Industrial Application of On-line First Principle Dynamic Models using State Estimation


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Abstract:

Four industrial applications of State Estimation have now been successfully commissioned some in operation for more than a year. This paper describes the overall technology and software framework with examples from one of the applications. We focus on the use of first-principle, non-linear, dynamic models applied on-line and corrected to match current plant operation using state estimation techniques. This approach combines the rigor of the first principle modeling, for example, obeying heat and material balance constraints, using process engineering design and data relationships, with the ability to accurately match current operation by estimating states and parameters from measured process data.

The provision of large-scale state estimation applications is new to the process industries. To have successful applications based on first principle models, the state estimation technology has to accommodate:

- A modeling tool able to handle large-scale dynamic simulation;
- A physical property database with accurate thermodynamic methods;
- The ability to generate robust models that function through a wide range of operating conditions;
- The collection and processing of real time data;
- Provision of an interface for the user and engineer;
- Structuring and configuration of large-scale state and parameter estimation.

These capabilities recognize the demands for accurate round-the-clock operation required in the process environment. AspenTech® have applied their experience in modeling and control applications and utilized their existing software products to develop the State Estimation Module technology described in this paper.

Our original customers continue to work with this technology and are expanding its application scope. All applications have generated benefits to the user, some with validated studies, by fulfilling primary project objectives. Furthermore, in most instances, the encapsulation of knowledge in the process models has allowed use beyond the original project scope. A significant portion of the economic incentive for this
technology comes from using, on a continuous basis, deep process knowledge and understanding embedded into maintainable models.

The specific application described in this paper is on a polyethylene process at the Matagorda, Texas site of Equistar Chemicals, LP. In this application the objective is to predict polymer properties by tracking, in real-time, the moments of the polymer distribution and relating these to the resultant polymer physical properties for closed loop process control. The Polymers Plus® package is used for the reaction kinetics, physical properties and polymer characterization. In addition, Equistar is also using the technology to continuously validate sophisticated polyolefins process models for off-line use. Other applications have included the ability to “look-ahead” using the rigorous dynamic model based upon the current plant operating conditions. A feature of this technology is that the on-line model may also be used to predict component attributes, for example the polymer molecular weight distribution, which cannot be directly estimated using data-centric tools.
1.0 Background

From our own project experience, and that of others [1], there is a drive in this technology area. As background we look at the motivations for and requirements placed on this technology. Here we refer to the system used to place first principle dynamic models on-line with state estimation as Dynamic Shadow Plant Models (DSP Models). We use this to specifically reflect that the models are Dynamic and ‘shadow’ the plant operation.

The heritage of DSP Models is a direct combination of the process design, process simulator and process control experience. DSP Models use the best of our simulator technology to predict the behavior of the process and the best of our control experience to make the match between these predictions and the actual plant behavior. DSP Models are dynamic non-linear first principle models run continuously in parallel with the process plant. These self-consistent models are continually auto-calibrated using the available plant data, providing the best estimate of the current process conditions and behavior.

To be industrially accepted DSP Models require a ‘generic’ form that can be re-deployed. The features needed to address practical issues have to be captured in an environment where they are configured and used on an as-needed basis. The environment must support a successful execution methodology. Failure to do this results in unique custom applications that have support problems.

With the correct approach all the issues in successfully achieving DSP Models are addressed. We know from our control and simulation experience that although every plant is different, and the conditions on each plant are unique, a well-structured approach to building models and controllers allows consistency and reuse of the software.

DSP Models use dynamic first principle models as their basis. Using this approach to performing estimation is a more expensive route than data centric regression techniques. The model centric approach is
cost effective because its added value is in releasing encapsulating knowledge about the process in a form usable in a variety of ways. The value obtained is determined by the application. DSP Models provide the following:

- Generate a consistent heat and material balance
- On-line view inside the process
- Inferential variables for information and control of process
- On-line future prediction
- Using off-line models for design investigations

2.0 Theory

The focus of this section is to understand the theory behind a DSP Model. The role played by the modeling technology and the use of state estimation in a DSP Model are set out. There are many choices in structuring the technology and an explanation is given for the choices made.

The Kalman Filter (KF) was originally developed as a discrete time algorithm (mathematical program) to estimate the states of a stochastic process [2]. The algorithm combines the variance of the measurements and the variance of the model states to estimate the true process states and variance in a way that minimizes the variance of the true process state estimate. There is now a large body of established knowledge about the use of the KF for state estimation representing over 30 years of use.

The KF is a central element of the state estimation used in DSP Models. It is essential that we apply this correctly. There are a series of assumptions behind the derivation. We cannot claim that these assumptions are absolutely applicable in practice. However, they are either sufficiently close, or much smaller assumptions than we may make elsewhere, that they are not significant to the overall performance.
This section develops the equations as used in the state estimator part of a DSP Model. The equations are presented in the form that is most appropriate for our implementation, often referred to as standard form [3], although there are several others. These represent specific reductions, often embodying other assumptions. They can be useful in particular cases, but can take the unwary into areas where the implementation is no longer consistent with the assumptions. There is no attempt to make a formal derivation of the underlying equations, the details can be found in textbooks [4,5]. The notation here is loose. This is done deliberately to make the equations appear simpler. The focus is on giving an understanding of what the equations mean.

2.1 Structure

Two interpretations are considered here, a simple statistical analogy and the control engineering block diagram of the system.

2.1.2 Stochastic Process interpretation

This interpretation closely follows a description given by Maybeck [6]. The estimation involves two steps. The first step is the combination of measurement estimates from a number of sources. The model is one source of information, the direct process measurements are another. We assume that these are independent sources. These are combined together on the basis of Gaussian probability distributions giving a minimum variance estimate of the true measurement. The second step is to propagate this estimate, and its associated variance, to the next sample time. At this point new process measurement values are obtained and the exercise repeats.

A DSP Model predicts plant behavior (outputs) based on a dynamic model relating plant inputs to outputs. The prediction is the result of a set of independent plant measurements (inputs) passed through a model transformation. The outputs are independent of corresponding direct plant measurements. The model integrates in real-time continually updating the output prediction. By bringing the independent direct plant measurement into account it is possible to correct the model states to give a better match to the outputs.
Both the model output and the corresponding plant measurement have a distribution reflecting their accuracy. Many measurements have a Gaussian distribution and this is a standard assumption in these derivations. The resultant estimate result is a linear function that combines each measurement weighted by the variance of that measurement.

For two independent measurements with Gaussian probability density functions the measurements are combined together using the following rule:

\[
\mu = \left( \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2} \right) \mu_1 + \left( \frac{\sigma_1^2}{\sigma_1^2 + \sigma_2^2} \right) \mu_2
\]

where \( \sigma_1 \) and \( \sigma_2 \) are the standard deviation (\( \sigma \) squared is the variance) and \( \mu_1, \mu_2 \) are the two measurements.

The following should be noted:

- The new estimate of the measurement is weighted by the relative accuracy (or certainty) of the individual measurements. The most certain (that with the smallest variance) being given the highest overall weighting.

- The new estimate of the measurement is a linear combination of the original measurements, and must fall between the measurements.

The variance of the new estimate is obtained by combining the variances of the measurements in a way exactly similar to the total resistance of resistors combined in parallel:

\[
\frac{1}{\sigma^2} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}
\]
This can be rearranged in terms of standard deviations as follows:

$$\sigma = \frac{\sigma_1^2 * \sigma_2^2}{\sqrt{\sigma_1^2 + \sigma_2^2}}$$

The following should be noted:

- The variance of the new estimate is always less than the variance of any of the individual estimates—exactly like placing one resistor in parallel with another the overall resistance must fall. This means that no matter how poor a new piece of information is (large variance) it improves the estimate of the measurement.

There is a special rearrangement that makes the calculation of estimate and variance more direct. It is based on the ratio of the variances, or how much confidence we can have in one measurement relative to the other.

$$K = \frac{\sigma_1^2}{\sigma_1^2 + \sigma_2^2}$$

This simplifies the earlier equations to give:

$$\mu = \mu_1 + K * (\mu_2 - \mu_1)$$

$$\sigma = \sqrt{\sigma_1^2 - K * \sigma_2^2}$$
The construct $K$ is the Kalman Gain. It plays a special role as it tells us how much of each measurement to combine and how much of each variance to take. Figure 1 shows how two estimates with Gaussian distribution are combined together to provide a new estimate with reduced variance.

Because our models are dynamic we not only have to combine measurements but also have to estimate the variance after a time step. Again there is a simple relationship to propagate the variance into the future for variables governed by linear differential equations that have Gaussian distributions.

Representing in discrete terms a first order differential equation driven by a noise process then the process behaves as:

$$y(k + 1) = a^*y(k) + w(k)$$

For the process to be stable the value of $a$ must be less than 1. The variance estimate is given as:

$$\sigma^2(k + 1) = a^2 \sigma^2(k) + \sigma^2$$

For stable processes the variance achieves a natural limit determined by the dynamics of the process. The minimum value of the variance is set by the variance of the noise. Figure 2 shows the decay (free response) of a process variable described by a first order linear differential equation together with the way in which the variance of the estimate increases from the initial starting condition.

2.1.1 IMC/MPC controller interpretation

A DSP Model has many similarities with the IMC and MPC structure and are readily seen from a control engineering perspective. A dynamic model is run in parallel with the process and a model-process mismatch developed. This mismatch is the ‘error’ process that drives a ‘controller’, the KF. In the control law the states in the model are adjusted in a way that minimizes a quadratic cost criteria.
A DSP Model predicts plant behavior (outputs) based on measured plant inputs. The model integrates in real-time mimicking events as they unfold. There is no direct link between the predicted plant outputs and those measured from the plant. Modeling error and unmeasured inputs will cause inevitable deviations between measured and predicted outputs.

A closed loop model structure is applied to reduce or eliminate prediction errors. Closed loop modeling is similar to IMC or MPC in concept. The traditional roles of setpoints, manipulated variables and controlled variables are changed as shown in the figure 3.

The model sees measured plant inputs, labeled IN. Other inputs affect the plant but are unmeasured or their effects not modeled. These are disturbances, labeled DV. Plant outputs are labeled OUT and model outputs are labeled PV. From the perspective of a closed loop model, the prediction error (OUT minus PV) is fed back to the model via the CONTROL block. The signal OUT corresponds to the setpoint while the signal PV becomes the controlled variable. The manipulated variables (MV) from the control block update the model to close the gap between its prediction (PV) and the plant measurement vector. The measured inputs, IN, play the role of feedforward inputs in a control context.

A KF fits this overall structure. The MV signal is the updated state vector that is calculated by applying the Kalman gain matrix, the controller, to the prediction error. The model consists of two parts. The normal input-output relationship (IN-PV) with the corresponding states is one part. Normal states are augmented with additional states designed to ensure that steady state prediction error can be eliminated. The result is equivalent to having a controller with integral mode that eliminates offset due to unmeasured disturbances.

Definition of the augmented states is an important part of the modeling effort. We can view this somewhat like choosing manipulated variables (e.g., valves) in a control system but without the encumbrance of the physical world. Still, it is highly desirable to match the selection with our understanding of the process. The simplest option is to choose an augmented state that is a bias to an element of the prediction vector
(PV). The implication is that there is offset in the measurement of the output signal. Commercial MPC typically employ this structure to obtain integral mode. The bias absorbs both model error and unmeasured disturbance effects. An alternative is input bias, effectively modeling input measurement errors. Beyond these obvious options, augmented states may be unknown parameters (e.g., catalyst activity or heat transfer coefficients) or unmeasured disturbances (e.g., unmeasured feed composition or ambient heat loss).

Normal practice is to define no more augmented states than there are important measured outputs. Some outputs are predicted and physically measured that are not included in the structure (i.e., the outputs are treated as being not measured). The net result is that we have a square system with enough augmented states to completely eliminate long-term prediction offset. The augmented states must be observable. Equivalently, the system must be able to “control” the predicted states to reach their respective “setpoints,” the output measurements. In practice, choosing physically meaningful augmented states with independent dominant effects essentially ensures “controllability.” Large Kalman gains leading to large changes to the augmented states during normal operation indicate the need to redefine the augmented states. This could also be an indication that the model is inadequate in some fundamental way.

The real-world applications being reported in this paper all are based on rigorous nonlinear models generated from physical principles. In most cases we have sufficient understanding to define physically meaningful augmented states that result in good system performance. In the diagram above, the Kalman gain in the CONTROL block is calculated based on a linear state space approximation of the model. This approximation is updated periodically to account for changes induced by the nonlinear model. The net configuration is much like a linear controller being applied to a nonlinear process with periodic updates to the controller. This approach has proved to be robust in practice.

The control system analogy introduces another familiar issue. There are physical limits for manipulated variables in any practical controller (e.g., valve position limits). Likewise, augmented states sometimes have to be limited to satisfy physical constraints. As an example, feed composition would be an augmented state with physical limits. Numerical solution of the nonlinear model often prohibits introduction of
infeasibilities such as negative compositions. Alternatively, the nonlinear model (which imposes a set of physically motivated equality constraints) will re-converge to a solution that negates the intended change introduced by the augmented state.

In some MPC, constraints are explicitly handled using an optimization approach. The computational cost of an equivalent approach for the estimation applications being reported here (nonlinear systems with up to several thousand states, with even more algebraic equations) is prohibitive. The alternative solution is to limit the position and rates of change of the augmented states. There will be prediction offset when augmented states constraints are active. This can sometimes be avoided by defining additional augmented states that tend toward zero when the system is otherwise unconstrained. A non-square system results, much like a multivariable controller with extra degrees of freedom.

A subtle effect of the configuration (nonlinear model with a linear “controller”) is that the state updates from the CONTROL block destroy the equalities imposed by the nonlinear model. These equalities are re-established by the nonlinear model solver each time a state update occurs. This does not invalidate any results, but it does impose additional computational burden on the system when a state update occurs.

### 2.2 Established Results

Two elements of state estimation for large-scale problems are considered here. These look at:

- The KF used for estimation;
- The augmentation of the process model to accommodate model errors.

#### 2.2.1 Kalman Filter

The KF (KF) algorithm consists of four equations applied recursively. These equations consist of:
• The calculation of the Kalman Gain, a weighting matrix based on the relative variances of the model states and process measurements.

• A state correction equation that turns out to be a linear combination of the one step ahead prediction of the state based on the current state and known disturbances to the process, with a Kalman Gain driven by the innovation process.

• The estimate of the corrected state co-variance matrix.

• An estimate, one step ahead, of the model state variance based on the current estimate of the state variance, the system dynamics and the variance of the model states.

DSP Models use an Extended Kalman Filter (EKF). This means they allow for non-linearity induced by process changes in their computations. When we use the EKF we implement the state correction equation based on the local linear approximation of the model and apply the corrections to the states of the non-linear model. This means that the linear model form that is often seen in the textbooks as the estimator is only of use to here in constructing the Kalman Gain and the Covariance estimates – it is not the estimator. The estimator is the non-linear dynamic model.

We are fully equipped through the AspenTech® dynamic modeling tools to extract local linear representations of large algebraically constrained sets of non-linear differential equations. The method used is similar to that described in [7].

The set of SYSTEM equations are typically represented as:

\[ x(k + 1) = A^* x(k) + B^* u(k) + w(k) \]

The terms are:
A, the state transition matrix (for a linear discrete system the state transition matrix is the matrix exponential evaluated for the sample interval)

B, the control transition matrix (for a linear discrete system the control transition matrix can be computed from the corresponding state transition matrix and the continuous control matrix). We will see that we do not require this matrix in our approach to State Estimation – a computational advantage.

x, is the state vector

w, is the stochastic element of the model. It is a vector of independent white noise processes. Each of these element in the vector has it’s own variance.

The set of MEASUREMENT equations are typically represented as:

\[ y(k) = C \cdot x(k) + D \cdot u(k) + v(k) \]

The terms are:

C, the measurement matrix (this is identical in the discrete and continuous form)

D, the direct connection matrix (this is generally zero in most modeling work – however, it can be non-zero where parts of a process are modeled in steady state). We will see that we do not require this matrix in our approach to state estimation.

y, is the measurement vector
\(v\), is the stochastic element of the measurements. It is a vector of independent white noise processes. Each element in the vector has it’s own variance.

The INNOVATION process (often referred to as a residual or error) is the difference between the plant measurement and the estimated measurement. In strict terms the residual or error is difference seen after the state correction has been made.

\[
e(k) = h(k) - m(k)
\]

The terms are:

- \(h\), the vector of estimates of the process measurement. Note, this is not \(Y\) from the measurement equations but the response of the integrated non-linear differential equation.

- \(m\), the vector of measurements taken from the plant.

- \(e\), is the innovation.

If our model were perfect then the innovation would replicate the \(V\) process. The independent noise processes of the process measurements.

Rather than determine the form of the KF update equation it is simply stated here as a linear combination of the estimated state and a weighted correction driven by the innovation process. We assert that this is a reasonable form to select.

\[
X_{\text{new}}(k) = x(k) + K \cdot e(k)
\]
Xnew(k), is the corrected state, obtained after applying the update equation.

x(k), is the estimated state value. This has been obtained by integrating the DAE up to the current time point.

e(k), is the innovation at this same point in time, based on the predicted process measurement (obtained by integrating the DAE) and the actual process measurement.

K, is a weighting matrix.

The task now is to construct the best weighting matrix. A criteria for this is to minimize the means square error of the estimate. Constructing the variance of the estimated state leads to the following expression:

\[ P_{\text{new}}(k) = (I - KC)PK(k)(I - KC)^T + KRK^T \]

This requires the application of statistical rules for the independence of the noise processes and observations.

The terms are:

I, the identity matrix of dimension equal to the number of states

K, the weighting matrix from the update equation

C, the measurement matrix
P(k), the covariance estimate for the state prior to application of the correction (a priori), corresponds with $X_k$

$R$, is the measurement noise co-variance matrix. It is generated from the variances of the independent measurement noises processes.

$P_{\text{new}}(k)$, the covariance matrix for the corrected states (generally a posteriori).

To find the weighting matrix $K$ that minimizes this expression take derivatives with respect to $K$ and set to zero. Solving this results in the equation:

$$K = P(k) * C^T * (C * P(k) * C^T + R)^{-1}$$

These terms are all known from the previous expressions. The resultant optimal $K$, Kalman Gain matrix, has the special property of minimizing the mean square error. It is one instance of the updating matrix that could have been selected.

Finally, to predict the variance of the states one step ahead can be calculated as the covariance and becomes:

$$P(k+1) = A * P_{\text{new}}(k) * A^T + Q$$

The terms are:

$A$, the state transition matrix

$P_{\text{new}}(k)$, the covariance matrix for the states at time interval $k$, (a posteriori).
Q, the state noise co-variance matrix. It is generated from the variances of the independent noise processes.

P(k+1), the covariance matrix for the states at time interval k+1.

This concludes the equations used in the State Estimator. The [ABCD] matrices are updated at regular intervals. They are introduced into the KF equations that are applied in a recursive fashion in the following order:

1) Calculate the Kalman Gain

\[ K = P(k) * C^T * (C*P(k)*C^T + R)^{-1} \]

This is based on the co-variance of the states calculated from the last cycle together with the current measurement matrix.

2) Update the states in the DAE model

\[ X_{new}(k) = x(k) + K * e(k) \]

The state update is driven by the current innovations.

3) Calculate the co-variance matrix for these updated states

\[ P_{new}(k) = (I - K * C) * P(k) * (I - K * C)^T + K * R * K^T \]
The co-variance is based on the Kalman Gain matrix, the co-variance estimate carried for the last cycle together with the measurement matrix and the measurement covariance matrix.

\( P(k +1) = A^* P_{new}(k) * A^T + Q \)

This propagates the co-variance to the next time step. It is based on the current co-variance, the state transition matrix and the state co-variance matrix.

Figure 4 shows schematically the combination of the local linear state estimation with the integration of a non-linear model.

The combination of the local linear KF with the integration of the non-linear DAE model violate the requirements for optimality – no proof can be claimed for what is a non-linear system. However, we believe the we are improving the estimation by employing powerful modeling techniques and only sacrificing some of the finer points of the derivation of the more traditional KF.

2.2.2 Model Matching through Stochastic Variables

Stochastic variables are a key element in matching process models to plant data. This was initially established by McAuley & MacGregor [8] in work on polymer processes. The reason many early optimal controllers based on Modern Control Theory failed was not that there was something wrong with the theory but that the structure of the models was inadequate. Providing stochastic states, or augmenting the model, is the equivalent of giving integral action in a controller. Without these terms the states of the model are adjusted but the steady state solution is never changed. The model always returns to an underlying behavior. This is desired for transient disturbances but is not adequate to absorb persistent miss match
between the process and the model. Stochastic states applied to model parameters allow the model to reach new steady states for the same input set and permanently capture model corrections.

Consider the following non-linear differential equation:

\[
\frac{dx}{dt} = F(k, x; t)
\]

x are the states in the model

k are parameters in the function F()

F() is a non-linear function

Then the system is non-linear in x and potentially k. k is a parameter in the model. When solving the equations in steady state this is typically a design parameter in the model. The design parameters generally have time based dynamics, reflecting gradual change of the process. For example, this could be the activity of a catalyst or efficiency of a machine. Representing the parameter dynamics we extend the steady state relationship with a new differential equation:

\[
k = k_{design} + z
\]

where z is given some simple dynamics:

\[
\frac{dz}{dt} = \frac{1}{\tau} * z
\]

This is an arbitrary selection. It gives k the following properties:
• The perturbation from the design condition is by an addition (an arbitrary choice, it could be multiplicative);

• If disturbed from the design conditions it returns to the design with a time constant $\tau$;

This has generated an additional differential equation, and a corresponding additional state, in the model. $z$ is referred to as an augmented state, or stochastic state.

With the KF approach we can estimate this augmented state at the same time as the ‘normal’ states in the model. We can see that setting a non-zero value for the stochastic state $z$ allows the system of equations to hold a new steady state.

We should strive to use a minimum set of stochastic states. It is possible to use many such states and the application will function, producing a solution point based on the weightings expressed, but it would seem good practice to use a minimum set.

These are very powerful and correctly selecting and structuring is an important exercise. Strangely the modeler often knows where these belong intuitively. They tend to be exactly those parameters that he is uncertain about in his model.

Our experience is that simultaneous parameter and state estimation, proportional and integral action, are requirements for successful large-scale state estimation.

3.0 Technology

In the previous section we the theory that underpins state estimation. There are a range of other practical real world issues that have to be addressed. We touch on these briefly. These are as important as solving the central equations to achieve a successful application.
3.1 Conversion of Theory to Technology

The following represent key implementation features that have to be solved in large-scale problems. Solving these make the theory applicable to practical application:

3.1.1 Linearisation

The DSP Model handles the non-linearities in the process in two ways. First as the estimator is a non-linear model the non-linearities are naturally captured. Further, the generation of the local linear model used in the state estimator is regularly updated. This is an EKF approach to the state estimation. This avoids the use of transformations in the state estimation.

In the state estimation described above the local representation of the non-linear process has to be generated. An efficient means of doing this is required. Numerical perturbation should be avoided as this can be ‘noisy’ and is prone to error. Analytical techniques should be used where possible.

3.1.2 State transition matrix

Large-scale computation of state transition matrices has to be performed. Simple tests demonstrate that Taylor series expansions are not stable, even retaining large numbers of terms.

The use of eigenvalue methods is accurate, however the computation of a full set of eigenvalues and vectors for systems with thousands of states is computationally prohibitive. Even obtaining this full description leaves further computation time problems working with complex number operations that inevitably result from practical sets of eigenvalues.

Our approach has been to directly integrate the continuous time linear equivalent model. This method is open to us and is successful because the continuous time linearisation is available from the open equations methods and the open equation solvers are particularly efficient at solving the resulting LU decomposition problem from integrating the linear system matrix.
3.1.3 Discrete and continuous approach

The selection of where to use continuous and where to use discrete methods in the structure of the DSP Model is very important. The use of a continuous integrator for the non-linear DAE allows the models to be build in the most natural way and provide a continuous representation of the process. This structure means that the future estimate of the process measurements is completely performed by the model, there is no requirement for the calculation of the control transition matrix. This is supplemented with a discrete KF, based on the local linearization. The discrete form of the KF is most efficient and has all the required information from the local linearization.

To keep the linearization accurate we repeatedly re-apply the linearisation – an Extended KF. The system is structured so that this is done on a regular basis. The timing of these operations and setting of the intervals is application dependent.

3.1.4 State Updates

We have already identified that it is necessary to apply validation to the updating of the states. We have chosen to apply a single filter across the whole model. Applying rules on the validation of the state updates (by maximum, minimum and incremental limits applied to the changes) is a pragmatic recognition that some states can be perturbed unduly by the action of the state estimation. This should be avoided. We accept that this type of validation can distort the optimum update into the model. Our experience is that a mechanism is required to prevent this distortion. If this is not done unusual effects occur as the convergence of the dynamic model takes place. It is these types of considerations that allow us to achieve a high degree of confidence in the convergence of the underlying model. We achieve on-line times (service factors) of the models well above 90%, with the models running continually for weeks.

3.2 Practical Issues

To date, application of state estimation to industrial chemical processes has been very limited. The reason is not that the equations are in some way difficult to understand or given the correct tools to solve. There are features in the nature of applications in the process industry that need to be handled with care.
3.2.1 Size

In typical large-scale practical applications our models have hundreds of states, possible thousands. Should all these states be updated using the state estimation? This leads naturally to questions of observability between the measurements and the states. The resulting answer is going to be no. It is highly unlikely that the measurement information covers, with sufficient strength, all parts of the process. It is necessary to be able to configure the state estimation so that only selected states are update and implement the calculations correspondingly. The selection of which states to update depends on strength of the measurement connection to the states.

3.2.2 Numerical implementation

For large-scale implementations with thousands of states, the ordering of the calculations in the KF is vital. There are orders of magnitude differences for inefficient implementation of the equations. For speed and efficiency the calculations should use BLAS routines [9] and the linear algebra implemented with efficient algorithms such as those available from LAPACK routines [10]. These routines represent the most robust implementation with the widest range of input of the linear algebra techniques available.

3.2.3 Loss of measurements

Practical applications have to be able to handle the unexpected loss of measurement information. The algorithm has to be able to restructure itself for reduced measurement information. This also means that it is not possible to implement a steady state Kalman Gain as the weightings given to the measurements need to change over time.

3.2.4 Changing measurement frequency

Practical applications must deal with measurement information that is not continuously available, but is available either at points in time or relating to earlier conditions. This has been allowed for so that the innovations of ‘old’ measurements can also be applied in the filter. This has a heuristic application rather than a theoretical one.
3.2.5 Modeling scope

The scope of the model is important in structuring the application. The following are typical questions is considering the model scope:

- How much of the control system to represent?
- Which measurements are significant in updating the model performance?
- Whether to include recycles?

The inclusion of recycles and controls is necessary when providing future prediction as these impact the operation of the process. For standalone estimation greater simplifications are possible.

Our experience has been that models naturally tend to have larger scope. There is a striving to capture as much detail as possible. Without doubt the fidelity of the model contributes to the success of the application. However, including additional detail is not always sensible. There is no point describing in detail something that has a high degree of uncertainty, it is better to simplify the model. Deep process knowledge, engineering judgment and collaboration between the modeler and process engineers are essential for successful model development and model validation. The challenge is always to know how simple a model can be and yet remain effective.

3.3 Structure and Tuning

Successful applications have to provide flexibility in structuring the application and a mechanism for tuning. Our approach places emphasis on the selection of states to be updated, the location of stochastic states, and the timing of the execution. This is the basis of an application and places emphasis on the understanding of the process behavior. The final performance is adjusted by tuning of Q/R weights.

3.3.1 Structural Considerations

In looking at the structure of the model each of the following has an impact:
• Model scope and fidelity;
• Selecting states to update;
• Location of stochastic states;
• Execution frequencies of the model components.

We have found that the necessary feature of a successful DSP Model is that it have the correct structure. The model equations should mimic the process behavior, however absolute accuracy is not required. Striving to include parameters based on poorly understood or complex physical relations is not necessary. The accuracy of the model is achieved through the use of the KF, however, no amount of ‘correction’ can make up for a poorly structured model.

The frequency of the linearization of the non-linear model and the KF execution rate are directly related to the dynamics and the degree of non-linearity of the process. In practical terms the real constraint is the CPU time to calculate the state transition matrix and the P-covariance matrix. For large applications (higher than 1500 states) the best that can be achieved is for these frequencies to be the mean value of the time required for the computations. If these frequencies are not sufficient then reducing the model order has to be considered. In general, a reduction in model order can be identified based on engineering judgment of the relative importance of the various states.

For the processes we have worked with the non-linearity is such that it is better to spend computer time performing KF calculations (feedback) correction rather than repeatedly re-linearising the process (feed-forward), although this cannot be ignored and is likely to be a characteristic of the particular process.

3.3.2 Tuning Considerations

Steady state and dynamic model validation based on multiple plant data sets are a central step. For tuning an environment separate from the execution one is required as large quantities of batch data have to be studied. We provide a simulation environment that can emulate, in faster than real time, the on-line performance of the DSP Model. This environment can be used off-line with plant data for:
• model validation;
• confirmation of structure;
• tuning of the KF performance.

We try to build from simple structures (small numbers of states) up to the complexity required. In this way
we minimize the number of states that need to be updated. We try to tune with the stochastic states first to
prove closure between plant measurements and model predictions.

Tuning is a simulation exercise and there are no absolute rules. We have some basic setting of the tuning
values to provide consistency from one variable to another.

Part of the model validation activity should be the identification of the inputs that will drive the dynamic
non-linear model and the outputs that will drive the KF corrections. These outputs are typically the plant
measurements that will be used as a performance index for the model validation. Selection of model
parameters to be included in the structure of the KF as stochastic states and their respective high, low and
incremental limits should also be part of the model validation activity.

Although the basic assumptions behind the KF formulation are realistic, the problem of determining the
constant covariance matrices Q and R for a specific application still exists. A specific methodology has
been elaborated in AspenTech® for estimating the Q and R variances.

The methodology is based on a decomposition of the global flowsheet into independent smaller sections
where the diagonal elements of Q variances related to the stochastic states can be tuned independently to
achieve an acceptable local performance. We assume that decoupling the covariance matrix can provide the
correct order of magnitude of those variances and only a fine tuning will be necessary when the entire
structure will be considered.
The diagonal elements of Q variances for the stochastic states were increased until the estimator responds quickly to changes in the state trajectories, yet was not producing changes beyond the incremental and low/high limits identified during the model validation phase. Their values have been adjusted in such a way that produces steady-state Kalman Gains with a reasonable physical understanding.

The diagonal elements of Q related to the normal states have been estimated by using the following formula:

\[ Q = 0.65 \cdot (V_{ss} \cdot f)^2 \]

where \( V_{ss} \) is the steady state value of the corresponding state and \( f \) is a steady-state deviation factor. This factor has been tuned based on the relative uncertainty of the states to the measurements.

The diagonal elements of R can be estimated from a qualitative information about the relative accuracy of the various plant measurements. It has been postulated [11] that without a noise adaptation mechanism and inexact a priori statistics, the filter might diverge. We have preferred to use an accurate model over the whole range of normal operating conditions. Our conclusion is that with relatively accurate modeling is very unlikely that the covariance matrix becomes unrealistically small (optimistic), the filter gain drops and subsequent measurements are ignored.

4.0 Application

Equistar Chemicals, LP (Equistar) operates four world-scale production lines at its Matagorda, TX manufacturing facility that produce injection, blow, and film grade high-density polyethylene (HDPE) resins. Matagorda runs the bimodal HDPE process offered jointly by Equistar and Maruzen (originally developed by Nissan), which is a slurry process with reactors in series utilizing a proprietary high performance catalyst technology.
Equistar has installed an Aspen Technology, Inc (AspenTech) DMCplus™ multi-variable controller on the Line 2 HDPE reactor systems at Matagorda [15]. The controller is being commissioned with a state estimation module (SEM), that consists of a rigorous dynamic process model which is semi-continuously reconciled to the operating plant for near real-time polymer property prediction and control. The dynamic model was developed using AspenTech’s SpeedUp™ dynamic simulation software, interfaced with a steady-state process model written with AspenTech’s Polymers Plus™ polymer modeling software.

The objective of the Matagorda Line 2 advanced process control (APC) project was to leverage the capabilities of DMCplus, specifically as means to move and hold the process against multiple operating constraints, while simultaneously maintaining high product quality, for optimum operating economics. The SEM provides essentially continuous real-time predictions of polymer physical properties. These predictions serve as controller inputs (process present values), and provide the DMCplus with information that is otherwise only available with intermittent laboratory analysis. At the time of this paper, the Matagorda Line 2 DMCplus/SEM has operated as a closed-loop process control application for several hundred hours. The Matagorda Line 2 APC project is now in the final stages of commissioning, and is expected to be deployed as a 24/7 application in 1Q 2000.

5.0 Model centricity

The modeling approach applied in a DSP Model is one that focuses on the physical understanding of the process. This application has used an approach where the model has been developed from basic physical property and polymer property information, into a steady state model of the process scope and then migrated into a dynamic model covering the range of process behavior. We observe at each step that the breadth of the model is expanded as new features expand the capability of the model.

A systematic development of the model, growing to meet the required scope, allows the re-use of the underlying components maximizing confidence in behavior and reducing effort in modeling. The end result is a robust model capable of operating over a wide range of conditions.
6.0 Conclusion

AspenTech®’s DSP Model is a new technology for the process industry [12,13]. To be successful not only must the technology be good but the infrastructure that it uses must also be solid and the user must be able to interact with the system. State Estimation is now a field based technology. The technology is moving quickly and techniques required for efficient engineering will be carried over to future applications. Here we summarize the factors that lead to this being a successful technology.

6.1 Real Time Platform

State Estimation technology is based on industry standard components developed for real-time applications. Products from AspenTech® for data collection (Connect™ software) and data management (InfoPlus™ software) are established and field proven. These have been broadly deployed in the use of DMCplus™ multivariable control technology.

6.2 Robust Implementation

Implementation of the State Estimation technology takes advantage of the lessons learnt in successful control application. The applications are robust to measurement behavior, control saturation and operator input. Indeed, the models go beyond this. The models are intended for use when the plant topology changes, when different components are fed to the plant and at different throughputs.

6.3 Modeling Technology

The model solving technology employs open equation solvers. These employ some of the currently most sophisticated tools for building and executing large-scale process models that can be solved in steady state, dynamic and optimization modes. The implementation of the state estimation has to be done in a way that is configurable so that the technology is easy to deploy to a range of models and can keep pace with plant changes.

6.4 State Estimation Calculations

State Estimation has been demonstrated in industrial applications outside the process industry. The technology provides a closed form solution to the estimation problem that is efficient. The calculations are
well defined and are used in many successful estimation applications. It is not enough to simply implement the calculations. The calculations have to be implemented in an efficient manner and the infrastructure has to be able to deal with real world considerations.

6.5 Project Methodology

There is an engineering methodology that spans the modeling and control applications worlds [14]. The best of both worlds are used to ensure the success of the applications. Successful control applications are based on a good understanding of the process behavior and relating this to the process measurements. Successful online modeling applications are also based on a good understanding of the process behavior and relating this to the underlying models.

6.6 Model scope

Making the correct simplifying assumptions about the process behavior remains an art. This means that there are good practices to be followed. This is similar to model identification where following some basic principles can make a big difference to the results obtained.

6.7 Benefits

State Estimation is delivering benefits to customers and achieving results they could not achieve in any other way. State estimation is being used to tackle specific process problems, providing benefits in a narrow and broad sense. It is being employed on tough problems beyond the scope of simple linear models and for uses that demand non-linear dynamic systems. Today these are the projects with significant benefits. As the technology becomes more established and the engineering capability expands we can expect to see more applications delivered faster into the process industry.
References


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