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An Aggregation Model Reduction Method for One-Dimensional Distributed Systems

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A method for deriving reduced dynamic models of one-dimensional distributed systems is presented. It inherits the concepts of the aggregated modeling method of Lévine and Rouchon originally derived for simple staged distillation models and can be applied to both spatially discrete and continuous systems. The method is based on partitioning the system into intervals of steady-state systems, which are connected by dynamic aggregation elements. By presolving and substituting the steady-state systems, a discrete low-order dynamic model is obtained. A characteristic property of the aggregation method is that the original and the reduced model assume identical steady states. For spatially continuous systems, the method is an alternative to discretization methods like finite-difference and finite-element methods. Implementation details of the method are discussed, and the principle is illustrated on three example systems, namely a distillation column, a heat exchanger, and a fixed-bed reactor. © 2011 American Institute of Chemical Engineers *AIChE J,* 58: 1524–1537, 2012
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Introduction

This article presents a method for deriving reduced dynamic models of spatially discrete or continuous one-dimensional distributed parameter systems. The reduced models are low-order systems of ordinary differential equations or differential-algebraic equations. For continuous systems, the method can be used as an alternative to common spatial discretization methods such as finite-difference, finite-volume, and finite-element methods.[1]

The method is based on the concept of aggregation, which was used by Lévine and Rouchon[2] for deriving reduced-order distillation models. Linhart and Skogestad[3] showed that this method can be used to increase the simulation speed several times, and extended the method to more complex distillation models.[4] In this case, the method is an alternative to other model reduction methods for this kind of one-dimensional separation processes such as orthogonal collocation methods[5,6] and wave propagation methods.[7,8]

The method presented here is a generalization from distillation columns to one-dimensional spatially distributed parameter systems. These systems can be discrete in space, like stagewise processes such as staged distillation columns, or continuous, like packed distillation columns, fixed-bed reactors, and heat exchangers. A special class of discrete systems are spatial discretizations, for example obtained by finite-differences, of continuously distributed systems. The reduction method can be applied to these systems in the same way as it is applied to spatially discrete systems. The reduction procedure for continuous systems can be derived as the limit case of the procedure for discrete systems, where the reduction method is first applied to the discretized system, and then the limit case when the discretization interval goes to zero is considered. For continuous systems, the method is limited to spatially second-order systems.

The reduction procedure starts with choosing several "aggregation points" on the spatial domain of the distributed system. To each of these aggregation points, dynamic "aggregation elements" are assigned. The ordinary or partial

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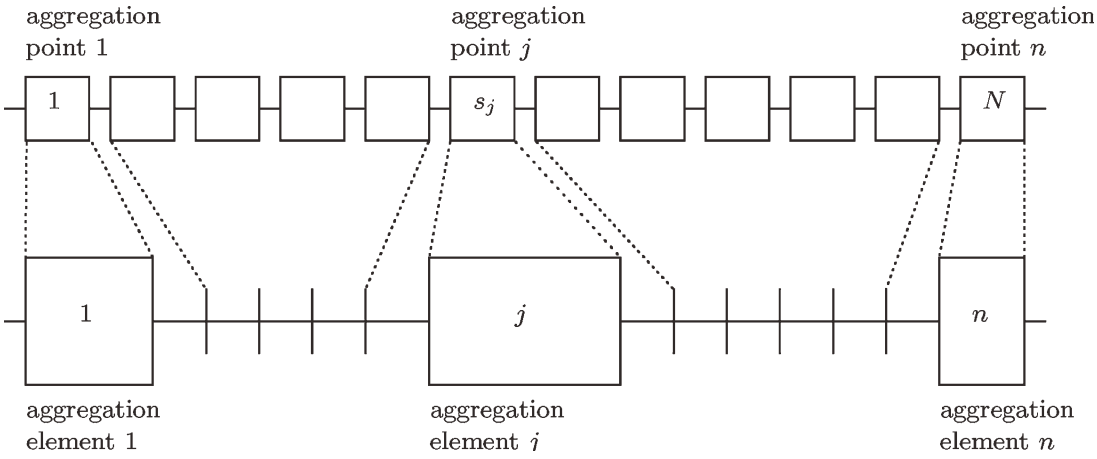

Figure 1. Schematic illustration of the reduction method for discrete distributed systems.

differential equations on the intervals between the aggregation points are treated as at steady-state. The values on the boundaries of the steady-state systems, which appear in the dynamic equations of the adjacent aggregation elements, are computed as functions of the states of the aggregation elements on both sides of each steady-state system. The thus obtained system is discrete and low-order in nature.

The main principle of the method is to replace the signal transport through the system by instantaneous transport through the steady-state intervals from aggregation element to aggregation element, where the dynamics are slowed down again by the large capacities of the aggregation elements.

The article is organized as follows. The "Method" section describes the mathematical structure of the one-dimensional systems that the method can be applied to. Subsequently, the main conceptual steps of the reduction procedure, which are the same for both spatially discrete and continuous systems, are explained. The detailed mathematical derivations of the reduction method for discrete and spatially first- and second-order continuous systems is described in the following subsections. In the last subsection, it is shown that both the original and the reduced models assume the same steady-state, which is a characteristic property of the method. The "Examples" section illustrates the reduction method on three example systems, namely a distillation column, a heat exchanger, and a fixed-bed reactor. In the first part of each example, the original and the derivation of the reduced model is explained. In the second part, a simulation study that demonstrates the approximation quality of the reduced models is presented. In the "Discussion" section, the advantages and limitations of the model reduction method are discussed. The similarities with and differences from reduced models derived via singular perturbation procedures are described subsequently, and a comparison of the method with alternative discretization schemes is given. Finally, a summary of the method and its performance is given in the "Conclusions" section.

Method

In the following, the mathematical structures of the two types of spatially distributed systems the method can be applied to are described. These are basically one-dimensional systems with spatially either discretely or continuously distributed variables. Subsequently, the reduction procedure is described, where the conceptual steps are the same for both types of systems.

Discrete distributed parameter systems

The first type of systems the reduction method can be applied to are discrete one-dimensional distributed systems. Figure 1 shows the principal structure of these systems.

The main characteristic of these systems is that they consist of a number of consecutive similar units that communicate with the respective neighboring units along one dimension. For a mathematically convenient notation, the dynamic and algebraic equations of each unit are expressed in vector notation:

$$\mathbf{M}_1\mathbf{x}_1(t) = \mathbf{f}_1(\mathbf{x}_1(t), \mathbf{x}_2(t), \mathbf{p}, t), \tag{1}$$

$$\mathbf{M}_i\mathbf{x}_i(t) = \mathbf{f}_i(\mathbf{x}_{i-1}(t), \mathbf{x}_i(t), \mathbf{x}_{i+1}(t), \mathbf{p}, t), \quad 2 \le i \le N-1, \tag{2}$$

$$\mathbf{M}_N\mathbf{x}_N(t) = \mathbf{f}_N(\mathbf{x}_{N-1}(t), \mathbf{x}_N(t), \mathbf{p}, t), \tag{3}$$

where i is the index of the unit, N is the total number of units, t is the time variable, $\mathbf{x}_i$ is the vector consisting of the dynamic and algebraic variables of unit i, $\mathbf{M}_i$ is a diagonal "mass" matrix that can be used to render some of the equations algebraic by setting the corresponding values to 0, $\mathbf{f}_i$ is a vector-valued function of the variables of unit i and the neighboring units, and $\mathbf{p}$ is a parameter vector. External inputs to the system are included in the notation above by the time-dependency of the functions $\mathbf{f}_i$.

Continuous distributed parameter systems

The second type of systems are one-dimensional continuous distributed parameter systems, where the spatial order is restricted to a maximum of two. These systems can be written as vector-valued partial differential equations:

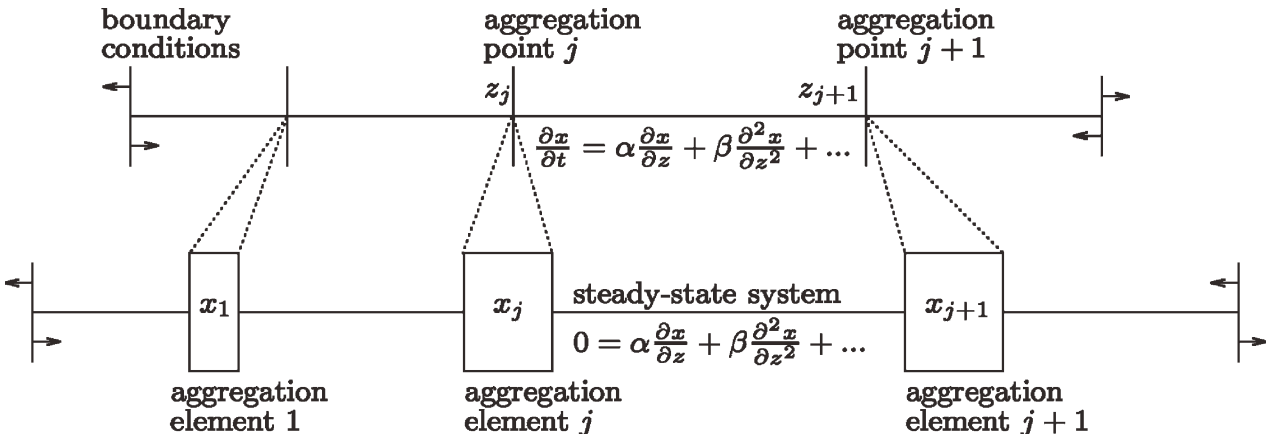

Figure 2. Schematic illustration of the reduction method for continuous distributed systems.

$$\frac{\partial \mathbf{x}(z,t)}{\partial t} = \mathbf{D}_z\mathbf{x}(z,t) + \mathbf{R}(\mathbf{x}(z,t),z,t), \qquad 0 \le z \le 1, \quad (4)$$

where $\mathbf{x}(z, t)$ is the vector of the distributed state variables, z is the spatial variable, t is the time, $\mathbf{D}_z$ is a spatial differential operator acting on the state vector $\mathbf{x}(z, t)$, and $\mathbf{R}(\mathbf{x}(z, t), z, t)$ is a local source term. A certain set of boundary conditions is needed to complete the description, which can also be time-dependent and thus contain external inputs to the system. For simplicity, the spatial domain of the partial differential equation is here chosen to be [0;1]. This is not a restriction, as any other spatial domain can be transformed into this by a simple scaling of the spatial variable z.

General reduction procedure

Figures 1 and 2 illustrates the principle of the method. The procedure can be divided into the following steps, which are the same for both discrete and continuous systems:

(1) **Derivation of reduced model equations**

(a) **Selection of aggregation points**

On the spatial domain of the system, n "aggregation points" are chosen. For discrete systems, these are n distinct indices of units s_j, $j = 1,\ldots, n$. For continuous systems, these are n points z_j with $0 \le z_j \le 1$, $j = 1,\ldots, n$.

The number and position of the aggregation points will affect the dynamic approximation quality of the reduced system but not the steady-states, and all choices will lead to a functional system.

(b) **Introduction of aggregation elements**

At every aggregation point, an "aggregation element" is positioned. For discrete systems, these elements are just the units at the aggregation points with a modified "capacity" H. For continuous systems, an aggregation element is positioned at every aggregation point. Their dynamics are governed by simple differential equations that are derived from the original partial differential equations. The derivation is explained in the later sections. The "capacity" H of an aggregation element refers to a factor that multiplies the left-hand sides of the dynamic equations of the element.

(c) **Steady-state approximation between aggregation elements**

For discrete systems, the left hand sides of the equations of all units that are not aggregation elements are set to 0. This results in systems of algebraic equations that depend on certain variables of the aggregation elements on both sides. For continuous systems, the partial differential equations on the intervals between the aggregation elements are treated as steady-state boundary value problems, where certain variables of the aggregation elements serve as boundary conditions.

(2) **Implementation**

(a) **Precomputed solution of steady-state systems**

The steady-state systems are pre-solved either numerically or analytically for a range of possible values of the states of the aggregation elements on both sides of each system. For the integration of the aggregation element equations, the solutions on the boundaries of the steady-state systems have to be known. They are therefore expressed as functions of the state variables of the neighboring aggregation elements and substituted into the aggregation element equations.

(b) **Substitution of steady-state solutions**

The functions computed in Step 2a are substituted into the equations of the capacity elements. The resulting system is a set of ODEs (or DAEs, if algebraic equations are present).

Steps 1a to c yield a model with reduced dynamics. This model is, however, of the same complexity as the original model. For discrete systems, a large number of dynamic equations have been converted into algebraic equations, but the total number of equations is unchanged. For continuous systems, the continuous system has been partitioned into dynamic aggregation elements and boundary value problems, which have to be solved simultaneously. A real reduction in model complexity and computational effort is therefore obtained only after implementing the precomputed steady-state solutions in Steps 2a and b.

In the following, details specific for either discrete or continuous systems are described.

Discrete systems

After Step 1c, the equations of the reduced system read

$$H_1\mathbf{M}_1\mathbf{x}_1(t) = \mathbf{f}_1(\mathbf{x}_1(t),\mathbf{x}_2(t),\mathbf{p},t), \quad (5)$$

$$H_j\mathbf{M}_{s_j}\mathbf{x}_{s_j}(t) = \mathbf{f}_{s_j}(\mathbf{x}_{s_j-1}(t),\mathbf{x}_{s_j}(t),\mathbf{x}_{s_j+1}(t),\mathbf{p},t), \quad j = 2,\ldots,n-1, \quad (6)$$

$$\mathbf{0} = \mathbf{f}_i(\mathbf{x}_{i-1}(t), \mathbf{x}_i(t), \mathbf{x}_{i+1}(t), \mathbf{p}, t), \quad i = 2, \ldots, N-1, i \neq s_j, j = 1, \ldots, n, \tag{7}$$

$$H_n \mathbf{M}_N \mathbf{x}_N(t) = \mathbf{f}_N(\mathbf{x}_{N-1}(t), \mathbf{x}_N(t), \mathbf{p}, t). \tag{8}$$

In the above equations, unit 1 and N are chosen to be aggregation elements ($s_1 = 1$ and $s_n = N$). Either of these could be steady-state systems as well.

Step 2a involves solving the systems 7 for the variables $\mathbf{x}_{s_j-1}$ and $\mathbf{x}_{s_j+1}$, $j = 1,\ldots, n$ (except for $\mathbf{x}_0$ if $s_1 = 1$ and $\mathbf{x}_{N+1}$ if $s_n = N$). These are needed in the equations of the aggregation elements 5, 6, and 8. The variables are expressed as functions of the variables of the aggregation elements on both sides. This means that, for example, for aggregation element j, the functions

$$\mathbf{x}_{s_j+1} = \phi_j(\mathbf{x}_{s_j}, \mathbf{x}_{s_{(j+1)}}, \mathbf{p}) = \phi_j(\overline{\mathbf{x}}_j, \overline{\mathbf{x}}_{j+1}, \mathbf{p}), \tag{9}$$

and

$$\mathbf{x}_{s_j-1} = \psi_j(\mathbf{x}_{s_{(j-1)}}, \mathbf{x}_{s_j}, \mathbf{p}) = \psi_j(\overline{\mathbf{x}}_{j-1}, \overline{\mathbf{x}}_j, \mathbf{p}) \tag{10}$$

are required. Here, the variable $\mathbf{x}_{s_j+1}$ is a function of the variables $\mathbf{x}_{s_j}$ and $\mathbf{x}_{s_{(j+1)}}$ of aggregation elements s_j and $s_{(j+1)}$. Note the difference between the variables $\mathbf{x}_{s_j+1}$ and $\mathbf{x}_{s_{(j+1)}}$. The former are the variables of the first unit after the aggregation element unit j, whereas the latter are the variables of the aggregation element unit $j+1$. To make this difference clear, the notation $\overline{\mathbf{x}}_j$ is introduced, where the bar denotes the state variables of the aggregation elements.

Generally, these functions are computed numerically and have to be implemented in a suitable way. A straightforward way is the tabulation of the solution values on a certain domain of the independent variables and the retrieval of the function values by interpolation of the table values. Whether the functions are implemented as look-up tables or in another way, they will be complex if the dimensionality of the $\mathbf{x}_i$ variables is high. It is therefore advisable to choose the independent variables carefully, because not necessarily all variables are needed to compute the function values. In addition, not the whole vectors of the variables $\mathbf{x}_{s_j-1}$ and $\mathbf{x}_{s_j+1}$ might be necessary in the aggregation element equations.

Step 2b implies the substitution of the functions 9 and 10 into the aggregation element equations 5, 6, and 8. The resulting system then reads

$$H_1 \overline{\mathbf{M}}_1 \overline{\mathbf{x}}_1(t) = \overline{\mathbf{f}}_1(\overline{\mathbf{x}}_1(t), \phi_1(\overline{\mathbf{x}}_1(t), \overline{\mathbf{x}}_2(t), \mathbf{p}), \mathbf{p}, t), \tag{11}$$

$$H_j \overline{\mathbf{M}}_j \overline{\mathbf{x}}_j(t) = \overline{\mathbf{f}}_j(\psi_j(\overline{\mathbf{x}}_{j-1}, \overline{\mathbf{x}}_j, \mathbf{p}), \overline{\mathbf{x}}_j(t), \phi_j(\overline{\mathbf{x}}_j, \overline{\mathbf{x}}_{j+1}, \mathbf{p}), \mathbf{p}, t), \quad j = 2, \ldots, n-1, \tag{12}$$

$$H_n \overline{\mathbf{M}}_n \overline{\mathbf{x}}_n(t) = \overline{\mathbf{f}}_n(\psi_n(\overline{\mathbf{x}}_{n-1}, \overline{\mathbf{x}}_n, \mathbf{p}), \overline{\mathbf{x}}_n(t), \mathbf{p}, t). \tag{13}$$

Here, the notation $\overline{\mathbf{M}}$, $\overline{\mathbf{x}}$, and $\overline{\mathbf{f}}$ is used to indicate a change of index of the variables and functions due to the elimination of the steady-state variables and equations. For every j, $\overline{\mathbf{x}}_j = \mathbf{x}_{s_j}$ holds.

Continuous systems: second-order systems

The differential equations of the aggregation elements for continuous systems can be derived by applying the reduction procedure to a finite-difference discretization of the partial differential equations, and considering the limit case of $\Delta z \to 0$, where Δz is the length of the finite-difference intervals. The result of this operation depends on the order of the spatial differential operator. The main derivation is demonstrated here for a system with second-order spatial derivatives, which represents a typical convection-diffusion-reaction system. The differences in the procedure for systems with first-order spatial derivatives are discussed in the next section.

The system discussed in this section reads

$$\frac{\partial x}{\partial t} = -\alpha \frac{\partial x}{\partial z} + \beta \frac{\partial^2 x}{\partial z^2} + R(x), \tag{14}$$

with a certain set of boundary conditions, and α and β being dimensionless numbers. For notational simplicity, a scalar system is used for the derivation of the reduced model equations.

A finite-difference discretization of the spatial derivatives yields

$$\frac{dx_i}{dt} = -\alpha \frac{x_i - x_{i-1}}{\Delta z} + \beta \frac{x_{i-1} - 2x_i + x_{i+1}}{\Delta z^2} + R(x_i), \tag{15}$$

where x_i are the states of the discretized system at the N distinct discretization points z_i, $i = 1,\ldots, N$, which span the spatial domain over intervals of length $\Delta z = 1/(N-1)$.

According to Steps 1a and b, a number of n aggregation points z_j, $j = 1,\ldots, n$, is chosen among all discretization points, and the differential equations of the corresponding states are modified by multiplying the left-hand side with a "capacity" H_j:

$$H_j \frac{dx_{s_j}}{dt} = -\alpha \frac{x_{s_j} - x_{s_j-1}}{\Delta z} + \beta \frac{x_{s_j-1} - 2x_{s_j} + x_{s_j+1}}{\Delta z^2} + R(x_{s_j}), \quad j = 1, \ldots, n. \tag{16}$$

Step 1c requires that the remaining equations are treated as in steady-state:

$$0 = -\alpha \frac{x_i - x_{i-1}}{\Delta z} + \beta \frac{x_{i-1} - 2x_i + x_{i+1}}{\Delta z^2} + R(x_i), \quad i = 1, \ldots, N, i \neq s_j, j = 1, \ldots, n. \tag{17}$$

The resulting model has the same steady-state as the original discretized model. The capacities H_j can be chosen freely, but should compensate for the missing capacities of the steady-state elements. A straightforward choice for a reduced model with equidistant aggregation points is therefore $H_j = N/n$, which distributes the capacities of the elements of the original discretized model equally among the aggregation points of the reduced model. N is expressed in terms of Δz as $N = 1/\Delta z + 1$, such that the equations of the aggregation elements read

$$\frac{\frac{1}{\Delta z} + 1}{n} \frac{dx_{s_j}}{dt} = -\alpha \frac{x_{s_j} - x_{s_j-1}}{\Delta z} + \beta \frac{\frac{x_{s_j+1} - x_{s_j}}{\Delta z} - \frac{x_{s_j} - x_{s_j-1}}{\Delta z}}{\Delta z} + R(x_{s_j}). \tag{18}$$

The second-order finite-difference approximation is here written as the finite-difference of two first-order finite-differences. Multiplying with Δz yields

$$\frac{1+\Delta z}{n}\frac{dx_{s_j}}{dt} = -\alpha(x_{s_j} - x_{s_j-1}) + \beta\left(\frac{x_{s_j+1} - x_{s_j}}{\Delta z} - \frac{x_{s_j} - x_{s_j-1}}{\Delta z}\right) + R(x_{s_j})\Delta z. \quad (19)$$

$\Delta z \to 0$ yields the continuous equations. As the system discussed here is a continuous second-order system, $x_{s_j-1} \to x_{s_j}$ for $\Delta z \to 0$. This is not the case if the system is first-order. This case will be discussed separately below. Thus, $\Delta z \to 0$ results in

$$\frac{1}{n}\frac{d\bar{x}_j}{dt} := \frac{1}{n}\frac{dx_{s_j}}{dt} = \beta\left(\left.\frac{\partial x}{\partial z}\right|_{z_j}^{+} - \left.\frac{\partial x}{\partial z}\right|_{z_j}^{-}\right). \quad (20)$$

The notation $\bar{x}_j$ is introduced here to express that the only remaining state variables are the states at the aggregation points, i.e., $\bar{x}_j = x_{s_j}$.

In Step 2a, the right derivative $\left.\frac{\partial x}{\partial z}\right|_{z_j}^{+}$ is calculated from the boundary value systems between the aggregation points z_j and z_{j+1},

$$0 = -\alpha\frac{\partial x}{\partial z} + \beta\frac{\partial^2 x}{\partial z^2} + R(x), \quad z_j \le z \le z_{j+1}, \quad (21)$$

with the boundary conditions

$$x(z_j) = \bar{x}_j, \quad (22)$$

$$x(z_{j+1}) = \bar{x}_{j+1}, \quad (23)$$

and the left derivative $\left.\frac{\partial x}{\partial z}\right|_{z_j}^{-}$ is calculated from the boundary value systems between the aggregation points z_{j-1} and z_j correspondingly. The solution can be obtained, for example, by using a finite-difference approximation as in Eq. 17. From the solution of a steady-state system 21 between the aggregation points z_j and z_{j+1} with the boundary conditions 22 and 23, the derivatives $\left.\frac{\partial x}{\partial z}\right|_{z_j}^{+}$ and $\left.\frac{\partial x}{\partial z}\right|_{z_{j+1}}^{-}$ can be calculated as functions of the states of the aggregation elements:

$$\left.\frac{\partial x}{\partial z}\right|_{z_j}^{+} = \phi_j(\bar{x}_j, \bar{x}_{j+1}), \quad (24)$$

$$\left.\frac{\partial x}{\partial z}\right|_{z_{j+1}}^{-} = \psi_{j+1}(\bar{x}_j, \bar{x}_{j+1}), \quad j = 2, \ldots, n-1. \quad (25)$$

For $j = 1$ or $j = n$, the boundary conditions of the original system can be used to solve Eq. 21. The resulting left and right derivatives depend then either on only one aggregation element variable and a possible input variable u, for example

$$\left.\frac{\partial x}{\partial z}\right|_{1}^{+} = \phi_N(\bar{x}_n, u_1) \quad (26)$$

for independent boundary conditions on the right side, or, for cyclic boundary conditions, on the states of the aggregation elements on both ends of the system in addition to a possible input variable u:

$$\left.\frac{\partial x}{\partial z}\right|_{0}^{-} = \psi_1(\bar{x}_1, \bar{x}_n, u_0). \quad (27)$$

Step 2b implies the substitution of these functions into Eq. 20 to yield the final reduced model

$$\frac{1}{n}\frac{d\bar{x}_j}{dt} = \beta\Big(\phi_j(\bar{x}_j, \bar{x}_{j+1}) - \psi_j(\bar{x}_{j-1}, \bar{x}_j)\Big), \quad j = 1, \ldots, n. \quad (28)$$

At steady-state, Eq. 28 are differentiability conditions for the steady-state profile at the aggregation points as they imply equality of the left and right derivatives.

Continuous systems: first-order systems

A partial differential equation with first-order spatial derivative reads

$$\frac{\partial x}{\partial t} = -\alpha\frac{\partial x}{\partial z} + R(x), \quad (29)$$

with a certain boundary condition on the left side, and α being a dimensionless number. This is a transport system with a source term R, with transport from left to right. The same procedure for Steps 1a to c as in the derivation for second order systems is applied. The equations for the steady-state systems 17 now read

$$0 = -\alpha\frac{x_i - x_{i-1}}{\Delta z} + R(x_i), \quad i = 1, \ldots, N, i \ne s_j, j = 1, \ldots, n. \quad (30)$$

These are discretizations of the continuous steady-state systems

$$0 = -\alpha\frac{\partial x(z)}{\partial z} + R(x(z)), \quad z_j \le z \le z_{j+1}, \quad (31)$$

with the single boundary condition on the left side

$$x(z_j) = \bar{x}_j, \quad (32)$$

where $x(z)$ denotes the spatially distributed states of the steady-state system j between the aggregation points z_j and z_{j+1}, and $\bar{x}_j$ is the state of aggregation element j on the left side of the system. This implies that the values of the variables on the right side of the steady-state systems are generally not the same as the variable values of the adjacent aggregation element but depend on the left boundary condition:

$$x(z_{j+1}) = \psi_{j+1}(\bar{x}_j). \quad (33)$$

The limit case of Eq. 19, which for first-order systems reads

$$\frac{1+\Delta z}{n}\frac{dx_{s_j}}{dt} = -\alpha(x_{s_j} - x_{s_j-1}) + R(x_{s_j})\Delta z,$$

is therefore

$$\frac{1}{n}\frac{d\bar{x}_j}{dt} = -\alpha(\bar{x}_j - \psi_j(\bar{x}_{j-1})). \quad (34)$$

Equations 34 for $j = 1,\ldots, n$ are the reduced model for first-order systems of the form 29. At steady-state, Eq. 34 are continuity conditions for the steady-state profile.

Steady-state preservation property

The characteristic property of the aggregation model reduction method is that the original and the reduced model assume identical steady states. This means that

(1) if the states of the reduced model assume the values of the steady-state profile of original system at the aggregation points, the reduced model is in steady-state, and

(2) if the reduced model is in steady-state, the profile of the aggregation elements with the interconnecting steady-state systems coincides with the unique steady-state profile of the original system.

To show this, it is assumed that there exists a unique steady-state for the original system. For continuous systems, the argument is restricted to systems with spatial derivatives of order up to two, and the steady-state profile of the original system is assumed to be differentiable.

The discrete case is trivial to show, because at steady-state, the equations of the original system 1–3 and the equations of the reduced system 5–8 are identical. As uniqueness of the solution is assumed, the solutions are identical as well.

In the continuous case, the two parts can be shown separately. The argument is given for second-order systems; first-order systems follow as a special case.

(1) As the states of the aggregation elements lie on the unique steady-state profile of the original system 14, the profiles of the steady-state systems between the aggregation elements coincide with the corresponding parts of the steady-state profile of the original model. Differentiability of the profile of the original system implies that the left and right derivatives at each aggregation point as in Eq. 20 coincide, and the equations are at steady-state.

(2) On the steady-state systems between the aggregation points of the reduced model 21, the equations of the original system 14 are satisfied at steady-state. As the boundary conditions of the steady-state systems are the states of the aggregation elements, the profile of the connected steady-state systems is continuous. As the reduced model is in steady-state, Eq. 20 implies that the first-order spatial derivatives of the steady-state systems on both sides of each aggregation points assume the same values. Then, by Eq. 21, the second-order derivatives of the steady-state systems assume the same values on both sides of each aggregation point. This means that the profile resulting from connecting all steady-state profiles satisfies the original system 14 at steady-state on the complete domain and is therefore the unique solution of the original system 14 at steady-state.

Examples

The method is illustrated on three simple example systems.

Distillation column

Model As an example for a discrete system, a staged distillation column is considered. This example system was used by Lévine and Rouchon[2] for the derivation of their reduction method, and has been discussed extensively in Linhart and Skogestad.[3] Therefore, the derivation of the model is described here only briefly.

The original model reads

$$H_1\dot{x}_1 = Vy_2 - Vx_1, \tag{35}$$

$$H_i\dot{x}_i = Lx_{i-1} + Vy_{i+1} - Lx_i - Vy_i, \quad i = 2,\ldots, i_F - 1, \tag{36}$$

$$H_{i_F}\dot{x}_{i_F} = Lx_{i_F-1} + Vy_{i_F+1} - (L+F)x_{i_F} - Vy_{i_F} + Fz_F, \tag{37}$$

$$H_i\dot{x}_i = (L+F)x_{i-1} + Vy_{i+1} - (L+F)x_i - Vy_i, \quad i = i_F + 1,\ldots, N-1, \tag{38}$$

$$H_N\dot{x}_N = (L+F)x_{N-1} - (L+F-V)x_N - Vy_N, \tag{39}$$

where H_i is the total liquid molar holdup, x_i and $y_i = k(x_i)$ are the concentrations of the first component in the liquid and vapor phase, respectively, of stage i, N is the number of stages including the condenser and reboiler, i_F is the index of the feed stage, V and L are the liquid and vapor flows in the column, respectively, and F and z_F are the feed flow rate and the feed concentration, respectively. The molar holdups, liquid and vapor flows are assumed to be constant. The energy balance is simplified using the constant relative volatility assumption

$$y_i = k(x_i) = \frac{\alpha x_i}{1 + (\alpha - 1)x_i}. \tag{40}$$

After applying Steps 1a to c of the model reduction method, the reduced model equations read

$$\bar{H}_1\dot{\bar{x}}_1 = Vk(\bar{x}_2) - V\bar{x}_1, \tag{41}$$

$$\bar{H}_j\dot{\bar{x}}_{s_j} = L\bar{x}_{s_j-1} + Vk(\bar{x}_{s_j+1}) - L\bar{x}_{s_j} - Vk(\bar{x}_{s_j}), \quad j = 2,\ldots, n-1, j \neq j_F, \tag{42}$$

$$\bar{H}_{j_F}\dot{\bar{x}}_{i_F} = L\bar{x}_{i_F-1} + Vk(\bar{x}_{i_F+1}) - (L+F)\bar{x}_{i_F} - Vk(\bar{x}_{i_F}) + Fz_F, \tag{43}$$

$$0 = L\bar{x}_{i-1} + Vk(\bar{x}_{i+1}) - L\bar{x}_i - Vk(\bar{x}_i), \quad i = 2,\ldots, N-1, i \neq s_j, j = 1,\ldots, n, \tag{44}$$

$$\bar{H}_n\dot{\bar{x}}_N = (L+F)\bar{x}_{N-1} - (L+F-V)\bar{x}_N - k(\bar{x}_N), \tag{45}$$

where n is the number of aggregation stages, $\bar{H}_j$ and s_j are the aggregated holdup and the index of aggregation stage j, respectively, and j_F is the index of the aggregation stage where the feed is entering. The terms "aggregation stage" and "aggregated holdup" are here used for the more general terms "aggregation element" and "capacity" as used in the "Method" section.

Steps 2a and b imply the solution of the algebraic equations and the substitution of the required solutions Y_j into the dynamic equations. Please note that in Eq. 44 as well as in Eq. 47 below, L should be replaced by $(L + F)$ as in Eq. 38 for stages below the feed stage.

$$\bar{H}_1\dot{\tilde{x}}_1 = VY_1(\tilde{x}_1, \tilde{x}_2, V/L) - V\tilde{x}_1, \tag{46}$$

$$\bar{H}_j\dot{\tilde{x}}_j = L\tilde{x}_{j-1} + VY_j(\tilde{x}_j, \tilde{x}_{j+1}, V/L) - L\tilde{x}_j - VY_{j-1}(\tilde{x}_{j-1}, \tilde{x}_j, V/L), \quad j = 2,\ldots, n-1, j \neq j_F, \tag{47}$$

Table 1. Parameters of the Distillation Column Model

Parameter	Value
N	74
n_F	36
H_1	20 mol
H_N	20 mol
$H_i, i = 2,\ldots,N-1$	1 mol
α	1.33
Input	**Nominal value**
z_F	0.45
F	0.04 mol/s
L	0.12 mol/s
V	0.14 mol/s

$$\bar{H}_{j_F}\dot{\tilde{x}}_{j_F} = L\tilde{x}_{j_F-1} + VY_{j_F}(\tilde{x}_{j_F}, \tilde{x}_{j_F+1}, V/(L+F)) - (L+F)\tilde{x}_{j_F} - VY_{j_F-1}(\tilde{x}_{j_F-1}, \tilde{x}_{j_F}, V/L) + Fz_F, \quad (48)$$

$$\bar{H}_n\dot{\tilde{x}}_n = (L+F)\tilde{x}_{n-1} - (L+F-V)\tilde{x}_n - VY_{n-1}(\tilde{x}_{n-1}, \tilde{x}_n, V/(L+F)). \quad (49)$$

The functions Y_j correspond to the functions ϕ_j in Eq. 9. Due to mass conservation of the steady-state systems 44, only the functions ϕ, but not the functions ψ are needed. The model parameters are given in Table 1. A reduced model of a more complex distillation model with complex hydrodynamic and thermodynamic relationships has been described in Linhart and Skogestad.[4]

Simulation study. Figure 3 shows the responses of the top and bottom concentrations of the full distillation model with 74 stages ($x^{top} = x_1$, $x^{bottom} = x_N$) and reduced distillation models with 3, 5, and 7 aggregation stages ($x^{top} = \tilde{x}_1$, $x^{bottom} = \tilde{x}_n$), to a step change in the feed concentration z_F from 0.45 to 0.55.

The reduced model parameters, i.e., the position of the aggregation stages and their aggregated holdups, are given in

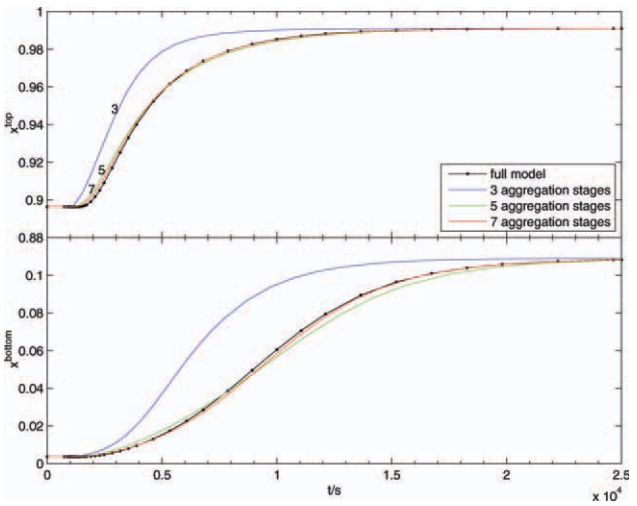

Figure 3. Distillation model top and bottom concentration responses to step change in feed concentration z_F from 0.45 to 0.55.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 2. Positions and Holdups of the Aggregation Stages of the Reduced Models

Aggregation Stage Index j	1	2	3	4	5	6	7
s_j (3 agg. stages)	1	36	74				
$\bar{H}_j$	20	72	20				
s_j (5 agg. stages)	1	14	36	60	74		
$\bar{H}_j$	20	21	28	23	20		
s_j (7 agg. stages)	1	8	20	36	53	67	74
$\bar{H}_j$	20	10	15	19	18	10	20

Table 2. They are taken from Linhart and Skogestad.[3] The parameter sets for the models with 5 and 7 aggregation stages are "optimized" to minimize the deviation from the original model over a broad range of changes in the feed concentration z_F and liquid and vapor flows L and V as described in Linhart and Skogestad.[3] However, the optimization is restricted to the position and the aggregated holdups of the aggregation stages except reflux drum and reboiler and constrained to the requirement that the sum of the aggregation stage capacities equals to the number of stages in the system. Consequently, there is no degree of freedom for the model with three aggregation stages. If these restrictions are lifted, better approximation quality, especially for the model with three aggregation stages, can be expected.

It can be seen that especially the approximation quality of the reduced model with seven aggregation stages is very good. This model has less than 10% of the states as the full model. The gain in computation time has been shown in Linhart and Skogestad[3] to be in the same order of magnitude as the reduction in the number of states.

Heat exchanger

Model. As an example of a continuous system described by (coupled) first-order partial differential equations, a tubular counter-current heat exchanger is considered (see Fig. 4).

A description of these types of heat exchangers can be found in Skogestad.[9] The partial differential equations of the system are of the form of Eq. 29 and read

$$A^h\rho^h\frac{\partial T^h}{\partial t} = -m^h\frac{\partial T^h}{\partial z} - \frac{Up}{c_p^h}(T^h - T^c), \quad (50)$$

$$A^c\rho^c\frac{\partial T^c}{\partial t} = m^c\frac{\partial T^c}{\partial z} + \frac{Up}{c_p^c}(T^h - T^c),\ 0<z<l, \quad (51)$$

$$T^h(t,0) = T^h_{in}, \quad (52)$$

$$T^c(t,l) = T^c_{in}, \quad (53)$$

where T^h, T^c, m^h, m^c, A^h, A^c, ρ^h, ρ^c, c_p^h, and c_p^c are the temperatures, mass flows, tube cross-sectional areas, densities, and heat capacities of the hot and the cold streams, respectively, U and p are the heat transmission coefficient and the perimeter of the surface between the hot and cold stream, respectively, l is the tube length, and T^h_{in} and T^c_{in} are the inlet temperatures of the hot and the cold stream, respectively. The main assumptions in this model are incompressible fluids, temperature-independent fluid properties, no diffusive heat transport, and negligible heat capacity of the tube walls. The parameter values are given in Table 3.

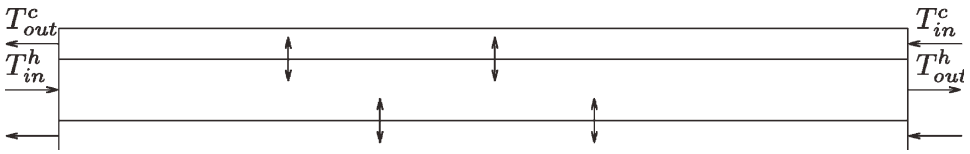

Figure 4. Schematic diagram of a tubular heat exchanger.

A straightforward choice of n aggregation points according to Step 1a of the reduction procedure is an equal-distribution of the aggregation points over the whole domain with the end points placed at the ends of the heat exchanger:

$$s_j = \frac{j-1}{n-1} l, \quad j = 1, \ldots, n. \tag{54}$$

The heat exchanger equations are a combination of two counter-current transport equations with a source term representing the heat exchange. The dynamic equations for the aggregation elements can therefore be derived from Eq. 34 to be

$$C_j \frac{d\bar{T}^h_j}{dt} = -\frac{m^h}{A^h \rho^h l}(\bar{T}^h_j - \psi_j(\bar{T}^h_{j-1}, \bar{T}^c_j)), \tag{55}$$

$$C_j \frac{d\bar{T}^c_j}{dt} = -\frac{m^c}{A^c \rho^c l}(\bar{T}^c_j - \phi_j(\bar{T}^h_j, \bar{T}^c_{j+1})), \tag{56}$$

where C_j is the capacity of aggregation element j, and ϕ_j and ψ_j are the solutions of the steady-state system right and left of aggregation element j, respectively. Figure 5 shows a schematic diagram of the reduced model.

A straightforward choice for the capacities is $C_j = 1/n$. This way, the continuously distributed heat capacity of the original model is equally distributed over the aggregation elements.

For heat exchangers, analytic steady-state solutions are available[10]:

$$\begin{bmatrix} T^h_{\text{out}} \\ T^c_{out} \end{bmatrix} = \frac{1}{1 - R^c a} \begin{bmatrix} 1 - R^c & R^c(1-a) \\ 1 - a & a(1-R^c) \end{bmatrix} \begin{bmatrix} T^h_{\text{in}} \\ T^c_{\text{in}} \end{bmatrix}, \tag{57}$$

where the parameters R^c and a are defined as follows:

$$R^c = \frac{m^c c^c_p}{m^h c^h_p}, \quad a = exp\left(-\frac{Up(1-R^c)}{m^c c^c_p}\right). \tag{58}$$

Expression 57 can be used in Step 2a of the reduction procedure to derive the steady-state functions ϕ and ψ:

$$\begin{bmatrix} \psi_j \\ \phi_{j-1} \end{bmatrix} = \frac{1}{1 - R^c a} \begin{bmatrix} 1 - R^c & R^c(1-a) \\ 1 - a & a(1-R^c) \end{bmatrix} \begin{bmatrix} \bar{T}^h_{j-1} \\ \bar{T}^c_j \end{bmatrix}. \tag{59}$$

Here, $\bar{T}^h_{j-1}$ and $\bar{T}^c_j$ are the temperatures of the neighboring aggregation elements $j-1$ and j of the steady-state system (compare figure 5). In Step 2b of the reduction procedure, the steady-state functions 59 are substituted into the dynamic equations 55 and 56 of the aggregation elements.

Simulation study. To demonstrate the approximation quality of the reduced models, Figures 6–9 compare the responses of reduced models with 2, 5, and 30 aggregation elements with finite-difference approximations with 100 and 2000 finite-differences. The simulation with 2000 finite-differences is referred to as the exact solution.

The variables that are compared are the outlet temperatures T^h_{out} and T^c_{out} of the hot and the cold stream, respectively. In the reduced model, they are the temperatures of the aggregation elements at both ends of the heat exchanger, i.e., $T^c_{\text{out}} = \bar{T}^c_1$ and $T^h_{\text{out}} = \bar{T}^h_n$. Figure 6 shows the responses to a step in the hot stream inlet temperature T^h_{in} from 360 K to 370 K.

It can be seen that the response of the cold stream outlet temperature T^c_{out}, which is located at the same side as the hot stream inlet, is approximated very well by the reduced models. The response of the model with 30 aggregation elements is almost indistinguishable from the exact solution. All reduced aggregation models perfectly reproduce the steady-state. The finite-difference approximation with 100 elements shows a certain steady-state deviation from the reference solution. For this heat exchanger model, this deviation can be corrected rather easily.[11] However, without any modification of the finite-difference models, the aggregated models achieve a certain approximation quality with much less dynamic states.

The response of the hot stream outlet temperature T^h_{out} (lower part of Figure 6) shows a dead-time period, which is characteristic for transport systems, since the hot stream outlet is located on the opposite side of the hot stream inlet where the change is applied. The approximation quality of the reduced models is rather poor here, since a dead-time system requires a model of high dynamic order for good approximation. Therefore, the 100 finite-difference approximation is superior to the aggregated model with 30 aggregation elements. Still, the aggregated models show a better approximation towards the steady state.

Figure 7 shows the responses to a 20% step change in the hot stream flow rate v^h.

Table 3. Parameters of the Heat Exchanger Model

Parameter	Value
$A^c \rho^c$	31.4 kg/m
$A^h \rho^h$	39.3 kg/m
c^c_p	3000 J/(kgK)
c^h_p	4000 J/(kgK)
U	0.5 kW/m^2
p	0.6283 m
Input	**Nominal Value**
m^c	2 kg/s
m^h	1 kg/s
T^c_{in}	320 K
T^h_{in}	360 K

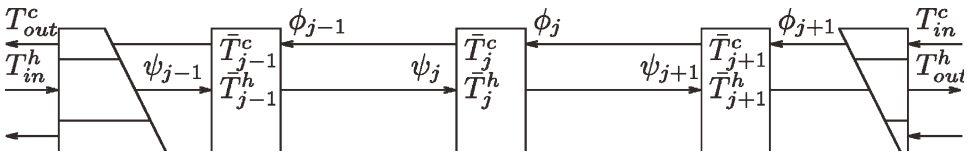

Figure 5. Schematic diagram of the reduced heat exchanger model.

This is approximated very well by the model with 30 aggregation elements. Since the fluid is assumed incompressible, the flow rate changes simultaneously throughout the whole system. Due to the increased velocity of the hot fluid, both the temperature of the hot and cold outlet streams rise. The transport characteristic of the system is still present in the response of the hot stream outlet temperature T^h_{out}, where the initial slope is flattened for the residual time of the hot fluid in the system.

Figures 8 and 9 show the responses to slow changes in T^h_{in} and v^h, respectively. Here, the input signal is a cubic spline curve with a transient time of 1000 s. Generally, the approximation quality of the reduced models with 5 and 30 aggregation elements is good. The approximation of the dead-time period of the hot stream outlet temperature T^h_{out} (lower part of Figure 8) is much better than in case of a step change. This is explicable by the diffusive character of the heat exchange between the counter-current flows, which is more dominant in this case.

Fixed bed reactor

Model. As an example of a second-order continuous system, an adiabatic fixed-bed reactor model is considered[12] (see Figure 10):

$$\sigma\frac{\partial\alpha}{\partial t} = -\frac{\partial\alpha}{\partial x} + \frac{1}{Pe_m}\frac{\partial^2\alpha}{\partial x^2} + DaR(\alpha,\theta), \tag{60}$$

$$\frac{\partial\theta}{\partial t} = -\frac{\partial\theta}{\partial x} + \frac{1}{Pe_h}\frac{\partial^2\theta}{\partial x^2} + DaR(\alpha,\theta), \tag{61}$$

which is in form of Eq. 14. Here, α is the conversion, θ a dimensionless temperature, and the reaction term is given by

$$R(\alpha,\theta) = (1-\alpha)^r exp\left(\gamma\frac{\beta\theta}{1+\beta\theta}\right). \tag{62}$$

The boundary conditions are

$$\alpha(0,t) = \frac{1}{Pe_m}\frac{\partial\alpha}{\partial x}\bigg|_{x=0}, \tag{63}$$

$$\theta(0,t) = f\theta(1,t) + \frac{1}{Pe_h}\frac{\partial\theta}{\partial x}\bigg|_{x=0}, \tag{64}$$

$$\frac{\partial\alpha}{\partial x}\bigg|_{x=1} = 0, \tag{65}$$

$$\frac{\partial\theta}{\partial x}\bigg|_{x=1} = 0. \tag{66}$$

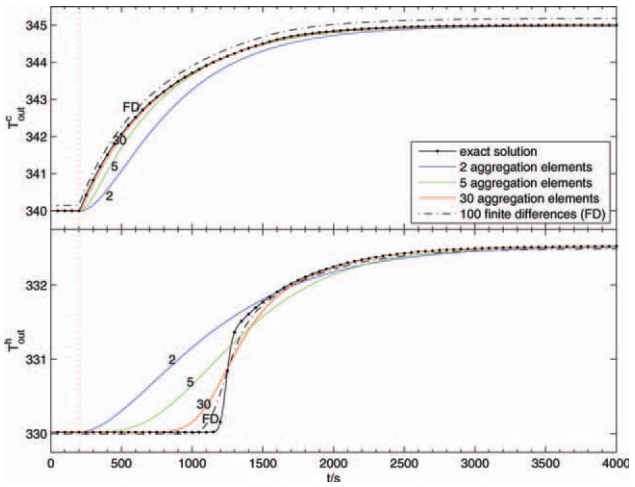

Figure 6. Heat exchanger outlet temperature responses of cold (upper plot) and hot (lower plot) streams to a step change in the hot inlet temperature T^h_{in}.

The dotted vertical line marks the time when the step change is applied. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

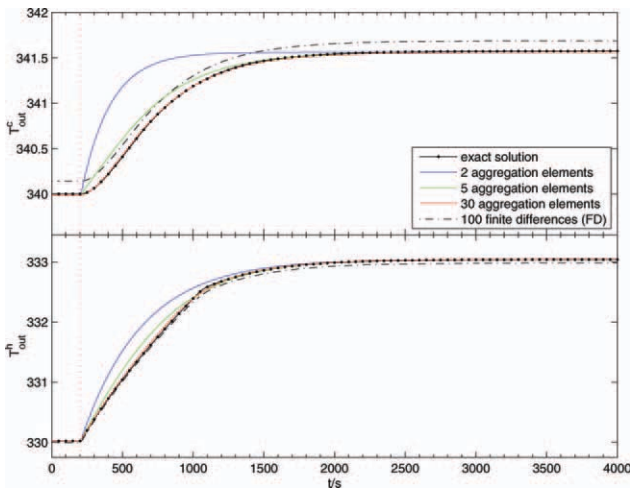

Figure 7. Heat exchanger outlet temperature responses of cold (upper plot) and hot (lower plot) streams to a step change in the hot stream flow rate v^h.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

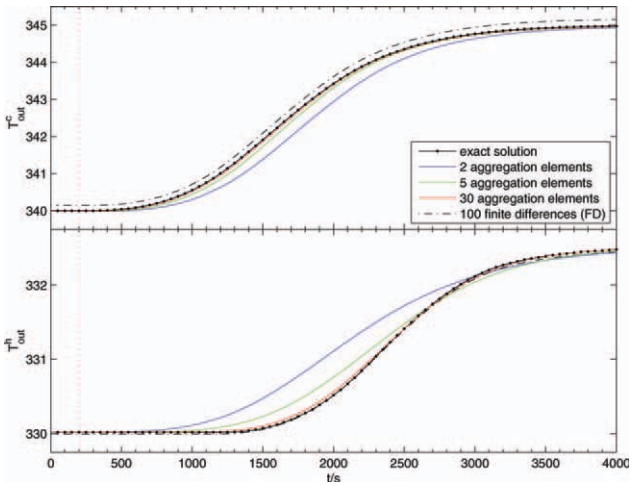

Figure 8. Heat exchanger outlet temperature responses of cold (upper plot) and hot (lower plot) streams to a slow change in the hot inlet temperature T^h_{in}.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

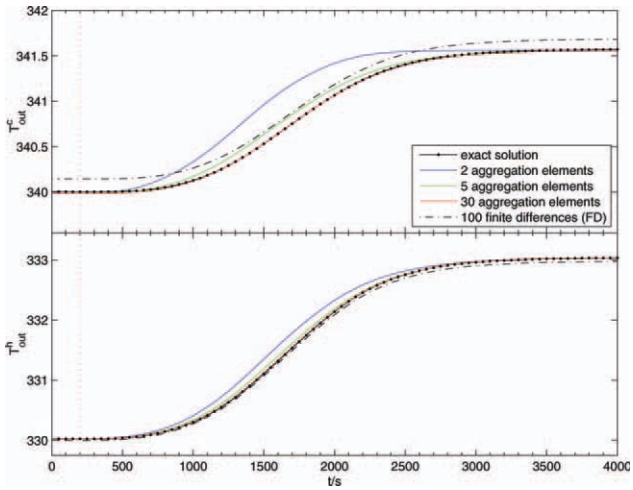

Figure 9. Heat exchanger outlet temperature responses of cold (upper plot) and hot (lower plot) streams to a slow change in the hot stream flow rate v^h.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

The derivation of a reduced model for this system is shown in detail in the "Method" section for second order systems. For the purpose of demonstrating the approximation quality of the reduced models, models derived using Steps 1a to c are sufficient. If a gain in computational performance is desired, the steady-state systems have to be eliminated from the model using Steps 2a and b. All aggregation points are chosen at locations x_j on inner points of the domain of the partial differential equation, i.e. $0 < x_j < 1$, $j = 1,\ldots, n$. Therefore, the boundary conditions of the original model have to be included in the solutions of the steady-state systems on the boundary of the system. The left boundary condition 64 is special in a way that it includes the state $\theta(1,t)$ on the right side of the system. This results in expressions of the form

$$\left.\frac{\partial \alpha}{\partial x}\right|_{x_1}^{-} = \psi_1^{\alpha}(\bar{\alpha}_1, \bar{\theta}_1), \tag{67}$$

$$\left.\frac{\partial \theta}{\partial x}\right|_{x_1}^{-} = \psi_1^{\theta}(\bar{\alpha}_1, \bar{\theta}_1, \bar{\alpha}_n, \bar{\theta}_n) \tag{68}$$

for the left side, and

$$\left.\frac{\partial \alpha}{\partial x}\right|_{x_1}^{+} = \phi_n^{\alpha}(\bar{\alpha}_n, \bar{\theta}_n), \tag{69}$$

$$\left.\frac{\partial \theta}{\partial x}\right|_{x_1}^{+} = \phi_n^{\theta}(\bar{\alpha}_n, \bar{\theta}_n) \tag{70}$$

for the right side of the system.

Simulation study. To demonstrate the approximation quality of the reduced models, Figures 11 and 12 compare the responses of reduced models with 5, 15, and 30 aggregation elements with finite-difference approximations with 100 and 2000 finite-differences. The simulation with 2000 finite-

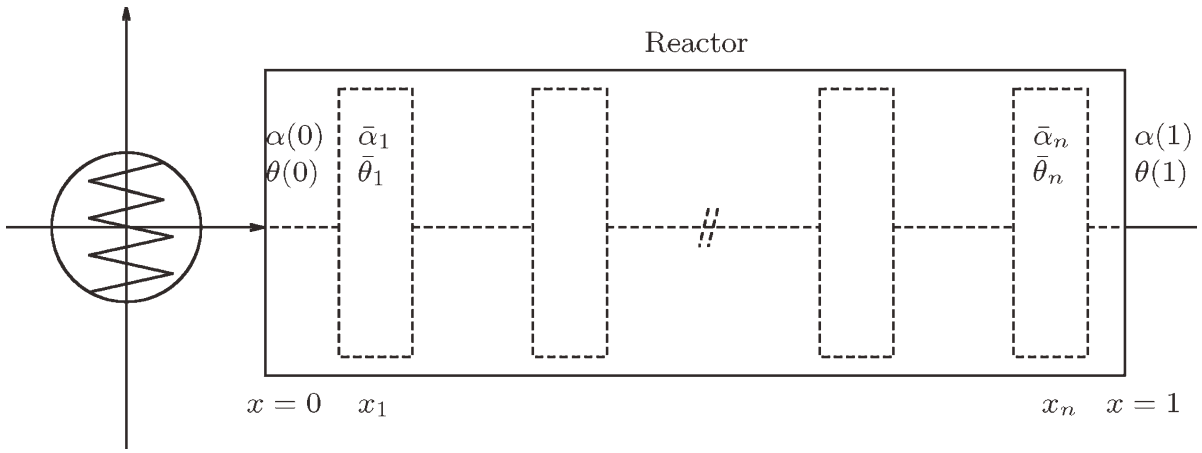

Figure 10. Schematic diagram of a fixed bed reactor with heat recycle.

The structure of the reduced model is schematically shown using dashed lines.

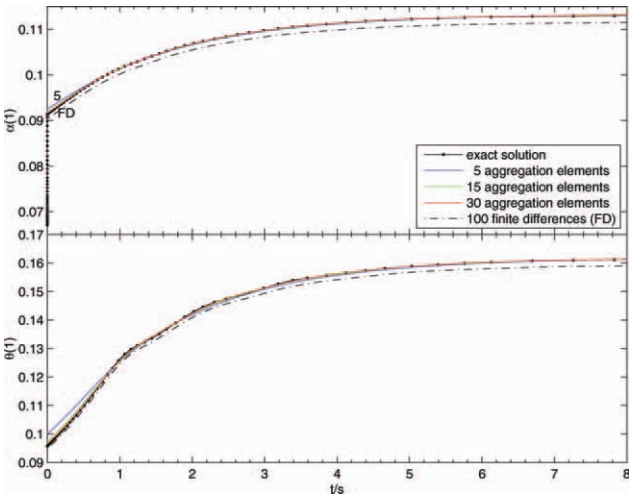

Figure 11. Responses of fixed-bed reactor conversion α and temperature θ at the right end to a change of *Da* from 0.05 to 0.07.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

differences is referred to as the exact solution. Liu and Jacobsen[12] show that the system exhibits a complex bifurcation behavior when *Da* is chosen as bifurcation parameter. At $Da = 0.05$ and $Da = 0.07$, the system has one stable steady-state, whereas at $Da = 0.1$, the steady-state is unstable, and the system performs limit cycle oscillations.

Figure 11 shows the trajectories of α and θ at the right end of the reactor, when a step change in *Da* from 0.05 to 0.07 is applied.

The trajectories show a fast initial change in α, which is due to the small parameter σ multiplying the left-hand side of Eq. 60. After that, the system performs a slow transient to a stable steady-state at $Da = 0.07$. It can be seen that the approximation quality of all reduced models is excellent, except for some deviation of the model with five aggregation elements in the beginning of the slow transient phase. While the reduced aggregation models perfectly reproduce the steady-state of the original system, the 100 finite-differences approximation shows a certain deviation.

Figure 12 shows the trajectories of the same variables, when a larger step change in *Da* from 0.05 to 0.1 is applied.

At $Da = 0.1$, the system exhibits high-frequency limit-cycle oscillations. It can be seen that the approximation quality of all reduced models of the slow motion towards the limit-cycle oscillations is excellent. The reduced model with 30 aggregation elements is also capable to reproduce the fast limit-cycle oscillations. It is remarkable that the reduced model can reproduce the fast movement despite its slow nature.

Discussion

Advantages and limitations of the aggregation method

The method presented in this article is conceptually straightforward. The good approximation quality of the reduced models has been demonstrated in several examples. The approximation quality can even be improved by optimizing the locations and capacities of the aggregation elements for the given problem.

The main limitation of the method lies in the implementation Step 2a of the reduction procedure. The problem is the high dimension of the functions that have to be substituted into the dynamic equations if the original system has a large number of spatially distributed state variables. In Linhart and Skogestad,[4] the method was applied to a complex distillation model containing energy balances and complex thermodynamic and hydraulic relationships. There, substitution was possible by using five-dimensional tables with linear interpolation. If, on the other hand, simple analytic solutions for the steady-state systems as in case for the heat exchanger model are available, the reduction method is easy to apply and yields models of good approximation quality.

Relationship to singular perturbation models

The presented method is not a singular perturbation method, but is closely related both structurally and in terms of approximation properties. In the following, the reduction procedure is therefore compared to the procedure to derive slow reduced models in singular perturbation theory.[13,14] The discussion is presented for discrete systems. As the continuous procedure is derived using the discrete procedure, the argument applies to continuous systems as well.

Singular perturbation procedure. In singular perturbation theory, systems with dynamics on two or more time-scales are analyzed mathematically. For this, a system

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{u}), \tag{71}$$

is transformed into the standard form of singular perturbations

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}, \mathbf{z}, \mathbf{u}), \tag{72}$$

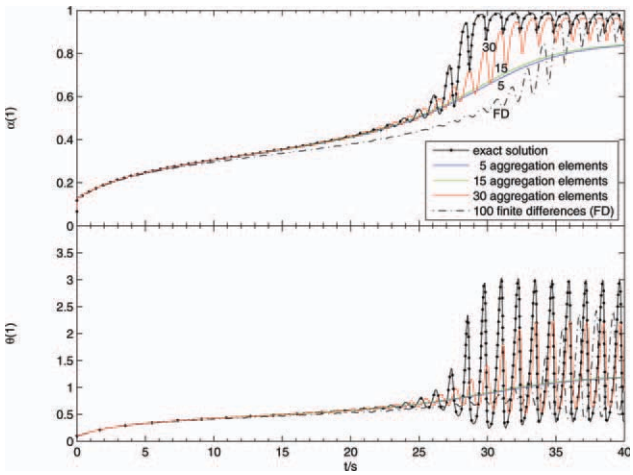

Figure 12. Responses of fixed-bed reactor conversion α and temperature θ at the right end simulated to a change of *Da* from 0.05 to 0.1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

$$\varepsilon \frac{d\mathbf{z}}{dt} = \mathbf{g}(\mathbf{y}, \mathbf{z}, \mathbf{u}), \tag{73}$$

where $\mathbf{y}$ is a vector of "slow" variables, $\mathbf{z}$ is a vector of "fast" variables, and $\varepsilon << 1$ is a small singular perturbation parameter. This is usually achieved by scaling the original equations and by a transformation of the state vector $\mathbf{x}$. In general, there is no unique procedure for choosing the scaling of the equations or the state transformation.

If the time-scales of the system are sufficiently separated, and the scaling and state transformation is suitable, then Eq. 72 and 73 represent the slow and the fast dynamics in the system, respectively. Then, these equations can be used for further analysis of the system. One common procedure is to apply the quasi-steady-state assumption $\varepsilon \rightarrow 0$ to Eq. 73, thus obtaining the reduced slow model

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}, \mathbf{z}, \mathbf{u}), \tag{74}$$

$$0 = \mathbf{g}(\mathbf{y}, \mathbf{z}, \mathbf{u}). \tag{75}$$

Here, the dynamic equations 73 are converted into the algebraic equations 75. This is one reason why ε is called the singular perturbation parameter. Depending on the time-scale separation and the appropriate transformation of the system, this system approximates the original dynamics more or less accurately. Due to the replacement of the fast equations by algebraic relationships, the fast dynamics are approximated by "instantaneous" dynamics. This is significant for changes in the inputs $\mathbf{u}$, where the response of the slow model is actually faster than the response of the original model. The term "slow model" therefore refers to the internal dynamics of the reduced model and not to its input-output behavior.

If a low-order model is desired and Eq. 75 can be solved explicitly for $\mathbf{z}$, then

$$\mathbf{z} = \mathbf{h}(\mathbf{y}, \mathbf{u}), \tag{76}$$

can be used to eliminate the fast variables $\mathbf{z}$ from the slow model

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}, \mathbf{h}(\mathbf{y}, \mathbf{u}), \mathbf{u}). \tag{77}$$

Comparison with aggregation method. To compare the singular perturbation procedure with the aggregation method proposed in this article, it can first be observed that after step 1c of the reduction procedure, the system is basically in the form of Eq. 74 and 75. Steps 2a and b correspond to the procedure in Eq. 76 and 77. The main difference between the procedures lies in the derivation of the form 74 and 75. In contrast to the singular perturbation procedure, the aggregation method does not use a state transformation and scaling of the equations to arrive at this form. Instead, the left-hand sides of the dynamic equations are manipulated in a way that cannot be achieved by a state transformation and scaling. The method does therefore not rely on the existence of a time-scale separation in the system. Instead, the method is based on approximating the spatial signal transport through the system by instantaneous transport through intervals connected by large capacity elements. This is an artificial construction, which deviates from the treatment of singular perturbation systems.

Lévine and Rouchon[2] derive their method for staged distillation columns, which ultimately leads to the reduction procedure for discrete systems described in this article, as a singular perturbation method. They partition the column into compartments of consecutive stages, and use a singular perturbation procedure to separate the time-scales created by the ratio of the large compartment holdups and the small stage holdups. This time-scale separation is, however, not present in the original model, since the compartments are introduced completely artificially. The reason that the resulting models still approximate the original model sufficiently well is the simplification of certain terms during the quasi-steady-state approximation due to the incorrect introduction of the singular perturbation parameter ε. As a consequence, the compartment boundaries do not appear anymore in the resulting models. If a reduced model is derived without this simplification, it shows some unphysical inverse response, which is clear evidence of the incorrect introduction of the singular perturbation parameter.[3]

The crucial property for the success of the aggregated models is the perfect reproduction of the steady-state. This property is also characteristic for slow singular perturbation models as Eq. 74 and 75. Both the derivation and the dynamic behavior of aggregated and singular perturbation models can therefore be said to be closely related.

Alternative numerical discretization schemes

As mentioned before, the method described in this article can be regarded as a discretization method for continuous systems. Classical methods for equations of the type of Eq. 14 are finite-difference and finite-element methods.[1] Direct comparisons with finite-element discretizations have been presented in the heat exchanger and fixed-bed reactor examples in the previous section. Below, a short comparison with finite-element discretizations is given. For certain classes of transport-reaction-diffusion systems in a control and optimization context, there exist more refined methods based on global spatial basis functions.[15,16]

Steady-state approximation. One difference between the aggregation method and other methods such as finite-volume and finite-element methods is immediately obvious: the aggregation method perfectly reproduces the steady-state even when the number of dynamic states is zero, while the above mentioned methods achieve this only in the limit case when the number of dynamic states goes to infinity. This is due to the incorporation of steady-state information into the aggregated models, which is not the case in the other methods.

Finite-element methods. In finite-element methods, the solution is approximated by weighted sums of basis functions, which usually are polynomials. The weights of the basis functions are determined by inserting the approximation into the original equations and weighting the residual over the spatial domain by certain functions. If these functions are the basis functions themselves, the method is called a Galerkin method. In collocation methods, the residual is required to vanish at certain discrete points, the so-called

collocation points. This method is popular in chemical engineering for the reduction of distillation models.[5,6] The efficiency of the method is based on the assumption that the solution profiles can be approximated by polynomials. To account for solution profiles that are difficult to approximate with polynomials over the whole spatial interval, the latter can be divided into finite-elements, on each of which a polynomial approximation by collocation is used. This procedure is therefore different from the aggregation procedure. Collocation models might be superior in approximating the fast responses of a system, whereas aggregation models will show better approximation of the behavior of systems that are close to steady state.

Eigenfunction decomposition methods. In many systems, a small number of spatio-temporal patterns dominate the system dynamics. In analogy to linear systems, these patterns can be regarded as eigenfunctions. The system dynamics can then be approximated by a time-dependent superposition of these patterns. Typically, the dominant patterns correspond to the slow dynamics of the system, because the fast dynamics settle quickly after some excitation. To approximate the dynamics of a given system, it is therefore often only necessary to consider the slow eigenfunctions. For nonlinear systems, proper orthogonal decomposition (also known as Karhunen-Loève method or principal component analysis) is a common method to derive empirical eigenfunctions from simulated trajectories.[17] It works by projecting the dynamics of a discretized distributed system on a lower-dimensional subspace containing the most dominant spatial patterns. While for many systems it is possible to obtain accurate low-order approximations for the dynamic range covered by the simulated trajectories, the original computational complexity is usually retained in the reduced models. This is because the complete set of equations is evaluated at the inclusion of the reduced state in the original state space.

There exist more specialized methods using eigenfunction decompositions for the treatment of distributed systems which combine several techniques to derive low-order reduced models. Christofides and Daoutidis[15] utilize the time-scale separation in quasi-linear PDEs marked by the differences in eigenvalue magnitude of the eigenfunctions of the linear spatial operator to derive approximate inertial manifolds, which contain the slow dynamics of the system. The obtained reduced models on basis of the approximate intertial manifolds are then used to derive nonlinear controllers. Baker and Christofides[16] extend the approximate inertial manifold method to nonlinear spatial operators using empirical eigenfunctions obtained by proper orthogonal decomposition. The time-scale separation and the slow dynamics are determined by the eigenvalues and eigenvectors of a linearization around a certain point, and the equations are transformed into a slow and a fast subsystem by a linear transformation using the eigenvectors.

The approximation quality of these approaches depends on how clearly the time-scales of a system are separated, and how well the separation into slow and fast variables reflects this time-scale separation. Due to the different complexities, these methods are difficult to compare with the aggregation method proposed in this paper. However, one main difference is that the methods described above are more specialized towards closed-loop controller design, while the aggregation method yields general-purpose reduced models. On the other hand, a similarity is that methods using spatial eigenfunctions typically work better for systems with strong diffusive characteristics (parabolic systems with important second-order spatial derivative) than for systems with strong transport characteristics (parabolic systems with weak second-order spatial derivative or hyperbolic systems). The aggregation method, as can be seen in the heat exchanger example in the Examples section, works also better for systems with stronger diffusive characteristics (large heat exchange due to low flow rates) than for stronger transport behavior (less heat exchange due to high flow rates). An important structural difference between methods relying on some sort of eigenfunctions and the method described in this paper is that in the former methods, the dynamic variables globally affect the whole spatial interval, while in the latter method, the dynamic variables are distributed over the spatial profile, having a more local effect.

Conclusions

An approach for deriving reduced models of one-dimensional distributed systems is presented in this paper. The approach extends the aggregated modeling method of Lévine and Rouchon[2] to general discrete and continuous one-dimensional systems. The main idea is the approximation of the spatial transport of signals through the system by instantaneous transport through intervals of steady-state systems connected by aggregation elements of large capacity, which slow down the system dynamics to match the dynamics of the original system. The most important property of the method is the perfect reproduction of the steady-state of the original system. The method has been demonstrated on three typical process engineering example systems. The method presents an alternative method to established spatial discretization methods such as finite-differences and finite-elements for spatially continuous systems, and to methods such as collocation or wave propagation methods for spatially discrete models. The approximation quality of the reduced models depends on the number, position and capacity of the aggregation elements. Generally, a good approximation quality can be achieved with a relatively low number of aggregation elements compared with other discretizations methods. The implementation effort of the reduced models depends on the difficulty to express the solutions of the steady-state systems as functions of the aggregation element variables in a suitable way.

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