Modeling and Optimization of Grade Changes for Multistage Polyethylene Reactors

Larsson, Per-Ola; Åkesson, Johan; Haugwitz, Staffan; Andersson, Niklas

2010

Modeling and Optimization of Grade Changes for Multistage Polyethylene Reactors

Per-Ola Larsson, Johan Åkesson, Staffan Haugwitz, Niklas Andersson

I. Introduction

Polyethylene reactors are today able to produce different grades by manipulating inflows of raw material. It is imperative for polyethylene manufacturers to change product grades to increase their profitability as market demands change, but also due to market competition and raw material pricing. During grade transitions it is of importance that production of off-specification material, raw material and time is minimized. We present an optimization procedure for grade change of a Borstar® polyethylene plant.

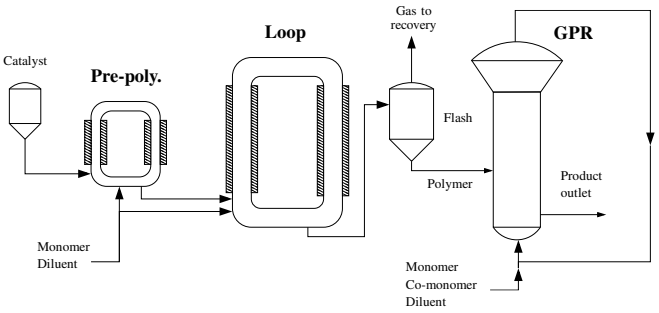

Fig. 1. Reactor chain of a Borstar® process: Pre-polymerization, Loop, and Gas phase reactor (GPR).

II. Plant Modeling

The Borstar® polyethylene plant at Borealis AB incorporates two slurry reactors, pre-polymerisation and loop reactor, and a gas phase reactor, see Figure 1. The model of the plant includes both first principles, semi-empirical, and empirical relations. A total of 12 inputs flows, denoted $\mathbf{u}$, are available at optimization and outputs such as masses of both fluid and solid components, reaction rates, instantaneous and bed averaged component concentrations, split factor, catalyst and polymer properties, denoted $\mathbf{y}$, can be used. Together with algebraic variables $\mathbf{w}$, the model can be written in the general non-linear index 1 differential algebraic equation form

$$\begin{aligned} \mathbf{0} &= F(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{w}, \mathbf{u}) \\ \mathbf{y} &= g(\mathbf{x}, \mathbf{w}, \mathbf{u}). \end{aligned} \tag{1}$$

and contains approximately 70 differentiated variables, 180 algebraic variables and 250 equations.

Sponsored by the Swedish Foundation of Strategic Research in the framework of Process Industry Centre at Lund University (PICLU).

P. Larsson and J. Åkesson are with the Department of Automatic Control, Lund University, Lund, Sweden, {perola|jakesson}@control.lth.se.

S. Haugwitz is with Borealis AB, Stenungsund, Sweden, Staffan.Haugwitz@borealisgroup.com.

N. Andersson is with the Department of Chmical Engineering, Lund University, Lund, Sweden. niklas.andersson@chemeng.lth.se.

Modelica, a high level language for encoding of complex physical systems, is used for plant modeling. The Optimica extension, see [1], gives constructs for cost functions, constraints and mechanisms to select inputs and parameters to optimize. Using JModelica.org, an open source project targeted at dynamic optimization, see [2], the optimization problem is translated into a non-linear programming problem using collocation on finite elements and solved using the large-scale NLP solver IPOPT [3].

III. Optimal Grade Transition

The grade transition example will change conditions in all three reactors and corresponds to two grades currently produced at Borealis AB. The main objectives are to change raw material concentrations and concentration ratios, split factor, and production rates. At transition start and end time, i.e., t_1 and t_2, the plant fulfills the static non-linear equations

$$\begin{aligned} \mathbf{0} &= F(\mathbf{0}, \mathbf{x}^\circ, \mathbf{w}^\circ, \mathbf{u}^\circ) \\ \mathbf{y}^\circ &= g(\mathbf{x}^\circ, \mathbf{w}^\circ, \mathbf{u}^\circ), \end{aligned} \tag{2}$$

which corresponds to Eq. (1) when all derivatives equal 0 and superscript $^\circ$ indicate constant value. Initial and end conditions of the transition for states, inflows and algebraic variables are given by solving the non-linear equations in Eq. (2), i.e., a DAE initialization problem is posed and contains approximately 280 equality constraints and 290 variables, of which 180 are algebraic and 230 have both upper and lower limits. Solving the NLP takes less than 10 seconds per grade.

A quadratic cost function that includes deviations from the grade to be are used, giving the possibility to emphasize the importance of different variables. Also the deviation from inflows yielding the new grade in stationarity will be used, removing too large over- and undershoots. Introducing the deviation vectors

$$\Delta\mathbf{u} = \mathbf{u} - \mathbf{u}_2 \qquad \Delta\mathbf{y} = \mathbf{y} - \mathbf{y}_2,$$

where $\mathbf{u}_2$ and $\mathbf{y}_2$ are inputs and outputs defining the new grade solved for in the DAE initialization problem, the dynamic grade transition optimization problem can be formulated as

$$\min_{\mathbf{u}} \int_{t_1}^{t_2} \begin{bmatrix} \Delta\mathbf{y} \\ \Delta\mathbf{u} \\ \dot{\mathbf{u}} \end{bmatrix}^T \begin{bmatrix} \mathbf{Q}_{\Delta\mathbf{y}} & 0 & 0 \\ 0 & \mathbf{Q}_{\Delta\mathbf{u}} & 0 \\ 0 & 0 & \mathbf{Q}_{\dot{\mathbf{u}}} \end{bmatrix} \begin{bmatrix} \Delta\mathbf{y} \\ \Delta\mathbf{u} \\ \dot{\mathbf{u}} \end{bmatrix} dt \tag{3}$$

$$\begin{aligned} \text{subj. to} \quad & \mathbf{0} = F(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{w}, \mathbf{u}), \quad \mathbf{y} = g(\mathbf{x}, \mathbf{w}, \mathbf{u}) \\ & \mathbf{y}_{\min} \le \mathbf{y} \le \mathbf{y}_{\max}, \quad \mathbf{u}_{\min} \le \mathbf{u} \le \mathbf{u}_{\max} \\ & \mathbf{w}_{\min} \le \mathbf{w} \le \mathbf{w}_{\max}, \quad \dot{\mathbf{u}}_{\min} \le \dot{\mathbf{u}} \le \dot{\mathbf{u}}_{\max}, \end{aligned}$$

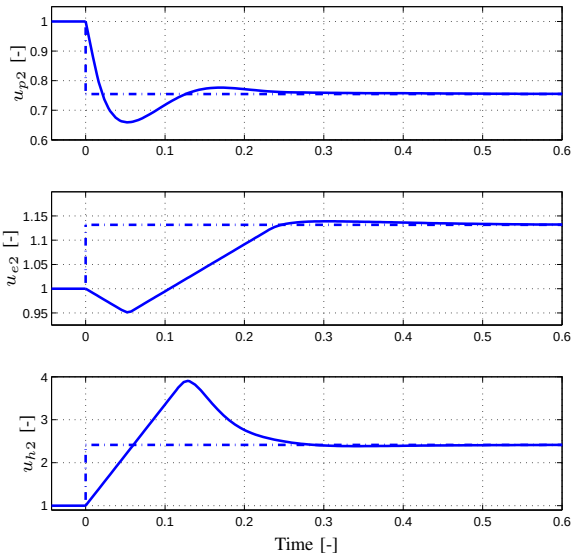

Fig. 2. Scaled optimal inflows to loop reactor at grade transition – propane u_{p2}, ethylene u_{e2} and hydrogen u_{h2}.

where also a cost of inflow derivatives is added such that smoothness of inflows can be controlled. The weights $\mathbf{Q}_{\Delta \mathbf{y}}$, $\mathbf{Q}_{\Delta \mathbf{u}}$ and $\mathbf{Q}_{\dot{\mathbf{u}}}$ are chosen diagonal for simplicity and the initial state of the plant is defined by the solution of the DAE initialization problem.

Over- and undershoots are accepted up to a certain limit for the instantaneous concentrations and ratios. However, for the bed average concentrations and ratios and the split S, no over- or undershoots are accepted in the grade change. The constraints on the algebraic variables $\mathbf{w}$ are for instance limits on volumes, component masses, and pressure, while constraints on inflows, both magnitudes and rates of changes, concern physical limits such as e.g., pump capacities.

After discretization, the NLP problem contains about 20.000–200.000 variables depending on number of elements and collocation points. Initial trajectories can be generated in JModelica.org via simulation using SUNDIALS, see [4], with inflows ramping from initial to end values found in the DAE intialization problem. With an Intel® Core™2 Duo CPU@3.00GHz, a solution is obtained in 5-90 minutes depending on number of variables and initial values.

Figures 2–3 show the resulting optimal inflows, component concentrations, and production rate of the loop reactor and the split factor between the loop reactor and GPR. Note the scaling, i.e., the transition is 1 time unit and all variables have initial value 1.

Since the production rate Q_2 is to be increased, the inflow of ethylene is increased in total and at the same time inflow of the diluent propane is decreased as shown in Figure 2. This results in a longer hold up time of the polymer and thus also a larger mass of polymer in the loop. The concentrations of ethylene and hydrogen in the loop are higher in the new grade and the decrease of diluent is not enough for the hydrogen specification to be met. Thus, the inflow of hydrogen is increased and to reach the specification of the hydrogen-ethylene ratio rapidly, the inflow of ethylene is initially

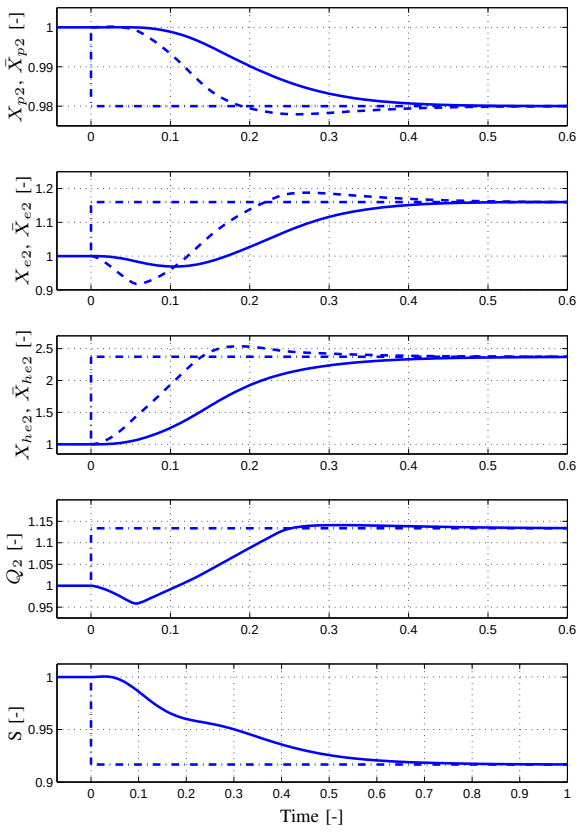

Fig. 3. Scaled key parameters for loop reactor and split factor at grade transition. Bed averaged (solid) and instantaneous (dashed) ethylene conc. $\bar{X}_{e2}$, X_{e2}, propane conc. $\bar{X}_{p2}$, X_{p2}, hydrogen-ethylene conc. ratios $\bar{X}_{he2}$, X_{he2}, production rate Q_2, split factor S.

decrased. Note that both the inflow of ethylene and hydrogen have their derivative constraints active in the beginning, seen by the linear decrease and increase. From Figure 3 it is seen that the over- or undershoot constraints on the averaged concentrations and ratios are obeyed and the instantaneous measures have over- or undershoots. The split, see Figure 3, which indirectly depends on the production rates in both loop and gas phase reactor, is decreased by lowering production rate in the GPR, i.e., decreasing the ethylene inflow to the gas phase reactor. The transition in loop reactor is completed after 0.5 time units. Similar trajectories for key parameters and inflows are available for the pre-polymerization and gas phase reactor.

References

[1] J. Åkesson, "Optimica—An Extension of Modelica Supporting Dynamic Optimization," in *In 6th International Modelica Conference 2008*. Modelica Association, Mar. 2008.

[2] J. Åkesson, K.-E. Årzén, M. Gäfvert, T. Bergdahl, and H. Tummescheit, "Modeling and optimization with optimica and jmodelica.org-languages and tools for solving large-scale dynamic optimization problem," *Computers and Chemical Engineering*, Jan. 2010, doi:10.1016/j.compchemeng.2009.11.011.

[3] A. Wächter and L. T. Biegler, "On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming." *Mathematical Programming*, vol. 106, no. 1, pp. 25–58, 2006.

[4] C. f. A. S. C. Lawrence Livermore National Laboratory, "SUNDIALS (SUite of Nonlinear and DIfferential/ALgebraic equation Solvers)," 2009, https: //computation.llnl.gov/casc/sundials/main.html.