

An aggregation model reduction method for one-dimensional distributed parameter systems

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Abstract

A new method for deriving reduced dynamic models of one-dimensional distributed parameter systems is presented. It inherits the concepts of the aggregated modeling method of Lévine and Rouchon [1] for simple staged distillation models, and can be applied to both spatially discrete and continuous systems. It 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, which asymptotically approaches the true steady-state of the original model. The method is an alternative to discretization methods like finite difference and finite element methods for spatially continuous systems, and collocation and wave propagation methods for spatially discrete systems. 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.

Keywords

Model reduction; Dynamic simulation; Distributed systems; Aggregated modeling; Distillation

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1 Introduction

This paper presents a new approach 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 (Hundsdoerfer and Verwer [2]).

The method is based on the concept of aggregation, which was used by Lévine and Rouchon [1] 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 complex distillation models (Linhart and Skogestad [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 (Cho and Joseph [5], Stewart et al. [6]) and wave propagation methods (Marquardt [7], Kienle [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 stage-wise 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 these 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 method is based on choosing several “aggregation points” on the spatial

domain of the distributed system. To each of these aggregation points, dynamic “aggregation elements” are assigned. The partial differential equations or the discretely distributed system on the intervals between the aggregation points is 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 is slowed down again by the large capacities of the aggregation elements.

The paper is organized as follows. Section 2 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 analog 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 the main characteristic property of the method. Section 3 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 respective 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 section 4, the advantages and limitations of the model reduction method are discussed. The similarities and differences to reduced models resulting from a singular perturbation procedure 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 section 5.

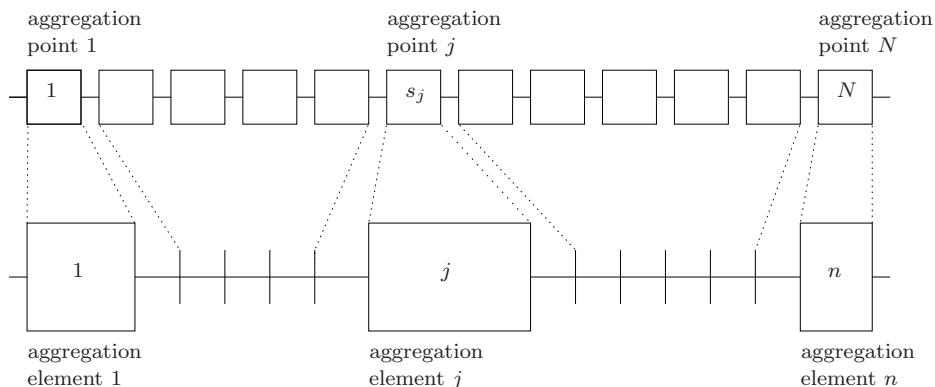


Figure 1: Schematic illustration of the reduction method for discrete distributed systems.

2 Method

In the following, the mathematical structure of the two types of spatially distributed systems the method can be applied to is described. These are basically one-dimensional systems, which are spatially either discrete or continuous. Subsequently, the reduction procedure, the conceptual steps of which are the same for all systems, is described.

2.1 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:

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

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

$$2 \leq i \leq N - 1,$$

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

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 value to 0, \mathbf{f}_i is a vector-valued function of the variable vectors of the current 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 .

2.2 Continuous distributed parameter systems

The second class 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:

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

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, since any other spatial domain can be transformed to this by simple scaling of the spatial variable z .

2.3 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 the discrete and continuous case:

1. Selection of aggregation points

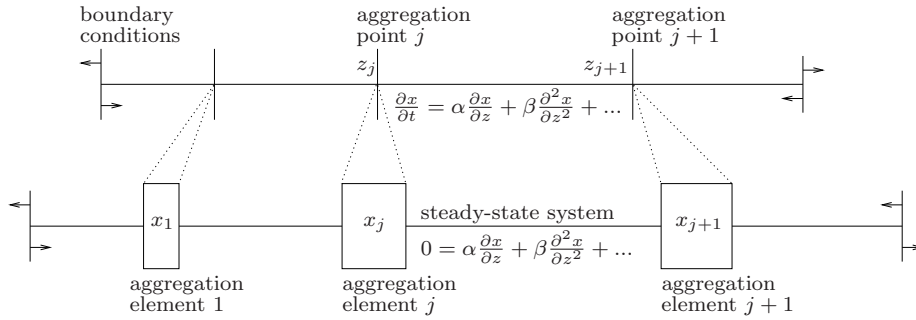


Figure 2: Schematic illustration of the reduction method for continuous distributed systems.

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

2. Introduction of aggregation elements

At every aggregation point, an “aggregation element” is positioned. In the discrete case, these elements are just the units at the aggregation points with a modified “capacity” H . In the continuous case, at every aggregation point, an aggregation element is positioned. Their dynamics are governed by simple differential equations that are derived from the original partial differential equations. The derivation is explained in sections 2.5 and 2.6. The “capacity” H of an aggregation element refers to a factor that multiplies the left-hand sides of the dynamic equations of the element.

3. Steady-state approximation of systems between aggregation elements

The equations on the intervals between the aggregation points are treated as in steady-state. In the discrete case, the left hand sides of all equations of the 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. In the continuous case, 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.

4. **Precomputed solution of steady-state systems**

The steady-state systems are 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.

5. **Substitution of steady-state solutions**

The functions computed in step 4 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 1 to 3 yield a model with reduced dynamics. It is, however, of the same complexity as the original model. In the discrete case, a large number of dynamic equations have been converted into algebraic equations. In the continuous case, 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 steps 4 and 5.

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

2.4 Discrete systems

After step 3, the equations of the reduced system read

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

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

$$j = 2, \dots, n-1,$$

$$\mathbf{0} = \mathbf{f}_i(\mathbf{x}_{i-1}(t), \mathbf{x}_i(t), \mathbf{x}_{i+1}(t), \mathbf{p}, t), \quad (7)$$

$$i = 2, \dots, N-1, i \neq s_j, j = 1, \dots, n,$$

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

Here, to simplify notation, a case is written where unit 1 and N are aggregation elements ($s_1 = 1$ and $s_n = N$). Either of these could be steady-state systems as well.

Step 4 involves solving the systems (7) for the variables \mathbf{x}_{s_j-1} and \mathbf{x}_{s_j+1} , $j = 1, \dots, n$ (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

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

and

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

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 $\bar{\mathbf{x}}_j$ is introduced, where the bar denotes the state variables of the aggregation elements.

Generally, these functions contain numerical solutions and have to be implemented in a suitable way. A straightforward way is the tabulation of the solution values over 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, since not all variables necessarily 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 5 implies the substitution of the functions (9) and (10) into the aggregation element equations (5), (6) and (8). The resulting system then reads

$$H_1 \bar{\mathbf{M}}_1 \dot{\bar{\mathbf{x}}}_1(t) = \bar{\mathbf{f}}_1(\bar{\mathbf{x}}_1(t), \phi_1(\bar{\mathbf{x}}_1(t), \bar{\mathbf{x}}_2(t), \mathbf{p}), \mathbf{p}, t), \quad (11)$$

$$H_j \bar{\mathbf{M}}_j \dot{\bar{\mathbf{x}}}_j(t) = \bar{\mathbf{f}}_j(\psi_j(\bar{\mathbf{x}}_{j-1}, \bar{\mathbf{x}}_j, \mathbf{p}), \bar{\mathbf{x}}_j(t), \phi_j(\bar{\mathbf{x}}_j, \bar{\mathbf{x}}_{j+1}, \mathbf{p}), \mathbf{p}, t), \quad (12)$$

$$j = 2, \dots, n-1,$$

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

Here, the notation $\bar{\mathbf{M}}$, $\bar{\mathbf{x}}$ and $\bar{\mathbf{f}}$ 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 , $\bar{\mathbf{x}}_j = \mathbf{x}_{s_j}$ etc. holds.

2.5 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 $\Delta z \rightarrow 0$, 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

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

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

A finite difference discretization of the spatial derivatives yields

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

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

According to step 1 and 2, a number n of aggregation points $z_{s_j}, j = 1, \dots, n$, 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 :

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

$$j = 1, \dots, n.$$

Step 3 requires that the remaining equations are treated as in steady-state:

$$0 = -\alpha \frac{x_i - x_{i-1}}{\Delta z} + \beta \frac{x_{i-1} - 2x_i + x_{i+1}}{\Delta z^2} + R(x_i), \quad (17)$$

$$i = 1, \dots, N, i \neq s_j, j = 1, \dots, n.$$

The resulting model has the same steady-state as the original discretized model. The capacities H_j can be chosen freely, but should compensate 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 discretized states 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

$$\begin{aligned} \frac{\frac{1}{\Delta z} + 1}{n} \frac{dx_{s_j}}{dt} &= -\alpha \frac{x_{s_j} - x_{s_{j-1}}}{\Delta z} + \beta \frac{\frac{x_{s_{j+1}} - x_{s_j}}{\Delta z} - \frac{x_{s_j} - x_{s_{j-1}}}{\Delta z}}{\Delta z} \\ &+ R(x_{s_j}), \end{aligned} \quad (18)$$

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

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

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

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

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 4, the right derivative $\frac{\partial x}{\partial z} \Big|_{z_j}^+$ is calculated from the boundary value systems between the aggregation points z_j and z_{j+1} ,

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

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 equations (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:

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

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

$$j = 2, \dots, n - 1.$$

For $j = 1$ or $j = n$, the boundary conditions of the original system can be used to solve equation (21). The resulting left and right derivatives depend then either only on 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 5 implies the substitution of these functions into equation (20) to yield the final reduced model

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

At steady-state, equations (28) are differentiability conditions for the steady-state profile at the aggregation points.

2.6 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 1, 2 and 3 as in section 2.5 is applied. The equations for the steady-state systems (17) now read

$$0 = -\alpha \frac{x_i - x_{i-1}}{\Delta z} + R(x_i), \quad (30)$$

$$i = 1, \dots, N, i \neq s_j, j = 1, \dots, n.$$

These are discretizations of the continuous steady-state systems

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

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 equation (19) of section 2.5, which now 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 $j = 1, \dots, n$ are the reduced model for first-order systems of the form (29). At steady-state, equations (34) are continuity conditions for the steady-state profile.

2.7 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, since at steady-state, the equations of the original system (1)-(3) and the equations of the reduced system (5)-(8) are identical. Since 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. Since 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 equation (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. Since 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. Since the reduced model is in steady-state, equation (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 equation (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.

3 Examples

The method is illustrated on three simple example systems.

3.1 Distillation column

3.1.1 Model

As an example for a discrete system, a staged distillation column is considered. This example system is was used by Lévine and Rouchon [1] 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 only very briefly.

The original model reads

$$H_1 \dot{x}_1 = Vy_2 - Vx_1, \quad (35)$$

$$H_i \dot{x}_i = Lx_{i-1} + Vy_{i+1} - Lx_i - Vy_i, \quad (36)$$

$$i = 2, \dots, i_F - 1,$$

$$H_{i_F} \dot{x}_{i_F} = Lx_{i-1} + Vy_{i+1} - (L + F)x_i - Vy_i + Fz_F, \quad (37)$$

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

$$i = i_F + 1, \dots, N - 1,$$

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

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

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

After applying steps 1 to 3 of the model reduction method, the reduced model equations read

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

$$\begin{aligned} \bar{H}_j \dot{\bar{x}}_{s_j} &= L\bar{x}_{s_{j-1}} + Vk(\bar{x}_{s_{j+1}}) - L\bar{x}_{s_j} - Vk(\bar{x}_{s_j}), \\ j &= 2, \dots, n-1, j \neq j_F, \end{aligned} \quad (42)$$

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

$$\begin{aligned} 0 &= L\bar{x}_{i-1} + Vk(\bar{x}_{i+1}) - L\bar{x}_i - Vk(\bar{x}_i), \\ i &= 2, \dots, N-1, i \neq s_j, j = 1, \dots, n, \end{aligned} \quad (44)$$

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

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 section 2.

Steps 4 and 5 imply the solution of the algebraic equations and the substitution of the required solutions Y_j into the dynamic equations.

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

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

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

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

parameter	value
N	74
n_F	36
H_1	20 mol
H_N	20 mol
$H_i, i = 2, \dots, N - 1$	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

Table 1: Parameters of the distillation column model.

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: Positions and holdups of the aggregation stages of the reduced models.

The functions Y_j correspond to the functions ϕ_j in equation (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].

3.1.2 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 table 2. They are taken from Linhart and Skogestad [3]. The parameter sets for the models with 5 and 7 aggregation stages are “opti-

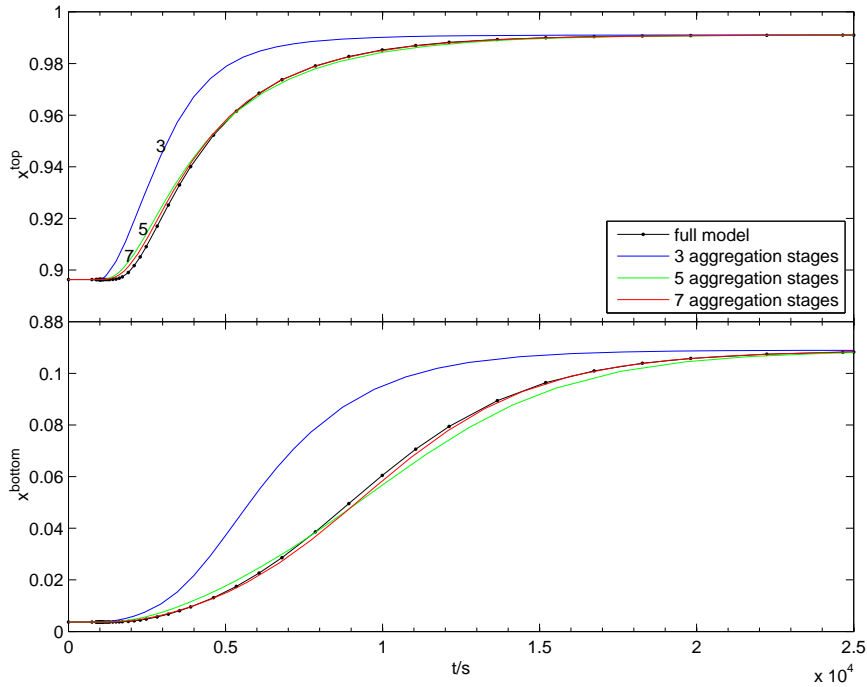


Figure 3: Distillation model top and bottom concentration responses to step change in feed concentration z_F from 0.45 to 0.55.

mized” 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 3 aggregation stages. If these restrictions are lifted, better approximation quality, especially for the model with 3 aggregation stages, can be expected.

It can be seen that especially the approximation quality of the reduced model with 7 aggregation stages is very good. This model has less than 10% of the states as the full model. The gain in computation time of the models has been shown in Linhart and Skogestad [3] to be in the same order of magnitude as the reduction in the number of states.

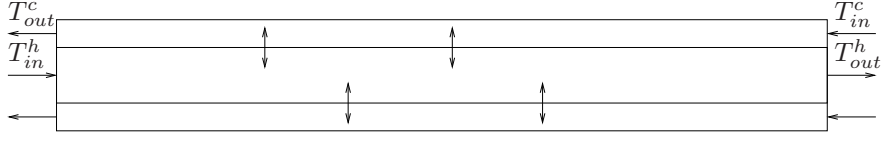


Figure 4: Schematic diagram of a tubular heat exchanger.

3.2 Heat exchanger

3.2.1 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 figure 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 equation (29) and read

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

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

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

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

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_{in}^h and T_{in}^c 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.

A straightforward choice of n aggregation points according to step 1 of the reduction procedure is an equal-distribution of the aggregation points over the

parameter	value
$A^c \rho^c$	31.4 kg/m
$A^h \rho^h$	39.3 kg/m
c_p^c	3 kJ/(kgK)
c_p^h	4 kJ/(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_{in}^c	320 K
T_{in}^h	360 K

Table 3: Parameters of the heat exchanger model.

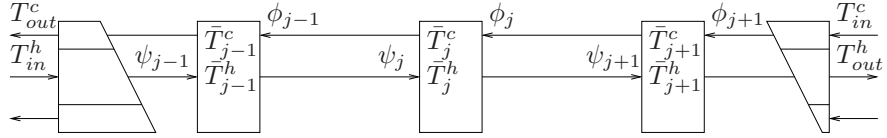


Figure 5: Schematic diagram of the reduced heat exchanger model.

whole domain with the end points placed at the ends of the heat exchanger:

$$s_j = \frac{j-1}{n-1}l, \quad j = 1, \dots, n. \quad (54)$$

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 equation (34) to be

$$C_j \frac{d\bar{T}_j^h}{dt} = -\frac{m^h}{A^h \rho^h l} (\bar{T}_j^h - \psi_j(\bar{T}_{j-1}^h, \bar{T}_j^c)), \quad (55)$$

$$C_j \frac{d\bar{T}_j^c}{dt} = -\frac{m^c}{A^c \rho^c l} (\bar{T}_j^c - \phi_j(\bar{T}_j^h, \bar{T}_{j+1}^c)), \quad (56)$$

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 (Kern [10]):

$$\begin{bmatrix} T_{out}^h \\ T_{out}^c \end{bmatrix} = \frac{1}{1 - R^c a} \begin{bmatrix} 1 - R^c & R^c(1 - a) \\ 1 - a & a(1 - R^c) \end{bmatrix} \begin{bmatrix} T_{in}^h \\ T_{in}^c \end{bmatrix}, \quad (57)$$

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

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

Expression (57) can be used in step 4 of the reduction procedure to calculate the steady-state functions ϕ and ψ :

$$\begin{bmatrix} \psi_j \\ \phi_{j-1} \end{bmatrix} = \frac{1}{1 - R^c a} \begin{bmatrix} 1 - R^c & R^c(1 - a) \\ 1 - a & a(1 - R^c) \end{bmatrix} \begin{bmatrix} \bar{T}_{j-1}^h \\ \bar{T}_j^c \end{bmatrix}. \quad (59)$$

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

3.2.2 Simulation study

To demonstrate the approximation quality of the reduced models, figures 6 to 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_{out}^h and T_{out}^c 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. $T_{out}^c = \bar{T}_1^c$ and $T_{out}^h = \bar{T}_n^h$. Figure 6 shows the responses to a step in the hot stream inlet temperature T_{in}^h from 360 K to 370 K. It can be seen that the response of the cold stream outlet temperature T_{out}^c , which is located at the same side as the hot stream inlet, is approximated very well by the reduced models.

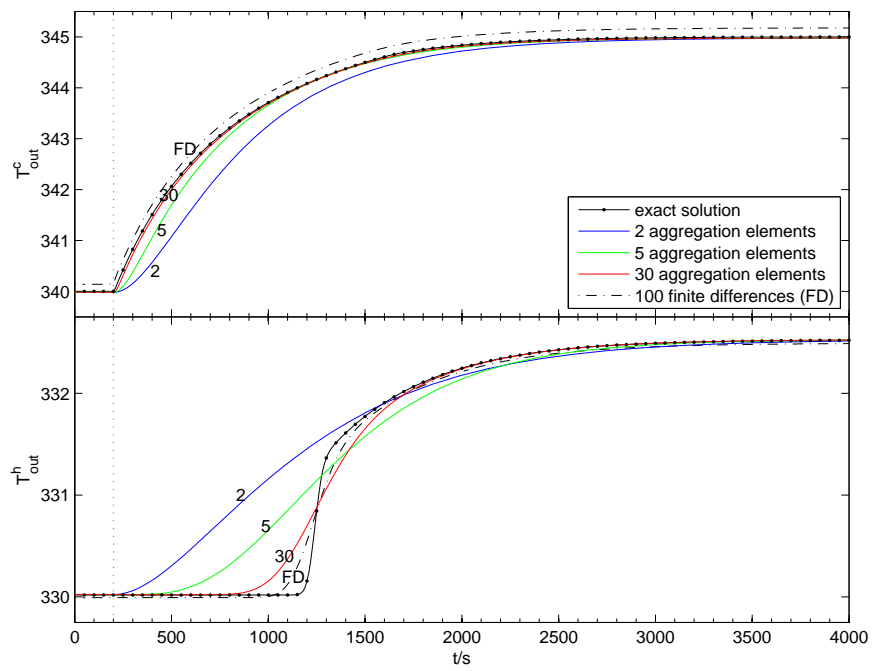


Figure 6: Heat exchanger outlet temperature responses of cold (upper plot) and hot (lower plot) streams to a step change in the hot inlet temperature T_{in}^h . The dotted vertical line marks the time when the step change is applied.

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 (Mathisen [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_{out}^h (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 . 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_{out}^h , 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_{in}^h 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_{out}^h (lower part of figure 8) is much better than in case of a step change. This is explicable by the diffusive character of

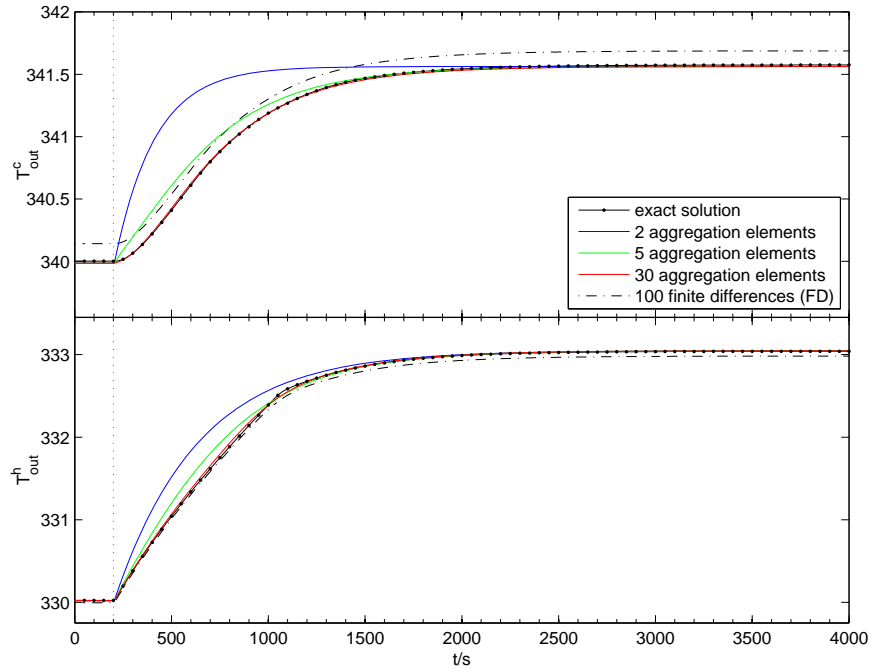


Figure 7: Heat exchanger outlet temperature responses of cold (upper plot) and hot (lower plot) streams to a step change in the hot stream flow rate v^h .

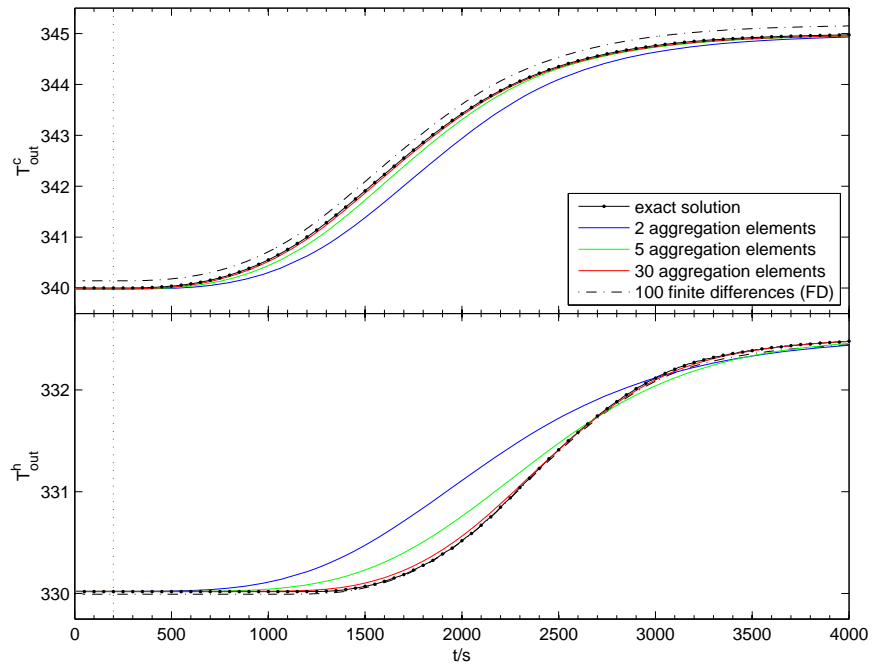


Figure 8: Heat exchanger outlet temperature responses of cold (upper plot) and hot (lower plot) streams to a slow change in the hot inlet temperature T_{in}^h .

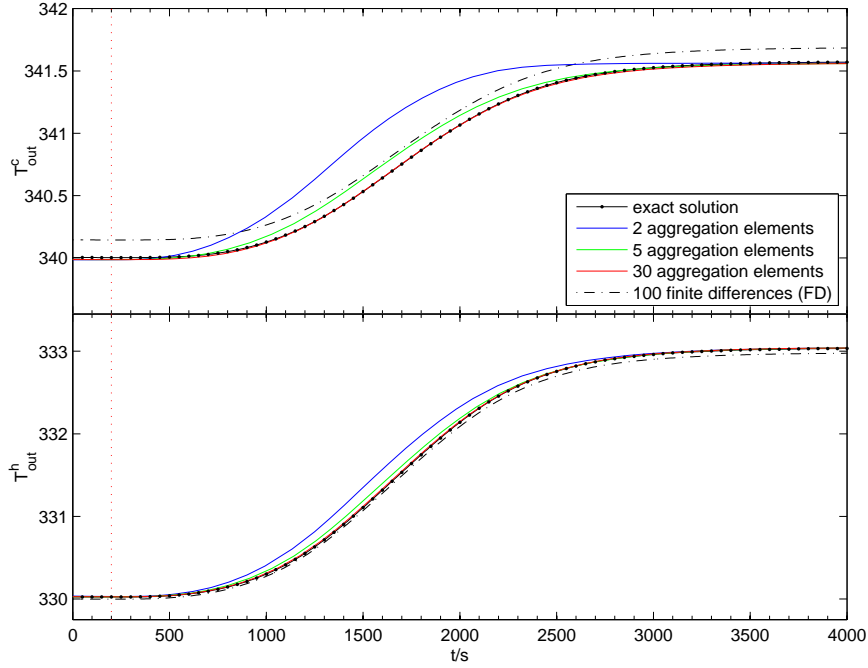


Figure 9: Heat exchanger outlet temperature responses of cold (upper plot) and hot (lower plot) streams to a slow change in the hot stream flow rate v^h .

the heat exchange between the counter-current flows, which is more dominant in this case, and is approximated better by the reduced models.

3.3 Fixed bed reactor

3.3.1 Model

As an example of a second-order continuous system, an adiabatic fixed-bed reactor model investigated by Liu and Jacobsen (2004) is considered (see figure 10):

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

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

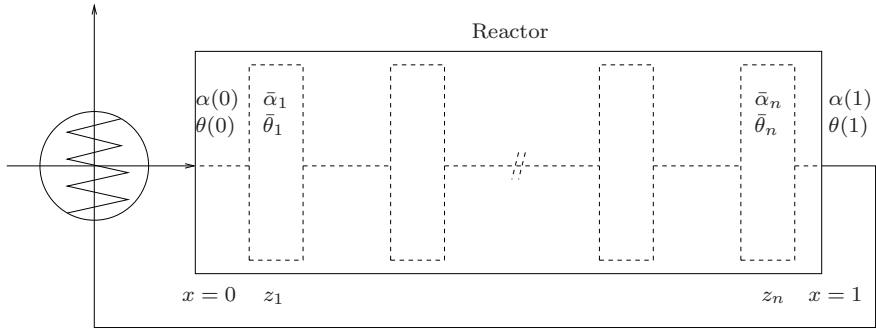


Figure 10: Schematic diagram of a fixed bed reactor with heat recycle. The structure of the reduced model is schematically shown using dashed lines.

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

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

The boundary conditions are

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

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

$$\frac{\partial \alpha}{\partial x} \Big|_{x=1} = 0, \quad (65)$$

$$\frac{\partial \theta}{\partial x} \Big|_{x=1} = 0. \quad (66)$$

The derivation of a reduced model for this system is shown in detail in section 2.5. For the purpose of demonstrating the approximation quality of the reduced models, models derived using steps 1 to 3 are sufficient. If a gain in computational performance is desired, the steady-state systems have to be eliminated from the model using steps 4 and 5. All aggregation points are chosen at locations z_j inside the domain of the partial differential equation, i.e. $0 < z_j < 1, j = 1, \dots, n$. 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

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

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

for the left side, and

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

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

for the right side of the system.

3.3.2 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 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 equation (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 5 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

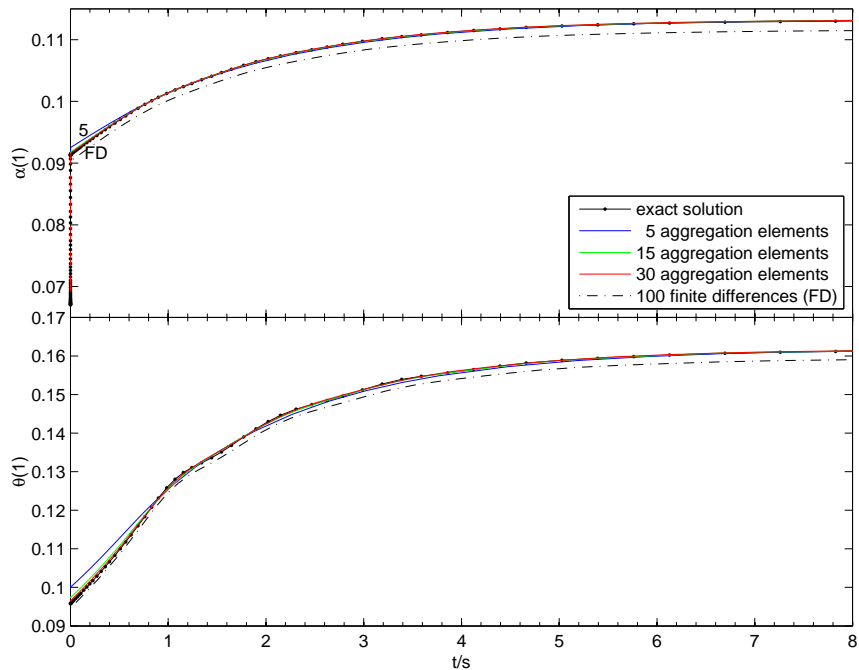


Figure 11: Responses of fixed-bed reactor conversion α and temperature θ at the right end to a change of Da from 0.05 to 0.07.

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 follow the fast movement despite its slow nature.

4 Discussion

4.1 Advantages and limitations of the aggregation method

The method presented in this paper is conceptually straightforward. The good approximation quality of the reduced models has been demonstrated in several

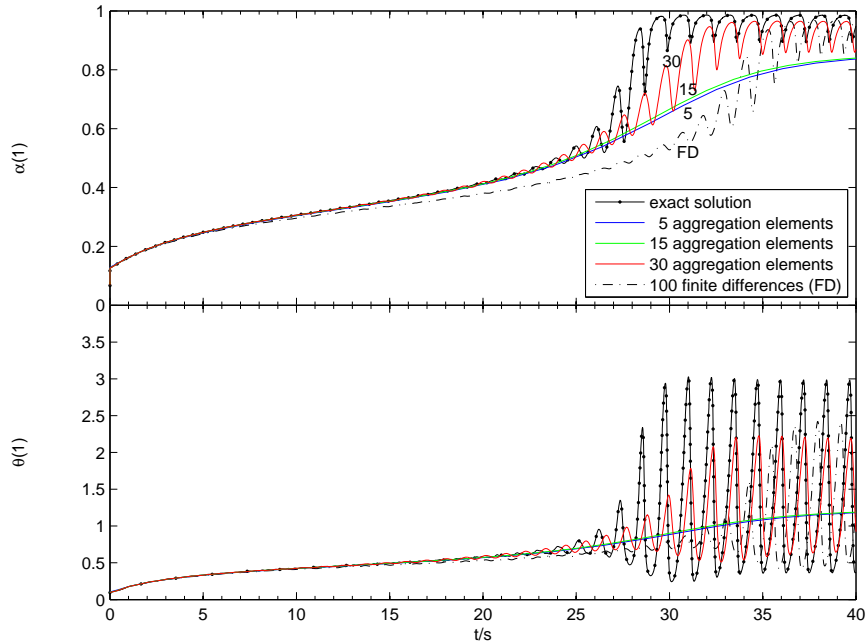


Figure 12: Responses of fixed-bed reactor conversion α and temperature θ at the right end simulated to a change of Da from 0.05 to 0.1.

examples. The approximation quality can even be improved by optimizing the location and capacities of the aggregation elements for the given problem.

The main limitation of the method lies in step 4 and 5 of the method. 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.

4.2 Relationship to singular perturbation models

In the following, the reduction procedure of this study is compared to the procedure to derive slow reduced models in singular perturbation theory (Kokotovic et al. [13], Lin and Segel [14]). This is done for discrete systems. Since the continuous procedure is derived using the discrete procedure, the argument applies to continuous systems as well.

4.2.1 Singular perturbation procedure

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

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

is transformed into the standard form of singular perturbations

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

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

where \mathbf{y} is a vector of “slow” variables, \mathbf{z} is a vector of “fast” variables, and $\varepsilon \ll 1$ 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 to choose 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 equations (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 apply the quasi-steady-state assumption $\varepsilon \rightarrow 0$ to equation (73), thus obtaining the reduced slow model

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

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

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 equations (75) can be solved explicitly for \mathbf{z} , then

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

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

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

4.2.2 Comparison with aggregation method

To compare the singular perturbation procedure with the aggregation method proposed in this study, it can first be observed that after step 3 of the aggregation method described in this study, the system is basically in the form of equations (74) and (75). Steps 4 and 5 correspond to the procedure in equations (76) and (77). The main difference of 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 trans-

formation 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 [1] derive their method for staged distillation columns, which ultimately leads to the reduction procedure for discrete systems described in this study, 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. This is discussed in detail in Linhart and Skogestad [3].

The crucial property for the success of the aggregated models is the perfect reproduction of the steady-state. This property the aggregated models have in common with slow singular perturbation models. Both their derivation and their dynamics can therefore be said to be related.

4.3 Comparison with other numerical discretization schemes

As mentioned before, the method introduced in this study can be seen as a discretization method for continuous systems. A good overview of these methods for equations of the type of equation (14) is given in Hundsdorfer and Verwer [2].

In the following, some qualitative similarities and differences will be discussed.

4.3.1 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 approaches infinity. This is due to the incorporation of steady-state information into the aggregated models, which is not the case in the other methods.

4.3.2 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 (Cho and Yoseph [5], Stewart et al. [6]). The efficiency of the method is based on the assumption that the solution profiles can be approximated by polynomials. In order 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.

5 Conclusions

A new 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 [1] 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 to 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.

6 Acknowledgment

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