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Modeling and Optimization of Grade Changes for a Polyethylene Reactor

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1. INTRODUCTION

In polymer industry, as in many other industries, there exist a problem of increasing the capital productivity while the market competition has increased the last decades. Manufacturers are forced to switch between different polymer grades to suit market demand, that is, running product campaigns on the same plant. It is important that the transitions are made in a way such that off-specification polymer is minimized at a low economical cost, van Brempt et al. (2004).

In this paper we will, using the Modelica and Optimica language, optimize a grade change for a polyethylene reactor.

2. MATHEMATICAL PLANT MODEL

The reactor considered is the first reactor in a Borstar® process, see Figure 1. Modeling a reactor is a task including both theoretical, but also empirical, challenges and has been accomplished at Borealis AB. Inputs used in the model are flows of propane, ethylene, and hydrogen, while several outputs such as masses, concentrations and densities are available as outputs.

The main equations of a reactor model includes material balances and non-linear equations for reaction kinetics, catalyst properties, and densities. The resulting model used for the grade change optimization can be written in the general non-linear differential algebraic form

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

where x is the internal state, w algebraic variables, u inputs, and y outputs.

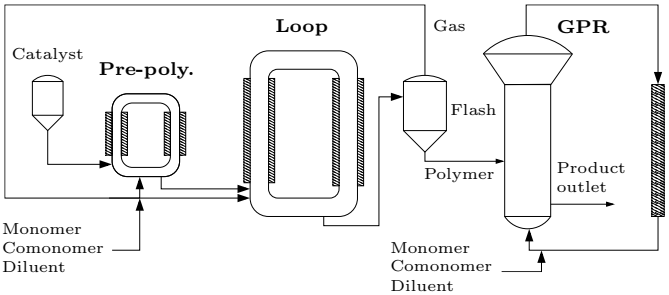

Fig. 1. Reactor chain of a Borstar® process

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3. MODELING LANGUAGES AND TOOLS

The Modelica modeling language is used to express the mathematical model of the reactor. Text-book style declarative equations can be expressed as well as acausal component connections representing physical interfaces, and differential and algebraic equations may be mixed resulting in differential algebraic equations. In order to strengthen the optimization capabilities of Modelica, the Optimica extension has been proposed, see Åkesson (2008). Optimica adds to Modelica a small number of constructs, enabling the user to conveniently specify dynamic optimization problems based on Modelica models.

JModelica.org is a novel Modelica-based open source project targeted at dynamic optimization, see Åkesson et al. (2009), and features compilers supporting code generation of Modelica/Optimica models to C, a C API for evaluating model equations and their derivatives and optimization algorithms. The platform contains an implementation of a simultaneous optimization method based on orthogonal collocation on finite elements, see Biegler et al. (2002).

4. OPTIMAL GRADE TRANSITION

The grade transition considered includes three main objectives,

(1) Increase production rate y_r by 20%.
(2) Increase hydrogen-ethylene ratio y_{he} by 20%.
(3) Keep amount of polymer in reactor y_s within specified bounds during grade transition.

which should be met using the following control variables,

u_p = propane input flow
u_e = ethylene input flow
u_h = hydrogen input flow.

Constraints on the inflows and their derivatives are set due to limitations on actuators and safety precautions.

The first step in the grade change solution procedure is to find the two stationary points corresponding to the two grades. These are initial value problems of the DAE, i.e., for $t = t_0$ and $t = t_f$ the system fulfills the static equations

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

for different values of the variables. The resulting NLP program contains approximately around 200 variables and is solved rapidly in the JModelica.org framework.

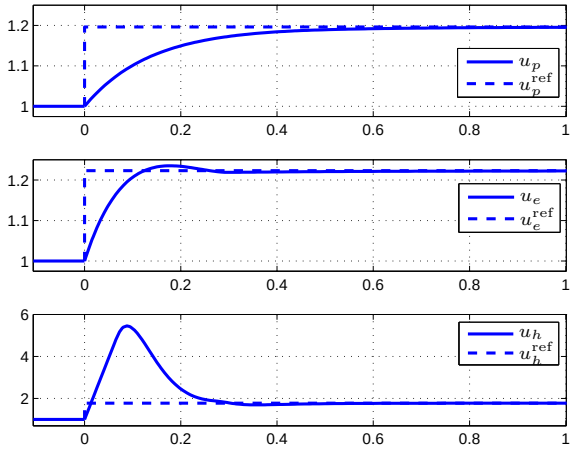

Fig. 2. Scaled optimal input flows at grade transition – propane u_p, ethylene u_e and hydrogen u_h.

In the dynamic optimization problem, the optimal transition trajectories between the two grades are found.

A quadratic cost function is constructed that includes deviations from the end grade specifications and inflows, and also inflow derivatives giving an option to control the smoothness of the input signals. With the reference vectors

$$y^{\text{ref}} = \begin{bmatrix} y_s^{\text{ref}} & y_r^{\text{ref}} & y_{he}^{\text{ref}} \end{bmatrix}^T, \quad u^{\text{ref}} = \begin{bmatrix} u_p^{\text{ref}} & u_e^{\text{ref}} & u_h^{\text{ref}} \end{bmatrix}^T,$$

comprising the stationary solution of the end grade, and the diagonal weighting matrices $Q_{\Delta y}$, $Q_{\Delta u}$ and $Q_{\dot{u}}$, the optimal control problem representing the transition can be formulated as

$$\min_{u_p,u_e,u_h} = \int_{t_0}^{t_f} \begin{bmatrix} \Delta y \\ \Delta u \\ \dot{u} \end{bmatrix}^T \begin{bmatrix} Q_{\Delta y} & 0 & 0 \\ 0 & Q_{\Delta u} & 0 \\ 0 & 0 & Q_{\dot{u}} \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta u \\ \dot{u} \end{bmatrix} dt \qquad (3)$$

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

where the deviation vectors are defined as

$$\Delta y = y - y^{\text{ref}}, \quad \Delta u = u - u^{\text{ref}},$$

and the initial values at time $t = t_0$ are defined by the steady state solution in Eq. (2).

Using the JModelica.org framework and the Modelica model resulted in an NLP problem containing approximately 20.000–40.000 variables depending on collocation point selection. Using an Intel® Core™2 Duo CPU@3.00GHz, a solution is obtained in about 5–30 minutes depending on number of variables and initial values.

Figures 2–4 show the resulting optimal trajectories for the grade transition problem. Note that the trajectories have been scaled, either such that initial value is 1 or by constraint. Both inflows u and controlled outputs y tend to the desired reference values specified by the static optimization problem while all constraints are fulfilled.

5. FUTURE WORK

Due to the modularity of the Modelica language, the optimization problem can easily be extended to the full Borstar® process. Successfull attempts at performing a grade change for all three reactors using up to 12 different inflows has been done. Future work include reactor model calibration using measurements and modeling of distillation towers for recycling of outflows.

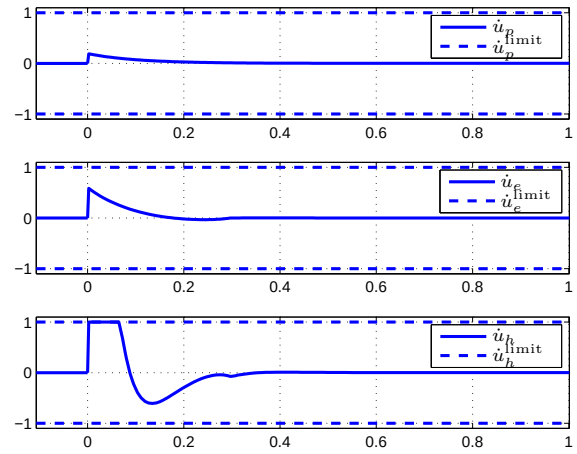

Fig. 3. Scaled time derivatives of optimal input flows at grade transition – propane $\dot{u}_p$, ethylene $\dot{u}_e$ and hydrogen $\dot{u}_h$.

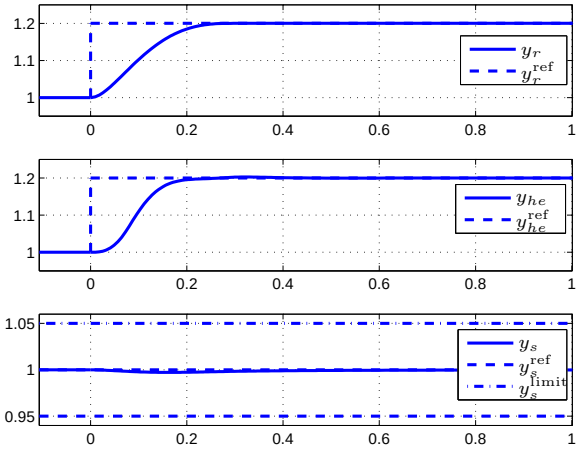

Fig. 4. Scaled optimal outputs at grade transition – mass of polymer in reactor y_s, reaction rate y_r and hydrogen-ethylene ratio y_{he}.

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