D-RM Builder: A Software Tool for Generating Fast and Accurate Nonlinear Dynamic Reduced Models from High-Fidelity Models

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Abstract

Dynamic reduced models (D-RMs) derived from rigorous models are highly desired for speeding up dynamic simulations. A useful software tool named D-RM Builder was developed to automatically generate data-driven D-RMs from high-fidelity dynamic models. It allows a user to configure input/output variables, sample input space and generate sequences of step changes, launch high-fidelity model simulations, fit simulation results to a D-RM, and finally visualize and validate the D-RM. The Decoupled A-B Net (DABNet) nonlinear system identification model was used as the main D-RM type and was enhanced to model nonlinear multiple input and multiple output dynamic systems with options for double-pole formulation to handle fast/slow time scales and pole value optimization. The D-RM Builder tool has been successfully used to generate D-RMs for a highly nonlinear pH neutralization reactor system and a two-time-scale bubbling fluidized bed adsorber-reactor for CO₂ capture.

Keywords: Data-driven dynamic reduced models, Nonlinear system identification models, Dynamic simulation, Model predictive control, Engineering software development, Carbon capture

1. Introduction

The development, scale-up, and commercialization of an innovative process such as a power generation system with carbon capture has historically required multiple steps ranging from laboratory prototype to pilot scale to demonstration and, finally, to large-scale deployment. Computer simulations have been playing a more important role in optimizing designs of individual devices and entire integrated systems. With increased confidence in computational models, some intermediate steps that are traditionally required in scaling up innovative processes, could potentially be shortened, thereby reducing the time, resources, and cost needed for process commercialization. Modern simulation models cover a wide range of length and time scales, from molecular- to device- to system-scales. The multiscale modeling challenges for carbon capture simulations have been discussed by Miller et al. (2014a). Model reductions

are sometimes needed to bridge the gap between scales such that a fast, small-scale model can be used in a large-scale model without sacrificing the speed of the simulation (Agarwal et al., 2014). In the time domain, steady-state models are used to optimize process designs while dynamic models are used to optimize process operations such as the transient response of the process in the presence of disturbances. Dynamic process models based on first principles of single or multiple unit operations require the solution of complex systems of differential algebraic equations (DAEs) involving thousands to hundreds of thousands of state variables. Typically, such DAE-based dynamic models are computationally expensive, particularly if the high-fidelity model contains a large number of stiff equations. Also, it is sometimes impractical to apply the high-fidelity models directly in dynamic simulations for off-line operator training systems (OTS) and on-line implementations of advanced process control (APC) and real-time optimization (RTO). For such applications, a fast and accurate dynamic reduced model (D-RM) must often be generated from the rigorous dynamic model.

Two major approaches exist for generating a dynamic reduced model from a DAE-based dynamic model. The first approach involves the simplification of the DAEs in the original high-fidelity model and the transformation of the model into projected space, resulting in a new set of DAEs with fewer unknowns and hence faster solution times (Yu et al., 2015). This type of D-RM is known as a reduced-order D-RM with order referring to the number of dynamic variables to be solved. The second approach treats the original rigorous model as a black box model. The transient relationship between the input and output variables of the system is obtained by using results from repeated simulation of multiple step changes in controlled input variables to fit a plant identification model using methods such as nonlinear regression and artificial neural networks (Sjöberg et al., 1995). A D-RM obtained in this way is known as a data-driven D-RM. While the order reduction approach is usually application specific and requires the detailed knowledge of the DAEs involved, the data-driven D-RMs can be generated automatically through a software tool that integrates with DAE solvers.

This paper discusses the generation of data-driven D-RMs through a software tool named D-RM Builder, developed under the auspices of the U.S. Department of Energy's Carbon Capture Simulation Initiative (CCSI) (Miller et al., 2015). The goal of CCSI is to develop models and software tools to help accelerate the scale-up and commercialization of carbon capture technologies. D-RM Builder is a module within the CCSI Framework for Optimization, Quantification of Uncertainty and Surrogates (FOQUS) (Eslick et al., 2014; Miller et al., 2014b). The following sections of the paper describe D-RM Builder's plant identification models, model fitting algorithms, overall software design and structure, typical user workflow, and available features. Finally, two case studies, including a carbon capture case, are provided to illustrate the features and capabilities of D-RM Builder.

2. Development of D-RM Builder

Development of an engineering software application usually involves the implementation of numerical algorithms and the presentation of commands with workflow for human-machine interaction. The development of D-RM Builder follows the same paradigm. First, advanced data-driven D-RMs and their required data structures are identified along with their training algorithms. These nonlinear D-RMs must provide fast and accurate simulations of nonlinear systems for fossil-fired power generation plants with carbon capture. Then, the graphical user interface under a specific development environment is outlined including menus, toolbars, dialog windows, and other widgets through which a user can select parameters and options for model generation, prepare required data, and finally train and validate the D-RM. These commands and dialogs need to be designed such that a user can follow a recommended workflow to generate the D-RM step by step from repeated simulation of the high-fidelity model. In the following sections, the physical models involved are discussed followed by the design and implementation from a software engineering perspective.

2.1 Data-Driven Dynamic Models

Plant identification models fall into two major categories: linear and nonlinear. A linear model is used to describe a system consisting of linear ordinary differential equations (ODEs) while a nonlinear model is used for a system consisting of nonlinear ODEs. A classical discrete-time state-space-based linear model can be expressed as:

$$\mathbf{x}(k+1) = \mathbf{A}\mathbf{x}(k) + \mathbf{B}\mathbf{u}(k) \quad \text{Eqn. 1}$$

$$\mathbf{y}(k) = \mathbf{C}\mathbf{x}(k) + \mathbf{D}\mathbf{u}(k) \quad \text{Eqn. 2}$$

where $\mathbf{x}(k) \in \mathcal{R}^{n_x}$ is the state-space vector of size n_x at time k , $\mathbf{u}(k) \in \mathcal{R}^{n_u}$ is the input vector of size n_u applied between time k and $k + 1$, and $\mathbf{y}(k) \in \mathcal{R}^{n_y}$ is the output vector of size n_y at time k . $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{D}$ in Eqns. 1 and 2 are time-invariant matrices. Commercial software packages such as MATLAB (Mathworks, 2015) have built-in functions to train linear models to find the optimal matrices given a set of transient data. Since most real-world processes such as those found in carbon capture systems are nonlinear, the objective of D-RM Builder is to generate nonlinear D-RMs. There are a variety of nonlinear system identification models in the literature including the Nonlinear Autoregressive Exogenous (NARX) model and the Hammerstein-Wiener model available in MATLAB (Mathworks, 2015). Two types of nonlinear discrete-time models have been implemented in D-RM Builder to date, including classical Nonlinear Auto Regressive Moving Average (NARMA) (Narendra and Mukhopadhyay, 1997) and Decoupled A-B Net (DABNet) (Sentoni et al., 1998). The NARMA model is a special NARX model that uses an artificial neural network (ANN) as the nonlinear function for mapping the finite number of previous inputs and outputs to the next future output. The DABNet model is

conceptually similar to the Wiener model since both are composed of a linear dynamic block followed by a nonlinear static map. The linear dynamic model of the DABNet is a state-space model based on discrete Laguerre systems while that of the Wiener model is a polynomial transfer function model. The Laguerre model incorporates a crucial process dynamic property – the process time-constant information – through “pole” definition, significantly reducing the number of model parameters compared to the Wiener polynomial model and hence is easier to be trained. Furthermore, the static mapping of the DABNet model is a nonlinear mapping from the state-space vector to individual outputs, while that of the Wiener model is a simple scalar-to-scalar nonlinear mapping, one for each output variable. This static mapping enables DABNet model to find the nonlinear correlations among multiple state variables within the state vector. The state-space dynamic formulation of the DABNet model makes it easy to implement the correction of the state variables inside a controller through various filtering algorithms such as extended Kalman filter and unscented Kalman filter when the measured output variables are available. The DABNet structure is well suited for embedding into a model predictive control (MPC) strategy, providing better long-term prediction than a NARX model in which the output errors are fed back into the model and amplified (Tsoi and Back, 1994). Since the NARMA model in D-RM Builder is similar to those found in commercial software tools, it will not be discussed further. This paper will focus on the DABNet model and its enhancements implemented in D-RM Builder.

2.1.1 DABNet Model

The DABNet model was originally proposed by Sentoni et al. (1998) to approximate nonlinear, causal, discrete time-invariant, multiple-input single-output (MISO) systems with fading memory. It is extended to a multiple-input multiple-output (MIMO) system inside D-RM Builder. Multiple independent DABNet models are used to simulate multiple outputs, one DABNet model for each output. In each DABNet model, linear dynamic mapping from an individual input u_j to its corresponding state-space vector $\mathbf{x}_{ij}$ for an output variable y_i is modeled by decoupled matrices $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$ (one set of matrices for each input-output pair, $j-i$) as described in Eqn. 3, where k represents current time and $k+1$ represents the next time step.

$$\mathbf{x}_{ij}(k+1) = \mathbf{A}_{ij}\mathbf{x}_{ij}(k) + \mathbf{B}_{ij}u_j(k) \quad \text{Eqn. 3}$$

Note that since u_j is a scalar, matrix $\mathbf{B}_{ij}$ contains only one column. If there are n_u input variables, then there are n_u sets of decoupled $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$ matrices with n_u sets of state vectors that form an augmented state vector $\mathbf{x}_i^{aug}$ as expressed in Eqn. 4.

$$\mathbf{x}_i^{aug} = \begin{bmatrix} \mathbf{x}_{i1} \\ \mathbf{x}_{i2} \\ \vdots \\ \mathbf{x}_{in_u} \end{bmatrix} \quad \text{Eqn. 4}$$

The nonlinear static mapping from the augmented state-space vector $\mathbf{x}_i^{aug}$ to an output variable y_i is modeled through a feedforward ANN with one hidden layer as described in Eqn. 5:

$$y_i(k) = f_i^{ANN}(\mathbf{x}_i^{aug}(k)) \quad \text{Eqn. 5}$$

where f_i^{ANN} represents the nonlinear function of the ANN for the output i .

The linear dynamic system with $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$ matrices is initially spanned by a set of discrete Laguerre systems (Sentoni et al., 1998). Figure 1 illustrates the discrete-time transfer function for an input-output pair j - i , where α_{ij} and n_{ij} are the pole and the order of the discrete Laguerre system for the input-output pair, respectively. According to Zervos et al. (1988), the pole value α_{ij} should match the main time constant τ_{ij} and sampling time interval Δt as shown in Eqn. 6.

$$a_{ij} = 1 - \frac{\Delta t}{\tau_{ij}} \quad \text{Eqn. 6}$$

The state-space vector for the pair $\mathbf{x}_{ij}$ is a collection of output signals after individual Laguerre blocks (see Figure 1). If a delay in the length of a sampling interval exists, a transfer function of $1/z$ can be added before the first Laguerre block, making the size of the state-space vector one state longer.

Figure 1. State-space variables for each input-output pair.

Given a Laguerre order n_{ij} and pole a_{ij} , the decoupled matrices $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$ can be readily obtained (see, for example, p. 65 of Zhou et al., 1996). If transient time series data are given for $\mathbf{u}(k)$ and $\mathbf{y}(k)$ where $k = 0, 1, 2, \dots, n_k$ and the first data point corresponds to a steady-state condition, the initial state-space vector for an input-output pair can be calculated based on Eqn. 7:

$$\mathbf{x}_{ij}(1) = \mathbf{x}_{ij}(0) = \mathbf{A}_{ij}\mathbf{x}_{ij}(0) + \mathbf{B}_{ij}u_j(0) \quad \text{Eqn. 7}$$

or Eqn. 8:

$$\mathbf{x}_{ij}(0) = [\mathbf{I} - \mathbf{A}_{ij}]^{-1} \mathbf{B}_{ij}u_j(0) \quad \text{Eqn. 8}$$

With the initial state vector determined, subsequent state variables at each time step can be calculated based on Eqn. 3. Using the augmented state vector $\mathbf{x}_i^{aug}$ at each time step, the output variable y_i at each time step can be calculated by Eqn. 5 if the structure and the weights of neuron connections of the ANN are given.

The weights inside the ANN can then be trained to match the actual response or, as in this case, to match data from the high-fidelity model. The matrices of the linear dynamic model initially obtained from the Laguerre series of finite terms ($\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$) can be reduced by balanced realization as outlined in Sentoni et al. (1998) using the weights between the input and the first hidden layer of the ANN. The reduction procedure is briefly described below.

While Eqn. 5 shows the nonlinear ANN function to map the state vectors $\mathbf{x}_i^{aug}$ to the system output variable y_i , the nonlinear sigmoid functions involved in the ANN are actually applied only at the first hidden layer neurons, after the weights between the input layer and the

first hidden layer are multiplied by the input state variables and the resulting products are summed. In other words, before applying the nonlinear sigmoid functions, the sums of the products of the weights and the state variables at the individual neurons in the first hidden layer can be considered as intermediate output variables in the DABNet model structure. The linear dynamic system with the intermediate variable $\mathbf{v}_{ij} \in \Re^{n_h}$ as the output vector for the decoupled j - i input-output pair can be described in Eqns. 9 and 10:

$$\mathbf{x}_{ij}(k+1) = \mathbf{A}_{ij}\mathbf{x}_{ij}(k) + \mathbf{B}_{ij}u_j(k) \quad \text{Eqn. 9}$$

$$\mathbf{v}_{ij}(k) = \mathbf{W}_{ij}\mathbf{x}_{ij}(k) \quad \text{Eqn. 10}$$

where n_h is the number of the neurons in the first hidden layer and $\mathbf{W}_{ij}$ is a time-invariant n_h by $n_{x,ij}$ matrix consisting of the weights between the input and the first hidden layers of the ANN. Because it is a linear dynamic system, all the theory of linear model reduction can be applied. To reduce the dimension of the state vector $\mathbf{x}_{ij}$ or the size of $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$ matrices, the balanced realization of the linear system (Zhou et al., 1996) and the truncation based on the Hankel singular values are applied. The observability Grammian $\mathbf{G}_{o,ij}$ and the controllability Grammian $\mathbf{G}_{c,ij}$ are matrices calculated based on the discrete-time Lyapunov equations as shown in Eqns. 11 and 12.

$$\mathbf{G}_{o,ij} - \mathbf{A}_{ij}^T \mathbf{G}_{o,ij} \mathbf{A}_{ij} = \mathbf{W}_{ij}^T \mathbf{W}_{ij} \quad \text{Eqn. 11}$$

$$\mathbf{G}_{c,ij} - \mathbf{A}_{ij} \mathbf{G}_{c,ij} \mathbf{A}_{ij}^T = \mathbf{B}_{ij} \mathbf{B}_{ij}^T \quad \text{Eqn. 12}$$

A similarity transformation $\mathbf{T}_{ij}$ can be obtained such that the system is in balanced form as shown in Eqn. 13:

$$\mathbf{G}_{o,ij,bal} = \mathbf{G}_{c,ij,bal} = \mathbf{\Sigma}_{ij} = \text{diag}(\sigma_{ij1}, \sigma_{ij2}, \dots, \sigma_{ijn_{ij}}) \quad \text{Eqn. 13}$$

where $\sigma_{ij1} \geq \sigma_{ij2} \geq \dots \geq \sigma_{ijn_{ij}}$ are Hankel singular values. The balanced system matrices can be expressed as:

$$\mathbf{A}_{ij,bal} = \mathbf{T}_{ij} \mathbf{A}_{ij} \mathbf{T}_{ij}^{-1} \quad \text{Eqn. 14}$$

$$\mathbf{B}_{ij,bal} = \mathbf{T}_{ij} \mathbf{B}_{ij} \quad \text{Eqn. 15}$$

Small Hankel values ($\sigma_{ijr} \gg \sigma_{ijr+1}$) indicate that the system can be reduced to an r -order model by truncating the $\mathbf{A}_{ij,bal}$ to an r by r square matrix $\hat{\mathbf{A}}_{ij}$ and $\mathbf{B}_{ij,bal}$ to an r by 1 matrix $\hat{\mathbf{B}}_{ij}$. Finally, the balanced nonlinear dynamic model becomes:

$$\hat{\mathbf{x}}_{ij}(k+1) = \hat{\mathbf{A}}_{ij}\hat{\mathbf{x}}_{ij}(k) + \hat{\mathbf{B}}_{ij}u_j(k) \quad \text{Eqn. 16}$$

$$y_i(k) = \hat{f}_i^{ANN}(\hat{\mathbf{x}}_i^{aug}(k)) \quad \text{Eqn. 17}$$

where $\hat{\mathbf{x}}_i^{aug}$ is the augmented state-space vector for output variable y_i , formed by combining the state-space vectors ($\hat{\mathbf{x}}_{ij}$) from all inputs in a similar way as shown in Eqn. 4. Using the balanced dynamic model of Eqn. 16, the new ANN function $\hat{f}_i^{ANN}$ in Eqn. 17 can be trained. Since the size of the state space is smaller, this balanced model is the final model exported from D-RM Builder.

Most nonlinear processes with a single time scale can be reduced to a DABNet model with a single set of Laguerre series associated with a single pole for each input/output pair as described above. However, for complicated processes with two different time scales (slow and fast), the Laguerre series with a limited number of terms was found to be unable to predict both the fast and slow responses as indicated by Mitsis and Marmarelis (2002). To resolve the fast mode, a short sampling time interval has to be used and a small pole selected to match the fast time scale. A large pole is required to match the slow process. Mitsis and Marmarelis (2002) used two Laguerre filter banks with two different poles coupled with a feedforward network with polynomial activation functions to form a Laguerre-Volterra network to model nonlinear physiological systems with both fast and slow dynamics. Their idea of using two Laguerre state vectors, one with a small pole value to match the fast response and the other with a large pole value, is adopted in D-RM Builder. The state-space vector for an input/output pair is now simply formed by combining the two state-space vectors as shown in Eqn. 18:

$$\mathbf{x}_{ij} = \begin{bmatrix} x_{ij,1}^{fast} \\ x_{ij,2}^{fast} \\ \vdots \\ x_{ij,n_f}^{fast} \\ x_{ij,1}^{slow} \\ x_{ij,2}^{slow} \\ \vdots \\ x_{ij,n_s}^{slow} \end{bmatrix} \quad \text{Eqn. 18}$$

where n_f and n_s are the orders of the Laguerre systems for the fast and slow responses, respectively. The corresponding $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$ matrices are also formed by combining the fast and slow ones as shown in Eqns. 19 and 20.

$$\mathbf{A}_{ij} = \begin{bmatrix} \mathbf{A}_{ij}^{fast} & 0 \\ 0 & \mathbf{A}_{ij}^{slow} \end{bmatrix} \quad \text{Eqn. 19}$$

$$\mathbf{B}_{ij} = \begin{bmatrix} b_{ij,1}^{fast} \\ b_{ij,2}^{fast} \\ \vdots \\ b_{ij,n_f}^{fast} \\ b_{ij,1}^{slow} \\ b_{ij,2}^{slow} \\ \vdots \\ b_{ij,n_s}^{slow} \end{bmatrix} \quad \text{Eqn. 20}$$

The double-pole approach provides a different formulation for the $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$ matrices. The algorithm for the balanced realization is the same as that for the single-pole formulation. D-RM Builder supports both the single-pole and double-pole formulations. It was found that the double-pole approach is capable of modeling processes with two time scales accurately, which can never occur using the single-pole approach. This is a major enhancement over the original DABNet model.

2.1.2 Model Parameters and Optimization of Pole Values

The model parameters in the DABNet model include the order of the discrete Laguerre system (i.e., the number of state variables n_{ij} in Figure 1), the pole value (a_{ij} in Figure 1) for each input-output pair j - i , and the number of neurons in the hidden layer of the ANN for output i . When the double-pole option is selected, there are two pole values for each input-output pair. As reported by Sentoni et al. (1998), the identification process is not very sensitive with respect to the order of the discrete Laguerre system n_{ij} . Typically, a Laguerre system of order six (the default input of D-RM Builder) produces a good fit for the D-RM. Note that the final order of the dynamic system is obtained by the balanced realization and truncation. In other words, D-RM Builder is able to remove high order terms for a low order system if a high order n_{ij} is initially specified. The pole values were sometimes found to be insensitive to the accuracy of the D-RM for simple dynamic systems while extremely sensitive for some complicated dynamic systems. To handle the latter case, D-RM Builder provides a derivative-free optimizer for selecting the best pole values around user-specified initial guesses. If the user knows the time constant of the process, Eqn. 6 can be used to calculate the pole value as the initial estimate. A default value of 0.5 is recommended if the user has no information about the time constant. When the double-pole option is selected, the user can also calculate the initial guesses for the first (fast) and the second (slow) poles based on Eqn. 6 if the user knows the two time constants. The value for the second pole must be higher than that of the first pole according to Eqn. 6. A

default value of 0.95 is recommended for the second pole if the user has no information about the time constants. Usually the optimum pole values obtained are not sensitive to the initial guesses. The built-in optimization feature is based on Nelder-Mead's simplex method (Nelder and Mead, 1965). The objective function that is minimized is the sum of the squared errors for the ANN function over individual time steps based on the Laguerre system matrices rather than the balanced matrices. The balanced realization and the subsequent ANN training are performed after the poles are optimized. Note that currently the number of neurons in the hidden layer of an individual ANN is not included in the optimization routine. The optimization of this input parameter remains to be explored in the future.

2.1.3 Uncertainty Quantification of Generated D-RM

When training a D-RM, the results of high-fidelity model simulations are assumed to be absolutely correct without any noise. In other words, the numerical errors in solving the DAEs are ignored. The accuracy of a D-RM can be measured by the relative error compared to the high-fidelity model used to generate it. A correlation plot of output variables predicted by the D-RM versus high-fidelity model results and the corresponding R-squared value also indicate D-RM accuracy. Those accuracy related measures can be applied to both training and validation data. However, they are more important for the validation data. Overfitting can usually be detected if the accuracy measures based on validation data are much worse than those based on training data.

The accuracy of a D-RM can also be measured in terms of uncertainties of state-space variables and measured output variables when the D-RM is used for advanced process control. In the control perspective, the state and output variables of the next time step are predicted based on the state and input variables at the current time. When the next time step is reached, the measured output data that contain measurement noise are fed to the control system, in which the state vector at the new time step predicted by the D-RM is corrected using a filtering algorithm such as a Kalman filter. The uncertainty can be quantified by the covariance matrices of the state and output variables. As a user option for a DABNet model, D-RM Builder can perform uncertainty quantification (UQ) based on an unscented Kalman filter (UKF) algorithm in which the generated DABNet model is used as the predictive model and the measurements of output variables are estimated by imposing white noise with user-defined signal to noise ratio (SNR) on the results of the rigorous model simulation. The UKF procedure is adopted from Hartikainen et al. (2011). For any nonlinear discrete-time dynamic system with Gaussian process noise and Gaussian measurement noise,

$$\mathbf{x}(k+1) = f[\mathbf{x}(k), \mathbf{u}(k)] + \mathbf{q}(k) \quad \text{Eqn. 21}$$

$$\mathbf{y}(k+1) = h[\mathbf{x}(k+1)] + \mathbf{r}(k+1) \quad \text{Eqn. 22}$$

1 where $\mathbf{x}$ and $\mathbf{y}$ are state and measured output vectors, respectively, $\mathbf{q} \sim N(0, \mathbf{Q})$ is the Gaussian
 2 process noise, and $\mathbf{r} \sim N(0, \mathbf{R})$ is the Gaussian measurement noise. For the DABNet model, $\mathbf{x}$
 3 is the collection of $\hat{\mathbf{x}}_i^{aug}$ in Eqn. 17 for all output variables ($i = 1, 2, \dots, n_y$), function f in Eqn.
 4 21 consists of multiple linear functions of Eqn. 17 decoupled among multiple input-output pairs,
 5 and function h in Eqn. 22 consists of multiple decoupled ANNs of Eqn. 17 for multiple output
 6 variables. In D-RM Builder, $\mathbf{Q}$ and $\mathbf{R}$ are diagonal matrices specified by the user for process
 7 (state variables) and measurement noises, respectively. Each diagonal element of $\mathbf{R}$ is related to
 8 the SNR (in terms of the ratio of signal variance to noise variance) of the corresponding
 9 measurement device. The UKF algorithm contains two calculation steps at each time step; one is
 10 a prediction step, and the other is an update step. UQ is performed on the transient high-fidelity
 11 model results for the validation sequence only. Since the first data point in the transient data
 12 represents a steady-state condition, the initial state-space vector $\mathbf{x}(0)$ can be calculated based on
 13 an equation similar to Eqn. 8 for the balanced model. Initially a small amount of process noise
 14 for state variables represented by a covariance matrix $\mathbf{P}_0$ is estimated. In the prediction step,
 15 unscented transformation (UT) is applied to the mapping of the current state vector to the state
 16 vector of the next time step. $2n_x + 1$ sigma points are created where n_x is the size of the state
 17 vector. Then decoupled linear dynamic functions are evaluated for individual sigma points and
 18 the mean $\mathbf{x}^-$ and covariance matrix $\mathbf{P}^*$ of the state vector at next time steps are calculated. The
 19 noise matrix $\mathbf{Q}$ is added to the covariance matrix $\mathbf{P}^*$ as the predicted process noise matrix $\mathbf{P}^-$.
 20 The measured output at the new step is assumed to be the results of the high-fidelity model plus a
 21 randomly sampled measurement noise from a normal distribution $N(0, \mathbf{Q})$. In the update step,
 22 UT is applied to the mapping of the new state vector to the new output vector. $2n_x + 1$ sigma
 23 points based on predicted noise matrix $\mathbf{P}^-$ is created and their corresponding outputs are
 24 calculated based on Eqn. 17. Then the mean $\mathbf{y}^-$ and covariance matrix $\mathbf{S}^*$ of the output vector
 25 are calculated. The measurement noise matrix $\mathbf{R}$ is added to the covariance matrix $\mathbf{S}^*$ as the
 26 new output noise covariance matrix $\mathbf{S}$. Then cross-covariance matrix $\mathbf{C}$ is calculated from the
 27 sigma points and the corresponding Kalman filter gain matrix $\mathbf{K}$ is calculated. Finally the mean
 28 of state vector $\mathbf{x}^-$ is updated or corrected based on the difference between the measured and
 29 modeled output $\mathbf{y} - \mathbf{y}^-$ and the gain matrix $\mathbf{K}$ while the covariance matrix $\mathbf{P}$ of state vector for
 30 the next step is updated from the predicted noise matrix $\mathbf{P}^-$. The prediction and update
 31 processes continue at each time step until all steps in the transient sequence are completed.
 32 Figure 2 shows the flow diagram of the UQ analysis procedure.

Figure 2. UQ Analysis Procedure

2.2 Software Architecture of D-RM Builder

D-RM Builder's architecture is integrated with the existing FOQUS platform and the required algorithms for fitting the transient data to system identification models and for validating the resulting models. FOQUS consists of several modules which enable multiple capabilities including simulation-based process optimization, UQ, optimization under uncertainty, generation of steady-state surrogate model for optimization (Cozad et al., 2014), and D-RM generation. FOQUS has a graphic user interface (GUI) written in Python using open PySide libraries (PySide Project, 2015). The main window of FOQUS contains a set of icons in the upper part and a set of stacked frames. Each icon corresponds to a stacked frame for an individual module. Figure 3 shows the FOQUS GUI with the D-RM Builder module activated; it contains a menu bar, a toolbar, a client area displaying the D-RM as a box connected by input and output variables as arrows and labels, and a client area displaying the messages.

Figure 3. Main window of FOQUS GUI with D-RM Builder activated

Figure 4 shows the workflow of D-RM Builder and the software components used in the process of building a D-RM. D-RM Builder uses three other FOQUS modules, which are shown in the box at the upper left corner of Figure 4. SinterConfigGUI is used to specify the input and output variables of a high-fidelity steady-state or dynamic process model. The high-fidelity dynamic model from which a D-RM is built may contain a large number of input and output variables. Some of the input variables may involve design parameters such as vessel dimensions or certain fixed feed stream data. If the system design and certain operating conditions remain invariant, it is possible that some input variables could be fixed and only a limited number of input variables in the high-fidelity model need to be included in the D-RM. In this paper, the high-fidelity dynamic models are implemented in the commercially available Aspen Custom Modeler (ACM) software package. SinterConfigGUI allows a user to browse ACM variables by querying the ACM model. The user can select a set of input and output (I/O) variables and save them in a file in the open-standard JSON format, which can later be used for scheduling a simulation job. The input variables listed in the JSON file can be assigned values during job execution (i.e., running the process model) and the output variables listed in the JSON file are returned after completion of the simulation. FOQUS provides different ways to run CPU-intensive dynamic model simulations via the Turbine module. Turbine also manages the multiple runs needed to build steady-state and dynamic reduced models, perform derivative-free

optimization or conduct a UQ analysis. Turbine provides the capability for job queuing and enables these jobs to be run in parallel using cloud- or cluster-based computing platforms or a single workstation. A data management framework can store and retrieve simulation files, data and their provenance.

Figure 4. D-RM Builder components and workflow

Generating a D-RM involves several CPU-intensive steps including high-fidelity model simulation, calculating and optimizing D-RM model parameters, and performing UQ analysis. While high-fidelity model simulation is handled by Turbine, some other CPU-intensive calculations need to be coded and compiled in other languages such that they can be run quickly. The two components in the box at the upper right corner of Figure 4 are Python extended components written in C++. They are compiled to dynamically linked libraries (DLLs) in a form that Python can call (with extension “pyd”). The advantage of compiling to a DLL over an executable is that no input and output files are required and all the data are passed in the form of Python tuples. The first Python extended component is for sampling the input space and generating the step change sequence for dynamic model simulation. The second Python extended component is for fitting the training data to a D-RM, including calculating the D-RM parameters and training the ANNs involved. For training ANNs, two types of training algorithms are provided. One is the back propagation (BP) method (Riedmiller, 1994), and the other is the interior point optimization (IPOPT) method (Wächter and Biegler, 2006). Both training options are very CPU-intensive, and there are no open Python libraries available for those algorithms. For the DABNet model, more linear algebra calculations are involved such as

those for solving Grammian matrices in the balanced realization of the liner system. Therefore, it is better to wrap all D-RM training calculations in a DLL written in C++.

The rest of the D-RM Builder components shown in the bottom box of Figure 4 are written as Python classes, representing I/O variables, step change sequences, transient ACM model simulation data, D-RM related objects (e.g. DABNet model, state-space variables, NARMA model, and ANNs), and UQ related objects (e.g. UKF related data and functions). The Python classes include calculations for predicting the response to a step change sequence using a D-RM in Python's runtime memory. Whenever there is a matrix-related calculation (e.g. in UKF), a fast Python library such as numpy is used. Additional Python classes developed for D-RM Builder (not shown in Figure 4) include the GUI classes and some classes to store user inputs. The widgets in the GUI classes are designed using Qt Designer (The Qt Company Ltd., 2015).

As shown in Figure 4, the workflow of D-RM Builder starts when a user selects the desired I/O dynamic variables from a high-fidelity model through SinterConfigGUI. Then the user specifies the ranges (lower and upper limits) of the input variables. The user also specifies the sampling interval for the discrete D-RM model and requests D-RM Builder to create two step change sequences by calling the DLL for step change sequence creation, one for training the D-RM and the other for validating the D-RM. The user is allowed to specify the length of the step change sequences by setting the number of Latin hypercube sampling (LHS) points and the duration (in terms of number of sampling time intervals) of holding the input constant before the next step change. Usually the sequence for validation can be much shorter than that for training. The resulting step change sequences can then be passed to Turbine to perform the dynamic simulations. The simulation results are passed back to D-RM Builder. Then the user needs to choose one of the system identification models, either DABNet or NARMA. Several training options such as number of neurons in the hidden layer of ANNs in the D-RM and the training methods (e.g. IPOPT or BP for ANN training) can be specified. The training data and options are passed to another DLL which constructs a Python object representing the D-RM in a D-RM container class. Validating the D-RM consists of predicting the responses of the training and validation sequences using the D-RM and comparing them to the high-fidelity model simulation results. The responses, along with the relative error can be plotted from FOQUS. R-squared values are also displayed as an indication of D-RM accuracy. For the DABNet model, the user is also allowed to specify the noise of the process and measurement and request D-RM Builder to perform UQ analysis on the validation data. If the D-RM is believed to be sufficiently accurate, the D-RM can be exported to a MATLAB script file, which can be used to construct a D-RM object for CCSI's APC Framework. If not, the user can either modify the model parameters or training options to generate a new D-RM or generate additional training data.

3. Case Study

Two example cases are presented in this section to demonstrate the features and capabilities of D-RM Builder. The first case is a continuous-stirred pH neutralization tank reactor system and the second case is a bubbling fluidized bed (BFB) reactor system for a solid sorbent-based CO₂ capture process.

3.1. pH Neutralization Reactors

The two-tank pH neutralization process is a highly nonlinear process that has been widely used as a benchmark dynamic problem in the literature and was also used by the original developers of the DABNet model (Sentoni et al., 1998). Figure 5 shows the schematic of the neutralization system.

Figure 5. Two-tank pH neutralization system

There are three feed streams to the first tank as shown in Figure 5. Q_1 and Q_2 are the volumetric flow rates of acetate acid (HAC) and Q_3 is the volumetric flow rate of sodium hydroxide (NaOH). The product stream of the first tank with a volumetric flow rate of Q_4 is fed to the second tank along with three extra feed streams (Q_5 , Q_6 and Q_7). Q_5 and Q_6 are the volumetric flow rates of the two HAC streams and Q_7 is the volumetric flow rate of NaOH.

The corresponding ODEs for the system are listed below:

$$A_1 \frac{dh_1}{dt} = Q_1 + Q_2 + Q_3 - C_{v1} \sqrt{h_1} \quad \text{Eqn. 23}$$

$$A_1 h_1 \frac{d\alpha_1}{dt} = Q_1 C_A + Q_2 C_A - C_{v1} \alpha_1 \sqrt{h_1} \quad \text{Eqn. 24}$$

$$A_1 h_1 \frac{d\beta_1}{dt} = Q_3 C_B - C_{v1} \beta_1 \sqrt{h_1} \quad \text{Eqn. 25}$$

$$A_2 \frac{dh_2}{dt} = Q_5 + Q_6 + Q_7 + C_{v1} \sqrt{h_1} - C_{v2} \sqrt{h_2} \quad \text{Eqn. 26}$$

$$A_2 h_2 \frac{d\alpha_2}{dt} = Q_5 C_A + Q_6 C_A + C_{v1} \alpha_1 \sqrt{h_1} - C_{v2} \alpha_2 \sqrt{h_2} \quad \text{Eqn. 27}$$

$$A_2 h_2 \frac{d\beta_2}{dt} = Q_7 C_B + C_{v1} \beta_1 \sqrt{h_1} - C_{v2} \beta_2 \sqrt{h_2} \quad \text{Eqn. 28}$$

where α , β , A , h , and C_v are acetate ($\text{HAC} + \text{AC}^-$) concentration, sodium (Na^+) concentration, cross section area, liquid height, and valve coefficient of a tank, respectively, with the subscript 1 or 2 representing either the first or the second tank. C_A and C_B are concentration of HAC and NaOH in the feed streams, respectively. The algebraic equations related to chemical equilibrium and electroneutrality are listed below:

$$K_A = \frac{[\text{AC}^-][\text{H}^+]}{[\text{HAC}]} \quad \text{Eqn. 29}$$

$$K_w = [\text{H}^+][\text{OH}^-] \quad \text{Eqn. 30}$$

$$\alpha_2 = [\text{HAC}] + [\text{AC}^-] \quad \text{Eqn. 31}$$

$$\beta_2 + [\text{H}^+] = [\text{OH}^-] + [\text{AC}^-] \quad \text{Eqn. 32}$$

$$\text{pH} = -\log_{10}[\text{H}^+] \quad \text{Eqn. 33}$$

where $[\text{HAC}]$, $[\text{AC}^-]$, $[\text{H}^+]$, and $[\text{OH}^-]$ are concentrations of HAC, AC^- , H^+ , and OH^- in the second tank, respectively. The normal operating conditions and equilibrium constants are listed in Table 1.

Table 1. Normal operating conditions and constants for pH neutralization example

Symbol	Description	Value	Unit of Measurement
A_1	Cross section area of Tank 1	10	m^2

A_2	Cross section area of Tank 2	10	m^2
C_{v1}	Valve coefficient of Tank 1	113.1	$\text{m}^{2.5}/\text{hr}$
C_{v2}	Valve coefficient of Tank 2	226.2	$\text{m}^{2.5}/\text{hr}$
Q_1	Acid volumetric flow rate 1	2.46	m^3/hr
Q_2	Acid volumetric flow rate 2	2.4	m^3/hr
Q_3	Base volumetric flow rate 3	30.9	m^3/hr
Q_5	Acid volumetric flow rate 5	3.0	m^3/hr
Q_6	Acid volumetric flow rate 6	1.86	m^3/hr
Q_7	Base volumetric flow rate 7	30.9	m^3/hr
C_A	HAC concentration	0.32	kmol/m^3
C_B	NaOH concentration	0.05	kmol/m^3
K_A	HAC dissociation constant	1.8×10^{-5}	
K_B	H_2O dissociation constant	1.0×10^{-14}	

Eqns. 23-33 are coded in an ACM model with six feed streams (Q_1 , Q_2 , Q_3 , Q_5 , Q_6 , and Q_7) and one final product stream (Q_8). The first step for generating a D-RM for the dynamic system is to configure the I/O variables through SinterConfigGUI. In this example, only two input variables and two output variables are included as the dynamic variables in the D-RM while all other input variables are kept as constants at normal operating conditions. The two dynamic input variables are the acid flow rate Q_1 and the base flow rate Q_3 , both of which are volumetric flow rates of feed streams to Tank 1. The two output variables are the acetate ($\text{HAC} + \text{AC}^-$) concentration α_2 and pH value in the final product stream Q_8 . To generate the D-RM for the pH neutralization system, a sampling time interval of 0.005 hr is used. The two input dynamic variables are allowed to change within $\pm 10\%$ of the steady-state values at normal operating conditions as listed in Table 1. In other words, the lower and upper limits of Q_1 are 2.214 and 2.706 m^3/hr , respectively, and those of Q_3 are 27.81 and 33.99 m^3/hr , respectively.

To generate a step change sequence for training, five sets of LHS samples are randomly generated by D-RM Builder with each set containing five steady-state points in the 2-D input space. A total of 25 steady-state points are sampled. The step change sequence is obtained by making two step changes to move to a new steady-state point, one for each input variable. The holding times in terms of number of sampling time intervals after each step change are also specified as D-RM Builder input. For this example, the holding durations are 5, 10, 15, 5, and 10 sampling time intervals for the five sets of LHS samples, respectively. Different holding durations are needed to excite the system in a range of frequencies. After switching to 25 steady-state points from the first point to the last point, the process is reversed. Therefore, a total of

50x2=100 step changes are generated with different holding durations. The total time covered by those step changes including the initial holding times before the first step change is 3.52 hr or 704 sampling time intervals. Plots (a) and (b) in Figure 6 show the step change sequence created by D-RM Builder.

DABNet is used as the D-RM type. The options selected for generating the D-RM are listed in Table 2. The BP method is used for training ANNs of both Laguerre and balanced models. The number of neurons in the hidden layer is set to 5 for both output variables α_2 and pH . The number of Laguerre states is set to 6 and 7 for I/O pairs involving α_2 and pH , respectively. No time delays are applied for all I/O pairs. Single-pole Laguerre series is used for all I/O pairs. Initially all pole values are set to the default value of 0.5 and are then optimized by D-RM Builder.

It took approximately 0.5 hr to perform the ACM simulations to predict the response to the step change sequence for training. It took approximately 180 s to train the two DABNet models (one for each output) for the pH neutralization reactor system including the pole optimization. All computations including ACM simulation and D-RM training were conducted on a Dell Precision M3800 (2.2 GHz Intel Core i7) workstation. The required time for training the two DABNet models at a given set of pole values is approximately 6 s, including calculating the $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$ matrices of the Laguerre system, training the initial ANN, performing balanced realization to calculate $\hat{\mathbf{A}}_{ij}$ and $\hat{\mathbf{B}}_{ij}$ matrices, and finally retraining the ANN based on the reduced matrices. Approximately 40 to 70 iterations are required to optimize the pole values for each output variable. Note that the balanced realization and the ANN training for the balanced model are performed only once, after the completion of the pole optimization as described in Section 2.1.2.

(a) Step change sequence of Q_1 (b) Step change sequence of Q_3
(c) pH predicted by ACM and D-RM (d) Relative error of D-RM prediction

Figure 6. Step change sequences for training the D-RM of pH neutralization reactor system and comparison between ACM and D-RM predictions

Table 2. Options for training D-RM of pH neutralization example

Option	Selection
Model type	DABNet
Method for training Laguerre model ANN	BP

Method for training balanced model ANN	BP
Maximum number of iterations for training Laguerre model ANN	7000
Maximum number of iterations for training balanced model ANN	10000
Number of neurons in hidden layer for output α_2	5
Number of neurons in hidden layer for output pH	5
Optimize pole values for output α_2	Yes
Optimize pole values for output pH	Yes
Time delay applied for I/O pair Q_1 / α_2	No
Number of Laguerre states for I/O pair Q_1 / α_2	6
Time delay applied for I/O pair Q_3 / α_2	No
Number of Laguerre states for I/O pair Q_3 / α_2	6
Time delay applied for I/O pair Q_1 / pH	No
Number of Laguerre states for I/O pair Q_1 / pH	7
Time delay applied for I/O pair Q_3 / pH	No
Number of Laguerre states for I/O pair Q_3 / pH	7
Initial pole value for all I/O pairs	0.5

After optimization, the pole values used for the D-RM are listed in Table 3. The order of the model (number of state variables) for I/O pairs are reduced through balanced realization as shown in Table 3. On average, they are reduced by more than 50% from their initial values. The average ANN training errors E_{ANN} defined in Eqn. 34 for normalized output variables are also listed in Table 3:

$$E_{ANN} = \frac{(y_t - y_o)^2}{2} \quad \text{Eqn. 34}$$

where y_t is the target output value from ACM simulation and y_o is the D-RM predicted output value. Note that within an ANN, any output value y is normalized by the mean $\bar{y}$ and the standard deviation σ_y of all output data points in the training sequence based on Eqn. 35 and the normalized value $\hat{y}$ is actually used in Eqn. 34 to train the ANN.

$$\hat{y} = \frac{y - \bar{y}}{\sigma_y} \quad \text{Eqn. 35}$$

Table 3. Optimized pole values and other results for pH neutralization example

Optimized pole value of balanced model for I/O pair Q_1 / α_2	0.7794
Optimized pole value of balanced model for I/O pair Q_3 / α_2	0.8445
Optimized pole value of balanced model for I/O pair Q_1 / pH	0.8456
Optimized pole value of balanced model for I/O pair Q_3 / pH	0.8644
Number of states of balanced model for I/O pair Q_1 / α_2	3
Number of states of balanced model for I/O pair Q_3 / α_2	3
Number of states of balanced model for I/O pair Q_1 / pH	4
Number of states of balanced model for I/O pair Q_3 / pH	2
Average error of the balanced model ANN for output α_2	0.000105
Average error of the balanced model ANN for output pH	0.000783

If the training errors are small, the response calculated by the D-RM should match the response calculated by the ACM simulation. Plot (c) in Figure 6 shows a comparison between the two responses and Plot (d) in Figure 6 shows the relative errors of the D-RM predictions. Notice that the D-RM prediction, shown as red dashed curve, is almost superimposed on the ACM prediction, shown as blue solid curve, and there are only a few spikes in the relative error. Plot (a) in Figure 7 shows the correlation plot of all data points at individual times along with the R-squared value for the pH data predicted by the D-RM and the ACM models for the training sequence. It can be seen that most data points are located near the 45° line and the R-squared value is 0.99979, indicating a very good match between the two sets of the data.

(a) Training data

(b) Validation data

Figure 7. Correlation plot of pH values predicted by ACM and D-RM

Since the D-RM is generated by fitting the ACM model results, the D-RM prediction can usually match the ACM prediction quite well. To validate the model, a different step change sequence is generated and the dynamic response to the new step changes is simulated by ACM. The corresponding response is then predicted by the D-RM. The D-RM prediction is compared to the ACM result for the validation sequence in Figure 8, along with the relative errors and step changes. The corresponding correlation plot is shown in Plot (b) of Figure 7. It can be seen from Figure 8 that the D-RM prediction, the red dashed curve in Plot (c), matches the ACM result, the blue solid curve. The R-squared value of 0.99853 for the validation data is also close to unity, indicating a good match.

(a) Step change sequence of Q_1 (b) Step change sequence of Q_3

(c) pH predicted by ACM and D-RM

(d) Relative error of D-RM prediction

Figure 8. Step change sequences for validating the D-RM of pH neutralization reactor system and comparison between ACM and D-RM predictions

To perform UQ analysis in the context of the D-RM for advanced process control, UKF is applied to the validation data with noise specified for state-space and output variables. In this example, the noise for all state-space variables is specified as 1% of the standard deviation of individual state-space variables based on the training data. The measurement noises for pH and acetate ($\text{HAC} + \text{AC}^-$) concentration α_2 in the product stream Q_8 (see Figure 5) are assumed to be 5% of the standard deviations of the two output variables from the training data. The covariance matrix of the UQ analysis on the validation data is listed in Table 4. The two diagonal elements of the matrix represent the variances of the filtered output variables, from which their standard deviations can be calculated. The two off-diagonal elements are very small in this case, indicating that the two output variables are not correlated. Figure 9 shows the filtered response curves with a section of the curves in the dashed rectangular region of the upper plot enlarged and displayed in the lower plot. The blue solid curve in Figure 9 is the measured pH value in the product stream. Notice that the zigzag lines are due to measurement noise. The red dashed curve in Figure 9 is the filtered prediction, which is much smoother. The black dotted curve and black double dotted curve show the range of the filtered result with a standard deviation calculated from the diagonal of covariance matrix $\mathbf{S}$ added to and subtracted from the filtered result (red dashed curve).

Table 4. Final covariance matrix of output variables

	α_2 of Stream Q_8	pH of Stream Q_8
α_2 of Stream Q_8	1.7×10^{-9}	-3.46×10^{-18}
pH of Stream Q_8	-3.46×10^{-18}	0.01151

Figure 9. Response of the DABNet model for validation sequence

3.2. Bubbling Fluidized Bed CO₂ Adsorber-reactor

Solid-sorbent-based post-combustion CO₂ capture was one of the challenging industry problems considered by CCSI. An ACM model was developed for a bubbling fluidized bed (BFB) adsorber for capturing CO₂ from post-combustion flue gas (Lee and Miller, 2013; Modekurti et al., 2013; Mahapatra et al., 2014). The adsorber uses an amine-based solid sorbent, and the adsorber consists of two BFBs in countercurrent series with cooling tubes embedded in each reactor. The process flowsheet in ACM is shown in Figure 10. Detailed information about the ACM model can be found in Modekurti et al. (2013).

Figure 10. ACM flowsheet of BFB CO₂ adsorber-reactor system

In this case study, a D-RM is generated from the rigorous ACM model with the flow rate of flue gas fed to the system $\mathbf{F}$ and the flow rate of the sorbent stream $\mathbf{F}_m$ as the two input variables and the percentage of CO₂ captured as the only output variable. The gas/solid two-phase reaction/separation system has both a fast and a slow time scale. The fast time scale is on the order of a few seconds due to the rapid response of fluid dynamics of the two-phase flow while the slow time scale is on the order of hundreds of seconds due to the slow kinetics of the solid sorbent. Table 5 lists the normal operating conditions for the two input variables and their lower and upper limits. Again, $\pm 10\%$ of the normal operating conditions are defined as the valid range for the D-RM.

Table 5. Range of input variables defined for the D-RM of the BFB adsorber-reactor

Input Variable	Feed Flue Gas Flow Rate $\mathbf{F}$	Feed Sorbent Flow Rate $\mathbf{F}_m$
Unit of Measurement	kmol/hr	kg/hr
Normal Operating Condition	6,750	600,000
Lower Limit	6,075	540,000
Upper Limit	7,425	660,000

To resolve the fast time scale, a sampling time interval of 1.0 s is used. To generate the step change sequence for training, four sets of LHS samples are generated, each of which has five steady-state operating conditions randomly selected in the ranges listed in Table 5. The holding times are 20, 40, 60, and 80 s for the four sets of samples, respectively. Step changes are formed by marching the individual steady-state condition from the first sample to the last and then from the last to the first (selecting the option with reversed step changes from the GUI of D-RM Builder). To validate the D-RM, two sets of samples are generated, each of which has five steady-state operating conditions randomly selected in the same ranges. The holding times are 30 and 70 s for the two sets of samples, respectively. The option with reversed step changes is also selected. Figure 11 shows the step change sequence for validation. The step change sequences for both training and validation are sent to the ACM model through Turbine. The results of ACM simulations are returned to D-RM Builder for training and validating the D-RM.

Initially a single-pole option of the DABNet model is used to generate the D-RM. For a process with a single time constant around a few seconds (corresponding to the fast time scale of the BFB adsorber-reactor), a sampling time of 1.0 s, a pole value near 0.5 (see Eqn. 6), and a Laguerre order of 6 are usually good enough to train the DABNet model. However, the slow time scale of the BFB adsorber is on the order of a few hundreds of seconds. Therefore, a high

Laguerre order needs to be used. Note that Laguerre terms at lower orders (the first few blocks in Figure 1) tend to fit a faster response, and those at higher orders tend to fit a slower response. It was initially expected that the long Laguerre series can fit both the fast and slow responses. However, too long a Laguerre series is impractical; it is extremely hard to train the ANN involved. A single pole value with initial guess of 0.8 is optimized for a Laguerre order of 8 for the two I/O pairs. Figure 12 shows the transient profile of the output variable, the percentage of CO₂ captured, predicted by the D-RM with the single-pole option for the validation sequence, the red dashed curve, and the one calculated by the rigorous ACM model, the blue solid curve. It can be seen from Figure 12 that there is a fast response at every step change followed by a slow response. The fast responses due to the step changes in feed flue gas flow rate are more dramatic than those of the sorbent flow rate. Apparently the optimized single-pole model cannot capture both the fast and slow responses, especially the response due to the change in sorbent flow rate. The average error when training the ANN of the balanced model is 6.35×10^{-4} and the R^2 value for the validation data is 0.993.

Figure 11. Step changes for the validation sequence of the BFB adsorber-reactor

Figure 12. Output response to validation sequence predicted by single-pole DABNet model

To generate a better D-RM that captures both the fast and slow time scales, the double-pole option is used and both poles for each I/O pair are optimized. Table 6 shows the options and parameters used for training the DABNet model. The Laguerre order for the fast pole is set to 6, and that for the slow pole is also set to 6 for a total of 12 states for each I/O pair. The fast pole is set to 0.5 initially and the slow pole is set to 0.99 initially. Both are optimized by D-RM Builder. It took approximately 600 s to train the DABNet model and optimize the pole values. At a given set of pole values, the required time for training the DABNet model is approximately 10 s. Table 7 shows the results along with the state vector size of the balanced model. Figure 13 compares the responses of the validation sequence with D-RM results. It took approximately 4 hours for the ACM model to simulate the validation step-change sequence on the Dell workstation while it took less than 1 s for the D-RM model to predict the response on the same computer. The speedup by using the D-RM is at least four orders of magnitude. It can be seen from Figure 13 that both the fast and slow responses are matched quite well. The average error when training the ANN of the balanced model is 5.10×10^{-5} and the R^2 value for the validation data is 0.99935 as shown in Figure 14, indicating a much more accurate D-RM than the one generated with the single-pole option.

Table 6. Options for training the D-RM of the BFB adsorber-reactor

Option	Selection
Model type	DABNet
Method for training Laguerre model ANN	BP
Method for training balanced model ANN	BP
Maximum number of iterations for training Laguerre model ANN	5000
Maximum number of iterations for training balanced model ANN	10000
Number of neurons in hidden layer for output $y_{captured}$	2
Optimize pole values for output $y_{captured}$	Yes
Time delay applied for I/O pair flow $F/y_{captured}$	No
Number of Laguerre states for I/O pair $F/y_{captured}$	6
Time delay applied for I/O pair $F_m/y_{captured}$	No
Number of Laguerre states for I/O pair $F_m/y_{captured}$	6
Initial pole value for all I/O pairs (fast/slow)	0.5/0.99

Table 7. Optimized pole values and other results for the BFB adsorber-reactor

Optimized fast pole value for I/O pair $F/y_{captured}$	0.575
Optimized slow pole value for I/O pair $F/y_{captured}$	0.9941
Optimized fast pole value for I/O pair $F_m/y_{captured}$	0.525
Optimized slow pole value for I/O pair $F_m/y_{captured}$	0.9965
Number of states of balanced model for I/O pair $F/y_{captured}$	10
Number of states of balanced model for I/O pair $F_m/y_{captured}$	12
Average error of the balanced model ANN for output $y_{captured}$	5.1×10^{-5}

Figure 13. Response to validation sequence predicted by the double-pole DABNet model

Figure 14. Correlation plot of the percentage of CO₂ captured predicted by ACM and D-RM for the validation sequence

4. Conclusions and Future Work

A useful software tool, D-RM Builder, was developed to generate fast and accurate data-driven dynamic reduced models (D-RMs) automatically from rigorous dynamic models in Aspen

Custom Modeler (ACM). The state-space based Decoupled A-B Net (DABNet) model of Sentoni et al. (1998) was chosen as the main nonlinear system identification model to fit the dynamic data generated in response to a series of step changes of input variables in ranges near normal operating conditions with user-defined holding times. Multiple enhancements of the DABNet model have been made including (1) multiple input and multiple output option, (2) double-pole formulation to handle fast/slow time scales, and (3) pole value optimization. Built as a module within the Framework for Optimization, Quantification of Uncertainty and Surrogates (FOQUS) developed under the U.S. Department of Energy's Carbon Capture Simulation Initiative (CCSI), D-RM Builder allows a user to configure the input/output variables, sample input spaces to generate sequences of step changes, launch high-fidelity ACM simulations, fit simulation results to a D-RM, and visualize and validate the resulting D-RM. Once a D-RM is created from the training data, it can be used to predict transient responses and compare them with the corresponding high-fidelity model results. Relative errors and correlation plots can be displayed through the FOQUS GUI. Uncertainty quantification based on unscented Kalman filter can also be performed. The D-RM can be exported as a MATLAB script that works with MATLAB classes developed to perform dynamic simulations and to integrate with the CCSI Advanced Process Control framework. D-RM Builder has been used successfully to generate fast and accurate D-RMs for a highly nonlinear pH neutralization reactor system and a two-time-scale bubbling fluidized bed adsorber-reactor for CO₂ capture. Further improvements are expected to be achieved by optimizing additional model parameters such as the orders of Laguerre series and the number of neurons in the hidden layer of the ANN.

Acknowledgment and Disclaimer

This work was supported by the U.S. Department of Energy, Office of Fossil Energy as part of the Carbon Capture Simulation Initiative (CCSI). This technical effort was performed in support of the National Energy Technology Laboratory's ongoing research under the RES contract DE-FE0004000. This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Nomenclature

Symbols

a_{ij} pole value of Laguerre series for i th output and j th input

1	A	time-invariant state-space matrix
2	<i>A</i>	area (m ²)
3	B	time-invariant state-space matrix
4	C	time-invariant state-space matrix or cross-covariance matrix
5	<i>C_v</i>	valve constant (m ^{2.5} hr ⁻¹)
6	D	time-invariant state-space matrix
7	<i>E</i>	error of artificial neural network training
8	<i>f</i>	a function
9	G	Grammian matrix
10	<i>g</i>	a function
11	<i>h</i>	a function
12	I	identity matrix
13	<i>k</i>	time-discrete model time index
14	K	gain matrix of Kalman filter
15	<i>K</i>	dissociation constant
16	<i>n_u</i>	number of input variables
17	<i>n_x</i>	number of state-space variables
18	<i>n_y</i>	number of output variables
19	P	covariance matrix of state-space variables
20	q	Gaussian process noise vector
21	Q	diagonal matrix for process noise
22	<i>Q</i>	volumetric flow rate (m ³ hr ⁻¹)
23	r	Gaussian measurement noise vector
24	R	diagonal matrix for measurement noise
25	S	covariance matrix of output variables
26	T	Transformation matrix for balanced realization
27	u	input vector
28	x	state-space vector
29	y	output vector
30	<i>z</i>	Z-transfer variable
31		

32 Greek letters

33	α	acetate (HAC + AC ⁻) concentration (kmol m ⁻³)
34	β	sodium (N _a ⁺) concentration (kmol m ⁻³)
35	Δt	sampling time interval (s)
36	σ	standard deviation
37	τ_{ij}	time constant for <i>i</i> th output and <i>j</i> th input (s)
38		

39 Subscripts

40	bal	balanced
41	c	controllability

1	<i>f</i>	fast
2	<i>i</i>	output variable index
3	<i>j</i>	input variable index
4	<i>o</i>	observability
5	<i>r</i>	term index for truncation
6	<i>s</i>	slow
7	<i>t</i>	target

9 **Superscripts**

10	–	mean
11	<i>aug</i>	augmented
12	<i>ANN</i>	artificial neural network

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