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Abstract

A polyethylene plant model coded in Modelica and based on a nonlinear MPC model currently used at Borealis AB is considered for calibration. A case study of model calibration at steady-state for four different operating points are analysed, both when looking at one operating point separately, but also to calibrate several simultaneously. Both model parameters and reactor inputs are calibrated for true plant measurement data. To solve the parameter estimation problem, the JModelica.org platform is used, offering tools to express and solve calibration problems. Calibration was obtained with narrow confidence intervals and shows a potential to improve the model accuracy by changing the parameter values. The results will be used for dynamic optimisations of grade changes.[*]
Keywords: calibration, Modelica, grade change, chemical industry, polymerisation

1. Introduction

Polyethylene manufacturers are facing a market that is constantly changing, which create a demand to move between different grades cost-efficiently by manipulating the feeding of raw materials to the reactors. An existing Borstar® polyethylene plant at Borealis AB that produces bimodal polyethylene will be considered. Bimodal polyethylene products are polymerised in three cascaded reactors, pre-polymerisation, loop and gas phase reactors (GPR). The first and smallest reactor is the pre-polymerisation reactor, whose main purpose is to gently polymerise the surface of the catalyst particles since a fast reaction may damage the particles. In the subsequent loop reactor the first peak of the bimodal molecular weight distribution is formed. The last reactor in the chain, GPR, is a fluidised bed reactor wherein the second peak is mainly formed.

Accurate modelling of advanced chemical reactors is a difficult task, which if successful may help to cut expenses of raw materials. This requires calibration of the model to make the differences to the real process dynamics as small as possible. The main purpose of the calibration is to obtain valid model parameters for a model suitable for optimisation of grade changes, which has previously shown promising results in (Larsson, Andersson et al. 2010). Calibration of the model at four different steady-state operating points is shown; both when looking at one operating point separately, but also to calibrate several simultaneously.

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2. Modelling Languages and Tools

The modelling language used to express the mathematical model is Modelica, which is a high-level language for encoding of complex physical systems, supporting object-oriented concepts such as classes, components and inheritance. In addition, textbook style declarative equations can be expressed. This modelling paradigm has significant advantages over the block-based paradigm in the context of physical modelling. In particular, acausal modelling systems do not require the user to solve for the derivatives of a mathematical model. Instead, differential and algebraic equations may be mixed, which then typically results in a differential algebraic equation (DAE).

In order to strengthen the optimisation capabilities of Modelica, the Optimica extension has been proposed which adds a small number of constructs, enabling the user to conveniently specify optimisation problems based on Modelica models, see (Åkesson 2008). The calibrations in this paper has been performed using JModelica.org, which is a Modelica-based open source platform targeted at dynamic optimisation, see (Åkesson, Bergdahl et al. 2009). Calibration in JModelica.org relies on an interior point algorithm, called IPOPT(Wächter and Biegler 2006).

3. Mathematical Plant Model

Modelling a series of reactors is a task including theoretical and empirical challenges. A resulting model of such work at Borealis AB for the Borstar® process is today used on-site in a non-linear Model Predictive Control (MPC) software, OnSpot, see e.g. (Saarinen and Andersen 2003), which is the same model used in this paper. The model is described with more details in (Larsson, Andersson et al. 2010).

Each reactor is modelled from material balances, where either the inflow comes from a previous reactor or a fresh feed, and outflows go to subsequent reactor, a bleed, recycle, or product outlet. The reactions are modelled using extended Arrhenius expressions, depending on temperature, pressure, reactant concentrations and catalyst activity. The catalyst activity varies throughout the reactor series and demands careful modelling. Some assumptions are made to simplify modelling. Firstly, the reactor pressures are controlled by outlet valves holding the pressures constant. It is also assumed that the polymer and the fluids are well mixed and the temperatures are uniform in the reactors.

Inputs used in the model are measured flows of ethylene, hydrogen and propane, but also comonomer and catalyst flows. Several outputs are available including substance masses, mass ratios, mass flows, concentrations, pressures, densities, production rates and split factor. The model contains, apart from the mentioned equations additional algebraic equations. If the inputs and outputs of the model are denoted u and y, respectively, and the dynamic and algebraic variables are denoted x and w, the model can be written in the general non-linear differential algebraic equation (DAE) form

$$0 = F(z, u, p)$$
$$y = g(z, u, p) \tag{1}$$
$$z^T = [\dot{x}^T \; x^T \; w^T]$$

in the optimisation problems. Here z denotes the N_z DAE variables. The parameters to calibrate are both the model parameters p and the inputs u, for which measurements are available.

There are many parameters to calibrate in the model. Most parameters are kinetic parameters in reaction and catalyst deactivation rates, but also controlling parameters

affecting flows, pressures and levels. In this paper five parameters are chosen, namely (i) a settling leg parameter in the loop sl_2, (ii) a reference value for the fluidised bed level in the GPR bl_3, (iii)-(v) pre-exponential factors in the Arrhenius equations for ethylene and hydrogen in the loop and butylene in the GPR, k_{e2}, k_{h2} and k_{b3}. The settling legs are designed to transport the slurry to the next reactor, and its parameter rules the solid ratio of the reactor outflow.

The nominal model is calibrated in an *ad hoc* manner using process know-how, experiments and/or by trial and error. This is satisfactory for a model when used in a model predictive controller that can correct any discrepancies between actual and estimated output measurements by updating states or parameters. However, in offline grade change optimisation, there is no corrector, and model errors will immediately be penalised by taking unrealistic optimal paths, and therefore calibration is necessary.

4. Process Model Calibration

A grade change is accomplished by transferring the process from producing a product A to producing another product B, denoted transfer A-B. In the sessions between grade changes, where the process operates in steady-state, four data sets for the transfers A-B and C-D have been averaged and measurement noise covariance have been computed. The scaled measurements $\hat{y}$ and their standard deviations σ for some of the outputs can be seen in Table 1. The outputs are divided into input and state measurements, denoted $\hat{y}_u$ and $\hat{y}_z$ with 12 and 13 values respectively. Reactor hold-up masses are denoted m_{ij} and molar fractions x_{ij}, where the indexing i denotes the components propane (p), hydrogen (h) , ethylene (e), butylene (b) and nitrogen (n) while j denotes pre-polymerisation (1), loop (2) and GPR (3) reactors.

Table 1. Measurements ($\hat{y}$) and standard deviations (σ) for all data sets together with calibrated model outputs y^* and 95% confidence interval for all inputs y_u. Above the dots are 4 of 12 inputs shown and below 4 of the 13 states. All values are scaled to measurements of data set A.

	A $\hat{y}$ (σ)	$y^* \pm$ *konf*	**B** $\hat{y}$ (σ)	$y^* \pm$ *konf*	**C** $\hat{y}$ (σ)	$y^* \pm$ *konf*	**D** $\hat{y}$ (σ)	$y^* \pm$ *konf*	**AB-A** $y^* \pm$ *konf*	**AB-B** $y^* \pm$ *konf*
u_{p1}	1.00 (0.002)	1.00± 0.002	0.97 (0.002)	0.97± 0.003	0.97 (0.002)	0.97± 0.002	0.97 (0.001)	0.97± 0.002	0.98± 0.004	0.99± 0.005
u_{h2}	1.00 (0.041)	1.00± 0.047	2.51 (0.052)	2.51± 0.060	3.54 (0.043)	3.53± 0.050	3.67 (0.050)	3.67± 0.058	1.01± 0.060	2.47± 0.097
u_{e3}	1.00 (0.005)	0.83± 0.004	0.89 (0.004)	0.79± 0.003	1.31 (0.006)	1.05± 0.004	1.25 (0.005)	0.97± 0.003	0.83± 0.005	0.78± 0.004
u_{b3}	1.00 (0.015)	0.99± 0.017	1.18 (0.016)	1.17± 0.018	0.78 (0.009)	0.77± 0.011	0.70 (0.006)	0.69± 0.006	0.97± 0.029	1.19± 0.032
...	…	…	…	…	…	…	…	…	…	…
m_{s2}	1.00 (0.011)	1.02	1.00 (0.014)	1.03	1.37 (0.008)	1.37	1.37 (0.011)	1.41	0.95	1.08
x_{e2}	1.00 (0.033)	1.02	1.19 (0.015)	1.24	1.27 (0.009)	1.28	1.43 (0.008)	1.48	1.05	1.20
x_{b3}	1.00 (0.032)	1.02	1.04 (0.013)	1.06	0.53 (0.008)	0.54	0.41 (0.002)	0.42	1.05	1.03
x_{e3}	1.00 (0.031)	1.10	0.82 (0.008)	0.97	0.92 (0.013)	1.08	0.76 (0.005)	0.89	1.10	0.97

The calibration of the system (1) is formulated as an optimisation problem

$$\min_{p,u} Q_z + Q_u = \min_{p,u} (\hat{y}_z - y_z^o)^T W_z (\hat{y}_z - y_z^o) + (\hat{y}_u - y_u^o)^T W_u (\hat{y}_u - y_u^o)$$

$$subj.\ to \quad F_0(z^o, p^o, u^o) = 0$$
$$\dot{x} = 0 \tag{2}$$
$$y_z^o = g_z(z^o), \quad y_u^o = g_u(u^o)$$

where $^\circ$ denotes a steady-state solution for the system and the weighting matrices W_u and W_z is defined accordingly as diagonal matrices scaled with corresponding measurements as $1/\hat{y}^2$.

An investigation of two calibration cases follows where the first is a calibration of each data set separately while the second case looks at simultaneously calibration of data sets A and B, called AB. When one model instance is calibrated the degrees of freedom is $N_u + N_p$, where N_u and N_p is the number of inputs and parameters respectively. For calibration of two model instances simultaneously, the degrees of freedom is $2N_u + N_p$.

In order to assess the quality of the parameter estimates, confidence regions have been computed. An 1-α marginal confidence interval means that there is 1-α probability that the true parameter is within the estimated interval, which is derived from the parameter Jacobian that is obtained at steady-state as

$$J = \frac{dy}{dp} = \frac{\delta g}{\delta p} - \frac{\delta g}{\delta z} \cdot \left(\frac{\delta F}{\delta z}\right)^{-1} \frac{\delta F}{\delta p}. \tag{3}$$

The standard deviations σ of the measured outputs are needed to compute the covariance matrix $X = (J^T W_\sigma J)^{-1}$ where W_σ is the diagonal weighting matrix with each output weighted with $1/\sigma^2$. Now, the standard deviation of the parameters can be estimated by $s_p = \sqrt{diag(X)}$ and henceforth a parameter 1-α marginal confidence interval can be estimated with

$$p_{i,opt} \pm s_{p_i} T_{inv}(\alpha/2, n - p) \tag{4}$$

where T_{inv} is Student' T-distribution (Englezos and Kalogerakis 2001).

4.1. Case 1 – Calibration based on a single data set

The calibration results for A, B, C, D are shown in Table 1 and Table 2. When comparing model output y to the output measurements a good agreement is noticed for the pre-polymerisation reactor. This is probably because there are only input signals in the objective function, while there are bigger differences in the loop and GPR reactors, where a trade-off between input signals and states prevails. The calibration of x_{e2} and x_{b3} is better than x_{e3} for all calibrations because they are directly affected by their respective kinetic parameter k_{e2} and k_{b3}. In addition, m_{s2} which are directly affected by sl_2 is nicely fitted. Table 3 shows how the optimal cost is distributed between inputs and states,

Table 2. The calibrated parameters p^* with a 95% confidence interval for all calibrations. All values are scaled to the original parameter values.

	A	**B**	**C**	**D**	**AB**
sl_2	1.02± 0.030	1.18± 0.033	0.90± 0.014	0.91± 0.015	1.21± 0.025
k_{e2}	0.99± 0.095	0.95± 0.043	0.73± 0.018	0.68± 0.019	1.00± 0.051
k_{h2}	1.43± 0.248	1.76± 0.119	1.31± 0.058	1.41± 0.065	1.60± 0.163
bl_3	0.88± 0.068	0.83± 0.026	0.68± 0.023	0.78± 0.018	0.86± 0.040
k_{b3}	1.29± 0.119	1.17± 0.041	1.53± 0.071	1.78± 0.033	1.22± 0.040

where the inputs part is much smaller for all calibrations. This is probably due to the fact that inputs are easier to calibrate than for instance concentrations that depend on the other components.

4.2. Case 2 – Calibration of multiple data sets simultaneously
When comparing the single data set calibrations A and B to the calibration of multiple data sets AB-A and AB-B, in Table 1, all optimised output values have good agreement. The parameters k_{h2} bl_3 and k_{b3} in Table 2 shows calibrated values in between those of the single calibrations for A and B, while sl_2 and k_{e2} values lies somewhat above, probably due to model non-linearity. The total optimal cost of A, B and AB is 1.12, 0.97 and 2.46. The sum of the optimal costs in A and B (2.09) is as expected less than that of AB because the number of freedoms are higher when separately calibrated, because p can obtain different values.

Table 3. The part of objective function that is u and z for all calibration sets.

	A	B	C	D	AB
Q_u	10%	7%	20%	20%	9%
Q_z	90%	93%	80%	80%	91%

5. Summary and Conclusions

The paper shows an application of calibrating a Modelica model, of an existing Borstar® plant used at Borealis AB, with the Optimica extension in JModelica.org platform. The calibration results show a huge reduction of the optimal cost compared to that obtained with nominal parameter values and the model accuracy could be improved by applying the calibrated parameters. It also shows narrow confidence intervals both for parameters and inputs which is comparable to the standard deviation of the measurements. A comparison between the optimised parameters for the different data sets shows that at least k_{h2}, bl_3 and k_{b3} have values distinctly different from the nominal parameter values (1) and a parameter adjustment should be beneficial for the model accuracy at all studied operating points. Some measurements have not equally good agreement, which may be explained by model errors or measurement sensors of various qualities, which need to be followed up. More work is to be done in the future by extending the model to also consider the recycle part of the plant, including distillation towers. Also, there are more parameter sets to examine and a single value decomposition analysis of the model parameters to additional investigate their identifiability, remains to be done. While the focus is to optimise grade transitions, it would be interesting to make an offline calibration on dynamic data for different cases.

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