

# Non-linear model order reduction using input to state Hammerstein structures

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**Abstract:** In this paper, the focus will be on approximating original model of process systems using block-structured models. The context of model reduction is to improve the computational efficiency (simulation time). The reduced order models are important for online applications. Hammerstein structures have been used to approximate a mathematical non-linear model of a process. Input-Output Hammerstein structure can be defined as classical Hammerstein model but the technique is extended here to Input-State Hammerstein structure. It is shown that Input-State Hammerstein structure can be derived from Taylor series. Approximation accuracy has been improved by approximation for second term. The approximated Input-state Hammerstein block structure model gives good approximation of the original non-linear system. Over an operating domain of a process, the Input-State Hammerstein structure provides opportunities for reducing the computational load by order reduction of states and Jacobians. The methodology has been applied to a high purity distillation benchmark and satisfactory results are obtained as far as approximation is concerned. Reduction in states and Jacobian size by 70% is attained.

*Keywords:* Nonlinear model order reduction, Hammerstein, Taylor series, high purity distillation column

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## 1. INTRODUCTION

First order principle models (rigorous models) are stiff and large, thus are computationally inefficient. Since the (rigorous) NL models are not always exact match of real processes and there is mismatch at some point between the two, reduced models can be very useful if they match the rigorous NL model over a certain operation window. Advantage of reduced mathematical models for NL processes include low computational effort, better approximation of process within the operating window and beneficial for the real-time applications (e.g; control and optimization purposes).

The rigorous models available for large industrial processes can be characterized as a set of differential and algebraic equations (DAE). DAE class of models is capable to express the majority of processes. Thus the methodology to achieve a reduced model should be capable of handling DAE models. The transformation from DAE to ordinary differential equation (ODE) format is regarded as a major model reduction step; but it is not possible generally. A methodology which involves this step is advantageous for the process models of DAE class.

There is not much literature available on model reductions when it comes to model reduction in context of computational load. Balasubramhanya and Doyle (2000) developed a reduced order model of batch distillation column using travelling waves. The closed loop simulation of this reduced model was six times faster than original model in closed loop. Aling et al. (1997) used POD to get reduced

model for rapid thermal processing system. Reduction of computational load by a factor ten was reported. Hahn and Edgar (2000) elaborated on model reduction by balancing empirical Gramians and showed model order reduction but reduction in computational effort and time was limited. Perregaard (1993) simplified and reduced chemical processes models for simulation and optimization purposes. He achieved the reduction by simplifying the calculation of algebraic equations, which resulted in computational effort reduction. Gani et al. (1990) replaced the true (symbolic) Jacobian by approximated Jacobian (from local models). They reported the reduction of computational times by factor of 20 ~ 60. Empirical modelling has been one of the major approaches for achieving low computational complexity (which allows fast simulations). Ling and Rivera (1998) used a Hammerstein structure for model reduction, but did not report reduction in computational load (on polymerization benchmark). Berg (2005) reported that if computational load has to be reduced, not only model order reduction is to be targeted but the complexity (and stiffness) of reduced model has to be lower; as Gani (Gani et al. (1990)) achieved the computational load reduction by reducing the complexity (discussed above). Block structure models have been used for the identification purposes (see Eskinat et al. (1991); Billings and Fakhouri (1977), Norquay et al. (1999), Harnischmacher and Marquardt (2007) etc.). Though block structure models have been used for the identification purposes, but the block structure models have not been used for the model reduction purposes.

As the literature review shows, there is no reduction technique available directly related to reduction of computational load. Each model reduction technique has its specific purposes which is completely understandable. Not every model reduction methodology works for every process, but it is desired to have a model reduction methodology which is generic and applicable to wide class of processes (represented by DAE class of models). Moreover the literature review indicates that there is not much research material available on model reduction subject; whatever is available, mostly addresses the model order reduction and it does not focuses the reduction in complexity of reduced model (which is major component for computational load). Not many model reduction methodologies have addressed the problem of simplification of reduced model. The field is open for research to achieve reduced models, which are simple and reduced order to achieve computational load reduction.

Block structure models have an advantage over other model approximation methodologies; the structure of approximation model gives insight to the complexity of the process and breaks down the complexity of the NL process. This give handles to feel for the complexity and reduce it. Use of block structure enhances the chances to get a reduced model, which is uncomplicated and is computationally efficient.

In this paper, a block structure (Hammerstein) has been used to achieve reduced model for nonlinear chemical process. In the subsequent section, Hammerstein structure is discussed. In section 3, reduction methodology is discussed. In section 4, implementation on high purity distillation column and its results are considered. The last section 5 concludes the paper with key points and future work.

## 2. HAMMERSTEIN STRUCTURE

There are different block structures which are known for model reduction (and empirical modeling); Wiener, Hammerstein etc. Chen (1995) has introduced and discussed a wide variety of such block structures. Wiener and Hammerstein block structure models are most widely used structures in literature for the representation of nonlinear physical processes and will be shortly discussed here. Wiener models have limitations (specifically for chemical processes) which give edge to Hammerstein structure for identification purposes ( Harnischmacher and Marquardt (2007)). Wiener models not only limit the nonlinearity measure to be approximated, but they also increase the complexity involved in identifying or approximating the process. Harnischmacher (2007) investigated that Wiener models restrict the dynamic NL behavior that can be approximated and identified in comparison to Hammerstein structure.

Hammerstein structure is used for the approximation of NL processes in this study. The methodology is extended further to I/S Hammerstein structure to improve the approximation.

### 2.1 Classical (Input-Output I/O) Hammerstein structure

Classical Hammerstein model can be seen as nonlinear static gain, followed by linear dynamics.

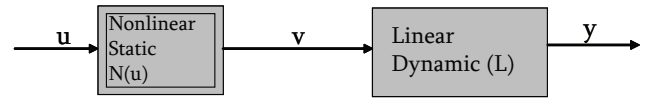


Fig. 1. Classical Hammerstein structure (input-output)

The classical I/O Hammerstein structure shown in figure 1 represents the continuous system/process. A procedure to get Hammerstein structure approximation for a process is to represent the nonlinear static block by interpolation table (lookup table), neural network or spline scheduling (the steady states) and represent linear dynamic block by linear time invariant (LTI) model. The intermediate variable  $v$  is a low dimensional vector. Mathematically, classical Hammerstein structure is given as;

$$\begin{aligned} \dot{x} &= A x + g(\mathbf{u}) \\ y &= C x \end{aligned} \quad (1)$$

where,  $A$  is the state matrix,  $C$  is the output matrix which can be identified from process data or can be obtained by linearizing the nonlinear system at 'nominal operating point'. Nominal operating point is an operating point within the operating domain, chosen by the input design (discussed in later section 3.1).

The input-output (I/O) Hammerstein model shown can be modified to Input-state (I/S) Hammerstein model under few assumptions (Naeem et al. (2008)). I/S Hammerstein model can be derived from expansion of Taylor series (shown in section 2.3)

### 2.2 Taylor Series

The Taylor expansion of a function  $f(x)$  that is differentiable in the neighborhood of real or complex number 'a' is mathematically given as:

$$f(x) = f(a) + \frac{1}{1!} \left. \frac{\partial f}{\partial x} \right|_a (x - a) + \frac{1}{2!} \left. \frac{\partial^2 f}{\partial^2 x} \right|_a (x - a)^2 + \dots \quad (2)$$

Typically process models are of DAE format and transformation from DAE to ODE is a model reduction step (for a large scale process). The ODE can be approximated by I/S Hammerstein structure.

Given an ODE  $\dot{x} = f(x, y)$ , which is modeled in an environment (gPROMS, MATLAB, SIMULINK), the first order Taylor expansion around point  $(x^*, u^*)$  is given mathematically as:

$$\dot{x} = f(x, u) = f(x^*, u^*) + J_x|_{x^*, u^*} (x - x^*) + J_u|_{x^*, u^*} (u - u^*) + \dots \quad (3)$$

Equation 3 evaluates the function  $f(x, u)$  given linearization at  $f(x^*, u^*)$ . Figure 2 shows the equation 3 in block diagram.

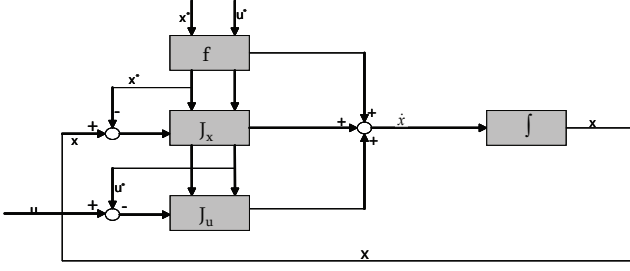


Fig. 2. Block structure for Taylor series of  $\dot{x} = f(x, u)$

### 2.3 Taylor Series expansion

Taylor series illustrated in preceding section can be extended to I/S Hammerstein structure (at steady-state point  $(x^*, u^*)$ ) under following assumptions:

- It is assumed, within the operating domain that every  $u^*$  leads the system finally to steady-state ' $x_{ss}$ ' which means a stable process is considered. Moreover, it is assumed that steady-state is calculated by  $u$ . Mathematically,  $x_{ss} = g(\mathbf{u})$ . Setting  $x^* = x_{ss}$  results in output of the (constant) block ( $f$ ) zero (the system is being evaluated at steady-state  $x^*$ ).
- Input  $u$  is chosen freely, but is chosen such that it is equal to the input at steady-state, mathematically;  $u = u^*$ ; this implies that gradient input to block ( $J(u)$ ) becomes zero; (since  $u - u^* = 0$ ).

Under above assumptions, adding  $g(\mathbf{u})$ , removing blocks  $f$  and  $J_u$  and rearranging the block structure in figure 2, we get the block structure shown in figure 3. Observing this structure it can be considered an *I/S Hammerstein structure*; it has two blocks, a NL steady-state mapping block, followed by linear dynamic block.

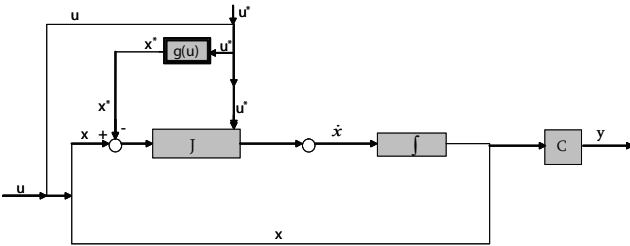


Fig. 3. Taylor series extension to I/S Hammerstein structure

For a linear system, state-space model can be mathematically given as below:

$$\begin{aligned} \dot{x} &= A x + B u \\ y &= C x \end{aligned} \quad (4)$$

For the state-space linear model (in equation 4), I/S Hammerstein structure can be shown as figure 4.

The block structure shown in figure 4 can be extended for NL processes, shown in figure 5. I/S Hammerstein structure shown in figure 5 is similar to the structure derived by Taylor series expansion (shown in figure 3).

The block structure shown in figure 3 and figure 5 is I/S Hammerstein block structure, with separated NL stat-

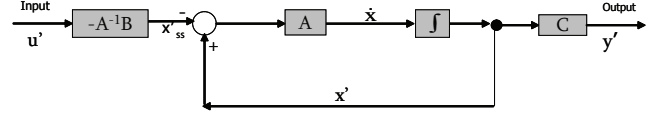


Fig. 4. Input-state Hammerstein structure for linear system

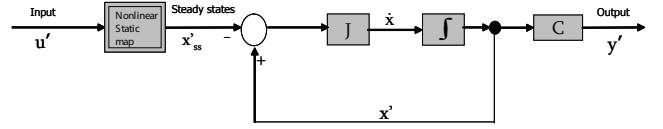


Fig. 5. Input-state Hammerstein structure for non-linear system

ics (where NL static mapping takes place), followed by linear dynamic block. The dynamic linear block is driven by difference between the steady state ' $x_{ss}$ ' and current state ' $x$ '.

Mathematically, for NL case, I/S Hammerstein structure can be given as:

$$\begin{aligned} \dot{x} &= J (x - x_{ss}) + g(\mathbf{u}) \\ y &= C x \end{aligned} \quad (5)$$

where,  $J = \text{Jacobian}$ ;  $C = \text{output state matrix}$ ;  $y = \text{output}$ ;  $x_{ss} = g(\mathbf{u})$  is steady-state, scheduling (implemented by lookup table).

The I/S Hammerstein block structure shown in figures 3 and 5 is used for the approximation of NL processes. The accuracy of approximation of I/S Hammerstein structure is improved by estimating Jacobian online. Jacobian is estimated (and updated) based on information of Jacobian basis  $J_b$ , reduced state  $z$  and input  $u$ . Jacobian basis  $J_b$  are calculated by SVD analysis of Jacobian data. Jacobian data is collected by taking snapshots of Jacobians over the operating domain ('input design') by exciting the NL system with inputs to acquire most information in operating envelope. Similarly the reduced order states  $z$  is calculated by transformation matrix ( $U_1$ ), obtained by SVD analysis of steady-state and dynamic state (snapshot) data, taken over the operating domain.

First order I/S Hammerstein approximation structure (with updated Jacobian), is shown in figure 6. As figure shows, the Jacobian estimation is based on (reduced) current state information ( $z$ ).

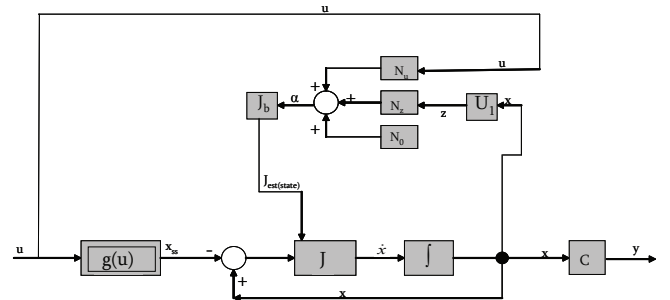


Fig. 6. First order I/S Hammerstein approximation structure

In the figure 6,  $J = \text{Jacobian}$ ;  $U_1 = \text{transformation matrix to transform full state } x \text{ to reduced state } z$ ;  $J_b =$

Jacobian basis obtained by SVD analysis of snapshots of Jacobians (within operating domain);  $N_0, N_1, N_2$  = the parameters relating Jacobian with reduced-state  $z$ , input  $u$  and constant.

It is to be noted, I/S Hammerstein can be derived by extending Taylor expansion as proved above. This is not possible for Wiener structure.

#### 2.4 Accuracy improvement by higher order approximation

First order approximation of NL system by expansion of Taylor series to I/S Hammerstein structure is shown in above section. The approximation accuracy can be improved with higher order terms.

The Taylor series is extended to second order. Taylor series around (steady-state) point  $(x^*, u^*)$  is given as:

$$f(x, u) = f(x^*, u^*) + \left. \frac{\partial f}{\partial x} \right|_{x^*, u^*} (x - x^*) + \frac{1}{2!} \left. \frac{\partial^2 f}{\partial^2 x} \right|_{x^*, u^*} (x - x^*)^2 \quad (6)$$

Similarly, Taylor series expansion around any point  $(x, u)$  is given as below:

$$f(x^*, u^*) = f(x, u) + \left. \frac{\partial f}{\partial x} \right|_{x, u} (x^* - x) + \frac{1}{2!} \left. \frac{\partial^2 f}{\partial^2 x} \right|_{x, u} (x^* - x)^2 \quad (7)$$

Equation 6 and equation 7 are the Taylor series expansions at two points ( $x^*$  and  $x$ ), given by Taylor series extension to second order. Rearranging equation 7, we get;

$$f(x, u) = f(x^*, u^*) + \left. \frac{\partial f}{\partial x} \right|_{x, u} (x^* - x) + \frac{1}{2!} \left. \frac{\partial^2 f}{\partial^2 x} \right|_{x, u} (x^* - x)^2 \quad (8)$$

Adding equation 6 and equation 8 (while higher order terms are canceled, assuming  $\frac{1}{2!} \left. \frac{\partial^2 f}{\partial^2 x} \right|_{x, u} = \frac{1}{2!} \left. \frac{\partial^2 f}{\partial^2 x} \right|_{x^*, u^*}$ ), we get;

$$f(x, u) = f(x^*, u^*) + \frac{1}{2} \left[ \left. \frac{\partial f}{\partial x} \right|_{x^*, u^*} + \left. \frac{\partial f}{\partial x} \right|_{x, u} \right] (x - x^*) \quad (9)$$

Equation 9 is the approximation of  $f(x, u)$  using higher order terms. There are two Jacobian evaluations involved in this approach, an approximation using knowledge at steady-state ( $x^*$ ) and approximation using current state ( $x$ ) knowledge. The block structure representation of this approximation is shown in figure 7.

### 3. REDUCED ORDER HAMMERSTEIN STRUCTURE

Approximation block structure shown in figure 7 is full state model. Since it is a prerequisite for the approximation block structure, to be valid within certain operating domain.

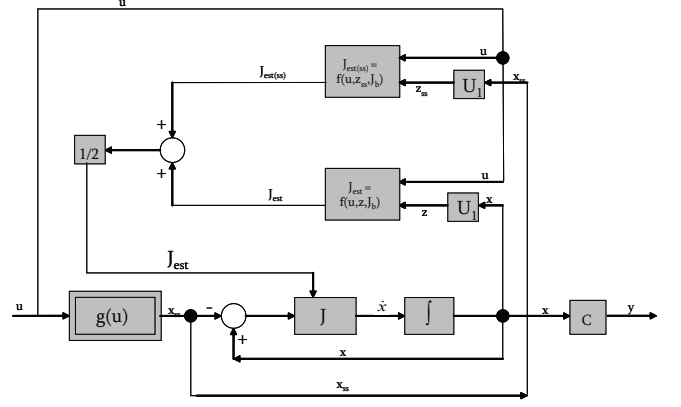


Fig. 7. Approximation model (I/S Hammerstein); Higher order approximation)

#### 3.1 Operating domain/Input Design

Within defined domain, inputs are designed with the purpose to define an input trajectory that travels through complete domain. The process is known as 'input design'. As the name indicates, it is the process of designing inputs based on constraints on input or output (depending upon a process). In summary, the operating domain is a region, where the approximated model is supposed to be valid, once identified (based on data from the physical process) and input design is the procedure, which defines the boundaries of this operating domain.

The steady-state and dynamic state data is obtained by taking snapshots over the operating domain. Similarly, Jacobian data is collected by taking the snapshots of Jacobians over the operating domain. Jacobian basis  $J_b$  are computed by SVD analysis of Jacobian data.

The I/S Hammerstein block structure gives scope to get the reduced order structure by;

- i. Reduction in state size.
- ii. Reduction in Jacobian size.

##### i. Reduction in state size.

The singular value analysis on data of states indicates that there is a low dimensional space, such that low order state ( $z$ ) can represent the whole operating domain. The state reduction is performed by transformation matrix. The transformation matrix  $U_1$  (to obtain reduced state 'z') is obtained by SVD analysis of data over the operating domain. Reduced states are back-transformed to full state by back transformation matrix  $\hat{U}_1$ . The block structure of the reduced approximation model is shown in figure 8. The Jacobian reduction takes place online (in the block  $U_1 * J * U_1^T$ ).

##### ii. Reduction in Jacobian size.

The scheme in figure 7 shows that Jacobian estimation takes place using Jacobian basis  $J_b$ , state  $z$  and input  $u$  information. The estimated Jacobian  $J_{est}$  is full order Jacobian. There is possibility to obtain reduced size Jacobian, by using reduced order Jacobian basis ( $J_{b,red}$ ) and reduced state ( $z$ ). With reduced basis  $J_{b,red}$  and reduced states  $z$ , estimated Jacobians are also reduced sized and the block structure is a reduced order I/S

Hammersteins approximation model. The block structure is shown in figure 9.

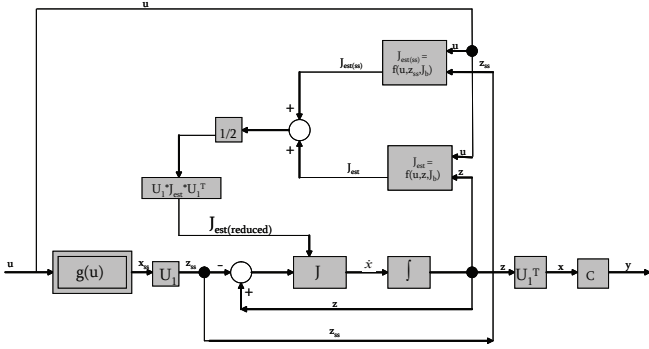


Fig. 8. Reduced order approximation model (I/S Hammerstein); Higher order approximation

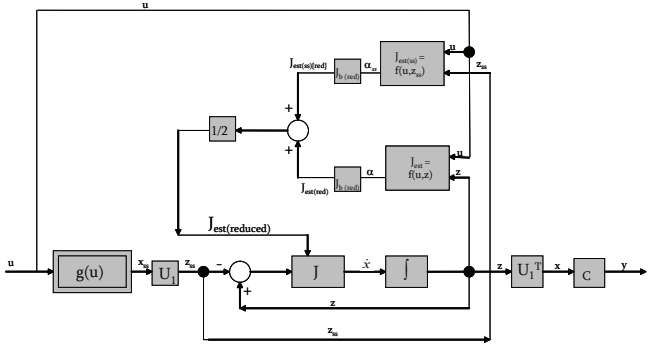


Fig. 9. Approximation block structure with reduced Jacobian and state size

#### 4. APPLICATION TO HIGH PURITY DISTILLATION COLUMN

The approximation block structure and reduced block structure model has been applied to the benchmark. A benchmark is high purity distillation column, and its properties will be discussed in subsequent sections. But before the methodology is implemented on benchmark, a prerequisite for the methodology is to define the operating domain, within which the approximation/reduced model is valid. Input design, discussed in section 3.1 is designed for distillation column; the operating domain has been finalized by constraint in output purity. A set of input variables (reflux (L) and vapour boilup (V)) is chosen, for which output variables are observed. The product purity for output variables sets the boundary for operating domain.

##### High purity distillation column

A high purity distillation column is used as test case, on which the approximated and reduced model estimation is applied. The distillation column has following properties; The column has 72 trays, a total condenser and partial reboiler. It is a nonlinear system. The thermodynamics of the column are governed by constant relative volatility. The relative volatility for this specific system is 1.33. Pressure is assumed to be constant. Vapour holdups are considered negligible and liquid holdups are considered

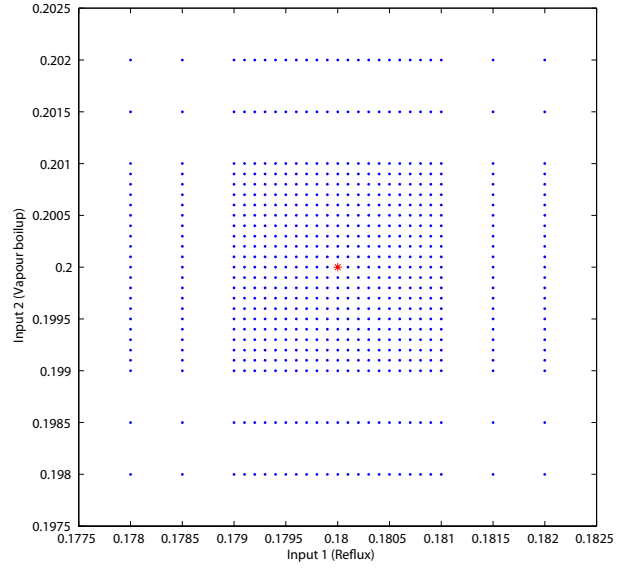


Fig. 10. Figure of operating domain 'input design'

to be constant. Moreover, the column is assumed to be working with equimolar flow (which results in eliminating energy balances). The distillation benchmark model has been explained in detail by Lévine and Rouchon (1991).

The benchmark is modelled in gPROMS while the approximation model is modelled in MATLAB and SIMULINK. The approximation technique is implemented on the benchmark. The operating domain is finalized (input design) shown in figure 10. The static part consists of lookup table which interpolates the steady-states. The steady-states are fed into the dynamic part. The difference between current state and steady-state is fed to Jacobian block, which is estimated based on state and steady-state data. This represents the linear block as bilinear system.

##### Two types of changes

There are two types of input signals tested for the validation of approximated (and reduced) model.

- a) 'Separation index' (SI) is change in distillation, when both the input variables (reflux rate (L) and vapour boilup (V)) are given *same* steps at the same time, or the rate of flow of distillate *D* and bottom *B* does not change.
- b) 'Effective Cut Point' (ECP) is change in distillation, when one input variable (reflux rate (L) or vapour boilup (V)) is kept constant and step change is given to the other input variable. This change is known to be highly non-linear for high purity distillation column (in process industry).

Figure 11 show the step in both inputs at the same time (separation index). The approximation model structure (in full state) and reduced order model structure approximate the behavior very well. The mismatch between the approximations and original is cause by offset form lookup table (NL block of approximated model).

Figure 12 show the result comparison of original, full order approximated model and reduced order model, when step in vapour boilup (V) input (effective cut point) is

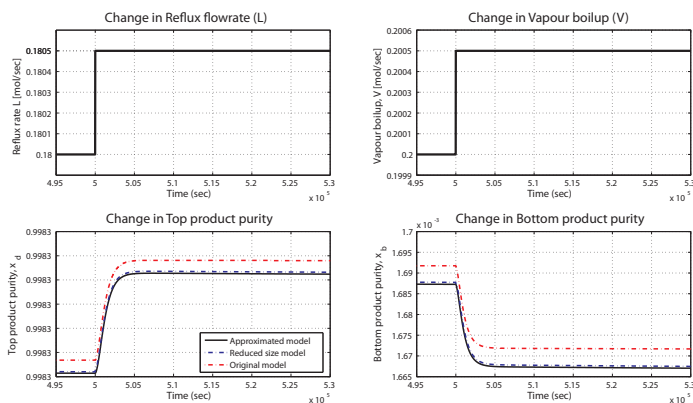


Fig. 11. Results for comparison of SI change between original, approximation 'full' and 'reduced' model

applied. The approximation model structure (in full state) and reduced order structure approximates the behavior satisfactorily. There is a very small mismatch in dynamics between the approximation model and original. The offset is acceptable (and sufficiently accurate) for this application.

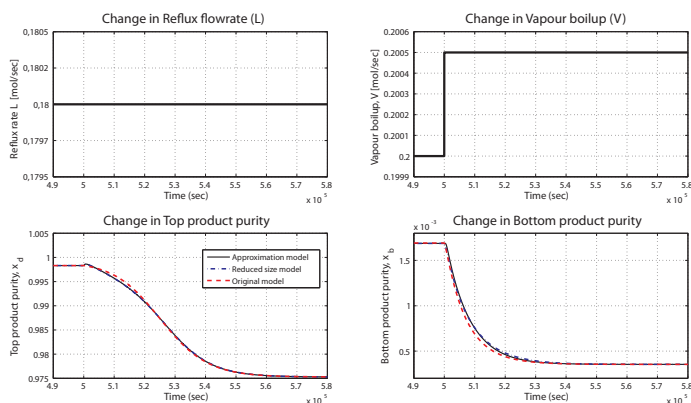


Fig. 12. Results for comparison of ECP change between original approximation 'full' and 'reduced' model

## 5. CONCLUSIONS & FUTURE WORK

In this paper, it is shown that Input-State Hammerstein structure can be derived from a Taylor expansion. The approximation model's accuracy can be improved by including higher order terms. The approximation results were shown for a high purity distillation benchmark and are acceptable for the kind of application. Order reduction of 70% is possible using the methodology with satisfactory results (high accuracy).

Work on the following tasks is done presently or is to be considered in future:

- i) The computational load reduction for the benchmark example (high purity distillation column) is to be investigated. The computational load and simulation time reduction has to be compared with original NL model.
- ii) It is planned to extend the methodology to industrial case. The industrial models make use of dynamic link library (dll) files (as foreign process) to compute different task (such as thermodynamic properties). Such foreign

processes buildup overhead costs, resulting in increased computational load. It is anticipated, that transformation of large DAE model to ODE structure will reduce the computational effort (and simulation time), since the algebraic computations are vanished in ODE structure, replaced by NL mapping.

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