A new method for deriving reduced models of one-dimensional distributed systems

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One-dimensional distributed systems:

- Staged/discrete (ODE/DAE systems)
- Continuous (PDE systems)

Examples of one-dimensional distributed systems in chemical engineering:

- Separation/Purification columns (staged or continuous)
- Tubular reactors (continuous)
- Heat exchangers (continuous)

Basic idea of model reduction method:

- Partition system into steady-state subsystems
- Connect steady-state subsystems by dynamic elements with large time-constants
- Solve steady-state subsystems off-line and substitute solutions

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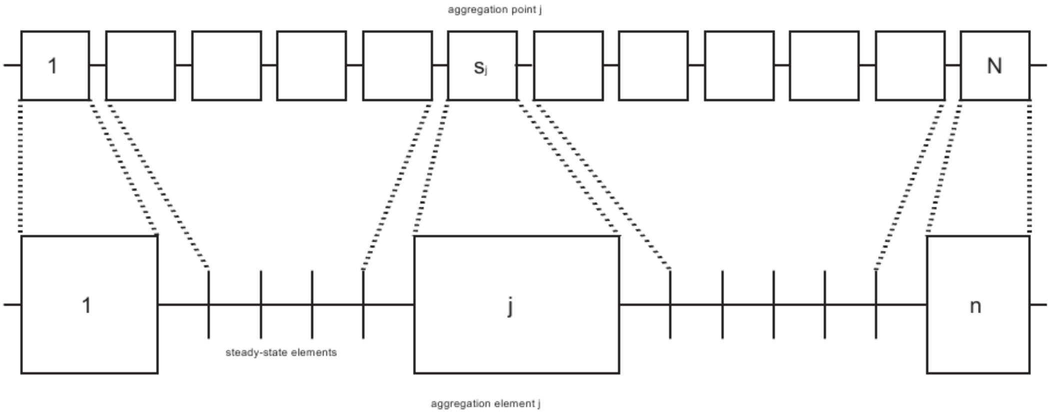
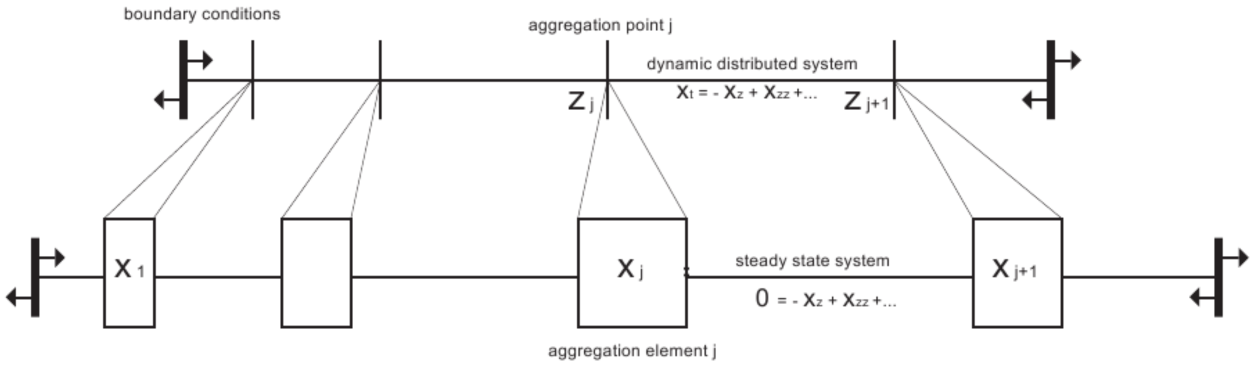
Discrete Systems:



Continuous systems:



Example: Distillation column

- 94 stages
- binary mixture
- SRK thermodynamics
- nonlinear hydraulic equations
- 286 differential equations
- 188 algebraic equations

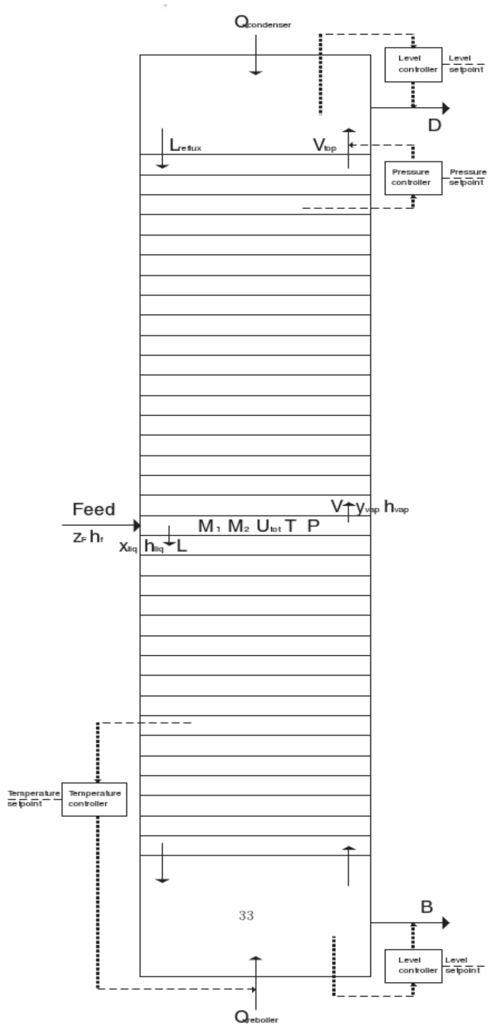
Reduction procedure:

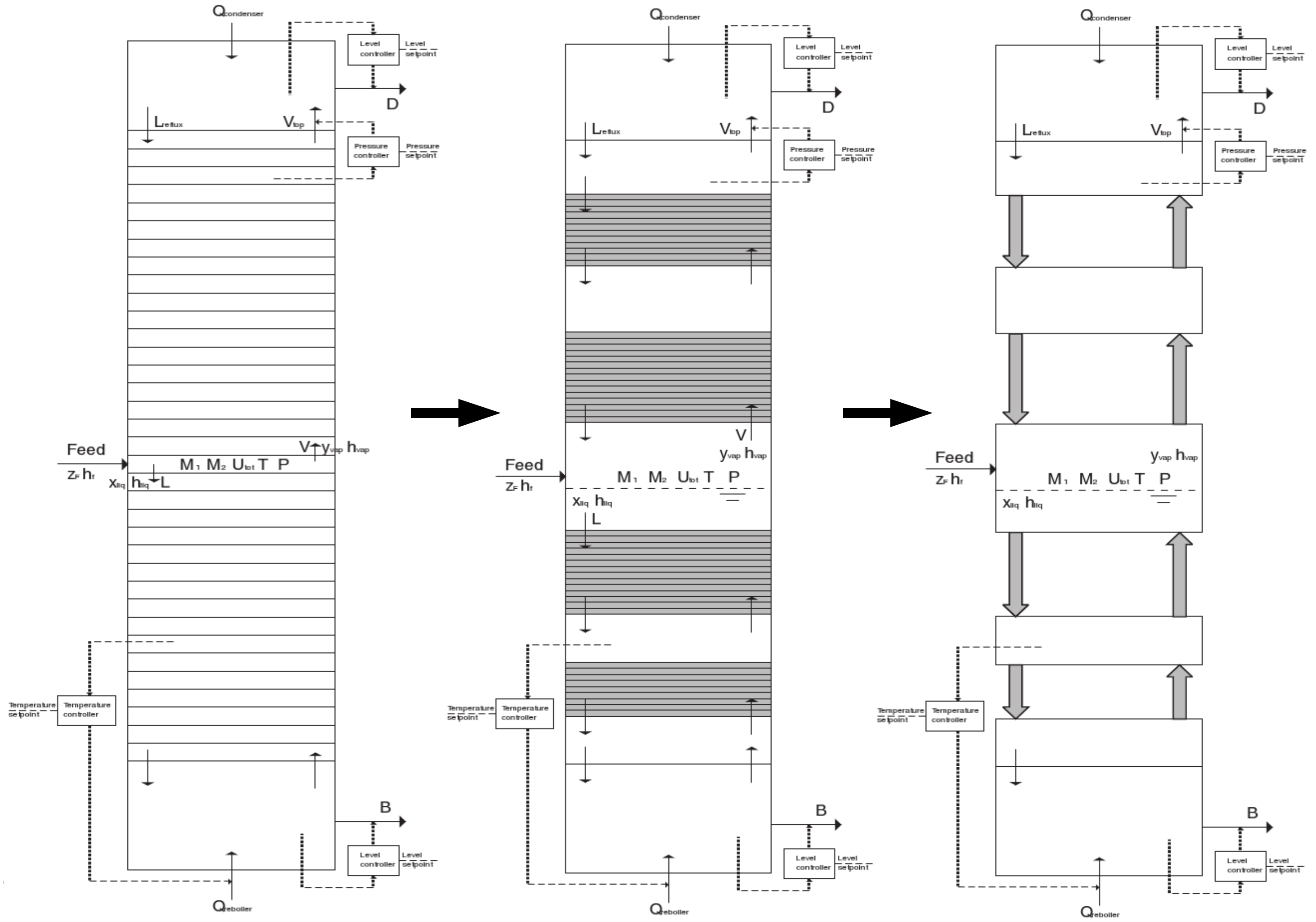
Step 1:

- select several dynamic stages and make their time-constant large
- model remaining stages as steady-state by setting their left-hand sides to 0.

Step 2:

- Eliminate resulting algebraic equations from model by off-line solution





Related work:

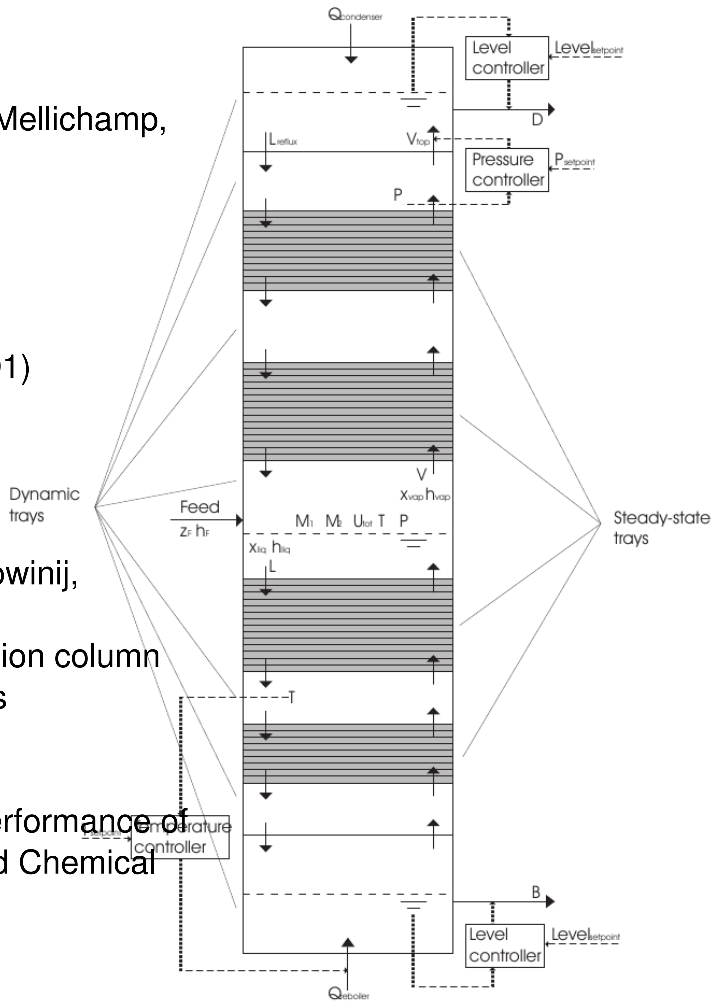
- Compartment models (Benallou, Seborg, & Mellichamp, 1986):
  - Definition of “compartments”
  - Yields structurally different models
  - Incorrect inverse responses

- Aggregated models (Levine & Rouchon, 1991)
  - Definition of compartments
  - Yields structurally identical models
  - Notion of “compartments” is imprecise

- Application of aggregated models (Bian, Khowinij, Henson, Belanger, & Megan, 2005)
  - Application of aggregation method to distillation column with simplified thermodynamics and hydraulics

Discussion:

Linhart, A., & Skogestad, S. Computational performance of aggregated distillation models. Computers and Chemical Engineering (2008), doi:10.1016/j.compchemeng.2008.09.014



Model stage equations

Full model:

$$\dot{M}_{i,k} = L_{i-1}^{out} x_{i-1,k} + V_i^{in} y_{i+1,k} - L_i^{out} x_{i,k} - V_{i-1}^{in} y_{i,k}, \; k = \{1,2\},$$
$$\dot{U}_i^{tot} = L_{i-1}^{out} h_{i-1}^{liq} + V_i^{in} h_{i+1}^{vap} - L_i^{out} h_i^{liq} - V_{i-1}^{in} h_i^{vap},$$

Reduced model: aggregation stages

$$H_j \dot{M}_{s_j,k} = L_{s_j-1}^{out} x_{s_j-1,k} + V_{s_j}^{in} y_{s_j+1,k} - L_{s_j}^{out} x_{s_j,k} - V_{s_j-1}^{in} y_{s_j,k},$$
$$k = \{1,2\},$$
$$H_j \dot{U}_{s_j}^{tot} = L_{s_j-1}^{out} h_{s_j-1}^{liq} + V_{s_j}^{in} h_{s_j+1}^{vap} - L_{s_j}^{out} h_{s_j}^{liq} - V_{s_j-1}^{in} h_{s_j}^{vap},$$

Reduced model: steady-state stages

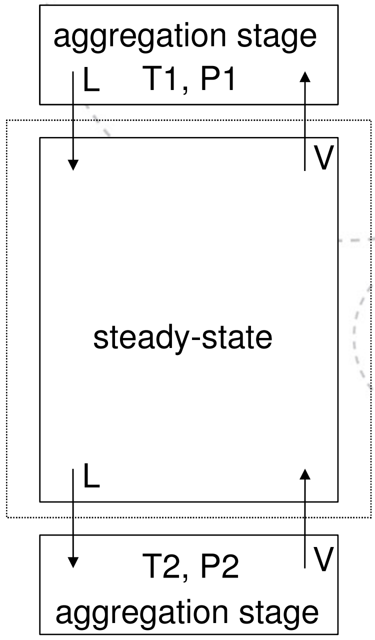
$$0 = L_{i-1}^{out} x_{i-1,k} + V_i^{in} y_{i+1,k} - L_i^{out} x_{i,k} - V_{i-1}^{in} y_{i,k}, \; k = \{1,2\},$$
$$0 = L_{i-1}^{out} h_{i-1}^{liq} + V_i^{in} h_{i+1}^{vap} - L_i^{out} h_i^{liq} - V_{i-1}^{in} h_i^{vap},$$
$$i = 1 \ldots N, i \neq s_j \; (j = 1 \ldots n).$$

Reduced model in DAE-form:

- Most of dynamic equations of full model are converted into algebraic
- Gives reduced dynamics
- No gain in computation speed
- Can be used for analysis of reduced dynamics, parameter estimation etc.

Elimination of steady-state tray equations:

- Equations for consecutive steady-state trays between two aggregation trays can be solved off-line in dependence of states of neighbouring aggregation trays
- Solutions depend on T, P and L of the upper aggregation stage, and T and P of the lower aggregation stage



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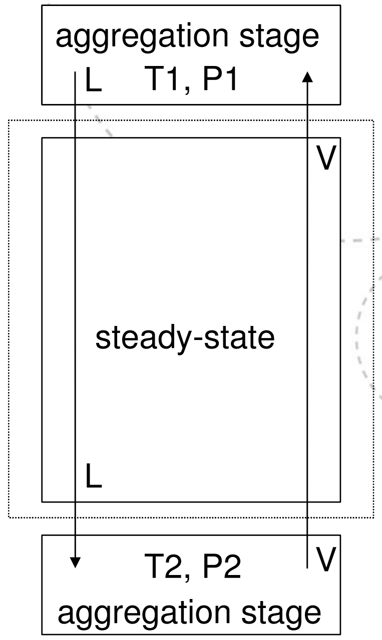
- Equations for consecutive steady-state trays between two aggregation trays can be solved off-line in dependence of states of neighbouring aggregation trays
- Solutions depend on T, P and L of the upper aggregation stage, and T and P of the lower aggregation stage
- As dependent variables, only T and P of the top-most steady-state stage is needed



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Representation of function values:

1) Tabulation and retrieval with suitable interpolation scheme

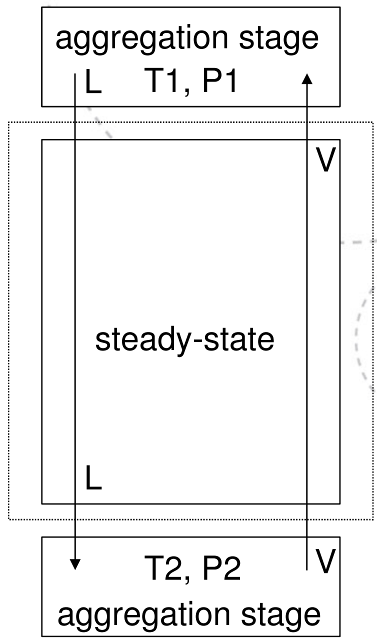
- Can handle the nonlinearities of the function
- Gives rise to very large tables
- Number of independent variables restricted

2) Polynomial approximation using linear regression

- Limited accuracy
- Number of independent variables restricted
- Gives rise to large terms

Substituting functions into reduced model:

$$
\begin{aligned}
H_j \dot{M}_{j,1} &= \underline{L}_j \underline{x}_j + \overline{V}_{j+1} \overline{y}_{j+1} - L_j^{out} x_{j,1} - \underline{V}_{j-1} y_{j,1}\,, \\
H_j \dot{M}_{j,2} &= \underline{L}_j (1 - \overline{x}_j) + \overline{V}_{j+1} (1 - \overline{y}_{j+1}) - L_j^{out} x_{j,2} \\
&\quad - \underline{V}_{j-1} y_{j,2}\,, \\
H_j \dot{U}_{s_j}^{tot} &= \underline{L}_j \underline{h}_j^{liq} + \overline{V}_{j+1} \overline{h}_{j+1}^{vap} - L_j^{out} h_j^{liq} - \\
&\quad \underline{V}_{j-1} h_{s_j}^{vap}\,.
\end{aligned}
$$



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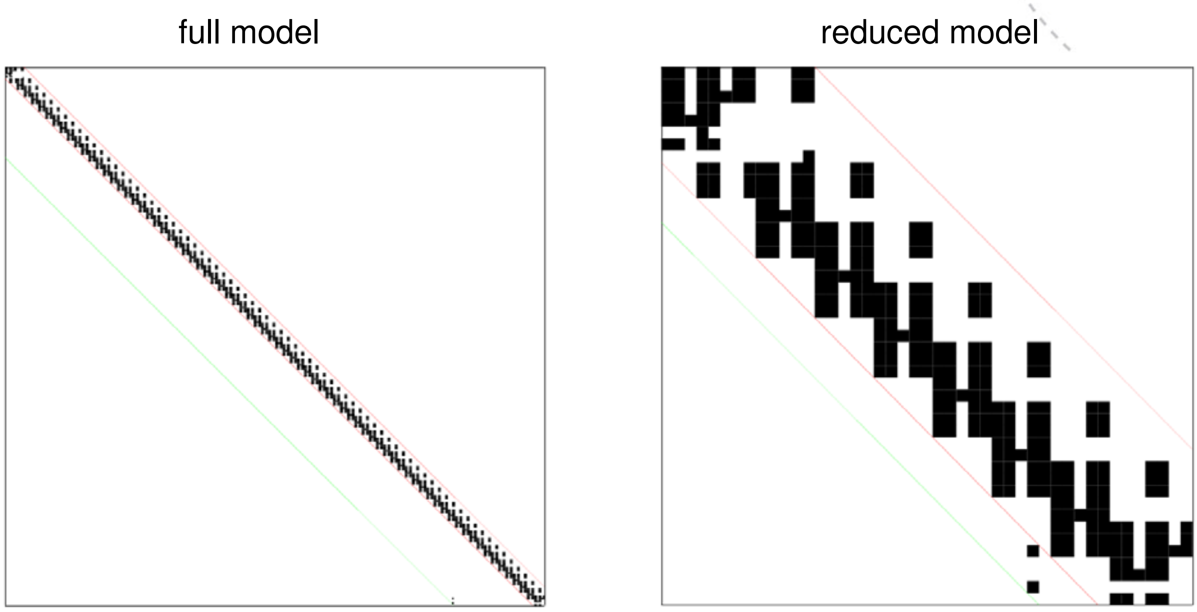
Jacobian structures

The reduced model has the same Jacobian structures as the full model.



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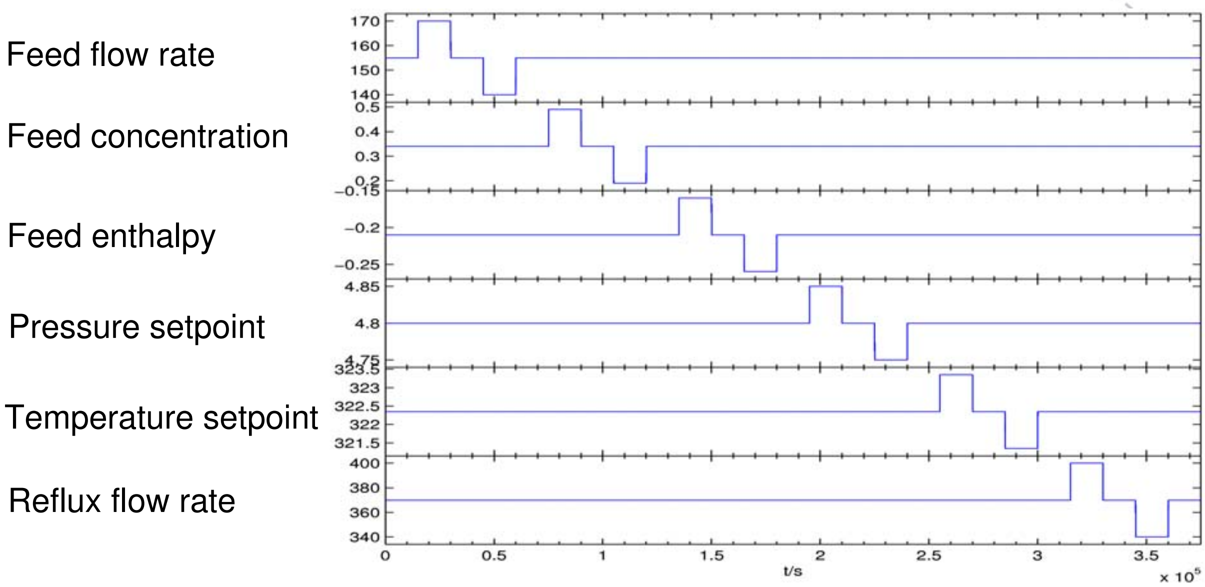
Performance test:

- Fast implementation of full and reduced model with DAE solver DASPK
- Test input trajectories:



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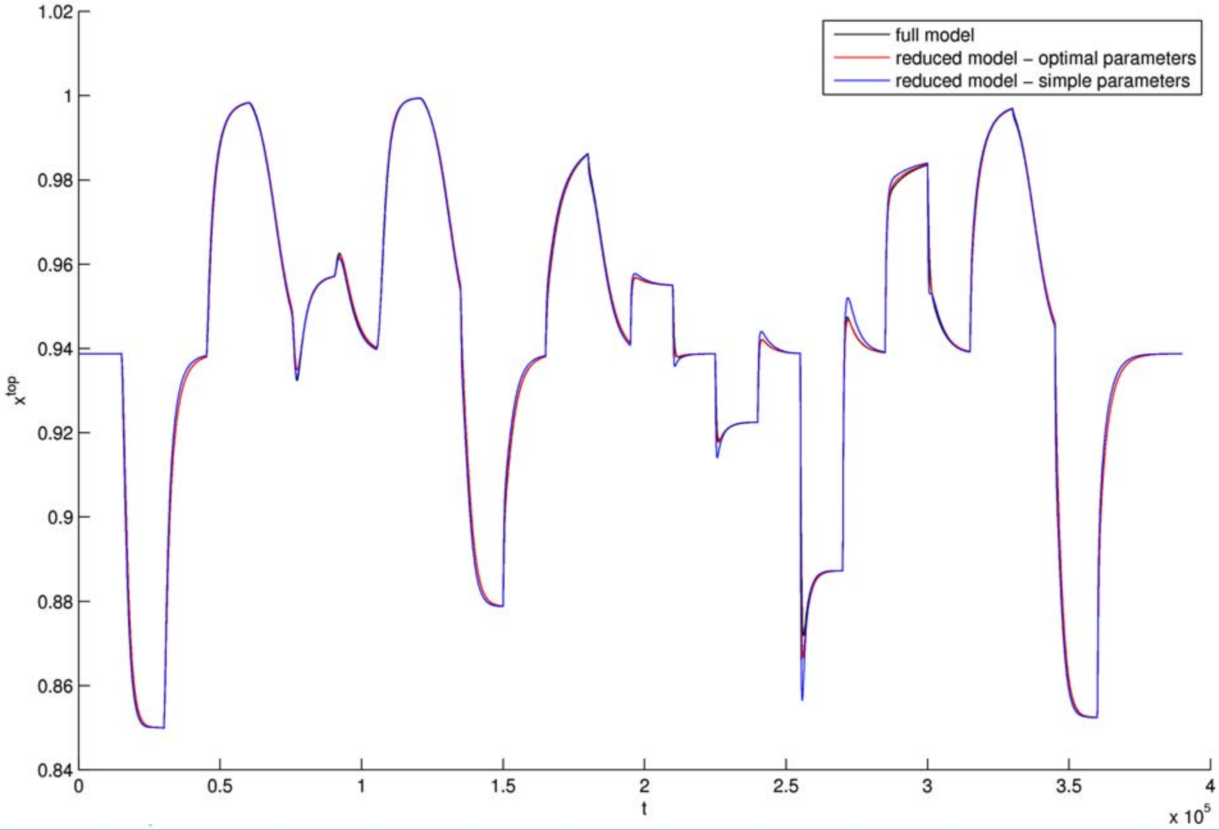
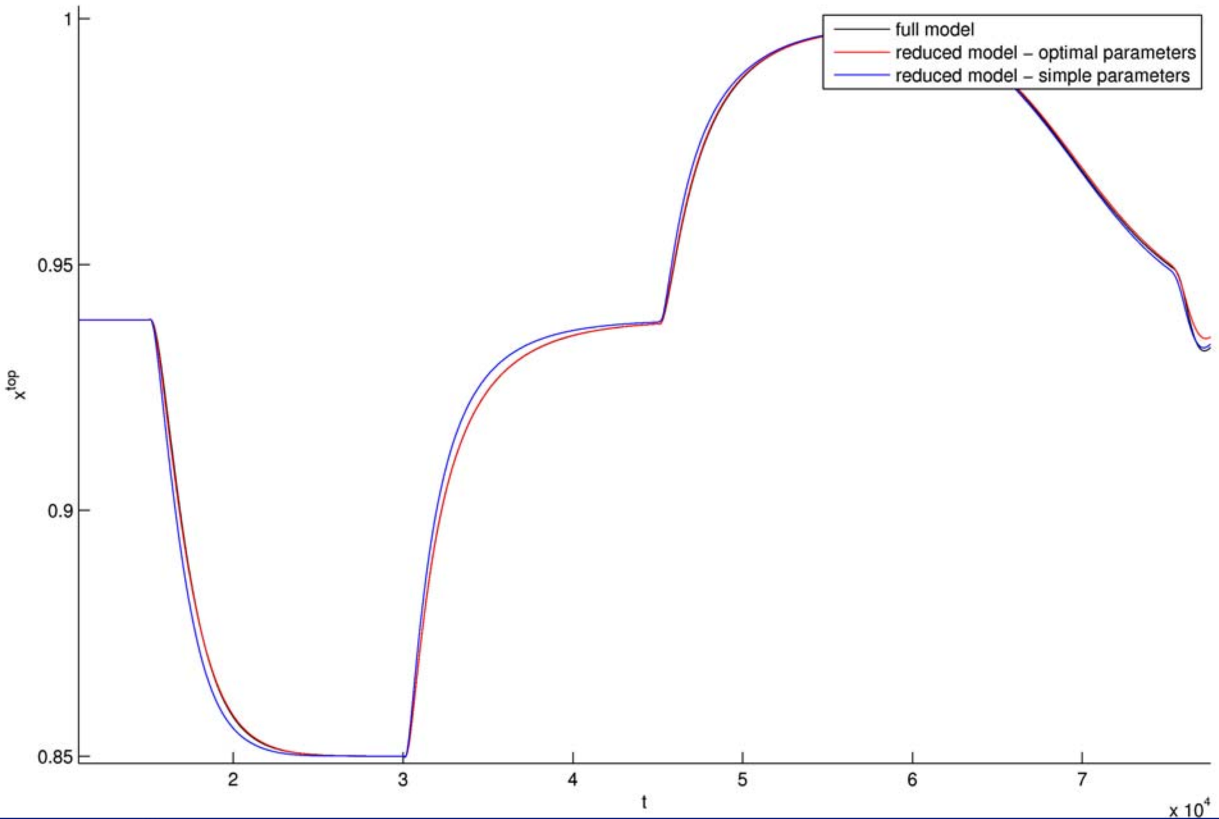
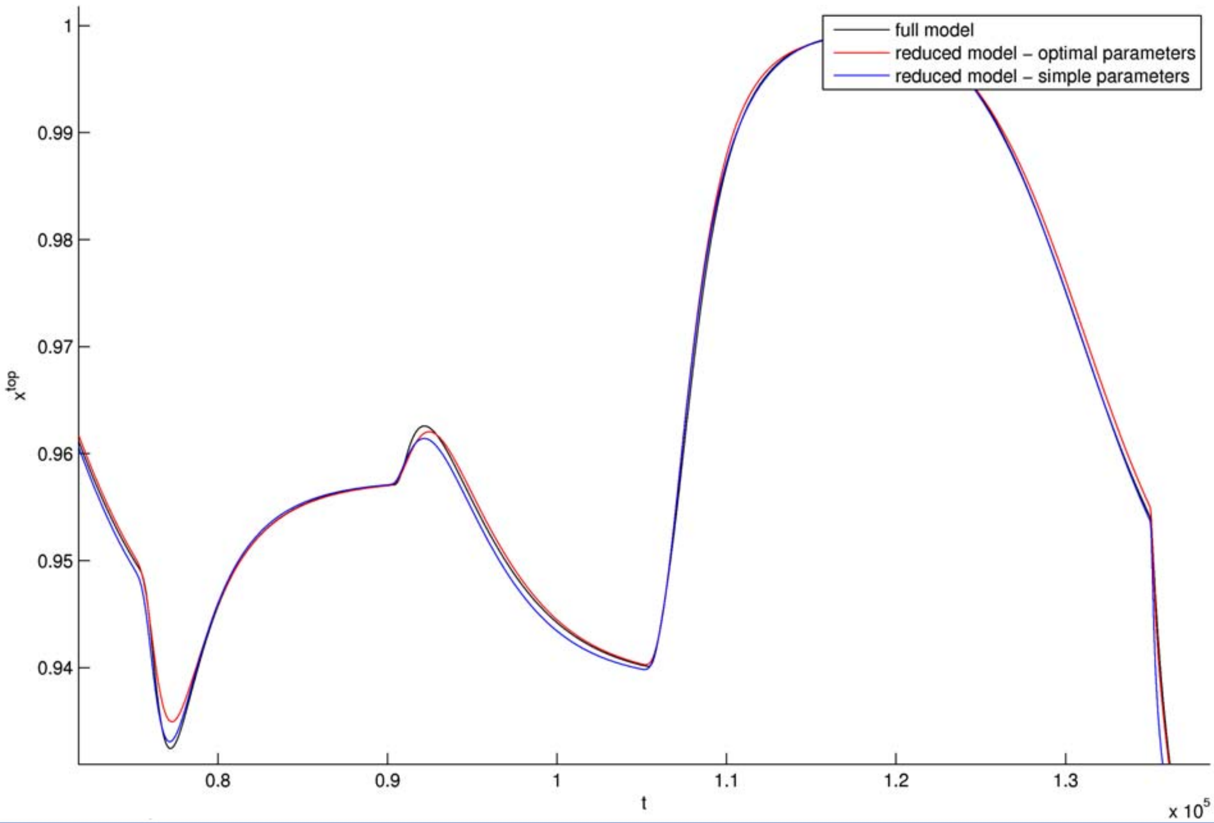
Response of top concentration to step changes in inputs



Feed flow 155 -> 170 -> 155 -> 140 -> 170



Feed concentration 0.34 -> 0.49 -> 0.34 -> 0.19 -> 0.34



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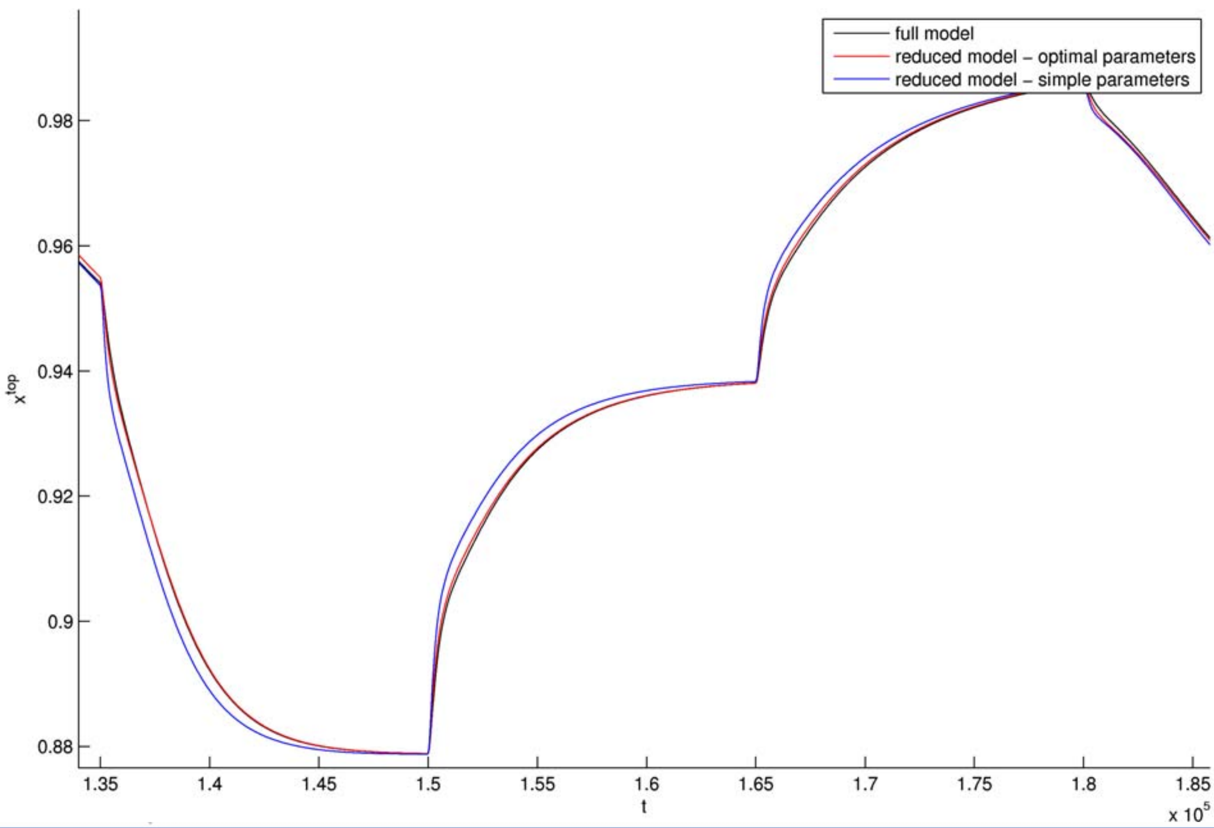
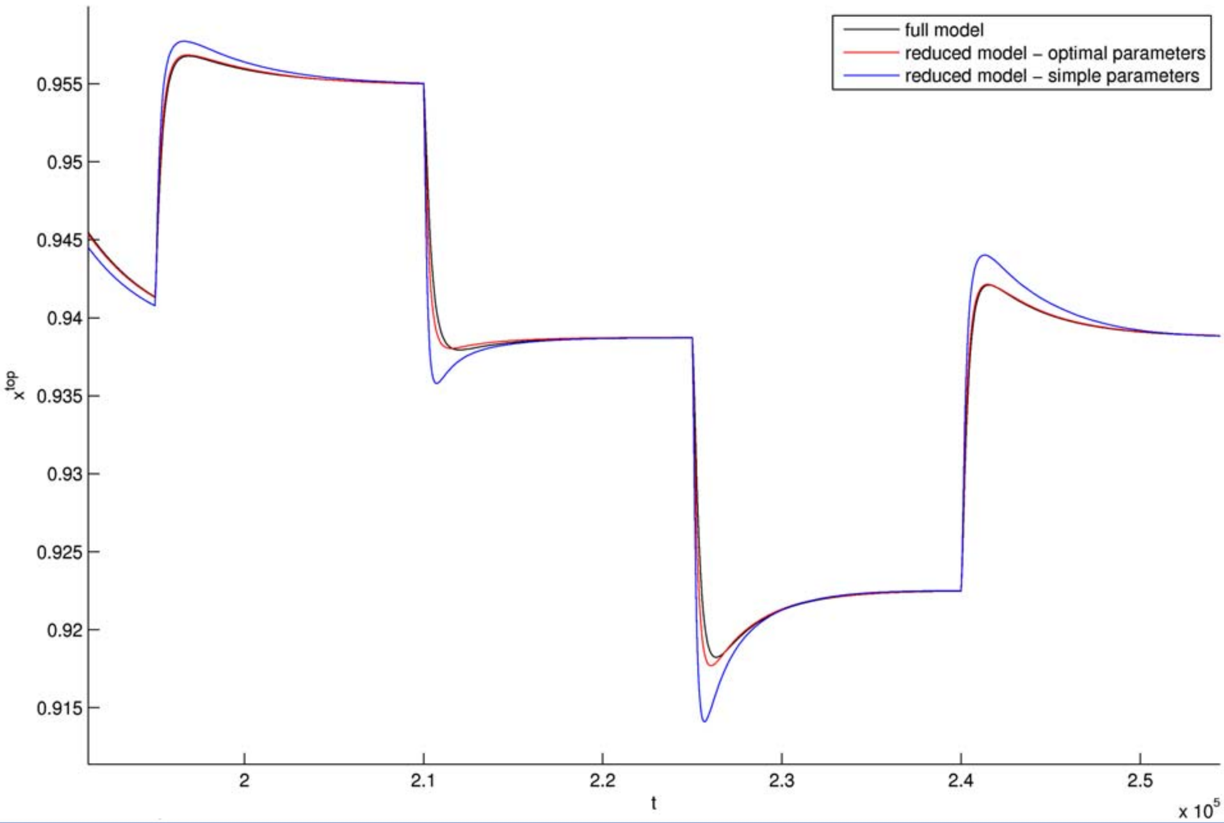
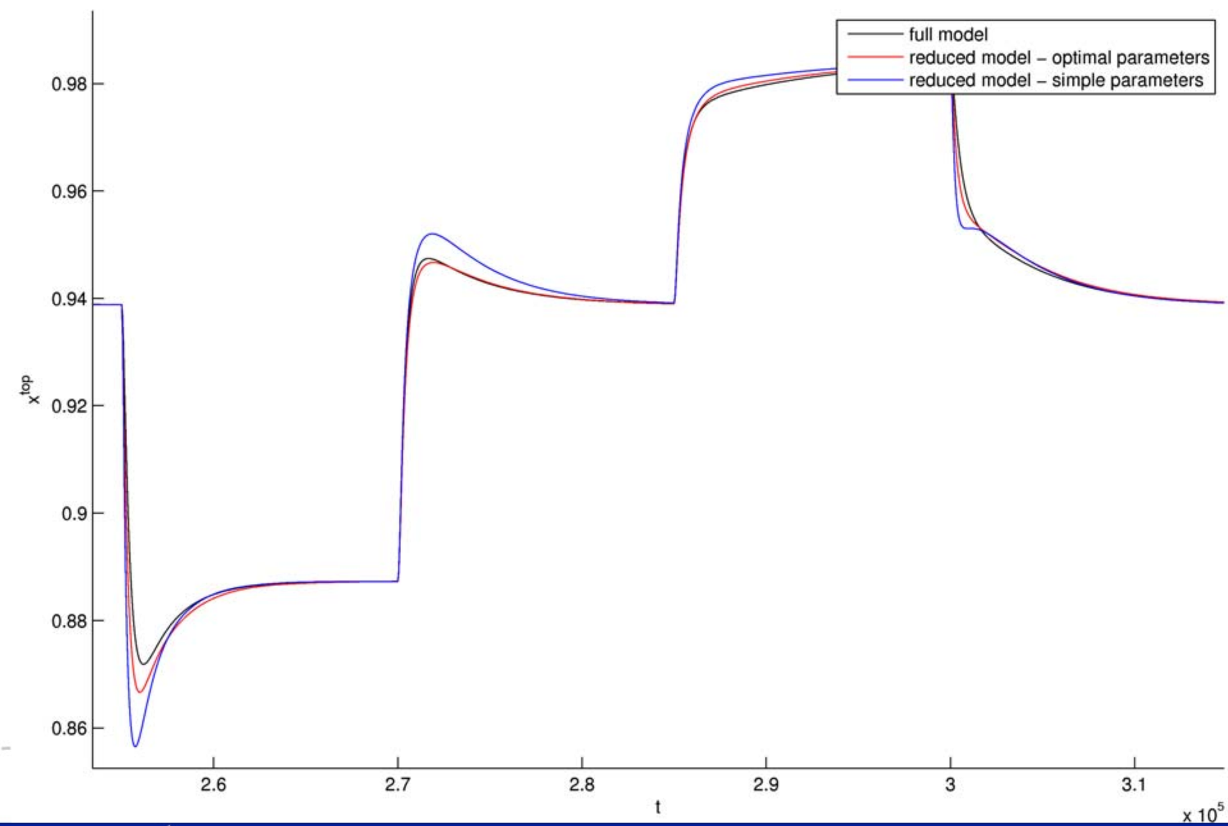


www.ntnu.no Andreas Linhart, A new method for deriving reduced models of one-dimensional distributed systems, REDUCIT, 4/5 Nov. 08

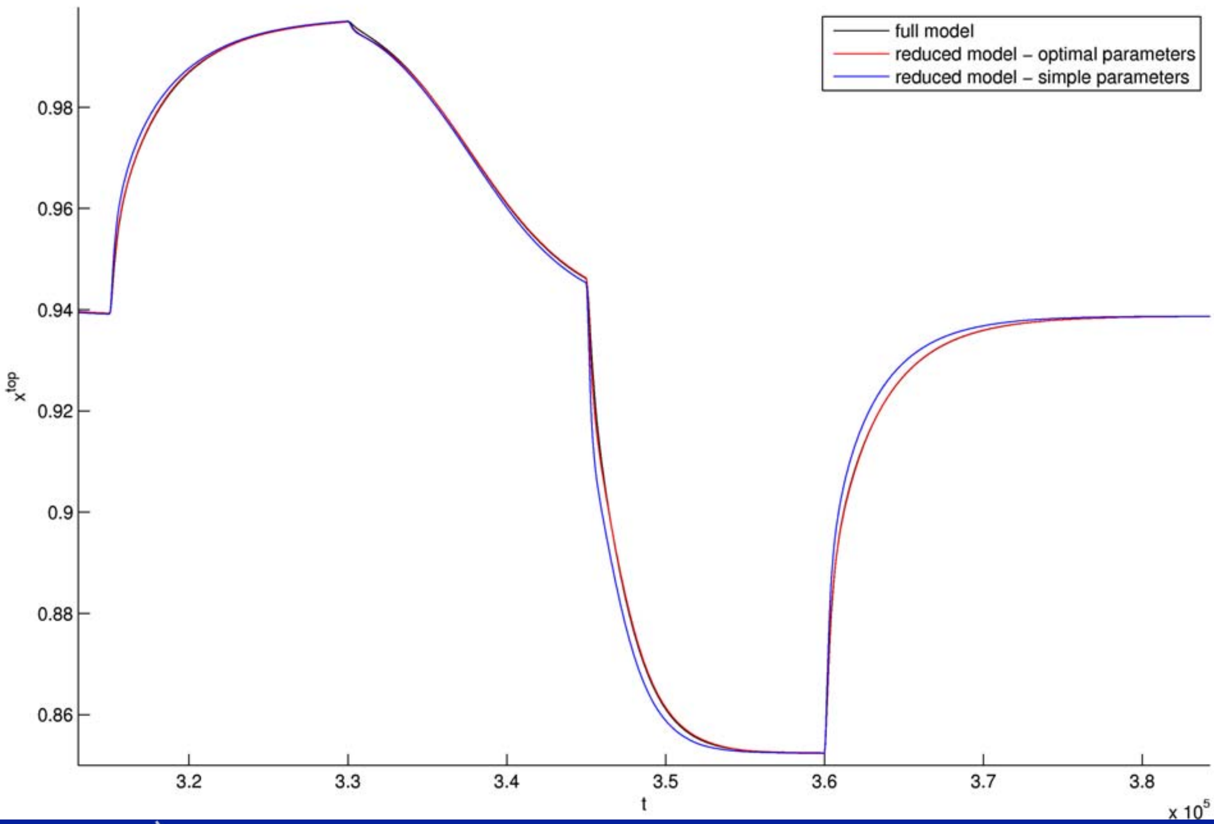
Pressure controller setpoint 4.8 -> 4.85 -> 4.8 -> 4.75 -> 4.8



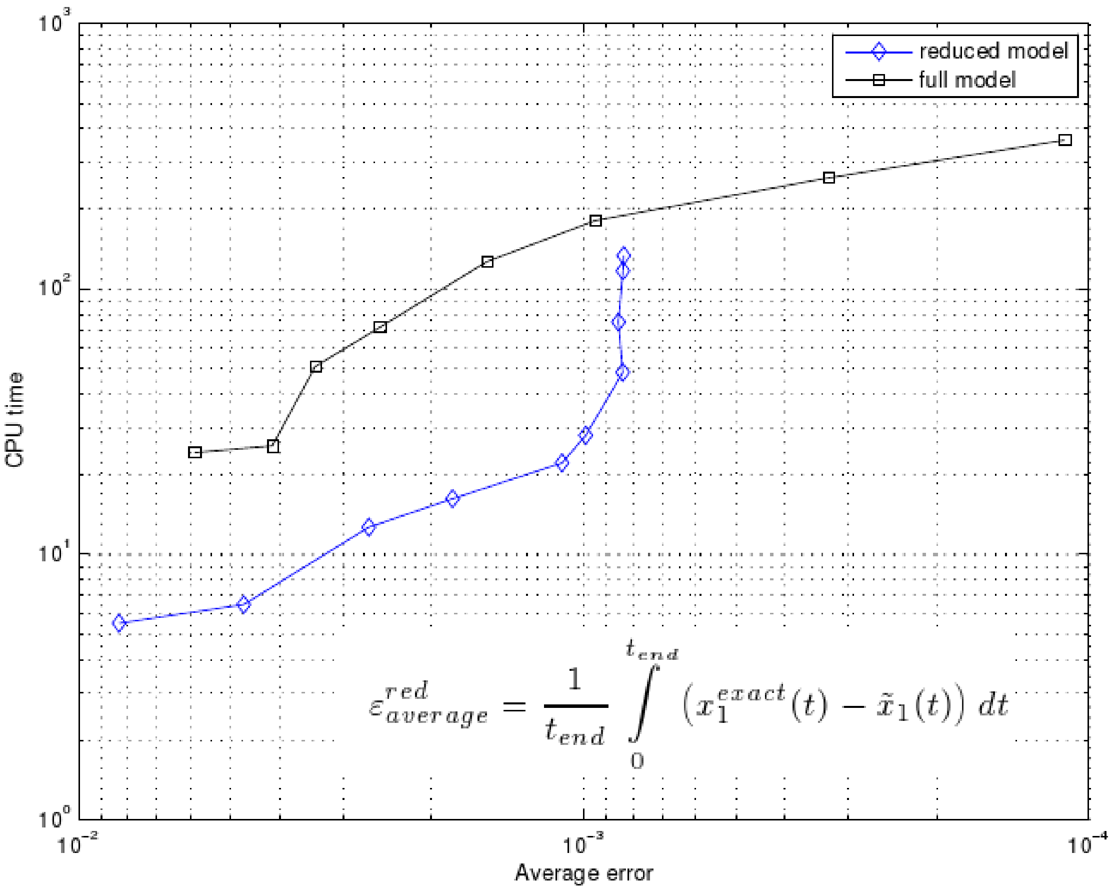
Temperature controller setpoint 322.35 -> 323.35 -> 322.35 -> 321.35 -> 322.35



Reflux flow rate 370 -> 400 -> 370 -> 340 -> 370

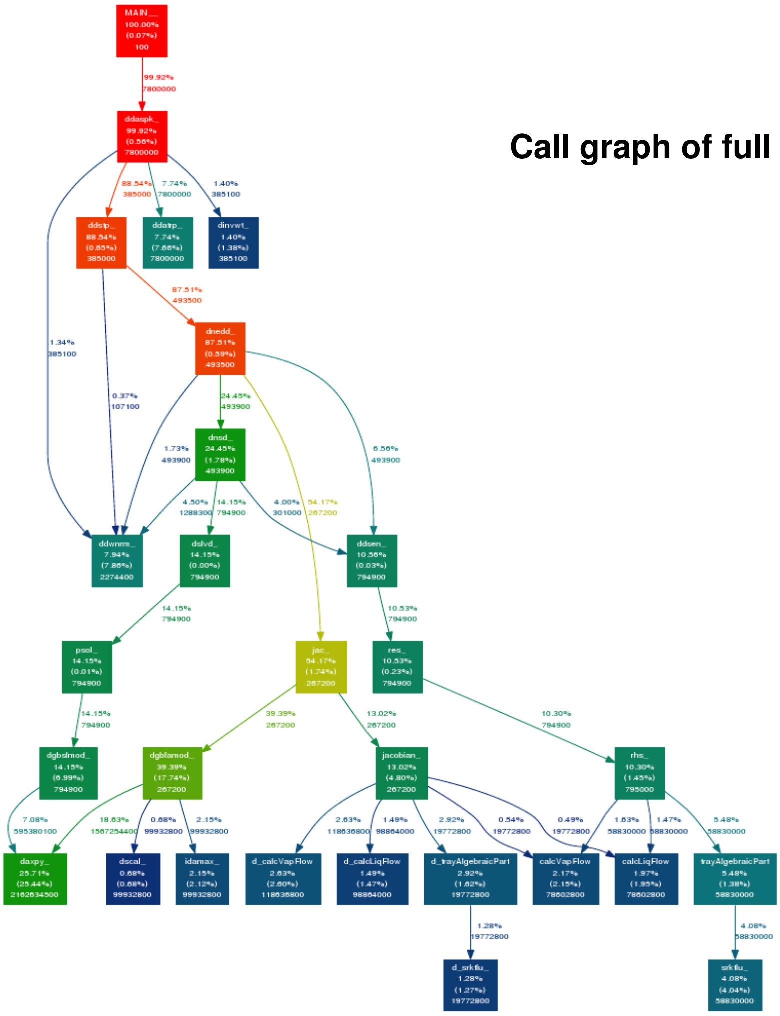


Performance comparison



$$\varepsilon^{red}_{average} = \frac{1}{t_{end}} \int_0^{t_{end}} \left(x_1^{exact}(t) - \tilde{x}_1(t) \right) dt$$

Call graph of full model simulation with DASPK



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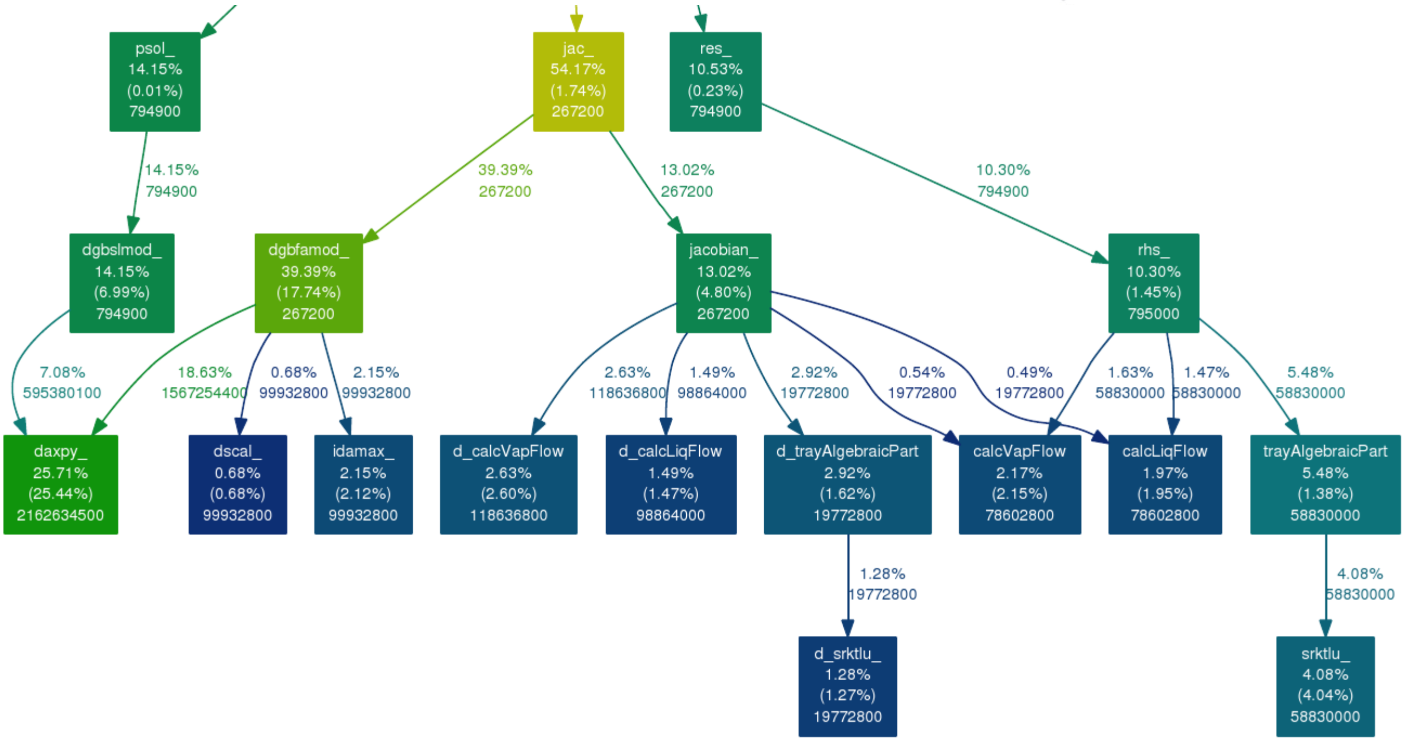
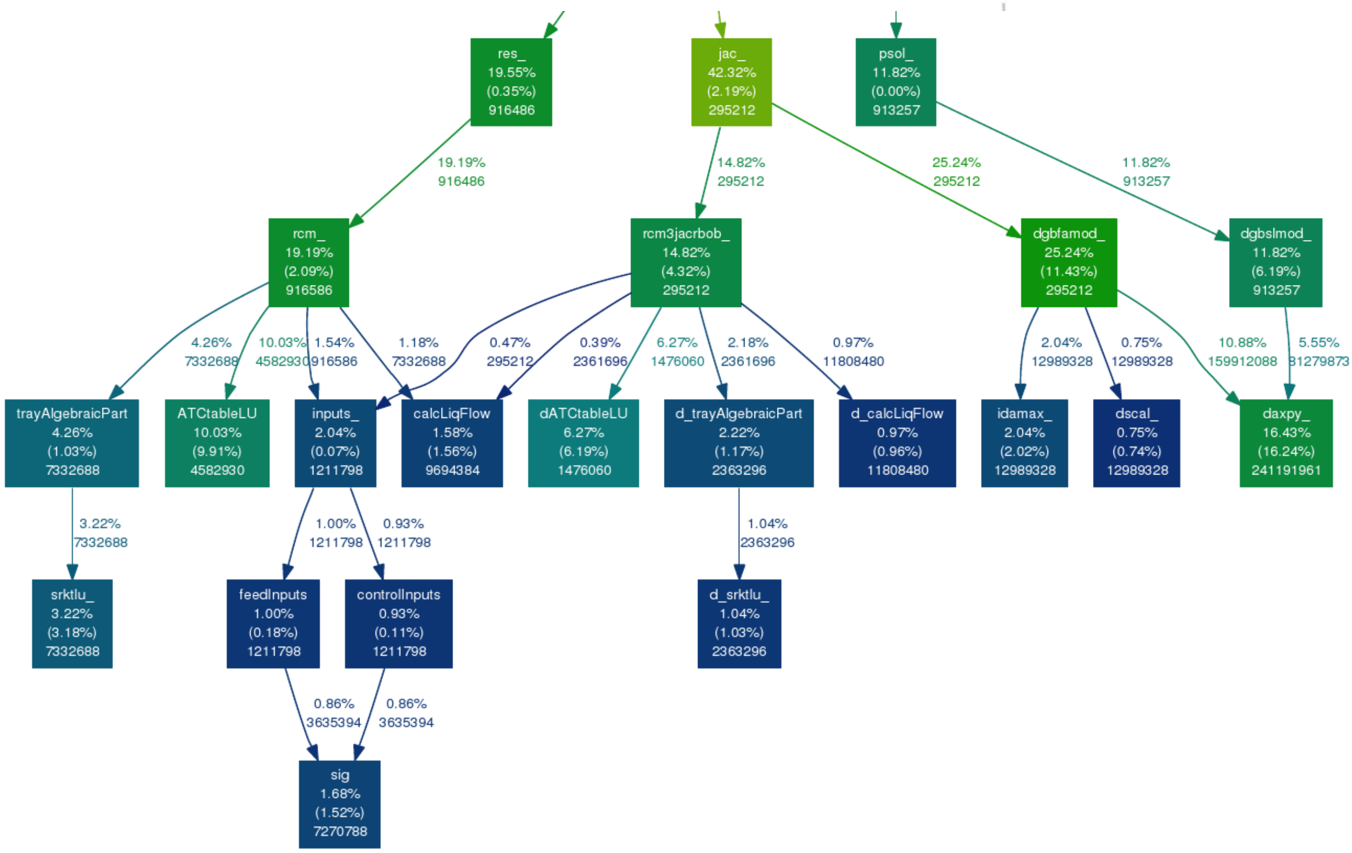
Call graph of full model simulation with DASPK



Call graph of reduced model simulation with DASPK



Discussion Distillation model:

- Simulation time proportional to number of stages
- Very good accuracy achievable
- Perfect steady-state agreement
- Bottleneck of procedure: functional approximation of steady-state stage solutions
  -if look-up tables are used, interpolation time limits model performance (here ~15%)
- Large number of degrees of freedom for selection of reduced model parameters

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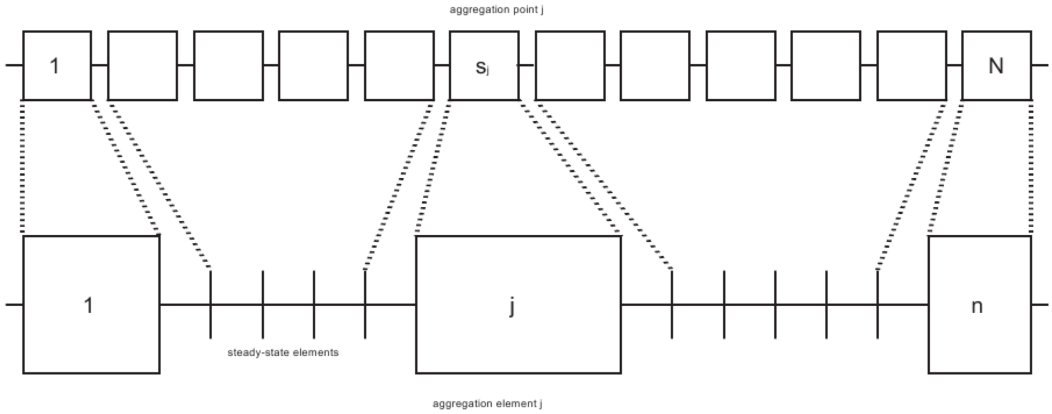
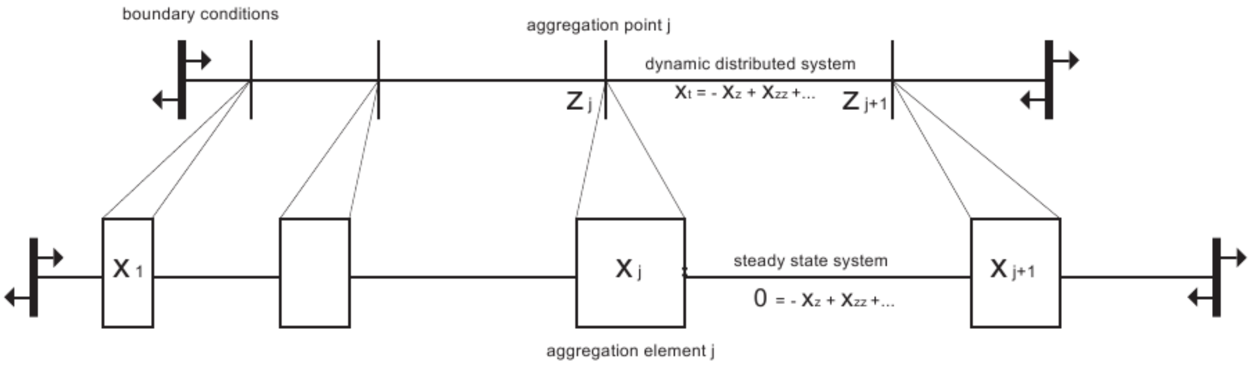
Discrete Systems:



Continuous systems:



Derivation of dynamic equations for continuously distributed systems:

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

Idea: apply model reduction method to discretised system, and let discretisation go to 0.

Example: Advection – Diffusion – Reaction equation:

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

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Finite difference approximation:

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

Multiply left-hand side of aggregation elements with large constant:

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

Set left-hand sides of steady-state systems to 0:

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

Use constants $H_j = N/n$

Rewrite equations with $\Delta z = 1/(N-1)$:

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

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

Consider limit to continuous case $\Delta z \rightarrow 0$:

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

Obtain left and right derivatives from solution of steady-state systems:

$$0 = -\alpha\frac{\partial x}{\partial z} + \beta\frac{\partial^2 x}{\partial z^2} + \gamma R(x) \qquad \begin{aligned} x(z_{j-1}) &= \bar{x}_{j-1}, \\ x(z_j) &= \bar{x}_j, \end{aligned}$$

Write solutions as functions of the dynamic variables:

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

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

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

Insert in aggregation element equations to obtain reduced model:

$$\frac{1}{n}\frac{d\bar{x}_j}{dt} = \beta\left(\phi_j(\bar{x}_j, \bar{x}_{j+1}) - \psi_{j+1}(\bar{x}_{j-1}, \bar{x}_j)\right)$$

$$j = 1, ..., n.$$

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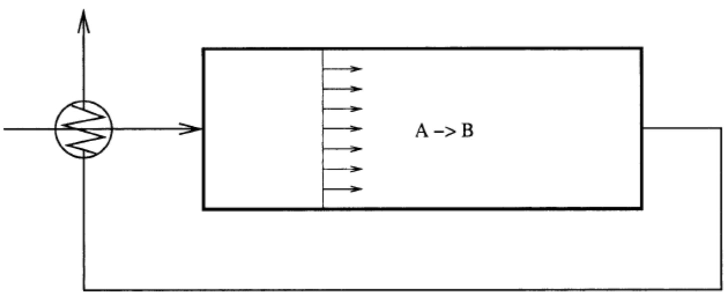
Example: Adiabatic fixed-bed reactor with heat recycle
(Liu and Jacobsen, 2004)



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

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

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

Boundary conditions

$$\alpha(0,t) = \left.\frac{1}{Pe_m}\frac{\partial \alpha}{\partial x}\right|_{x=0},$$

$$\theta(0,t) = f\theta(1,t) + \left.\frac{1}{Pe_h}\frac{\partial \theta}{\partial x}\right|_{x=0},$$

$$\left.\frac{\partial \alpha}{\partial x}\right|_{x=1} = 0,$$

$$\left.\frac{\partial \theta}{\partial x}\right|_{x=1} = 0.$$

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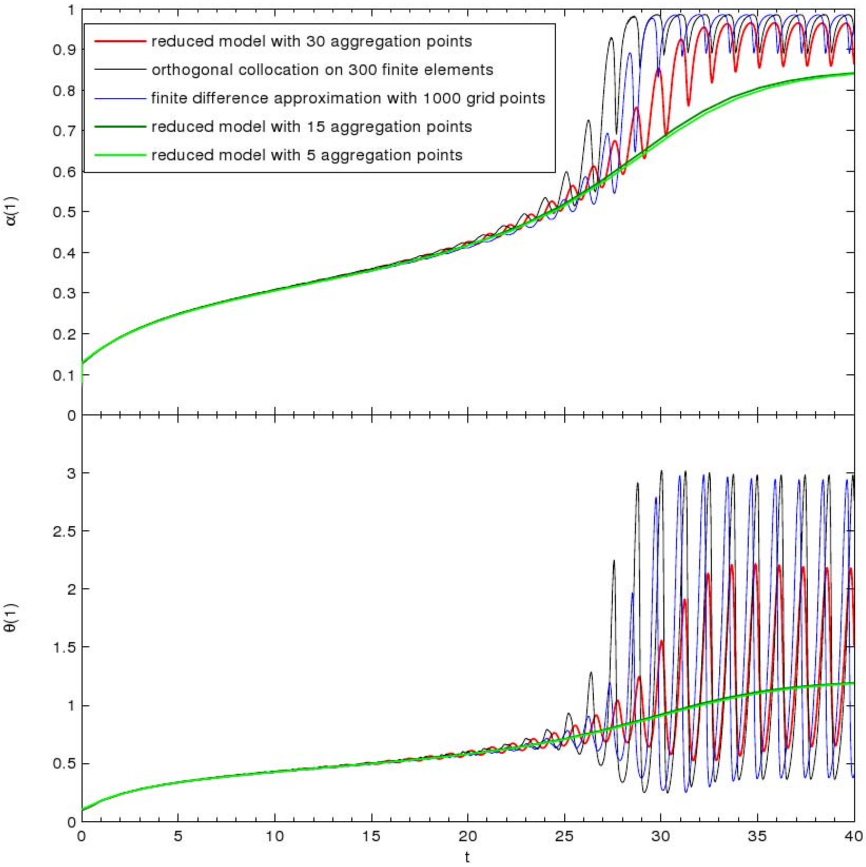
Limit cycle oscillations at change Da from 0.05 to Da=0.1:



- The reduced model reproduces oscillations for more than 15 aggregation elements
- Transient behaviour before oscillations is reproduced already with 5 aggregation elements

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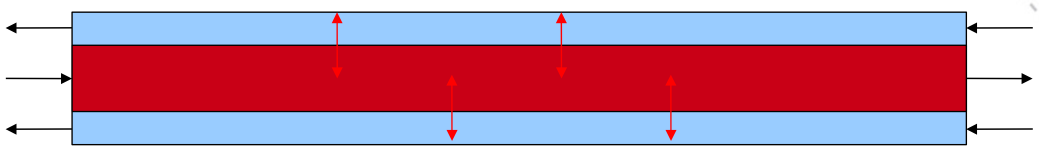
Example: Heat Exchanger



$$
\begin{aligned}
\frac{\partial T^h}{\partial t} &= -v^h \frac{\partial T^h}{\partial z} - \frac{Up}{A^h \rho^h c_p^h}(T^h - T^c), \\
\frac{\partial T^c}{\partial t} &= v^c \frac{\partial T^c}{\partial z} + \frac{Up}{A^c \rho^c c_p^c}(T^h - T^c), \; 0 < z < l, \\
T^h(t,0) &= T^h_{in}, \\
T^c(t,l) &= T^c_{in},
\end{aligned}
$$

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Reduced model:

Equations for dynamic element j:

$$C_j \frac{d\bar{T}_j^h}{dt} = -\frac{v^h}{l}(\bar{T}_j^h - \psi_j(\bar{T}_{j-1}^h, \bar{T}_j^c)),$$
$$C_j \frac{d\bar{T}_j^c}{dt} = -\frac{v^c}{l}(\bar{T}_j^c - \phi_j(\bar{T}_j^h, \bar{T}_{j+1}^c)),$$

Analytic solutions of steady-state subsystems:

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

$$a = exp(-N_{TU}^c(1 - R^c)), \quad R^c = \frac{m^c c_p^c}{m^h c_p^h}$$

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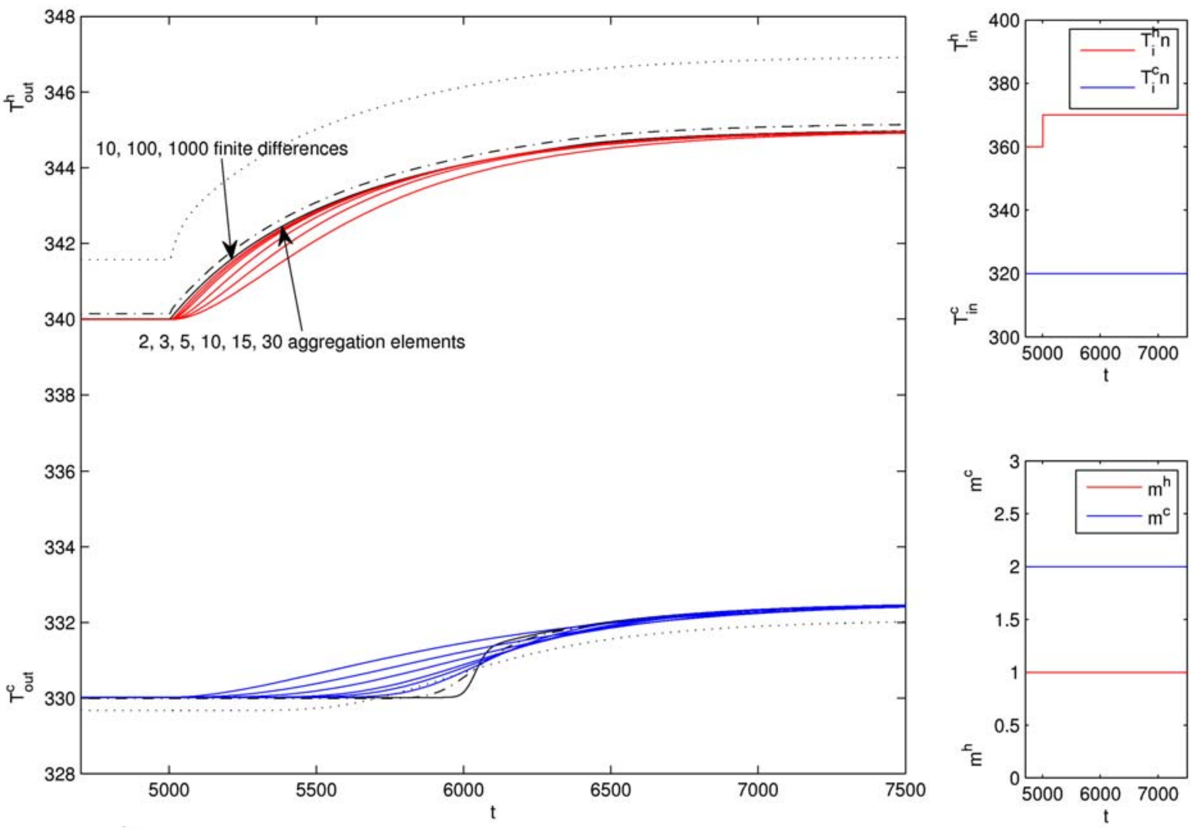
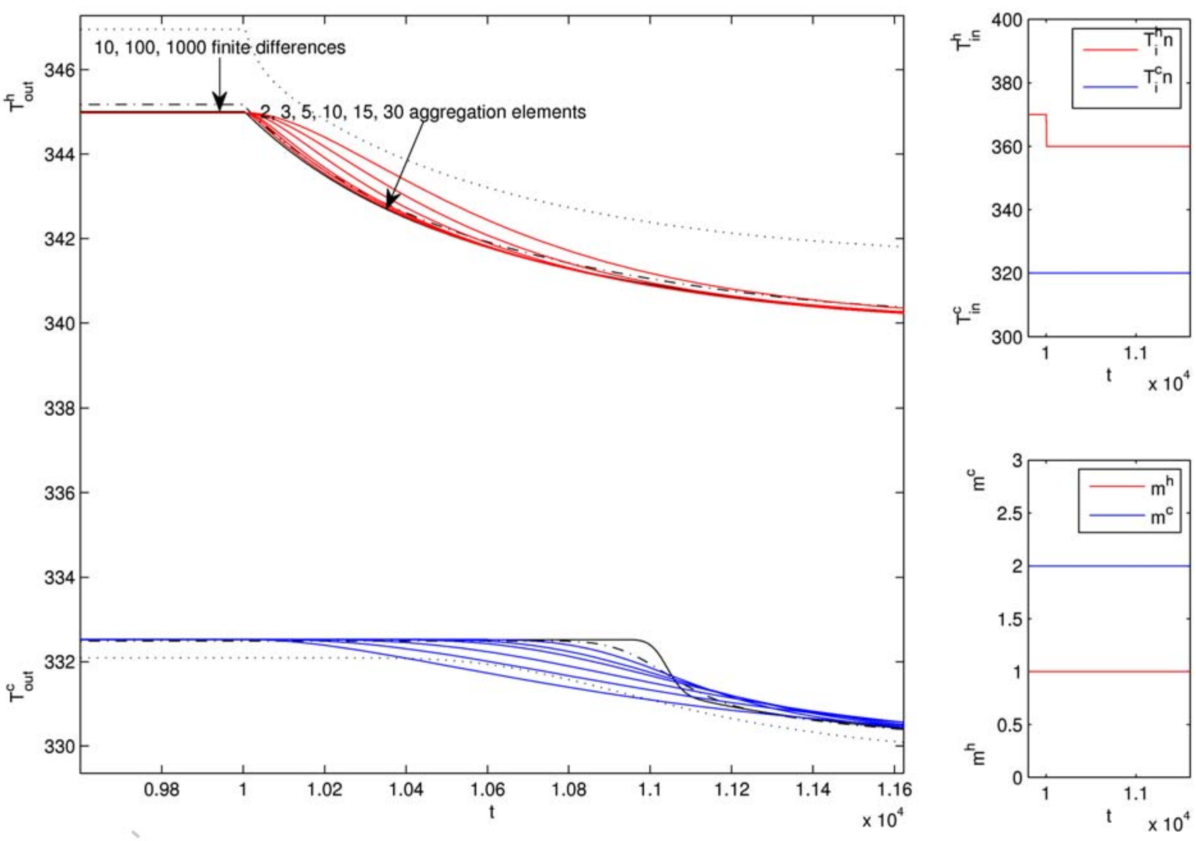
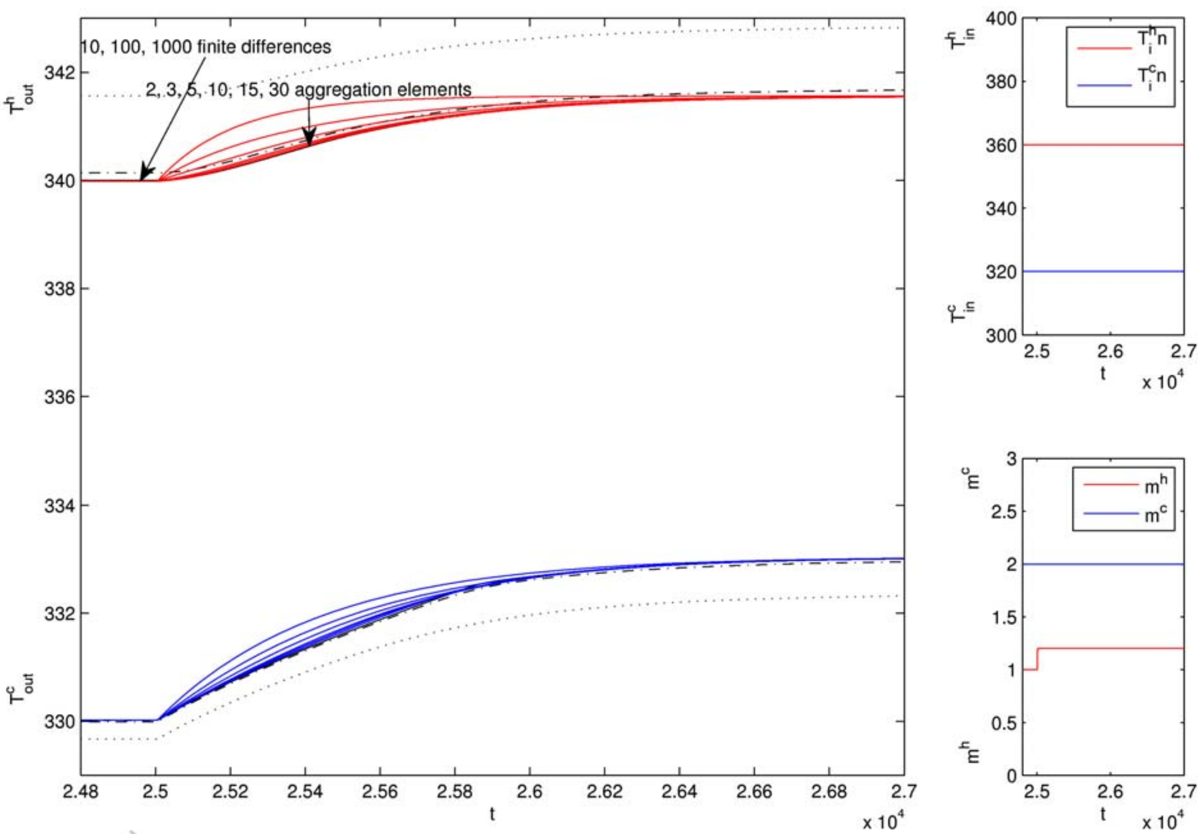
Response of hot and cold outputs to step change in hot inflow temperature



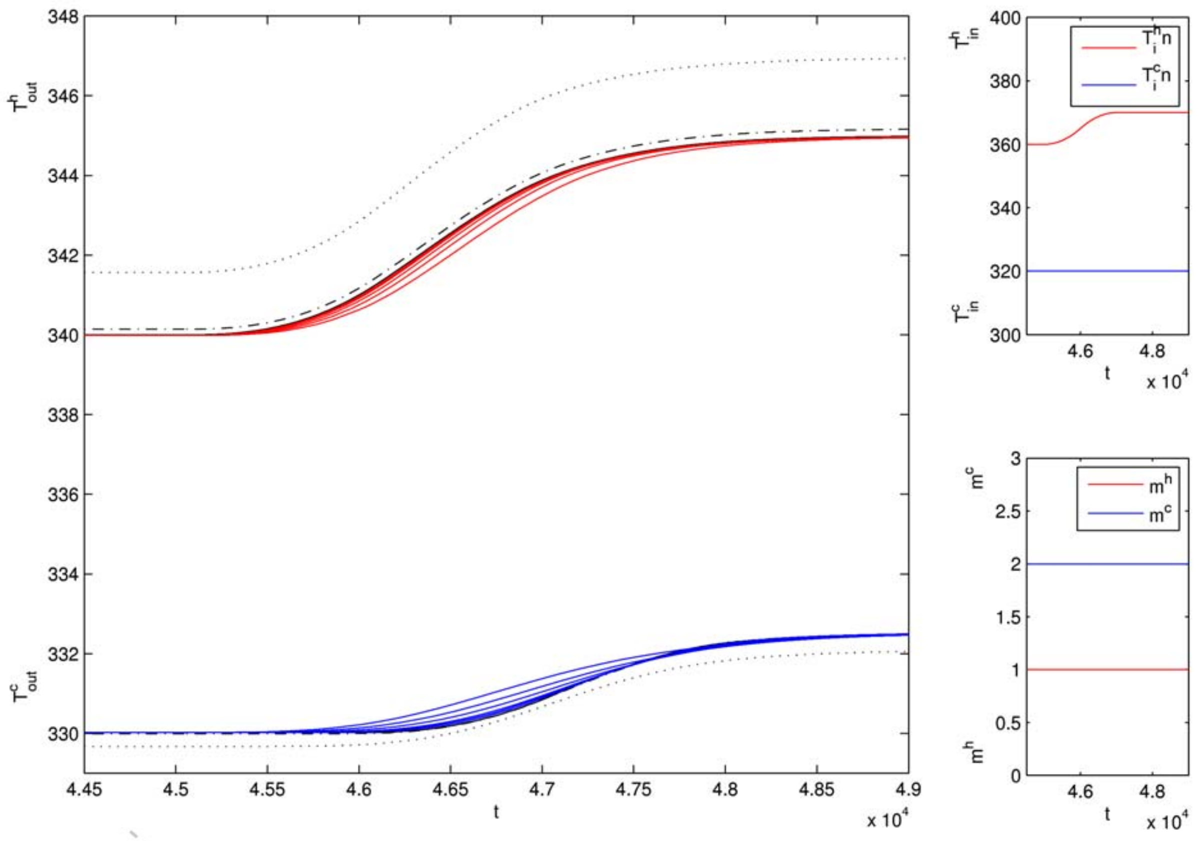
Response of hot and cold outputs to step change in hot inflow temperature



Response of hot and cold outputs to step change in hot inflow rate



Response of hot and cold outputs to slow change in hot inflow temperature



Conclusions:

- Very simple model reduction method for discrete and continuous one-dimensional distributed systems
- Good dynamic accuracy and perfect steady-state agreement of reduced models
- In discrete case, reduction to DAE gives no computational advantage
- Suitable treatment of resulting algebraic equations can speed up simulations significantly
- Method is limited to system with a low number of distributed variables
- Method for continuous case is alternative to other discretisations (finite differences, finite volumes, orthogonal collocation)

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