Model-Based Optimization of Economical Grade Changes for the Borealis Borstar® Polyethylene Plant

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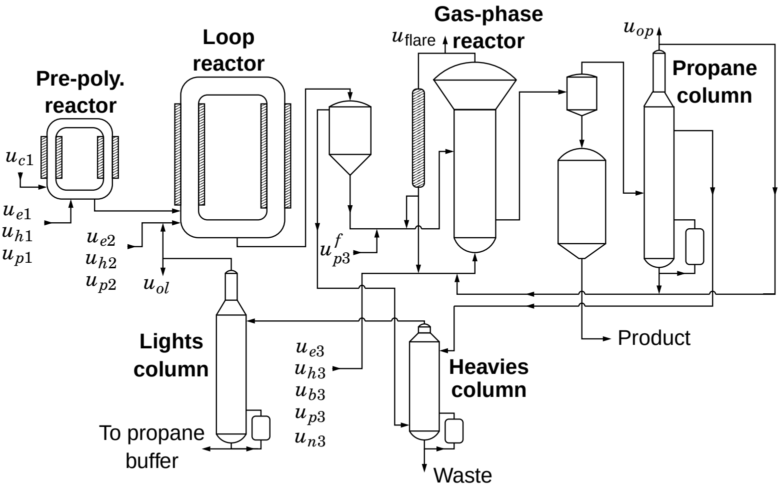
Background

- Polyethylene
  - Most widely used plastic in the world
  - Several different grades, i.e., types
  - Specified by quality variables:
    - density
    - melt index
    - molecular weight distribution
    - ...
- Why Grade Changes?
  - Market demands
  - Raw material and product pricing
  - Technology supports several grades
- How to Perform a Grade Change
  - Manipulate inflows of raw material in a continuous manner
    - No “stop-and-go”
  - Desired: Economically optimal
  - Obey safety and constraints on e.g., flows, conc., grades.

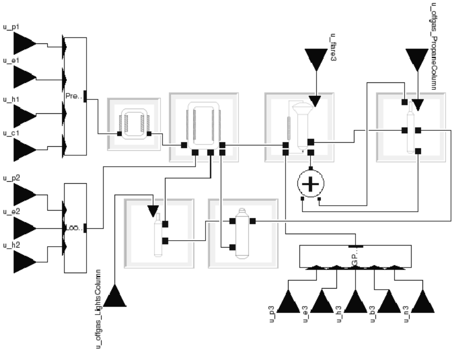
PE3 at Borealis AB, Stenungsund



- Inflows: catalyst, ethylene, hydrogen, propane and nitrogen
- Outflows: propane, off-gases, flare, product, (and waste)

Modelica Model and Model Size

- Modelica library constructed



- Number of
  - states $\mathbf{x}$: 46
  - algebraic variables $\mathbf{w}$: 167
  - inputs $\mathbf{u}$: 15
  - equations in $\mathbf{F}(\cdot)$: 213
  - quality variables $\mathbf{y}$: 7
  - operational variables $\mathbf{z}$: 2

$$\mathbf{0} = \mathbf{F}\left(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{w}, \mathbf{u}\right)$$

$$\mathbf{y} = \mathbf{g}_{\mathbf{y}}\left(\mathbf{x}, \mathbf{w}, \mathbf{u}\right)$$

$$\mathbf{z} = \mathbf{g}_{\mathbf{z}}\left(\mathbf{x}, \mathbf{w}, \mathbf{u}\right)$$

$$\mathbf{x}(t_0) = \mathbf{x}_0$$

Grade Definitions and Prices/Costs

Grade	$\overline{X}_{he1}$	$\overline{MI}_2$	$\overline{MI}_{\text{mix}}$	$\overline{\rho}_{\text{mix}}$	$\overline{S}_1$	$\overline{S}_2$	$\overline{S}_3$	E_j
A	1.00	1.00	1.00	1.000000	1.000	1.000	1.000	1.24
B	0.37	6.50	3.51	1.001065	1.000	1.132	0.917	1.46
$\pm\%$	± 5	± 5	± 5	± 0.1	± 0.5	± 0.5	± 0.5	-

- Grade definitions have *target values* and *intervals*.
- Inside intervals = *on-grade* $\Rightarrow$ sell price E_j.
- Outside intervals = *off-grade* $\Rightarrow$ sell price E_{off}.
- Costs C_i of inflows, offgas sell price E_{og} and off-grade polymer sell price E_{off}.

C_c	C_e	C_h	C_b	C_p	C_n	E_{og}	E_{off}
214.6	1.000	8.003	1.419	0.501	0.044	0.266	0.880

Stationary Optimization Problem

- Instantaneous profit R_j in stationarity production of grade j

$$R_j = \overbrace{E_j w_{s3}}^{\text{production revenue}} + \overbrace{E_{og} u_{ol} + E_{og} u_{op}}^{\text{offgas revenue}} + \overbrace{C_p w_{p6}^b}^{\text{propane revenue}}$$
$$\underbrace{- \sum_{i \in \{c,e,h,p\}} C_i u_{i1} - \sum_{i \in \{e,h,p\}} C_i u_{i2} - \sum_{i \in \{e,h,b,p,n\}} C_i u_{i3} - C_p u_{p3}^f}_{\text{inflow costs}}$$

- Optimization problem solved using JModelica.org

$$\max_{\dot{\mathbf{x}},\mathbf{x},\mathbf{w},\mathbf{u}} R_j$$
$$\text{s.t. } \mathbf{0} = \mathbf{F}(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{w}, \mathbf{u}) \quad \text{(dynamics)}$$
$$\mathbf{y}_j = \mathbf{g}_{\mathbf{y}}(\mathbf{x}, \mathbf{w}, \mathbf{u}) \quad \text{(on specification)}$$
$$\mathbf{z}_j = \mathbf{g}_{\mathbf{z}}(\mathbf{x}, \mathbf{w}, \mathbf{u}) \quad \text{(pressures in GPR)}$$
$$\dot{\mathbf{x}} = \mathbf{0} \quad \text{(stationarity)}$$
$$\mathbf{x}_{\text{min}} \leq \mathbf{x} \leq \mathbf{x}_{\text{max}}, \mathbf{w}_{\text{min}} \leq \mathbf{w} \leq \mathbf{w}_{\text{max}}, \ \mathbf{u}_{\text{min}} \leq \mathbf{u} \leq \mathbf{u}_{\text{max}}$$

Stationary Optimization – Some results

- Specifications on grade variables sets reactant ratios.
- Profitable to produce $\Rightarrow$ production level at maximum.
- Off-gases at minimum and flare closed.
- Minimizes expensive components in off-gases.
- Gives economically optimal operating points for grade j.

Dynamic Optimization – Ideal Profit

- Ideal instantaneous profit R_j for grade j

$$R_j = \overbrace{\big((E_j - E_{\text{off}})\theta_j(\mathbf{y}) + E_{\text{off}}\big)}^{\text{Effective sell price}} w_{s3} + E_{og}u_{ol} + E_{og}u_{op} + C_p w_{p6}^b - \sum_{i\in\{c,e,h,p\}} C_i u_{i1} - \sum_{i\in\{e,h,p\}} C_i u_{i2} - \sum_{i\in\{e,h,b,p,n\}} C_i u_{i3} - C_p u_{p3}^f,$$

where $\theta_j(\mathbf{y})$ is the ideal on-grade function for grade j

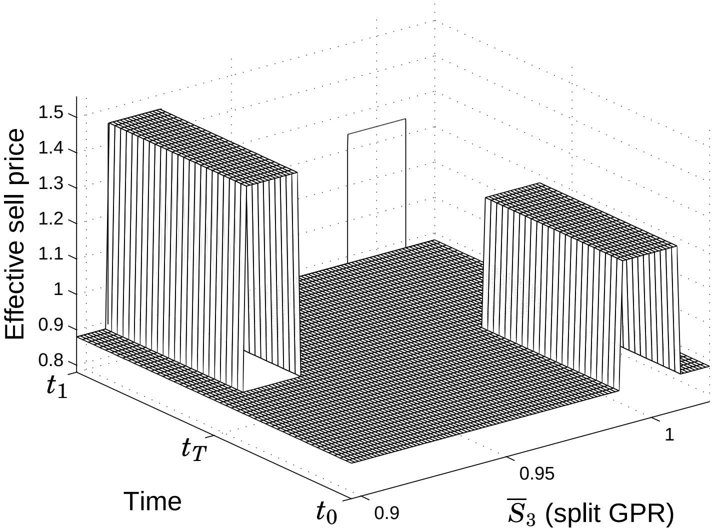
$$\theta_j(\mathbf{y}) = \begin{cases} 1 & \text{if } y_{ji}^{\text{min}} \le y_i \le y_{ji}^{\text{max}}, \quad i \in \{1, \ldots, 7\} \\ 0 & \text{otherwise,} \end{cases}$$

- Define a time interval $[t_0,\ t_1]$ and a transition time t_T

$$R = \begin{cases} R_{\text{A}}, & t_0 \le t \le t_T \\ R_{\text{B}}, & t_T < t \le t_1. \end{cases}$$

- Goal: Maximize cumulative profit $V_{\text{eco}} = \int_{t_0}^{t_1} R\, dt.$

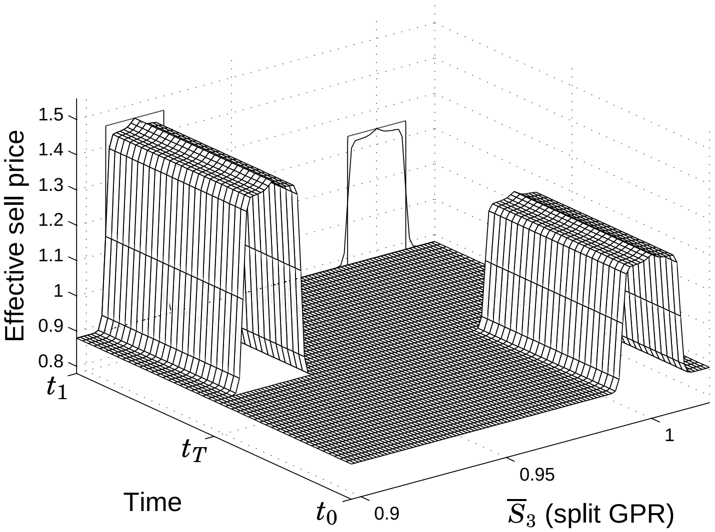
Ideal Effective Sell Price – Visualization



Dynamic Optimization – Difficulties and a Solution

- Difficulties
  - Cost function is *not differentiable.*
  - Might be optimal to be on quality variable *interval border*.
  - Desired to be *on-target* with grade variables.
  - Desired to be *on-target* with operational variables.
- A solution
  - *Smooth* approximation of ideal on-grade function $\theta_j(\mathbf{y})$.
  - *Economical* incentives, i.e., “price peaks” at target values.
  - Rational function of
    - grade variables
    - target values
    - grade intervals
  - Parameters in rational function control
    - Smoothness
    - Price peak

Smooth approximation with peaks – Visualization



Dynamic Optimization Problem

$$\max_{\dot{\mathbf{u}}} \int_{t_0}^{t_1} \left(\tilde{R} - \dot{\mathbf{u}}^T \mathbf{U}_d \dot{\mathbf{u}} \right) \, dt$$

$$\text{s.t. } \mathbf{0} = \mathbf{F}(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{w}, \mathbf{u}), \; \mathbf{u} = \int_{t_0}^{t} \dot{\mathbf{u}} \, d\tau$$

$$\mathbf{y} = \mathbf{g}_{\mathbf{y}} (\mathbf{x}, \mathbf{w}, \mathbf{u})$$

$$\mathbf{z} = \mathbf{g}_{\mathbf{z}} (\mathbf{x}, \mathbf{w}, \mathbf{u})$$

$$\mathbf{x}_{\text{min}} \leq \mathbf{x} \leq \mathbf{x}_{\text{max}}, \quad \mathbf{w}_{\text{min}} \leq \mathbf{w} \leq \mathbf{w}_{\text{max}}$$

$$\mathbf{u}_{\text{min}} \leq \mathbf{u} \leq \mathbf{u}_{\text{max}}, \quad \mathbf{y}_{\text{min}} \leq \mathbf{y} \leq \mathbf{y}_{\text{max}}$$

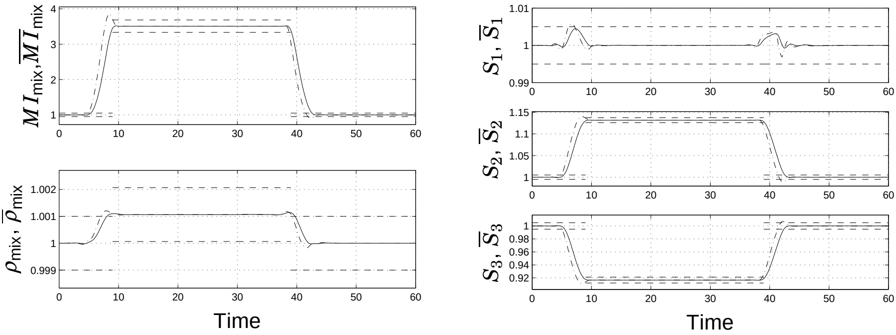
$$\mathbf{z}_{\text{min}} \leq \mathbf{z} \leq \mathbf{z}_{\text{max}}, \quad \dot{\mathbf{u}}_{\text{min}} \leq \dot{\mathbf{u}} \leq \dot{\mathbf{u}}_{\text{max}}$$

$$\mathbf{x}(t_0) = \mathbf{x}_s, \quad \mathbf{u}(t_0) = \mathbf{u}_s$$

$$\mathbf{u} = \mathbf{u}_e, \quad t_1 - T_c \leq \; t \leq t_1$$

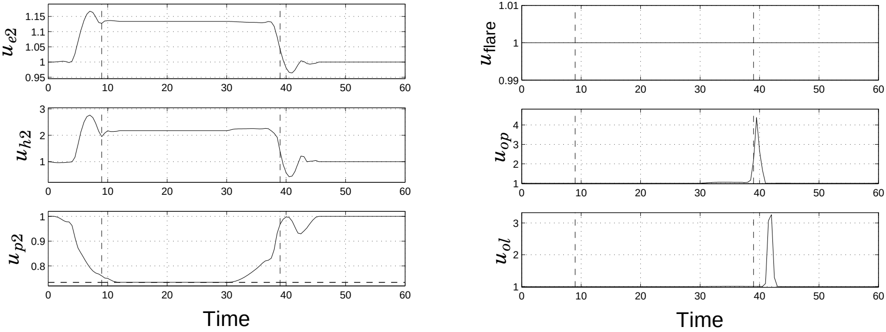
- Control flow derivatives $\dot{\mathbf{u}}$ as decision variables.
- $\dot{\mathbf{u}}^T \mathbf{U}_d \dot{\mathbf{u}}$ penalizing highly varying control flows.
- Control flows fixed at an end interval, avoiding all fresh inflows closing.
- Solved using JModelica.org.

Results – Quality variables



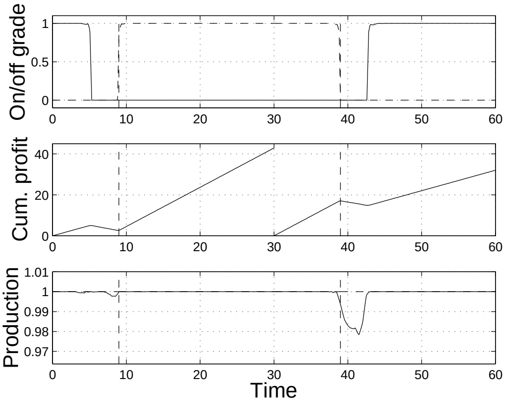
- Economical incentive for on-target production large enough.
- Over-/undershoots in instantaneous quality variables.
- Preparations performed prior grade change.

Results – Control flows



- Change for a longer time period than off-grade period.
- Significant over-/undershoots for rapid grade change.
- Flare never used due to pure economical loss.
- Off-gases remove hydrogen at economically beneficial times.

Results – Production and Profit



- Most profitable product produced the longest time.
- High production rate $\Rightarrow$ small reactor hold-up times.
- Economically optimal transition has three phases:
  1. Preparation
  2. Transition
  3. Completion

Summary

- A Modelica library has been constructed for the Borealis Borstar® Polyethylene Plant.
- Cost functions for optimization of economical grade changes have been designed.
- Economically optimal grade changes have been characterized.