill butene only to the bottom. The two remaining components, i.e., propane and ethylene, are present in all outtakes.

The off-gas flow u_{op} is taken from the top flow and may be used for control purposes since this flow has a higher concentration of light components than the gas in the GPR. The component-wise recycle flows back to the GPR, i.e., w_{i3}^{rec}, are thus,

$$w_{i3}^{\text{rec}} = w_{i4}^t + w_{i4}^b - w_{i4}^{op}, \quad i \in \{e, h, b, p, n\}, \tag{105}$$

where the component-wise off-gases are

$$w_{i4}^{op} = \frac{w_{i4}^t}{\sum\limits_{j \in \{e,h,b,p,n\}} w_{j4}^t} u_{op}, \quad i \in \{e, h, b, p, n\}. \tag{106}$$

The side flows w_{i4}^s are led to the heavies column for further processing.

4.2 Heavies Column

Since the reactor models do not include the production of heavier components such as pentane, hexane, etc., and oligomers, the bottom flow of the heavies column is assumed to be zero, and all inflow components are distilled to the column top. This assumption yields that no split factors are needed for the heavies column and the component flows are

$$\dot{w}_{i5} T_{i5} = -w_{i5} + w_{i2} + w_{i4}^s, \quad i \in \{e, h, p\}, \tag{107}$$

where w_{i2} and w_{i4}^s are the component flows from the loop reactor and the propane column, respectively, and T_{i5} is the associated time constant of the component. Since it is assumed that all nitrogen and butene in the propane column are recycled directly back to the GPR, the heavies column model incorporates only ethylene, hydrogen and propane.

4.3 Lights Column

The only inflow to the lights column is from the heavies column and it is therefore only necessary to model ethylene, hydrogen and propane. With measurement data support, it is assumed that the majority of propane is distilled to the column bottom, while all lighter components are distilled to the column top.

The model structure is similar to the propane column model, using an associated time constant and split factors for each component as

$$\dot{w}_{i6}T_{i6} = -w_{i6} + w_{i5} \tag{108}$$

$$w_{i6}^t = S_{i6}^t w_{i6} \tag{109}$$

$$w_{i6}^b = S_{i6}^b w_{i6}, \tag{110}$$

where $i \in \{e, h, p\}$. The split factors for the three different components are found in Table 2. The recycle inflow to the loop reactor is the top flow from the lights column except for the off-gas flow u_{ol}, which may be used for control purposes since the light component concentration is high in the recycle flow compared to the concentration in the loop reactor. The component-wise recycle flows are thus

$$w_{i2}^{\text{rec}} = w_{i6}^t - w_{i6}^{ol}, \quad i \in \{e, h, p\} \tag{111}$$

with the component-wise off-gas flows

$$w_{i6}^{ol} = \frac{w_{i6}^t}{\sum\limits_{j \in \{e,h,p\}} w_{j6}^t} u_{ol}, \quad i \in \{e, h, p\}. \tag{112}$$

5. Model Form and Size

If a state, algebraic variable and input vector are defined and denoted $\mathbf{x}$, $\mathbf{w}$ and $\mathbf{u}$, respectively, the plant model may be written as a general non-linear index-1 differential-algebraic equation (DAE) as

$$\begin{aligned} \mathbf{0} &= \mathbf{F}\left(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{w}, \mathbf{u}\right) \\ \mathbf{x}(t_0) &= \mathbf{x}_0, \end{aligned} \tag{113}$$

where $\mathbf{x}_0$ is the initial state. The number of states, algebraic variables and inputs are 46, 167 and 15, respectively.

6. References

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