Experiences in the Building of Dynamic Flowsheet Models for Embedded Nonlinear Control of Polymer Processes

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Abstract — **Controllers that directly incorporate an embedded first principles dynamic flowsheet model have been applied to a range of transition metal and free radical polymerization kinetics industrial processes. These controllers handle grade runs, transitions and constraint pushing. This paper discusses lessons learned from these applications, with reference to industrial examples, in the contexts of (i) scoping the flowsheet model; (ii) offline parameter estimation to match the model to process steady state; and iii) online state estimation for continuous and discontinuous process measurements. An emphasis is placed on (ii). The discussion in this paper is of a general nature, although the experiences were gained with specific tools not in the public domain.**

I. INTRODUCTION

TABLE 1 lists some generic challenges inherent to polymer process control.

TABLE 1: POLYMER PROCESS CONTROL CHALLENGES

Concept	Notes
Core challenge	Complex catalytic reaction.
No in-situ quality measurements	Quality properties such as melt index, density, % solubles, etc measured outside the reactor (often in the laboratory) with some time delay.
Process capability issues	Quality properties set tight relative to process sampling, laboratory measurement and consistent process operation capabilities given typical measured and unmeasured disturbances.
Transition control	Implementation of significant changes to property targets during which other operating conditions such as production rate may also be changed significantly to maximize process unit profitability.
Constraint pushing and turndown ratio	Controlling to unit constraints and/or through 60%+ turndown as apparent dynamics and gains change with different properties and/or production rate.
Adapting to process change	For example, handling new catalysts or quality properties.

Xie et al [1] were among the first to discuss nonlinear reactor modeling for gas phase polymerization processes with emphasis on control application. Subsequently, controllers that directly incorporate an embedded first principles dynamic flowsheet model have been applied for handling grade runs, transitions and constraint pushing to a range of transition metal and free radical polymerization kinetics industrial polymer processes. This paper focuses on issues associated with the development and implementation of the embedded dynamic flowsheet model.

II. CONCEPT OF PROCESS MODEL DESCRIPTION

By definition models both simplify a real system and also synthesize state-of-the-art knowledge. The bridging of these potentially contradictory definitions is the model description, the specific set of questions about the real world for which the model is required to provide an answer. Through a review of the model description, the model detail that can be sacrificed without reduction in relevant predictive capability can be identified. The process model description is influenced through the use of established tools in the problem realm and by applying generic model-building concepts during use of these tools.

Established problem-solving approaches within the process industries are the concepts of flowsheeting for modeling and online state estimation for control model update … and the evolution of tools that apply these concepts. For example, flowsheeting has evolved to support the generation of dynamic models through entry of actual equipment volumes and geometry. Also within the context of flowsheeting for polymer processes the framework has evolved to allow the engineer configuring the application to:

- Select the reactions to use from a library of reaction schemes (free radical or transition metal kinetics).
- Predict end-use properties based on the most common correlations proposed and validated in the open technical literature.

Online state estimation has evolved from constant or integrating output disturbance value through Extended Kalman Filter (EKF) to methodologies that have a more direct connection with a flowsheet model – such as Implicit Dynamic Feedback (IDF) and Moving Horizon Estimation (MHE) – see Hedengren et al [2].

Generic model-building concepts to be applied in conjunction with these established tools include:

- Clarify model objectives
- Start small
- Verify (test/debug) and validate (does the model adequately mimic reality?)
- Improve incrementally (prioritizing additions in terms of the greatest anticipated improvement in the model)
- Refactor frequently (backtrack and/or simplify)

III. DEFINING THE PROCESS MODEL DESCRIPTION FOR THE APPLICATION CONTEXT

For a process control application, the embedded flowsheet model must be both robust (provide a usable solution) and

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solve relatively quickly. Within the context of these generic constraints, the core requirement is to predict the effect of the manipulated (MV) and feed forward (FF) variables in the controller on the controlled variables (CV). This definition implies the exact objective is a function of controller design. However, for the general range of polymer production processes and reaction mechanisms, we can practically think of the CVs as falling into three groups:

- Polymer properties
- Polymer production rate
- Polymer production rate constraints

Real-time process values are typically available (measured directly or inferred through relatively simple calculation of direct measurements) for the latter two groups of CVs. Although this blurs defining the process model description, continuous state estimation algorithms can play a role in the overall prediction capability of the model for these CV groups. In actual practice, this becomes iterative in the sense of applying the generic model-building concepts of “Start Small”, “Validate” and “Improve Incrementally” until a model that is judged satisfactory for control objectives is obtained – section VIII reviews some selected examples.

However, the set of CVs in the first group are not typically continuously measured in real time and as such cannot be updated by continuous state estimation. As indicated in Table 1, these CVs are also the CVs associated with process capability issues i.e. constraints on these CVs are tight given typical measured and unmeasured disturbances. As such, prediction capability similar to the measurement capability is sought for these CVs – and this becomes part of the process model description. Measurement capability can be viewed from the context of examining the cumulative effect of sampling issues, sample pre-treatment variation, measurement system repeatability, etc. on the measurement variability. More practically, measurement capability can be looked at from the context of actual variability when the process is nominally steady. From experience, this is typically less than 5% (in terms of the actual measurement for properties such as polymer melt index or across the range of measurement for properties such as polymer density). As well as such base prediction capability, the prediction “error” should show no significant bias across the range of operating conditions e.g. not biased in terms of poor prediction for one product type, or when operating at high production rates, etc.

IV. IMPLICATION OF PROCESS MODEL DESCRIPTION

As implied earlier, the basis for prediction of polymer properties within a flowsheet model is as outputs of the “reactor” unit operation. Flowsheeting packages usually provide a continuous stirred tank reactor (CSTR) and, if appropriate, combinations of these CSTR are used to represent the reality. For example, a tubular reactor can be represented as a set of CSTR in series.

Quality properties of interest are correlated as functions of more fundamental properties such as polymer molecular weight distribution. These more fundamental properties are predicted subsequent to the solution of polymer kinetic expressions. The general rate expression is of the form:

$$r = k c_A^{\gamma} c_B$$

where:

C_A is the monomer, modifier, solvent, etc.
C_B is the live polymer site or radical concentration
γ is the reaction exponent
k is the rate constant and is of the form:

$$k = k_0 e^{\frac{-(EA + VA\ P)}{RT}}$$

where:

P is pressure
T is temperature
R is the gas constant
k_j is the rate constant for reaction j
$k0_j$ is the frequency factor for reaction j
EA_j is the activation energy for reaction j
VA_j is the activation volume for reaction j

For transition metal kinetics such rate expressions are applied to the following reaction classes:

- Site activation – monomer, hydrogen, cocatalyst, electron-donor, spontaneous, etc.
- Initiation – vacant active site to monomer with active site
- Propagation – monomer addition
- Chain transfer – monomer addition terminated (by monomer, hydrogen, cocatalyst, electon donor, spontaneous, etc.) and new vacant active site created.
- Site transformation – conversion of active site types by monomer, hydrogen, cocatalyst, electron donor, spontaneous, etc.
- Site deactivation – monomer, hydrogen, cocatalyst, electron donor, spontaneous, etc

For free radical kinetics such rate expressions are applied to the following reaction classes:

- Initiator decomposition
- Propagation – monomer addition
- Chain transfer – monomer, modifier, polymer
- Chain termination – combination, disproportionation
- Beta scission
- Backbiting

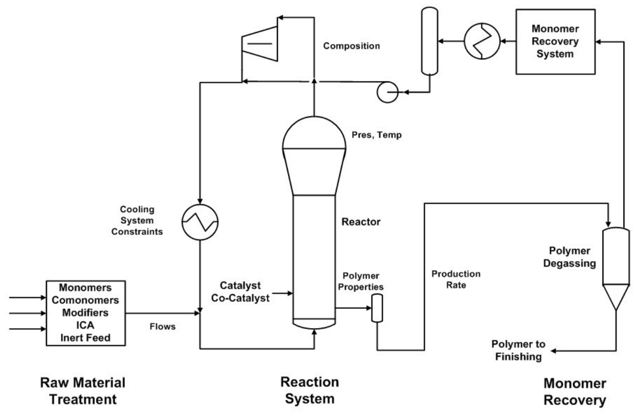
The relative rates of the different reactions determine the model predictions. For example, the relative rates of chain transfer and propagation reactions determine the length of the polymer chain. In turn, subsequent to transformation through the method of moments [3] to predict polymer molecular weight distribution, this is typically the primary correlating input for melt index prediction.

As each reaction class applies to a number of explicitly defined reactions, the implication of the process model description is that parameter determination approaches are required for the kinetic and additional correlating parameters. For multiple catalyst site types – maybe also multiple monomer systems – the number of different relevant parameters in the model may approach 100. Irrespective of the operation of the polymer process, there is insufficient information in the available process data to enable all these parameters to be treated as independent. As such the process of parameter determination requires application of engineering judgment in the context of the available body of knowledge in the open literature. A core objective of this paper is to provide an overview of the application of such knowledge for some specific examples.

V. PREDICTING QUALITY PROPERTIES FOR UNIPOL™ POLYETHYLENE (PE) PROCESS

Gas phase reactors are often discussed in the polymers technical literature. An example is UNIPOL™ technology, licensed through Univation – a process description is given in references [4] and [5] (interactive format). Figure 1 shows the main process equipment.

FIGURE 1: PROCESS FLOW DIAGRAM



Different product types (grades) are produced by selecting reaction conditions, comonomers and (transition metal) catalyst system. Each grade represents some balance in properties for different end uses. Grade specifications are typically quoted in terms of melt index and density as defined by ASTM measuring standards [6].

Steps involved in "identifying" the model are listed in Table 2 (next page). In practice, simultaneous manipulation of parameters that involves an obvious but difficult to define trade-off occurs only in step 8 (chain transfer to monomer as compared to chain transfer to hydrogen). In particular for such trade-off – but of general use especially for the latter steps in Table 2 – a multiple data-set reconciliation problem is auto-configured. The objective function is specified as:

$$\phi(\mathbf{y},\mathbf{p},\mathbf{w}) = \sum_{i=1}^{n_y}\left(\frac{w_i^y (y_i - y_i^{meas})}{y_i^{scale}}\right)^2 + \sum_{i=1}^{n_p}\left(\frac{w_i^p (p_i - p_i^{start})}{p_i^{scale}}\right)^2$$

where:

n_y	is the number of measured variables
n_p	is the number of parameter variables
$\mathbf{y}$	is the model predicted variable values
$\mathbf{y}^{meas}$	is the measured values
$\mathbf{y}^{scale}$	is the measurement scaling factor values
$\mathbf{w}^{y}$	is the measurement weights
$\mathbf{p}$	is the model parameter variable values
$\mathbf{p}^{start}$	is the initial model parameter variable values
$\mathbf{p}^{scale}$	is the parameter scaling factor values
$\mathbf{w}^{p}$	is the user supplied parameter weights

The weighting factors for the measured values and parameters in this objective function are defined by the user. Normally the $\mathbf{w}^p$ weights are zeroed out, but when non-zero they can help the regularization of the problem where weak observability may result in ill-conditioning (or solution non-uniqueness). This objective function is an L2-norm that penalizes "outliers". Some alternate objective function definitions have been utilized. An example is the automatic zeroing out of objective function contributions for predictions that fall within "tolerance" of the measurement: however from a mathematical perspective this is a more complicated implementation (non-smooth objective function changes for variation of parameters in certain ranges).

Generally, a valid model is not obtained just by matching process data. The use of the tool has to be "engineering smart". Engineering knowledge of the process gains are often incorporated into the estimation process – either directly through constraining the gains or indirectly by gain analysis – combined with parameter limits and data set adjustments. Also, unmeasured disturbances present in the process data can result in poor model sensitivities even though the model matches the process data quite well. If the structure and presence of unmeasured disturbances are known it can be appropriate to include simultaneous disturbance estimation in the parameter estimation problem through model specification changes to address this issue.

Typically the input multiple data-sets are recipes – typical operating data covering different grades (maybe production rates) – adjusted to be consistent with recent operating data. The change in operating conditions necessary to implement transition from grade to grade is of more importance than absolute values. Some of the key inputs for this example are cycle gas composition and reactor temperature.

An approach and tools to develop a kinetic model focused on prediction of polymer properties have been described. How good are such kinetic models? In our experience predictions for 70-80% of **consistent** data-sets are within the 5% criterion defined above; the remaining 20-30% are within 10%. Why not all predictions within the 5% criterion?

TABLE 2: STEPS TO DETERMINE KINETIC PARAMETERS FOR UNIPOL^{TM} PE PROCESS

Step	Activity	Observations	Outcomes
1	Literature search: tabulate reaction schemes and associated kinetic parameters.	Success reported based on modeling fluidized bed as single CSTR. Polydispersity not a typical input for correlations to predict bulk melt index and polymer density. Moderate, relatively constant pressure.	Fluidized bed modeled as CSTR. Only a single catalyst site type is considered (as a consequence, also no site transformation reactions). Activation volume kinetic parameters zeroed out.
2	General process observations	Single reactor. Site activation and initiation are "fast" (after adjusting catalyst flow to bed, the effect is seen in a few minutes).	Deactivation kinetics are zeroed out. Site activation and initiation reactions are made dependent on reactants always present in the model. Kinetic parameters for these reactions set to values that impart small sensitivity to production rate (made "fast").
3	From literature search, identify base activation energies.	Differences in activation energies (not absolute values) are important for predicting sensitivity of polymer properties to reactor temperature. For polymer density, differences for propagation of comonomer as compared to ethylene are important. For melt index, differences between chain transfer and propagation reactions are important.	Rough check is made to confirm that the predicted sensitivities of polymer properties to reactor temperature obtained with the selected activation energies are consistent with experience/observation.
4	Identify base propagation frequency factors	Match the general polymer production rate versus catalyst usage data for the process.	Initially the propagation frequency factors for the different reactions are all set equal.
5	Determine polymer density correlation	Several density correlation forms (usually relatively simple) available in the literature; primary correlated variable is percent comonomer incorporated. Some approximate data across operating range are available e.g. comonomer wt% incorporation is known from historical plant performance.	Several forms are fitted – the form and parameters with best fit and extrapolation relationship are selected. Note: willing to accept different correlation parameters for different comonomers.
6	Identify comonomer propagation kinetic parameters.	Recipes for different grades are input data. For fluidized bed reactor the recipes typically include cycle gas composition ratios, e.g. comonomer/ethylene ratio. Frequency factors and reaction order exponents are set equal for reactions with the same monomer with active reaction site in the polymer chain – to reduce the number of different parameters.	The propagation frequency factor for ethylene is held and the propagation frequency factors and (possibly) reaction order exponents for comonomer(s) are adjusted to improve the polymer density prediction. A check is made to determine if errors of the fit for polymer density are correlated with reactor temperature: if this is the case the activation energies for comonomer propagation are adjusted to eliminate this bias.
7	Select melt index correlation function	In the literature, melt index is normally correlated as a function of polymer weight average molecular weight. A few laboratory data may be available.	A correlation form and parameters are selected from the literature (form and parameter values independent of comonomer type). Parameters are fitted if sufficient lab data available.
8	Identify chain transfer kinetic parameters	Recipes for different grades are input data. For fluidized bed reactor the recipes typically include cycle gas composition ratios, e.g. comonomer/ethylene, hydrogen/ethylene ratios. Frequency factors and reaction order exponents are set equal for reactions with the same monomer with active reaction site in the polymer chain – to reduce the number of different parameters.	The propagation kinetic parameters are held and the chain transfer to hydrogen and chain transfer to monomer kinetics are adjusted. A check is made to determine if errors of the fit for polymer melt index are correlated with reactor temperature: if this is the case the activation energies for comonomer propagation are adjusted to eliminate this bias.
9	Check overall quality of model prediction and iterate to earlier step	Most common to iterate steps 4, 7 and 8.	Require fit of polymer melt index within 5% of target values and fit of polymer density to be within 5% of range of polymer density with no identified biases that are functions of operating conditions.

The model is an approximation: even though there are many available parameters, prediction limitations still exist. Are prediction discrepancies greater than 5% just accepted? The answer is “it depends”. Generally, if the predictions that are out by more than 5% also bias the model predictive capability, then additional modeling and parameter fitting of a different form will be implemented. Sometimes the form has a known process basis that is not covered by the detail of the model as generally described above. For example polymer density may be known to be a (weak) function of polymer melt index - in which case this relationship is added and correlating parameters identified.

Similarly, several mechanisms not initially in the model may be proposed for effects on production rate. Again, the model can be enhanced – although engineering judgment is needed regarding accepting the implementation costs, as online state estimation can also be utilized to “improve” the model prediction.

Otherwise, a purely statistical model can be added and parameterized that addresses the model prediction “deficiencies”. In our experience, this is not typically required but is better than catching model prediction deficiencies on feedback of irregular and delayed plant data.

Model-fitting as described above is abstracted from the actual process. If sufficient relevant historical data are available these data can be utilized relatively easily to provide a "feel-good" factor that connects with the actual process – the kinetic parameter optimization tool can be used to generate input data for identifying back-test success rate on predicting historical transitions. (As a steady state model is being used, some subjectivity is involved in identifying the pre- and post-transition "steady states".) Although it is a function of unmeasured disturbances (usually particularly associated with the catalyst) a success rate of higher than 75% is generally experienced.

What is the engineering effort involved for this model-fitting? On the basis of a good understanding of the engineering concepts and tools, the effort related to the process described herein is akin to model identification effort for traditional linear multivariable controllers. Generally, the major activity involves collating historical plant operation to provide the objectives of the model-fitting and ensure "coverage" is consistent with actual plant operations.

VI. PREDICTING QUALITY PROPERTIES FOR SINGLE REACTOR FREE RADICAL POLYMER PROCESSES

Although many of the reaction classes for free radical reactions have a parallel to the reaction classes for transition metals, there are some differences that impact the detail of the procedure for determining kinetic parameter values. For example, initiator decomposition kinetic parameters may be available – from open literature, or the manufacturer. As another example, usually deactivation reactions need to be active to enable reasonable prediction of production rate. Understanding the predictive effect of the different termination reactions (disproportionation and combination) may be difficult. One approach is to initially fix the ratio of these reaction rates at some literature value; then complete the overall model fit (in much the same way as reviewed in Table 2). Then the ratio is varied; the model re-fitted and the effects on the model prediction capability studied (i.e. an overall iterative step). As before, updated values for kinetic parameters are only accepted after analysis deems the steady state gain matrix remains reasonable.

VII. PREDICTING QUALITY PROPERTIES FOR MULTIPLE REACTOR POLYMER PROCESSES

Multiple reactor polymer processes bring challenges to controller design. However, a model-fitting advantage exists as there are effectively additional measurement data due to inference of production rates from each reactor. These data can be used to determine some of the kinetic parameters for reactions previously set primarily from engineering assumptions. For transition metal kinetics, this includes the deactivation and site activation or initiation reactions.

VIII. EXPANDING THE PROCESS MODEL DESCRIPTION

Sections IV to VII focused on achieving the requirements for prediction of quality properties CVs. However, section III also listed the CV "groups" of polymer production rate and production rate constraints. Reasonable prediction for polymer production rate effectively falls out of the approach discussed for kinetic parameter fitting. In the online environment, model-based state estimation such as IDF or MHE can use the instantaneous production rate, as determined by energy and/or material balance, to update an input disturbance of catalyst activity. This is particularly effective for multiple reactors in series. The CV group remaining for discussion is therefore polymer production rate constraints. In reality each CV within this group has unique aspects for a particular application. Some examples for a UNIPOL™ PE process controller are discussed below.

An important operability constraint is maintaining the cooled cycle gas returned with fresh monomer to the fluidized bed distributor as dry (no hydrocarbon condensation) or wet (including condensed hydrocarbon). If returned wet, then there is typically an upper limit on the liquid fraction. Polymer production rate is typically maximized at the intersection of maximum cooling constraint – such as valve position at output limit – and maximum liquid fraction of cycle gas (or minimum approach of cycle gas temperature to dew point for dry operation).

First, predicting the valve position constraint is discussed. The flowsheet approach for the process model conserves energy and material balances. Use of an exchanger model enables prediction of required cooling water flow, which has a relatively simple, direct relationship with cooling water valve position that can be determined in a spreadsheet using traditional linear regression on plant data. (This is akin to determining the "measured" valve characteristic.) Online state estimation can be used to update an output bias for the predicted valve position. It can also be noted that online state estimation can be used to update the input disturbance of exchanger UA thus facilitating use of a "simple" exchanger UA model within the flowsheet.

Now we turn to the cycle gas cooler exit liquid fraction constraint. An online measurement is not available so, as was the case for polymer properties, a more detailed flowsheet modeling approach is required. Given that the process may be operated in a high hydrogen concentration regime, for offline studies specialized thermodynamic relationships can be used to predict the process-side flash. However, there are concerns to incorporate such relationships within the control flowsheet model due to expectation of multiple roots from the relevant equations that may affect the solution robustness. Resolution of this issue is to emulate the specialized thermodynamic relationships by determining and using "k-value" multipliers that adjust base k-values predicted from a more basic equation of state such that the model predictions with these "k-value" multipliers result in a reasonably closed energy balance for various sets of process data. These "k-value" multipliers are determined using the offline tool discussed for determining kinetic parameters.

IX. MATCHING THE CONTROL MODEL TO THE PROCESS: ONLINE STATE ESTIMATION – CONTINUOUS MEASUREMENTS

Unmodeled features of a physical process pose a limitation, in particular, for model-based control. Before optimized manipulated variable (MV) moves can be computed, the current model states must reasonably match the measurements from the actual process. Several approaches are discussed in the technical literature for implanting this match (termed state estimation). We prefer more direct optimization approaches such as MHE because the real world nonlinear differential algebraic equation (DAE) model forms, including partial DAEs (PDAE), are easily accommodated in this formulation. This allows for the exploitation of sparsity, which is critical to success in using flowsheet models for process control/optimization applications. Constraints are also naturally handled in MHE approaches. Our focus is to use state estimation approaches that facilitate the use of less sophisticated models for predictive analysis as discussed in [2].

We have found that EKF is not appropriate for large sparse models such as those generated by flowsheet models as elimination of algebraic equations during the linearization process is required for the computation of Kalman gains. This typically destroys any sparsity present in the model. In addition, flowsheet models generally contain a large number of algebraic equations, usually precluding state reduction to reduce the problem size.

X. MATCHING THE CONTROL MODEL TO THE PROCESS: ONLINE STATE ESTIMATION – DISCONTINUOUS MEASUREMENTS

Section III discussed that measurements for the actual quality CVs are often only available on a delayed and discrete basis (for example as laboratory measurements). This was the argument for initially focusing model description on prediction of the quality property CVs. However, the CV measurement needs to be used to update the control model as it is this measurement (not model prediction) that determines whether the product is within quality specifications.

In the absence of an automated system the board operator uses human judgment to respond to a new laboratory measurement and the objective of automation is to match or exceed the judgment of the "best operator". Application of traditional Statistical Process Control (SPC) to the laboratory measurement tends to be insufficient as:

- The time to obtain the measurement subsequent to sampling is relatively long compared to reactor residence time.
- Inhibitors/poisons in small quantities can cause properties to drift at steady state.

Our experience has been to apply additive or multiplicative output biases to the underlying model-predicted values for polymer properties to generate the controller predicted value. On receipt of a new laboratory measurement, a new additive bias is calculated through:

$$\mathrm{A}\mathit{error} = \mathrm{CV}_{\mathrm{meas}} - \mathrm{CV}_{\mathrm{model}}$$

$$\mathrm{A}\mathit{bias} = \mathrm{A}\mathit{bias}_{\mathrm{old}} + \mathrm{Gain} * \mathrm{A}\mathit{error}$$

And a new multiplicative bias is calculated through:

$$\mathrm{M}\mathit{error} = \mathrm{Ln}\,(\mathrm{CV}_{\mathrm{meas}} - \mathrm{Offset}) - \mathrm{Ln}\,(\mathrm{CV}_{\mathrm{model}} - \mathrm{Offset})$$

$$\mathrm{M}\mathit{bias} = \mathrm{Exp}\,(\mathrm{Ln}\,(\mathrm{M}\mathit{bias}_{\mathrm{old}}) + \mathrm{Gain} * \mathrm{M}\mathit{error})$$

where:

$\mathrm{CV}_{\mathrm{meas}}$	New laboratory measurement value
$\mathrm{CV}_{\mathrm{model}}$	Controller unbiased model prediction value corresponding to the process time (sample time – process/sample dead time) the sample was taken.
Gain	Bias feedback gain term
Offset	Fixed offset value (typically zero)

A*error*, M*error*	Error
A*bias*, M*bias*	New bias
$\mathrm{A}\mathit{bias}_{\mathrm{old}}$, $\mathrm{M}\mathit{bias}_{\mathrm{old}}$	Previous value of bias

for which engineering judgment applies to:

- Selection of the model variable to be updated
- Choice of additive or multiplicative output bias
- Setting values for Gain

If the model prediction change for a step input is a fairly constant absolute delta, independent of the underlying model prediction value, an additive output bias is most appropriate. A multiplicative output bias is most appropriate when the model prediction change for a step input is generally a fairly constant fraction of the current measurement.

Melt index is known to be consistent with the expectations for using a multiplicative output bias – this can also be inferred from the relatively common practice described in the literature of using a logarithm transformation on the melt index to generate a variable more suitable to be handled with a more traditional linear multivariable controller. Thus model predicted melt index is updated using the multiplicative output bias approach (and this same bias is also applied to the instantaneous melt index which is a constraint controlled variable in the controller matrix).

For polymer density, the approach to update the model from the laboratory measurement has been varied – and the choice between additive and multiplicative biases has been application-specific. Multiplicative output biases have been applied on variables transformed from the base laboratory measurement, such as percent comonomer incorporated.

Our practice also uses a variable Gain set by a heuristic algorithm, nominally emulating the judgment of the "best operator". Inputs to the algorithm include the trend of the discrepancy between unbiased model prediction and actual laboratory measurement: if drift is detected the Gain is increased in order to catch up with the process. In the absence of drift the Gain is set lower. If the occasional "outlier" is sometimes present in the laboratory measurements, then the algorithm is set to use a low value for Gain on the first occasion of a significant discrepancy between model prediction and laboratory measurement.

XI. CONCLUSIONS

In the context of development and implementation of dynamic flowsheet models embedded within nonlinear controllers, this paper has discussed:

- Factors affecting choice of flowsheet modeling approach
- Determination of kinetic and other parameters for the flowsheet model
- Coupling use of continuous state estimation with less fidelity in the flowsheet model
- Use of delayed discrete measurements for state estimation

Much of the discussion has been based around engineering "common sense". As a very broad generalization, an argument has been made for a rigorous first principles approach for the reactor(s) coupled with simpler flowsheeting modeling that maintains energy and material balances for the remainder of the process. Practically some exceptions will occur to this generalization, as was discussed for the process side cooler for UNIPOL^{TM} PE process.

Our experience is that the effort to develop the flowsheet model embedded within the controller is akin to the effort required to develop empirical models for traditional linear multivariable controllers. As such, this approach to nonlinear control bears serious consideration as it brings the potential benefits listed in Table 3, some of which were discussed in [7].

TABLE 3: CONTROLLER EMBEDDED MODEL ADVANTAGES

Issue	Notes
Offline study	Dynamic chemical engineering control model from the online controller available for offline study use.
Regression validity concerns	Reduced engineering focus for regression evaluation due to the underlying nature of the control model.
Handling new grades	Validation exercise rather than a re-engineering exercise due to the nature of the control model.
Inferred measurements	All states in the control model are available, including intrinsic instantaneous polymer properties.

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