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

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Outline:

- General idea
- Reduction method for discrete distributed systems
- Example 1: staged distillation column
- Reduction method for continuous distributed systems
- Example 2: fixed-bed reactor with heat recycle
- Example 3: heat exchanger
- Conclusions

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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)

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- Tubular reactors (continuous)
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Basic idea of model reduction method:

- Approximate spatial transport through system by infinitely fast steady-state subsystems connected by slow dynamic elements

- Extends the concept of "Aggregated modeling" method of Levine & Rouchon (1991) for simple distillation models

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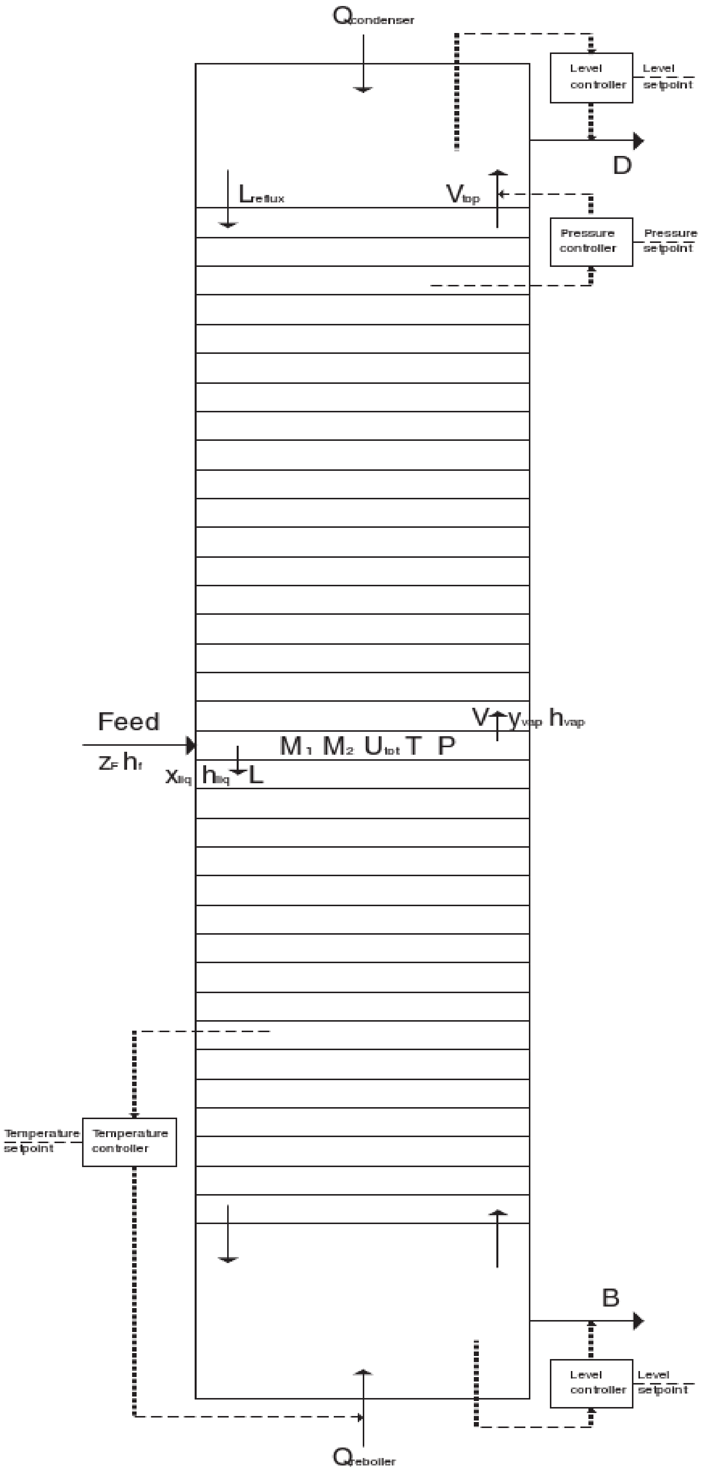

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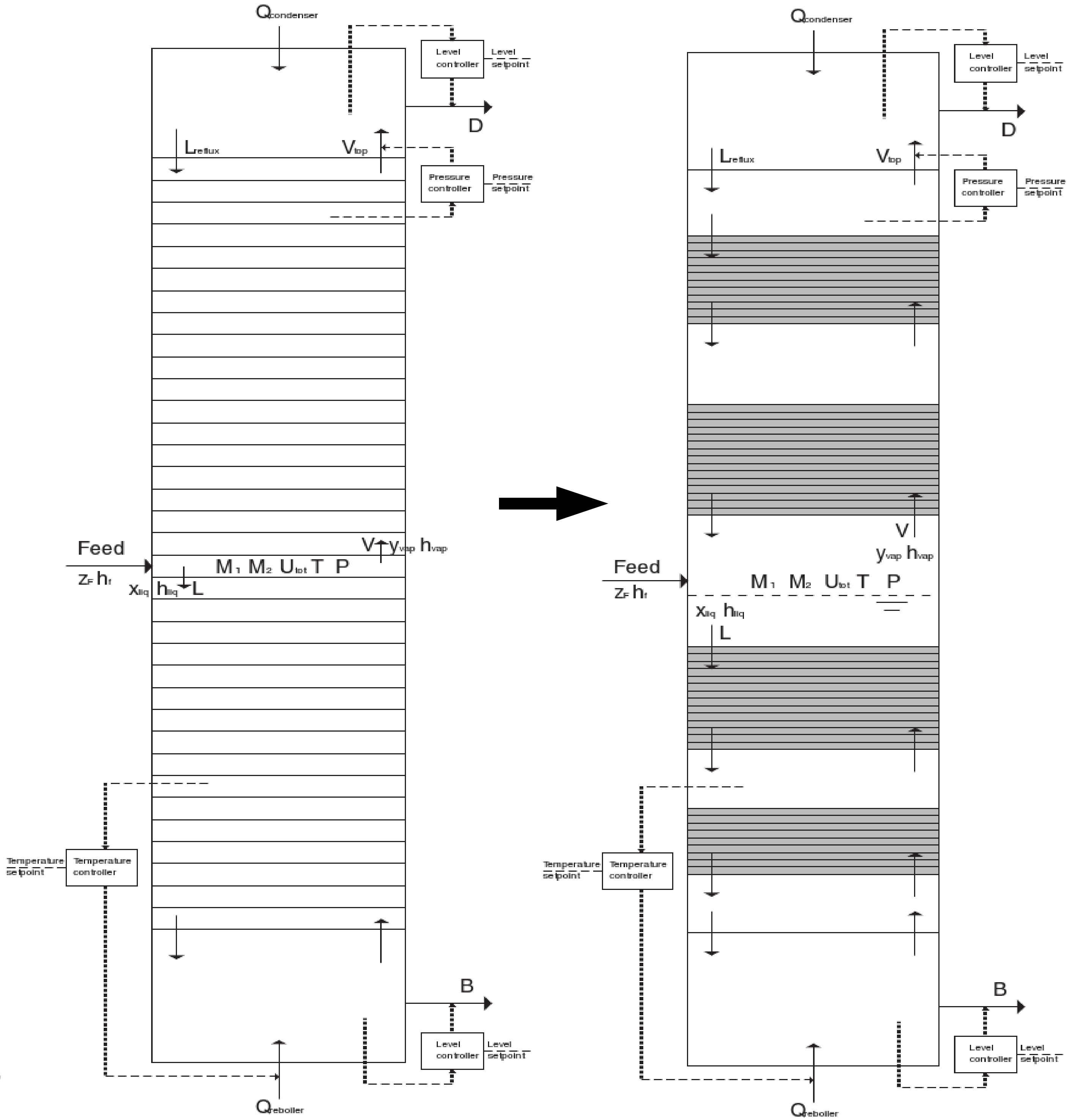

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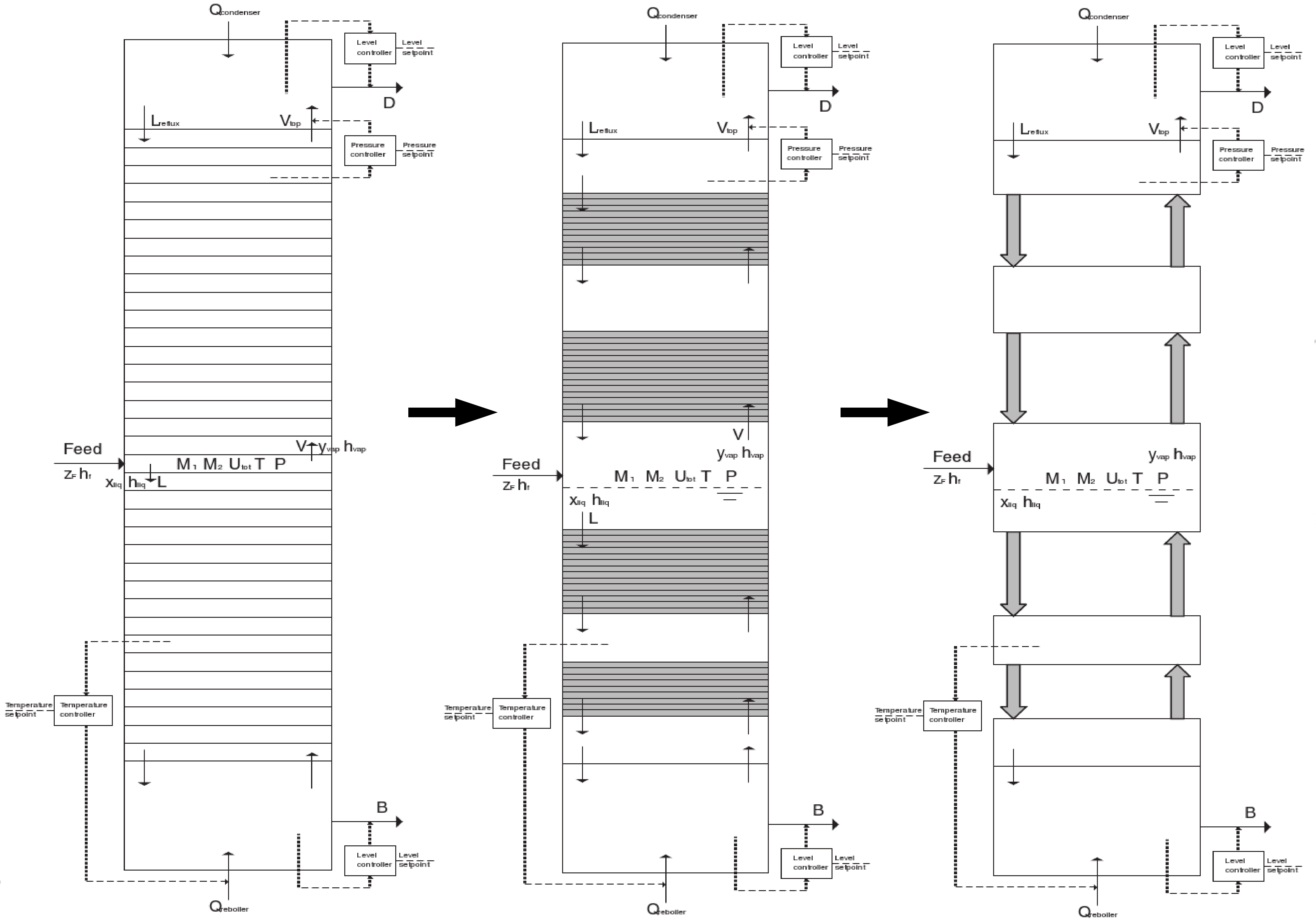
Q condenser
Level controller
Level setpoint
D
L reflux
V top
Pressure controller
Pressure setpoint
Feed
z F h f
V y vap h vap
M 1 M 2 U tot T P
x liq h liq L
Temperature setpoint
Temperature controller
B
Q reboiler

Simple distillation example:

Original system:

$$
\begin{aligned}
\dot{M}_1 &= V_2 y_2 - (R + D) x_1 \\
\dot{M}_2 &= L_1 x_{2-1} + V_3 y_3 - L_2 x_2 - V_2 y_2 \\
\dot{M}_3 &= L_2 x_2 + V_4 y_4 - L_3 x_3 - V_3 y_3 \\
\dot{M}_4 &= L_3 x_3 + V_5 y_5 - L_4 x_4 - V_4 y_4 \\
\dot{M}_5 &= L_4 x_4 + V_6 y_6 - L_5 x_5 - V_5 y_5 \\
\dot{M}_6 &= L_5 x_5 + V_7 y_7 - L_6 x_6 - V_6 y_6 \\
\dot{M}_7 &= L_6 x_6 + V_8 y_8 - L_7 x_7 - V_7 y_7 \\
\dot{M}_8 &= L_7 x_7 + V_9 y_9 - L_8 x_8 - V_8 y_8 \\
\dot{M}_9 &= L_8 x_8 + V_{10} y_{10} - L_9 x_9 - V_9 y_9 \\
\dot{M}_{10} &= L_9 x_9 - B x_{10} - V_{10} y_{10}
\end{aligned}
$$

Step 1:

$$
\begin{aligned}
H_1 \dot{M}_1 &= \ldots \\
0 &= \ldots \\
0 &= \ldots \\
0 &= \ldots \\
0 &= \ldots \\
H_2 \dot{M}_6 &= \ldots \\
0 &= \ldots \\
0 &= \ldots \\
0 &= \ldots \\
H_3 \dot{M}_{10} &= \ldots
\end{aligned}
$$

Step 2:

$$
\begin{aligned}
H_1 \dot{M}_1 &= V_2 y_2 - (R + D) x_1 \\
y_2 &= y_2(M_1, M_6) \\
x_5 &= x_5(M_1, M_6) \\
H_2 \dot{M}_6 &= L_5 x_5 + V_7 y_7 - L_6 x_6 - V_6 y_6 \\
y_7 &= y_7(M_6, M_{10}) \\
x_9 &= x_9(M_6, M_{10}) \\
H_3 \dot{M}_{10} &= L_9 x_9 - B x_{10} - V_{10} y_{10}
\end{aligned}
$$

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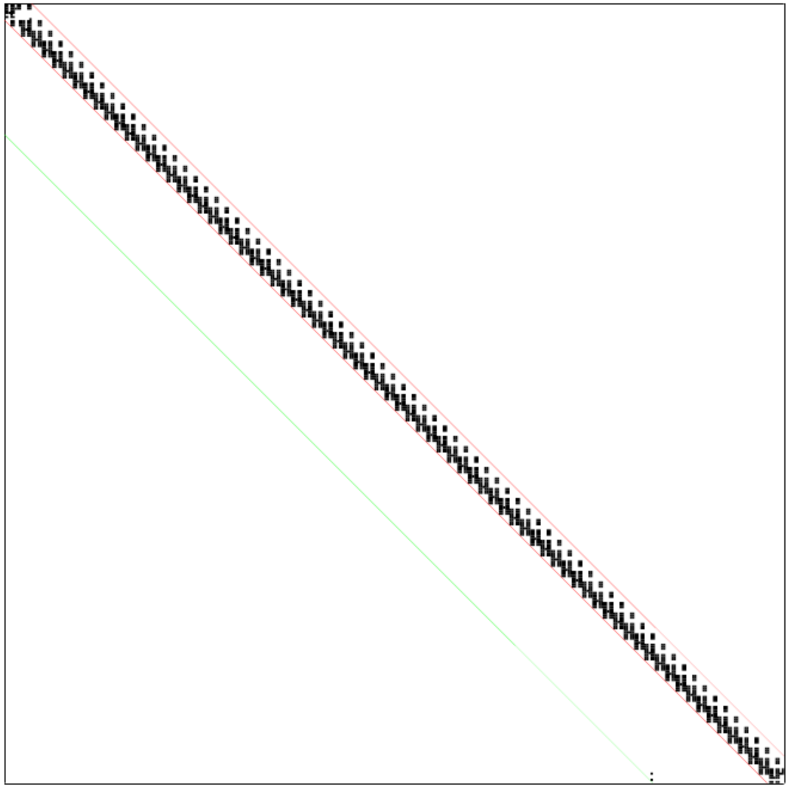
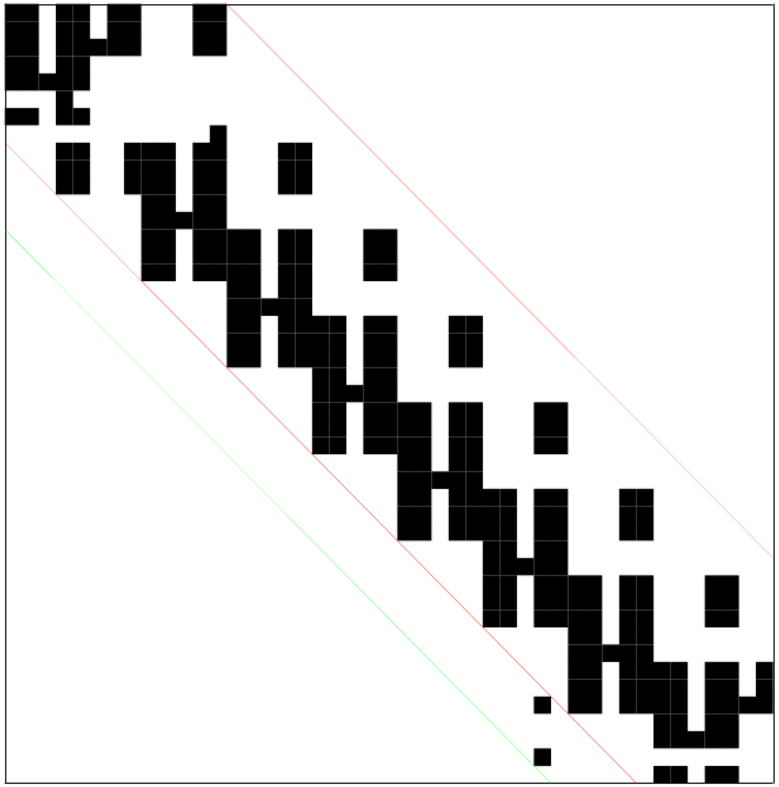
Jacobian structures

- Full and reduced models have same Jacobian structures
- Example: Distillation column with 94 stages and 5 variables per stage

full model (474 variables)

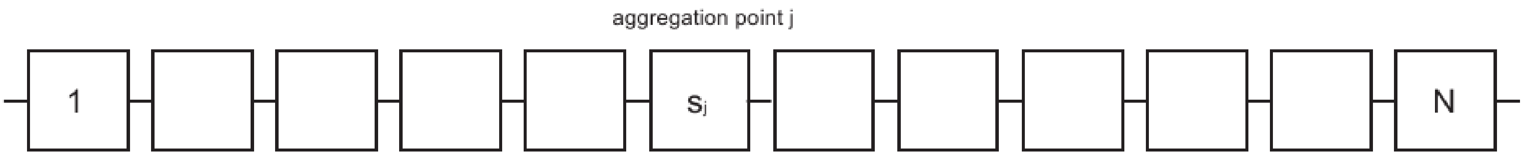


reduced model (49 variables)

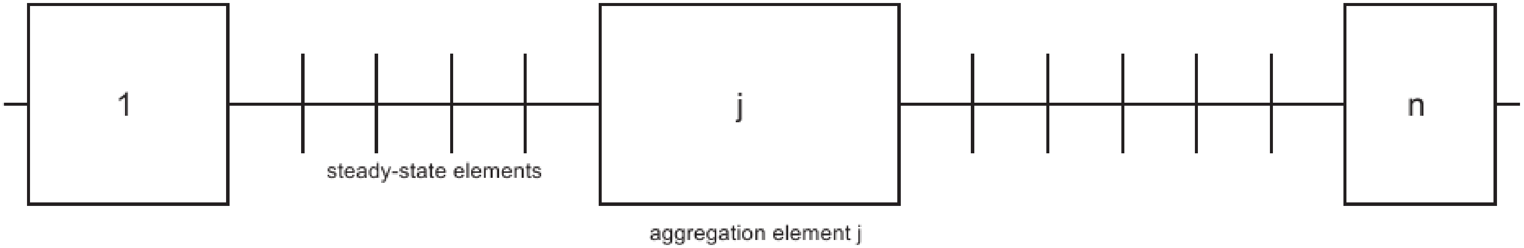


Reduction method for discrete systems:

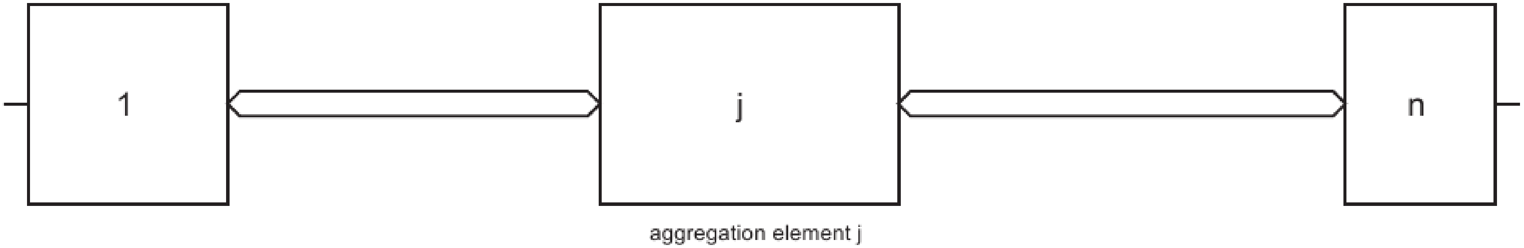
Original system:



Reduction step 1: Selection of aggregation and steady-state elements



Reduction step 2: Elimination of steady-state elements



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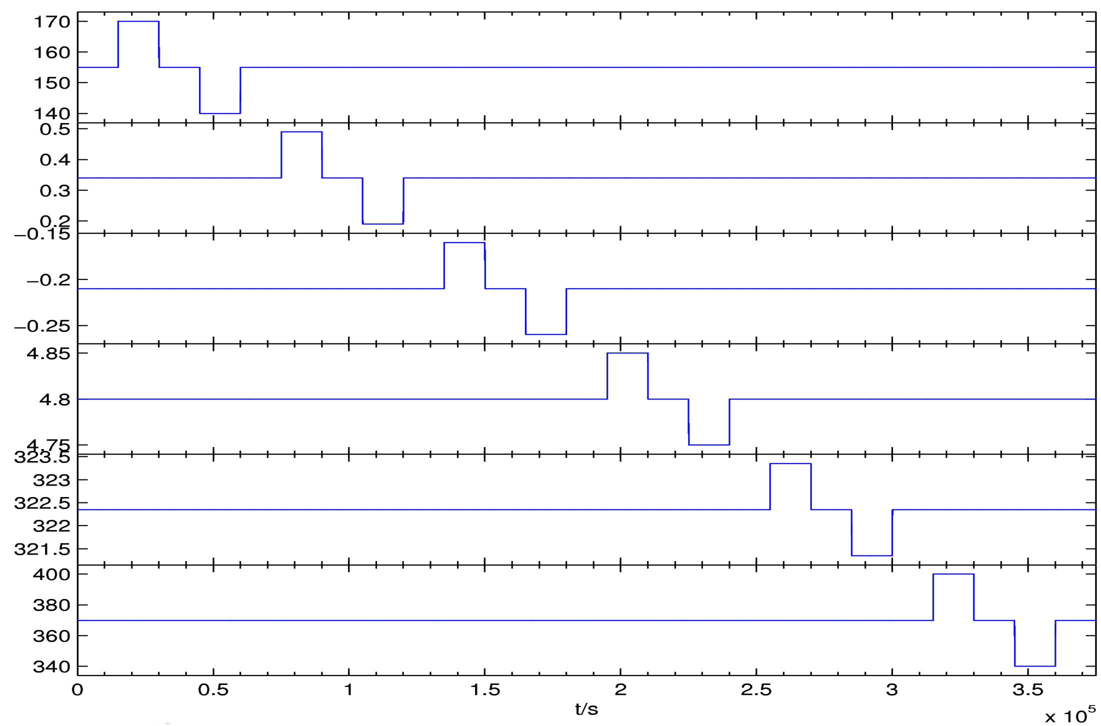
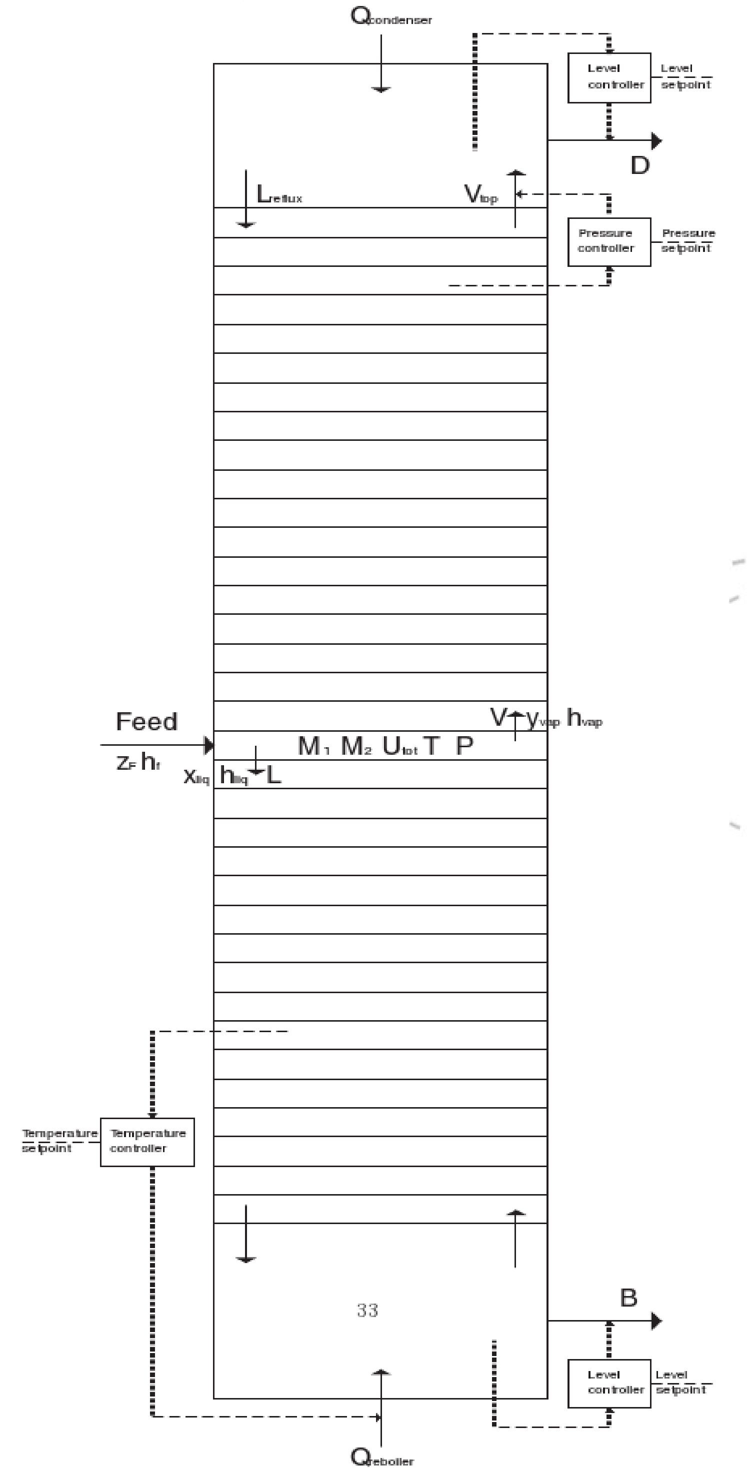
Example 1: Distillation column

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

Test inputs:





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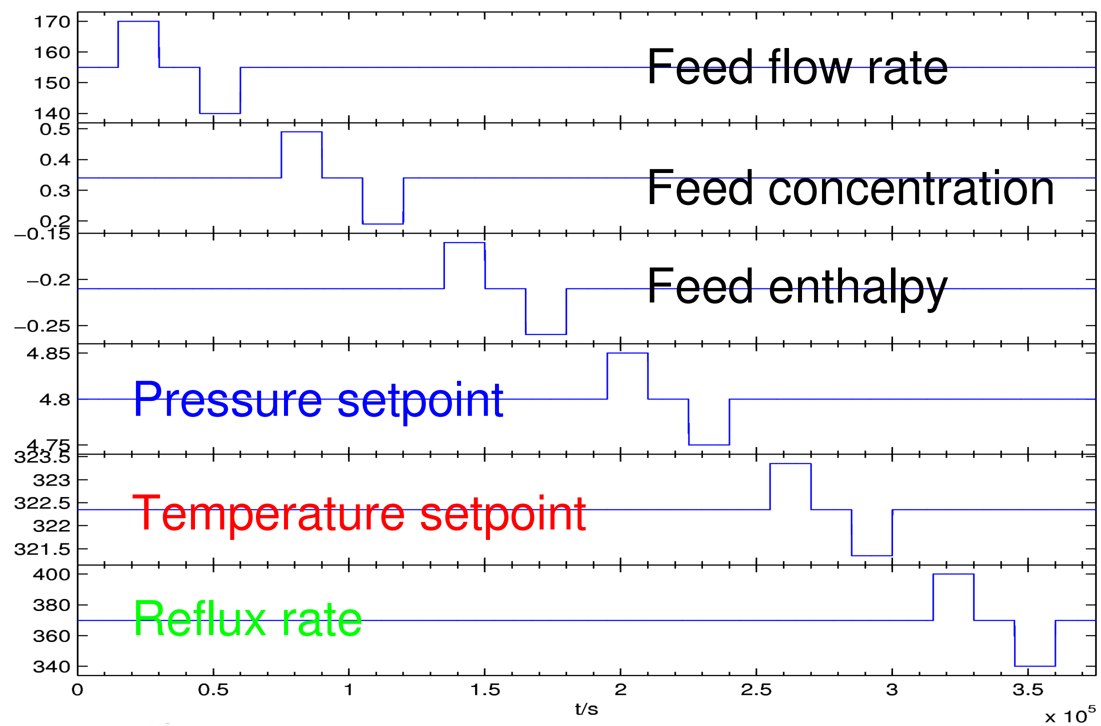
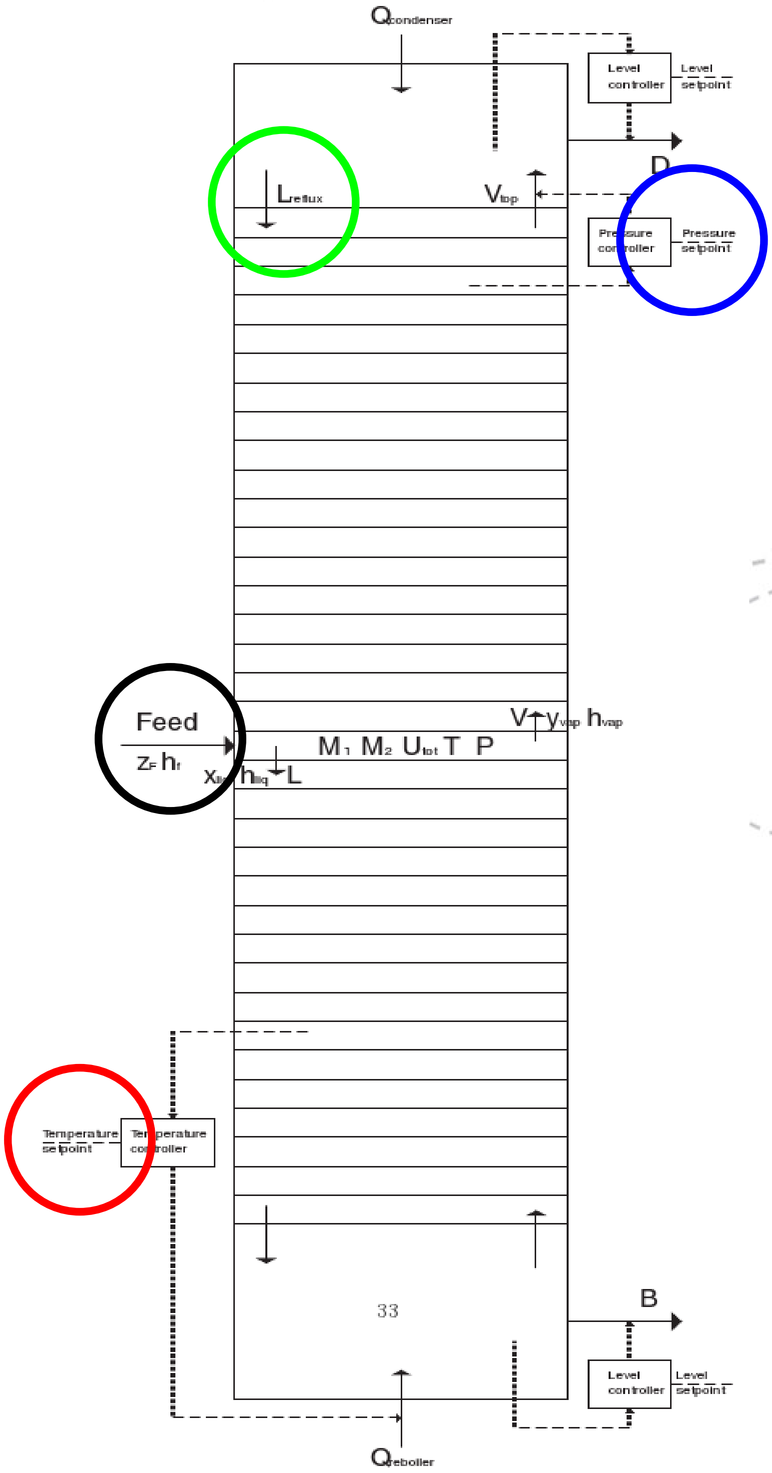
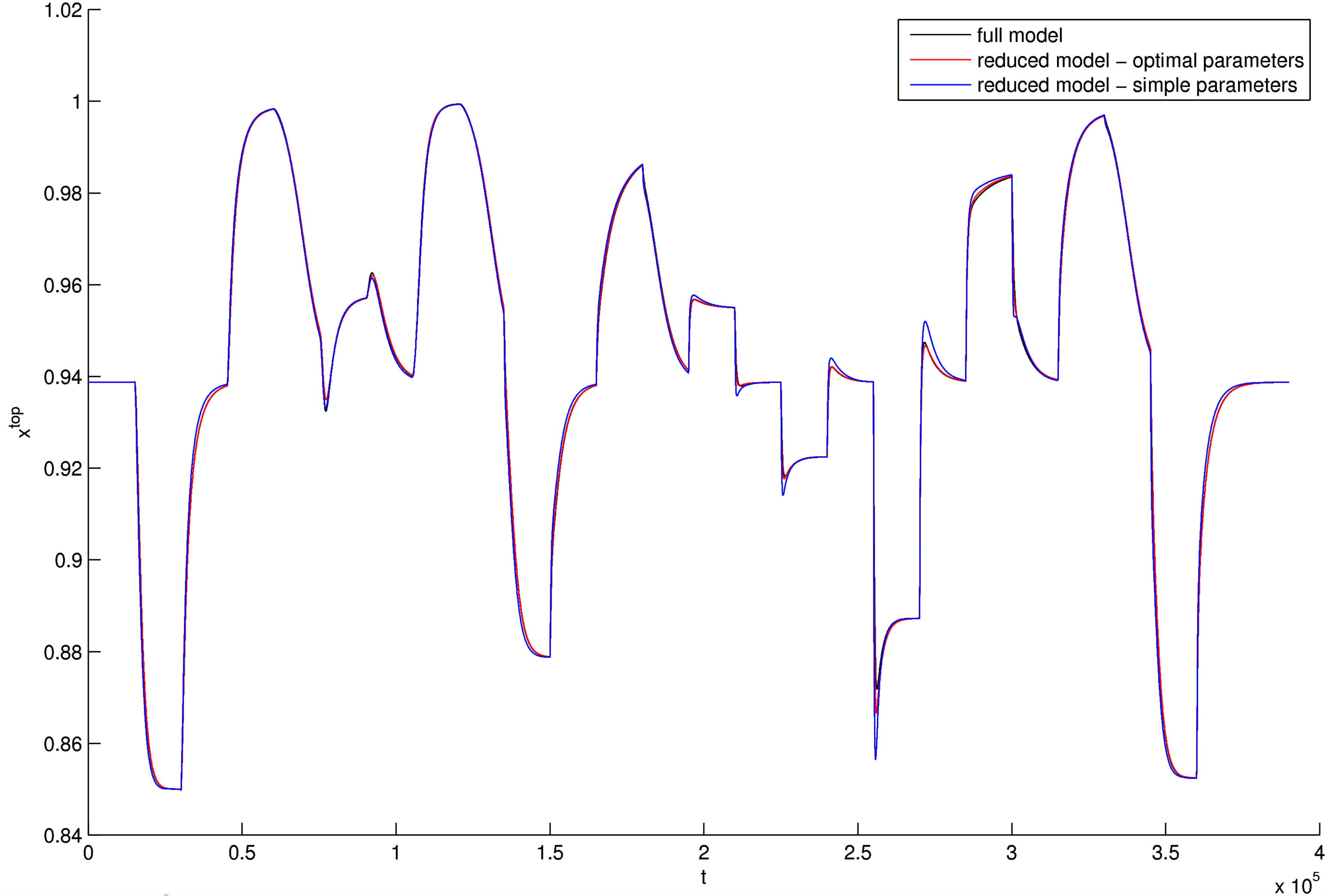
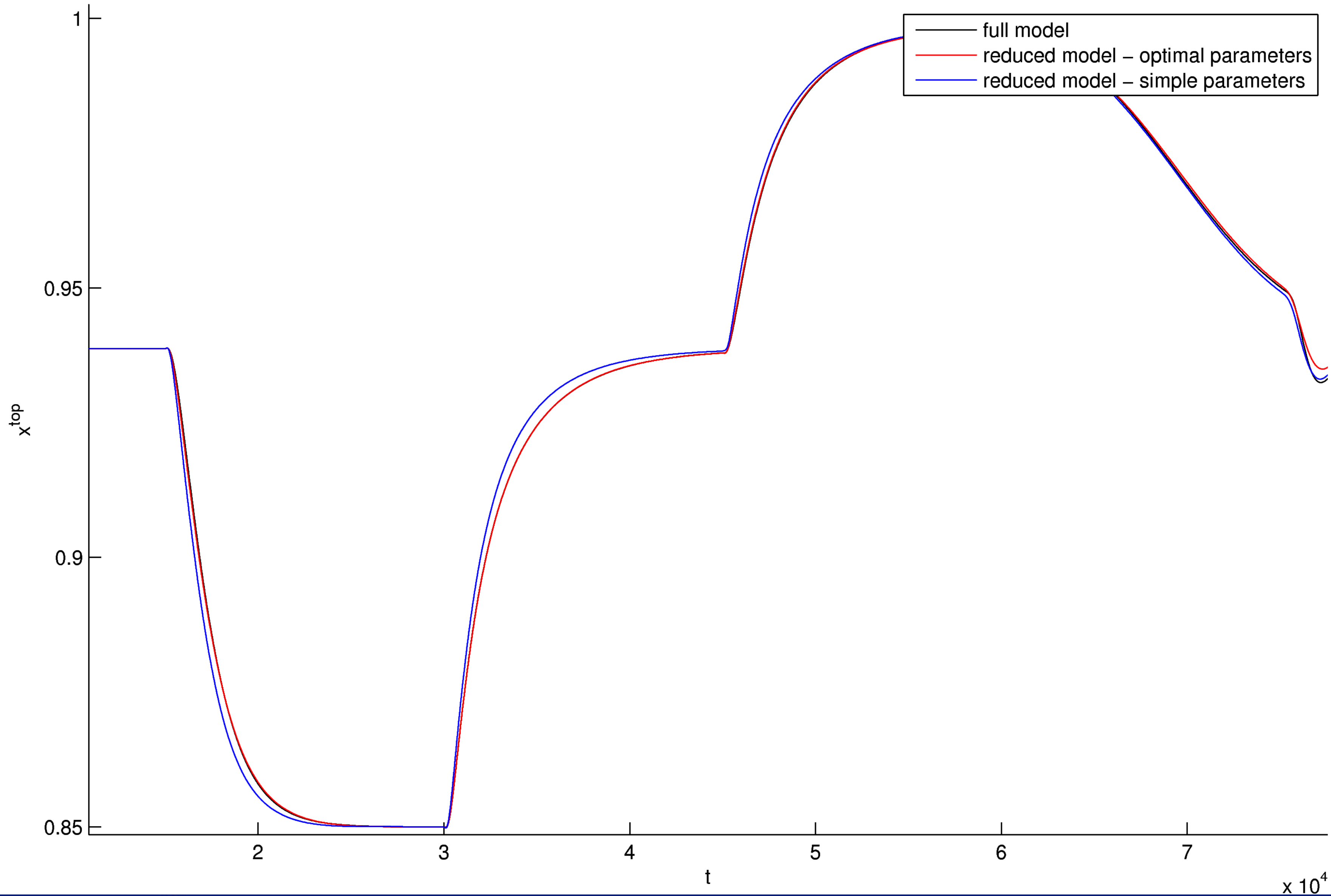




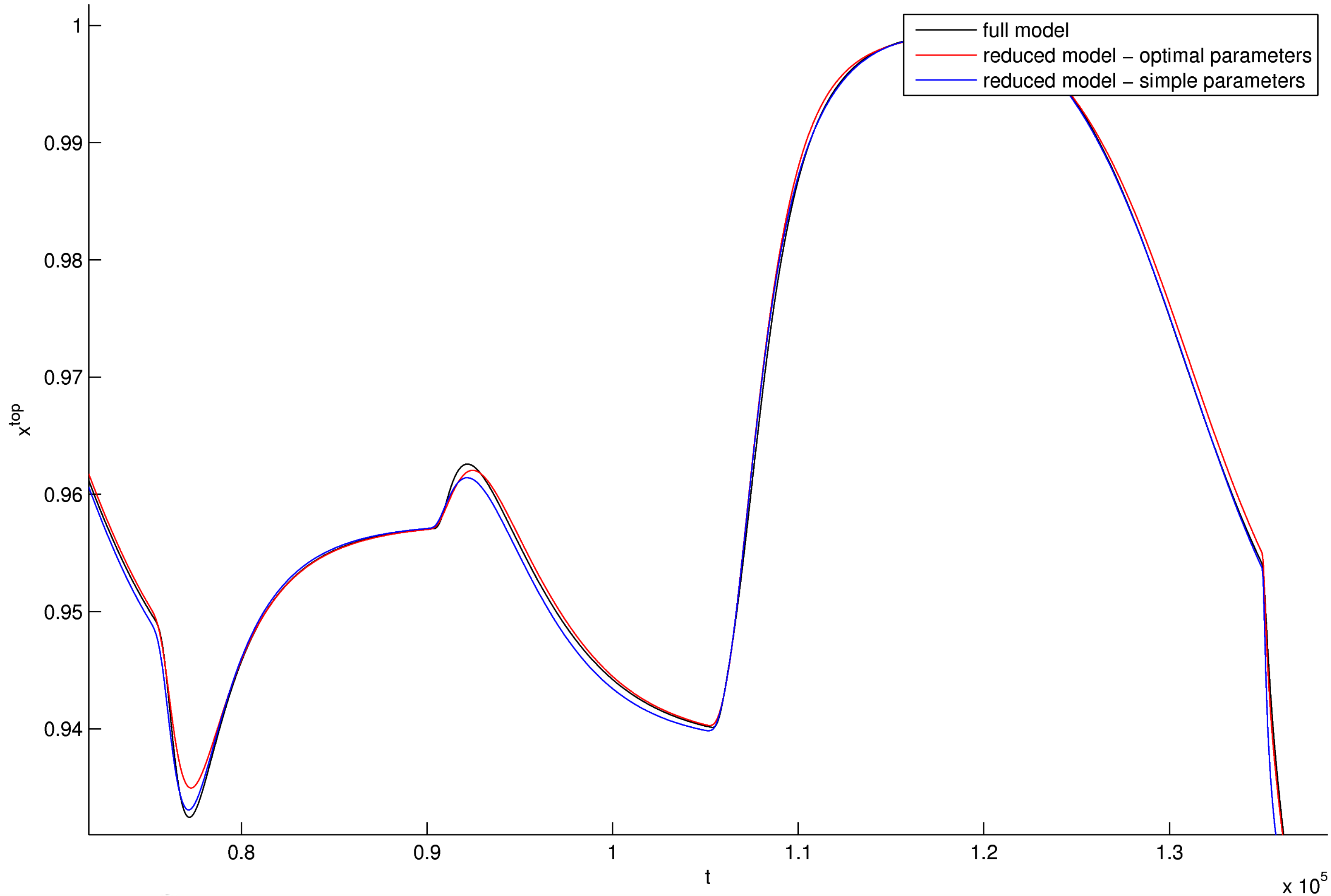
Response of top concentration to step changes in inputs



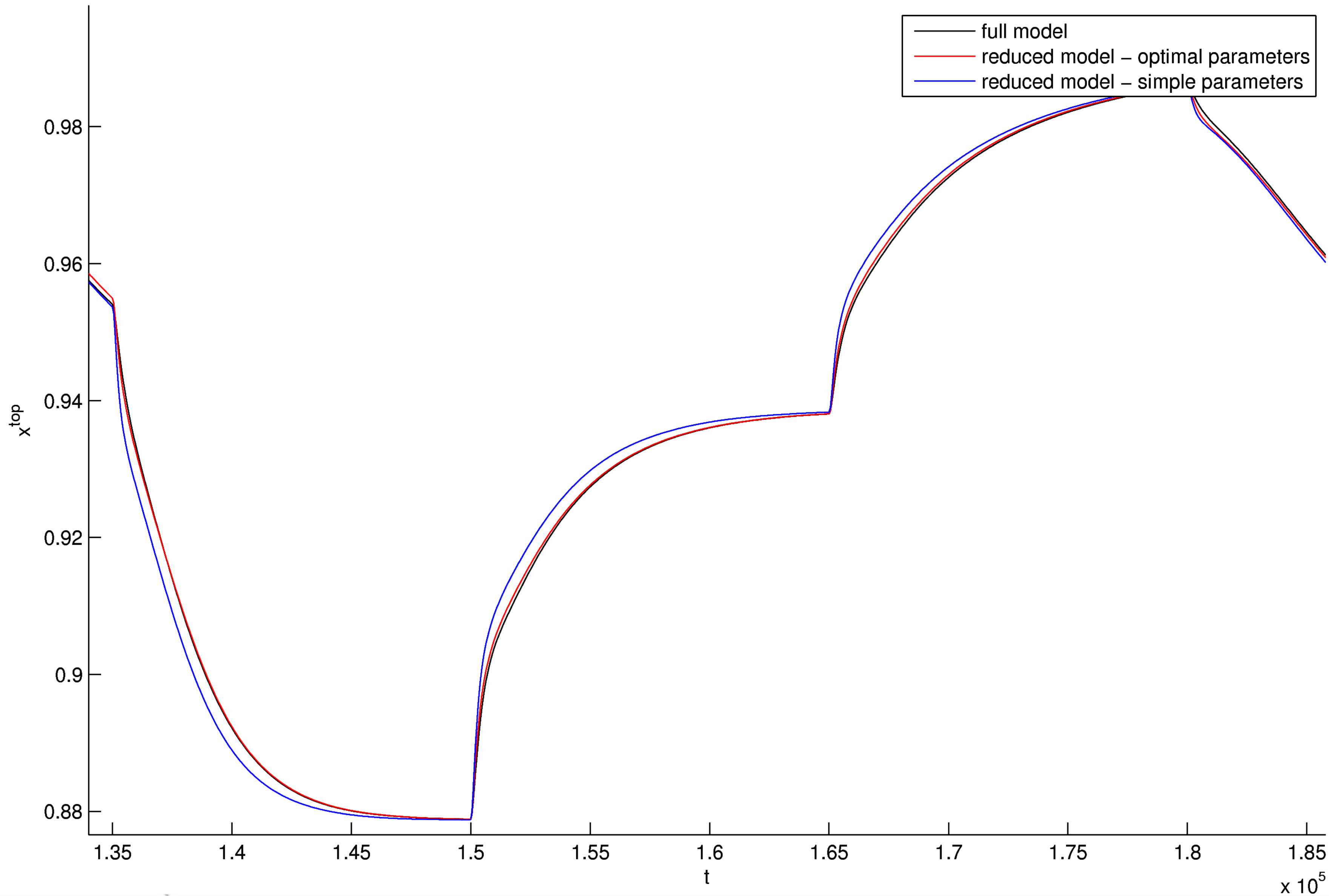
Feed flow rate 155 -> 170 -> 155 -> 140 -> 170



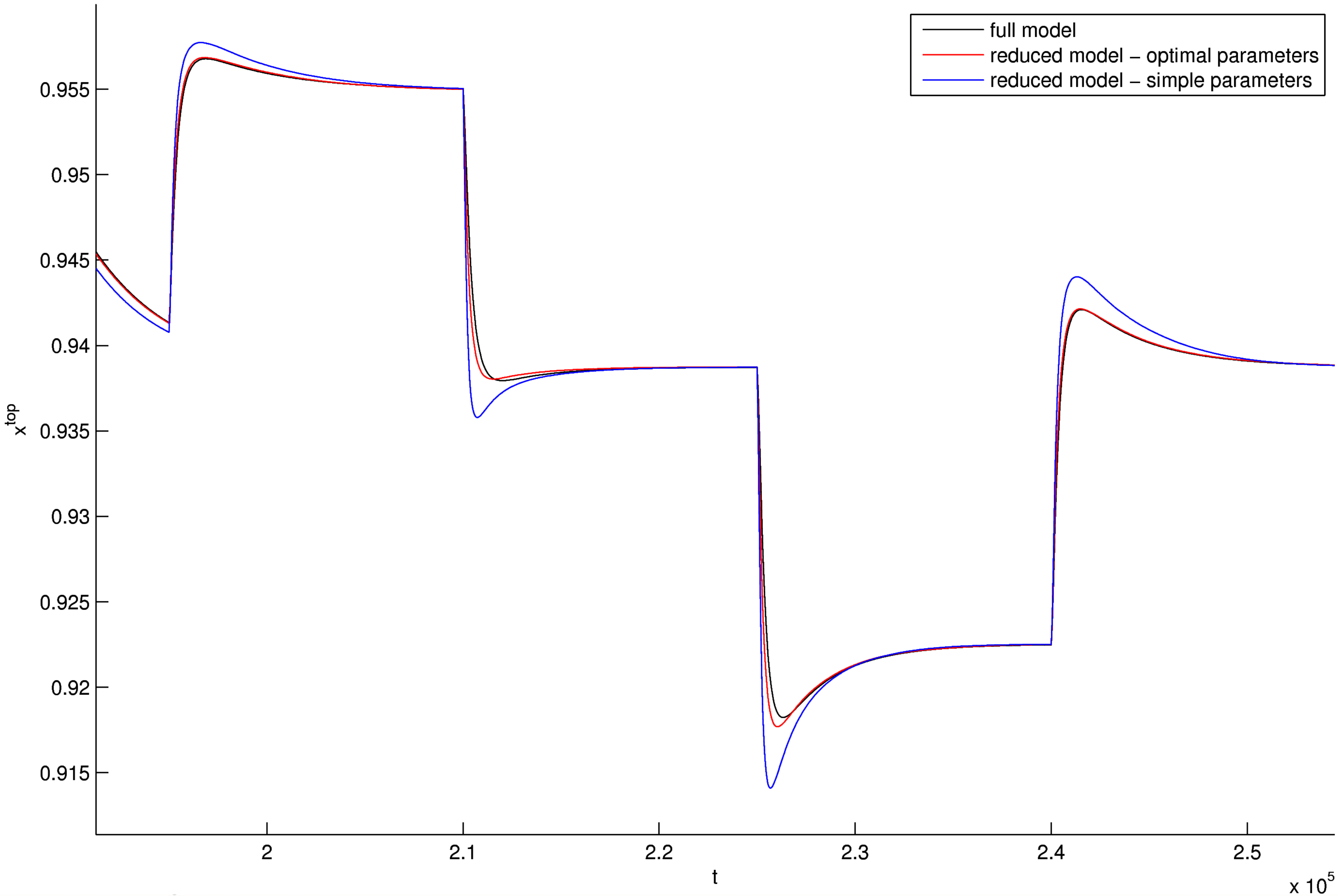
Feed concentration 0.34 -> 0.49 -> 0.34 -> 0.19 -> 0.34



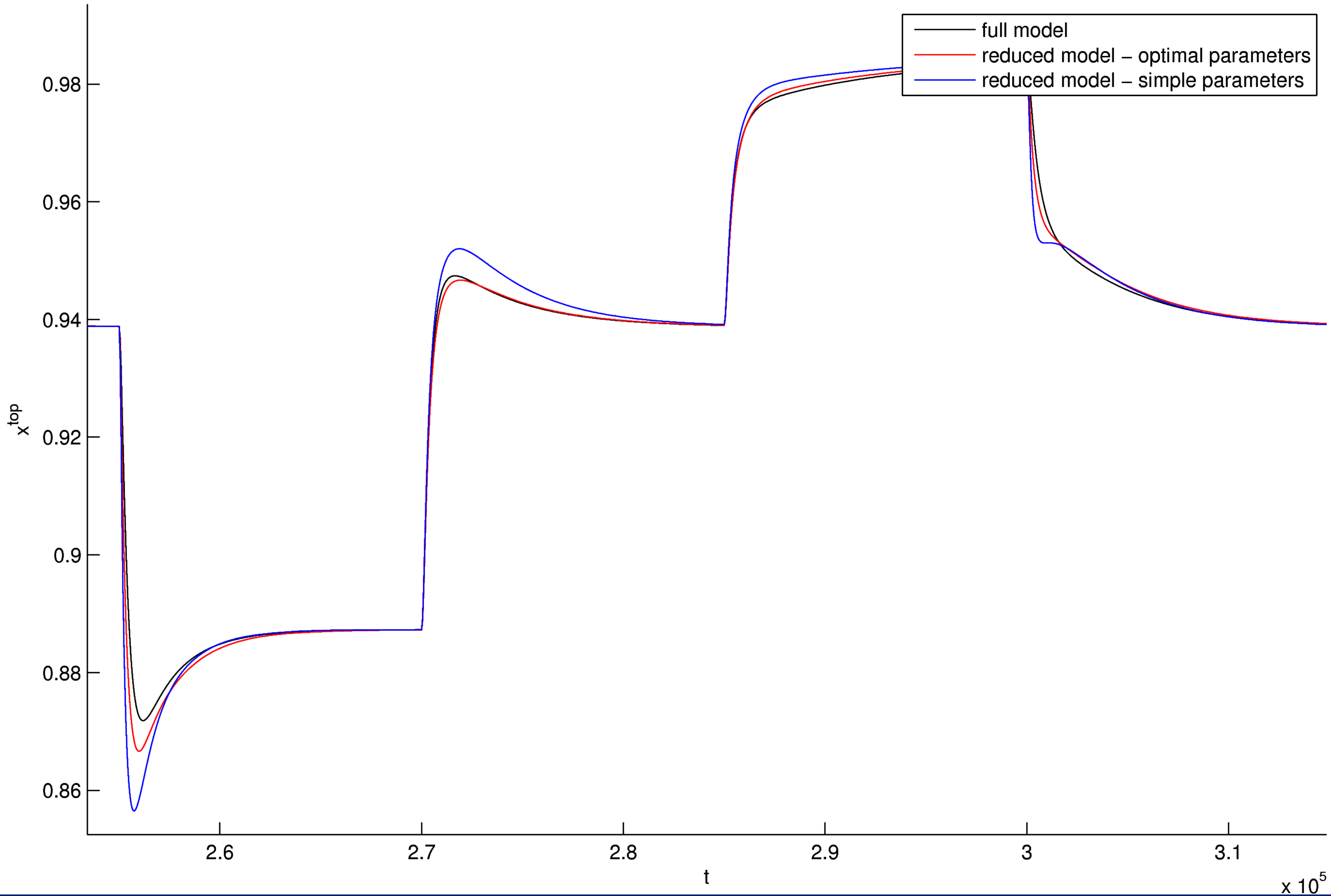
Feed enthalpy -0.21 -> -0.16 -> -0.21 -> -0.26 -> -0.21



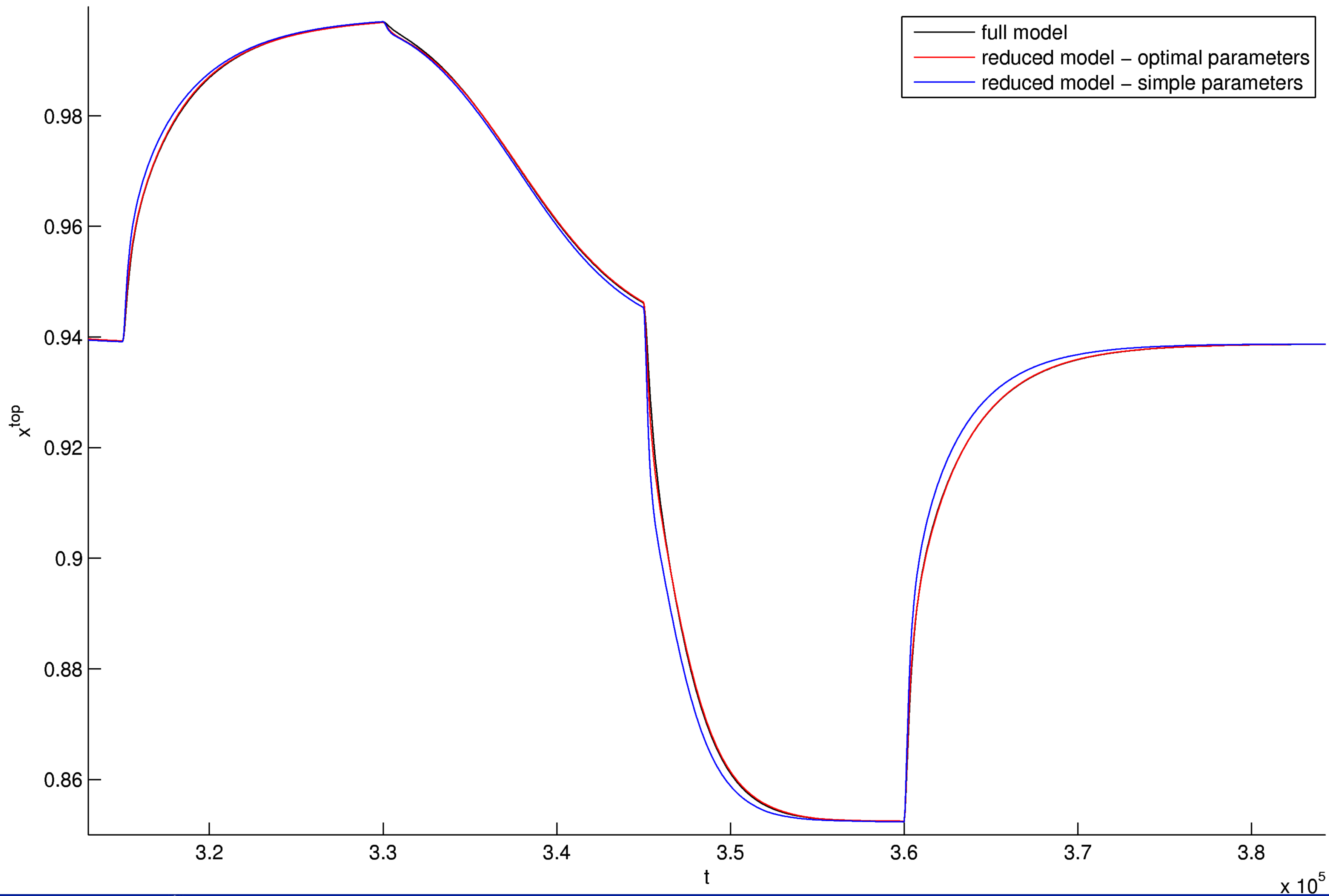
Pressure controller setpoint 4.8 -> 4.85 -> 4.8 -> 4.75 -> 4.8



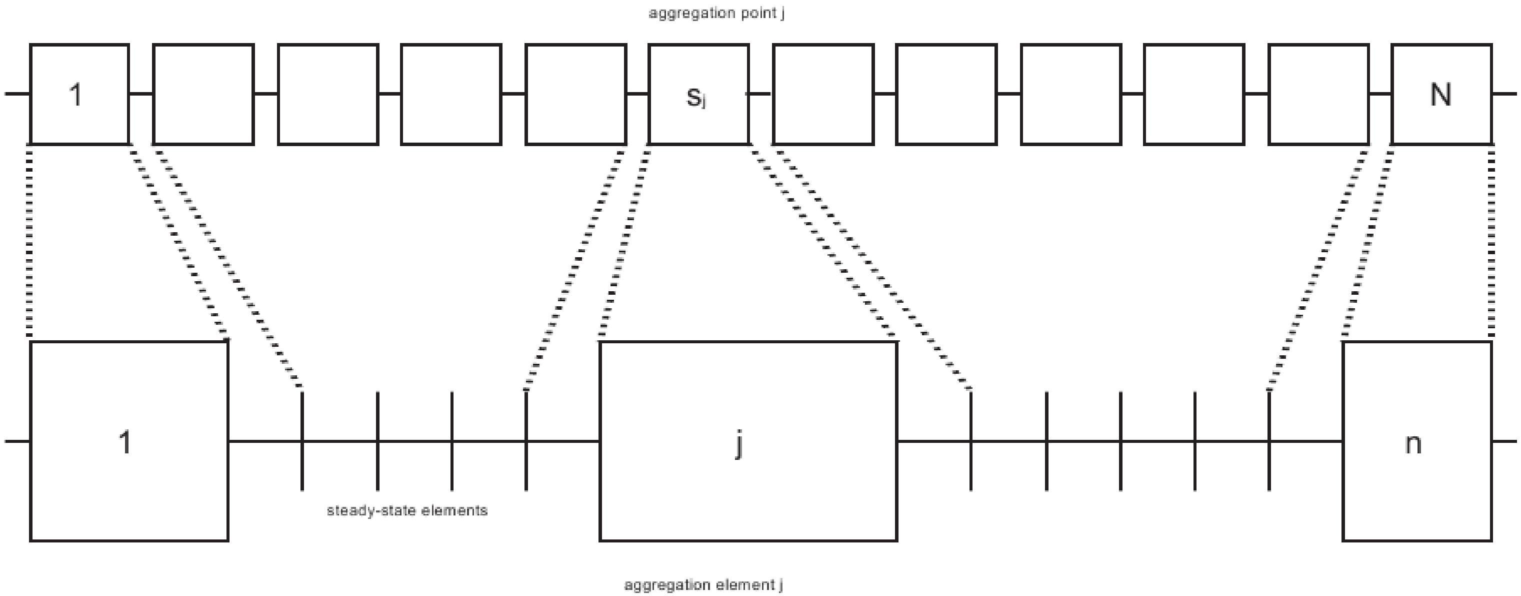
Temperature controller setpoint 322.35 -> 323.35 -> 322.35 -> 321.35 -> 322.35



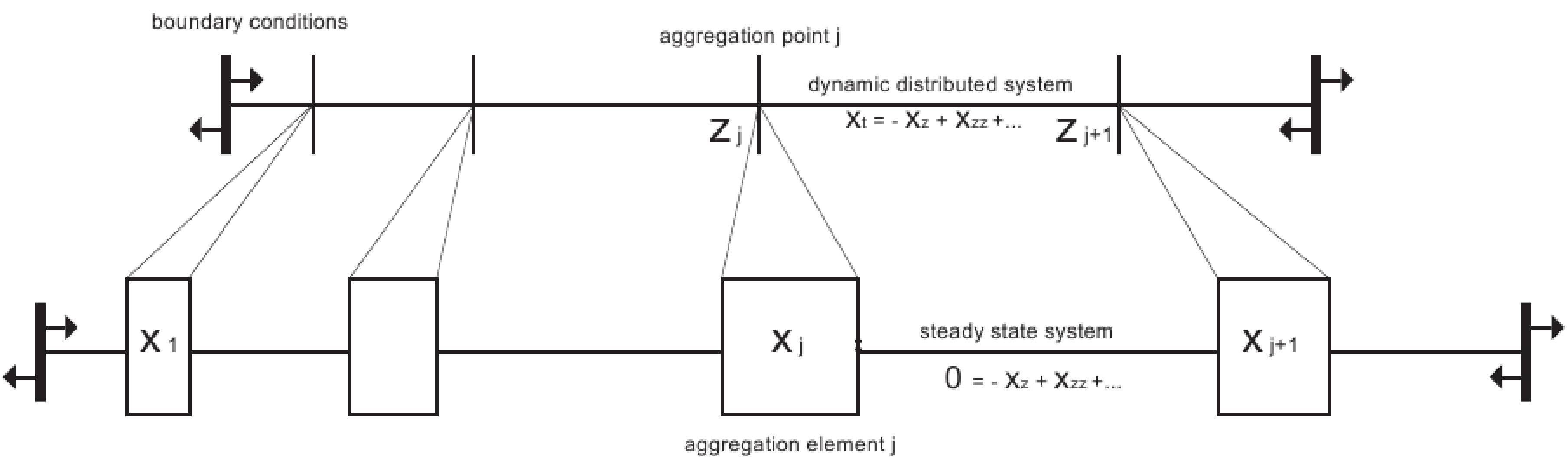
Reflux flow rate 370 -> 400 -> 370 -> 340 -> 370



For far: discrete Systems



Now: continuous systems



Derivation of dynamic equations for continuously distributed systems:

$$\frac{\partial \mathbf{x}(z,t)}{\partial t} = \mathbf{D}_z \mathbf{x}(z,t) + \mathbf{R}(\mathbf{x}(z,t), z, t)$$

+boundary conditions

Idea:
Apply model reduction method to discretised system, and let discretisation step 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:

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

Apply reduction procedure:

- Multiply left-hand side of aggregation elements with constant $H_j = N/n$:

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

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

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

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Go back to continuous system:

- Rewrite dynamic 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 $\Delta z \to 0$:

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

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- 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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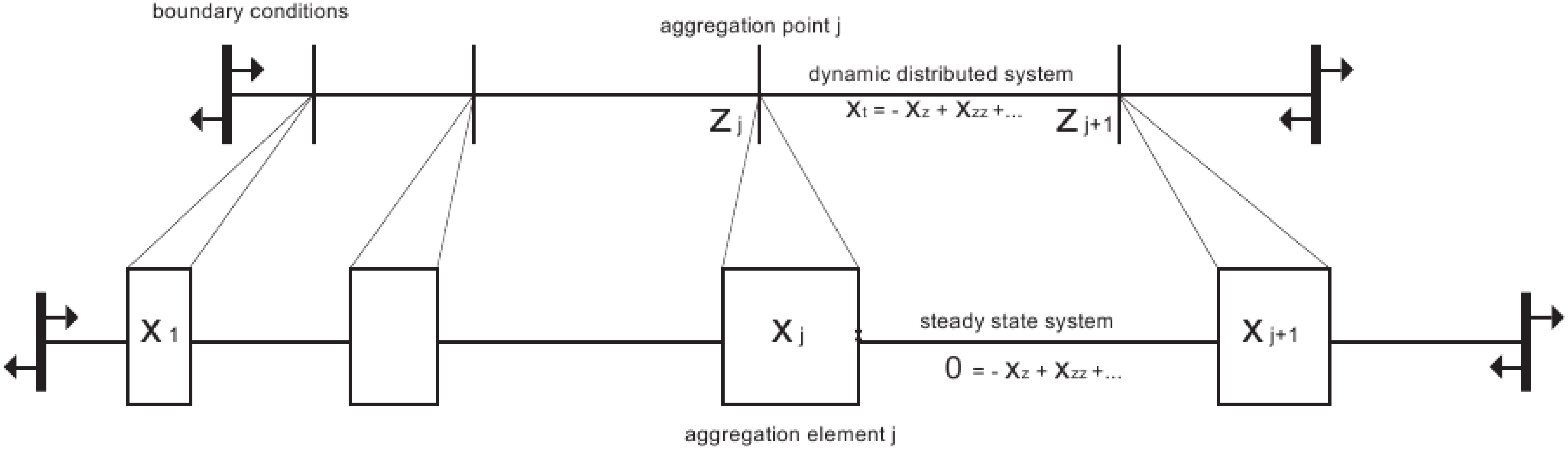

Steady-state subsystems:

$$0 = -\alpha \frac{\partial x}{\partial z} + \beta \frac{\partial^2 x}{\partial z^2} + \gamma R(x)$$

Solutions at boundaries:

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

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

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

Aggregation element equations:

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

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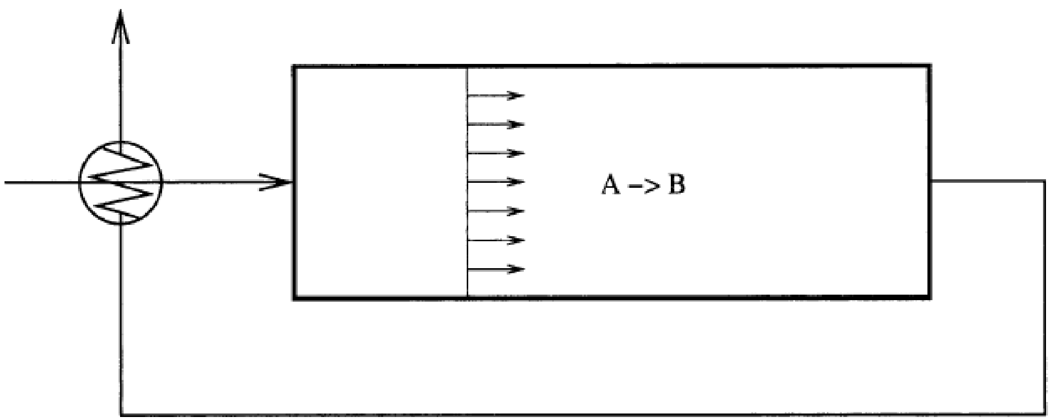
Example 2: Adiabatic fixed-bed reactor with heat recycle
(Liu and Jacobsen, 2004)



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

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

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

Boundary conditions:

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

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

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

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

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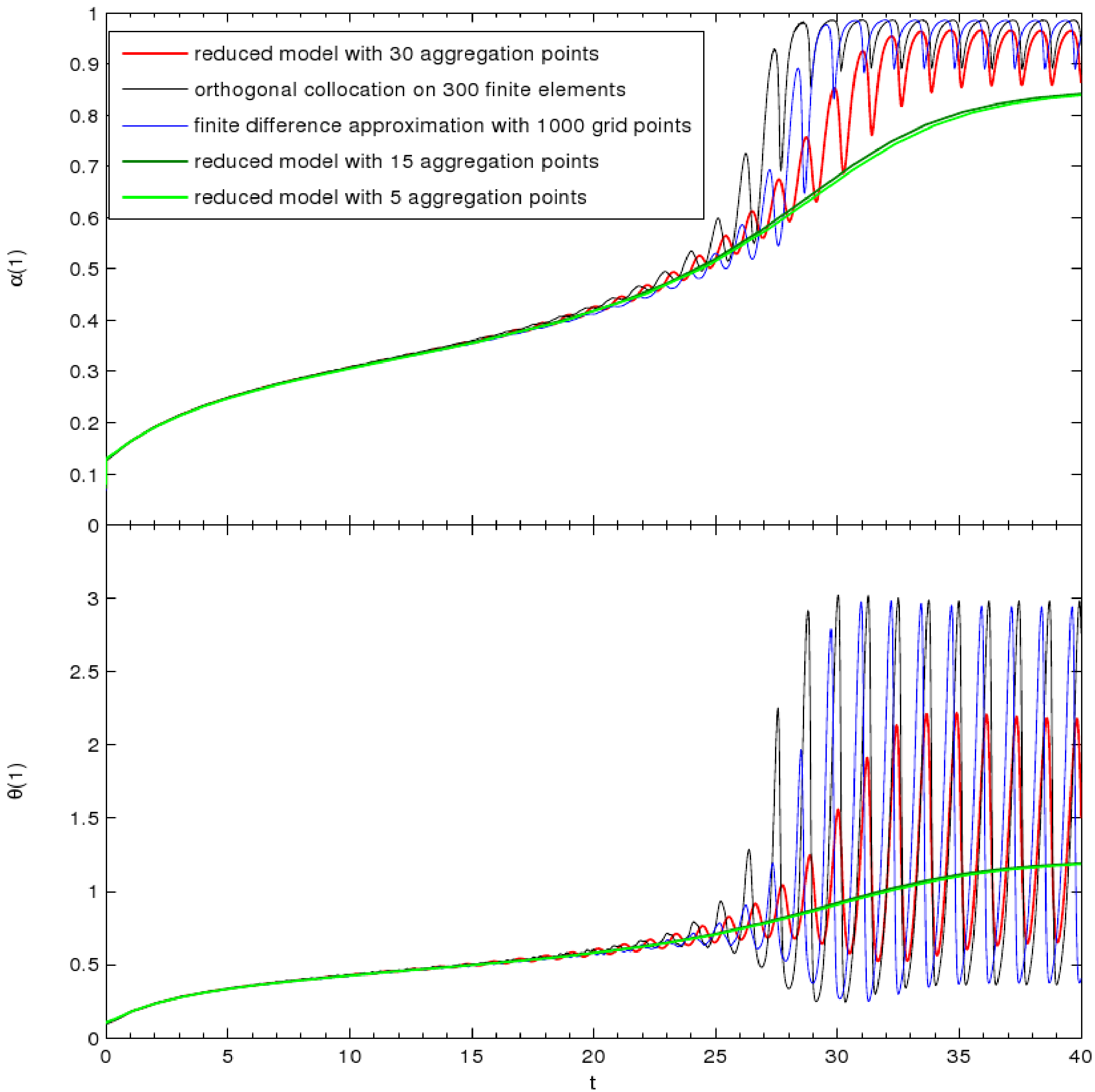
Limit cycle oscillations at right end for a change of Da from 0.05 to Da=0.1:



- 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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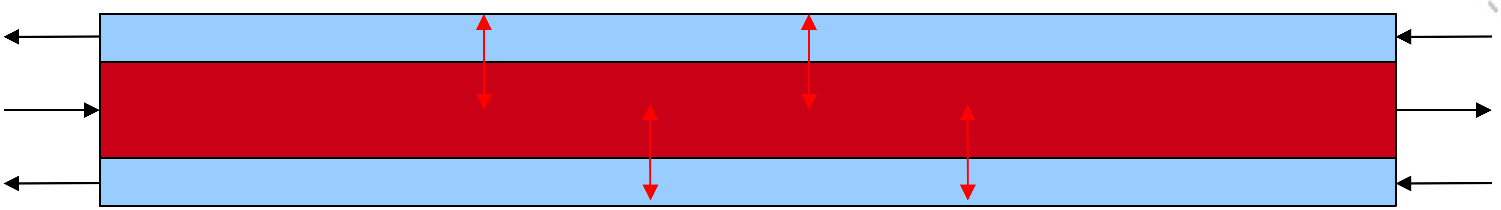
Example 3: Heat Exchanger



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

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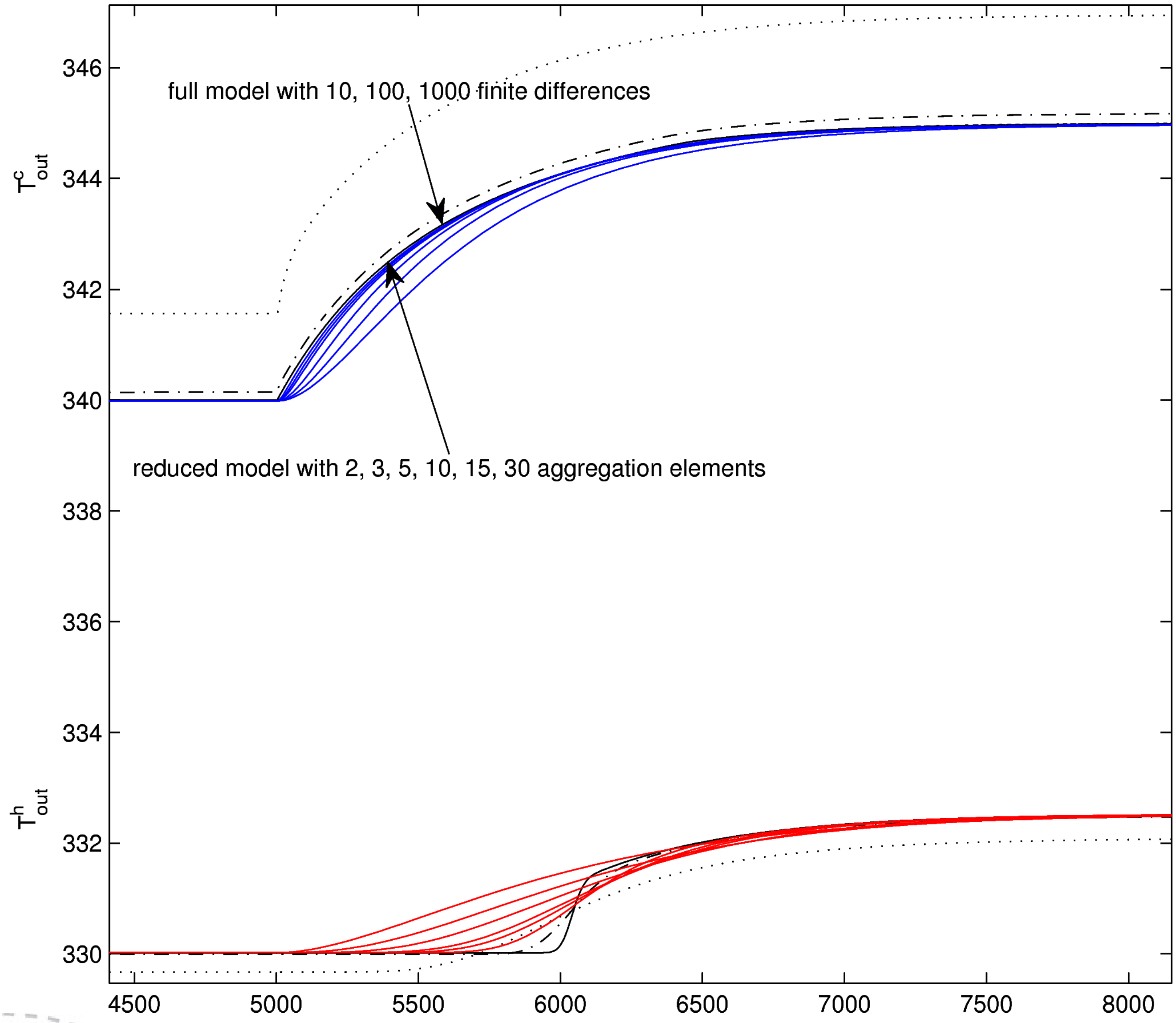
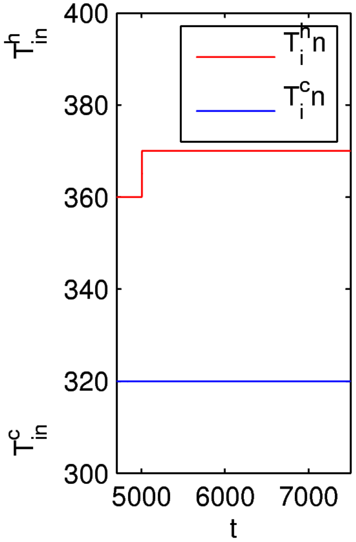
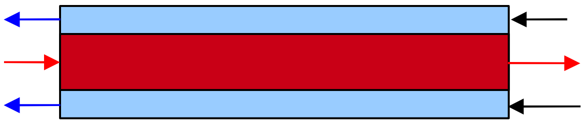
Response of hot and cold outputs to step change in hot inflow temperature

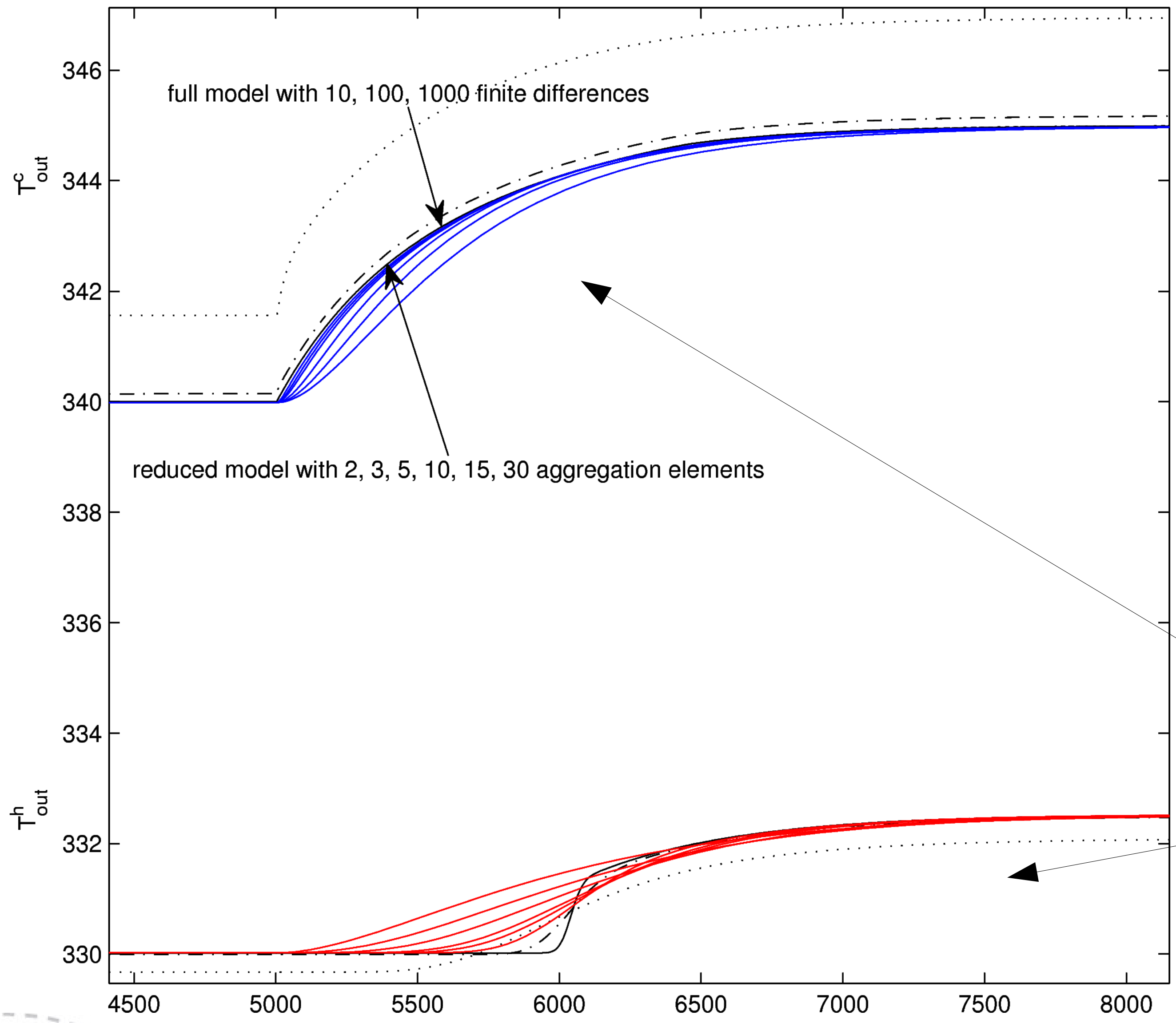


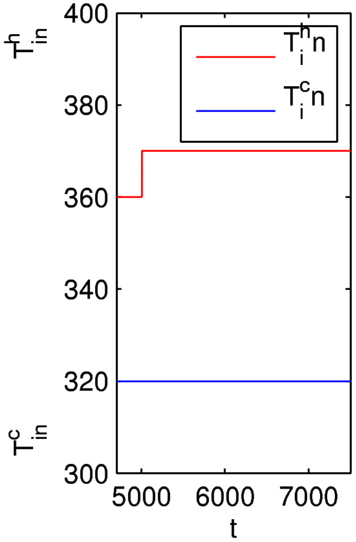


Step change in hot inflow temperature

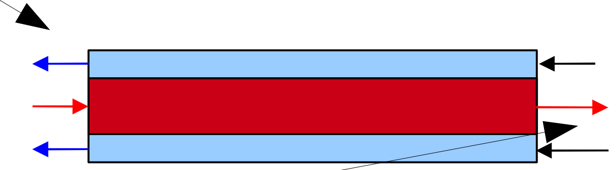


Response of hot and cold outputs to step change in hot inflow temperature

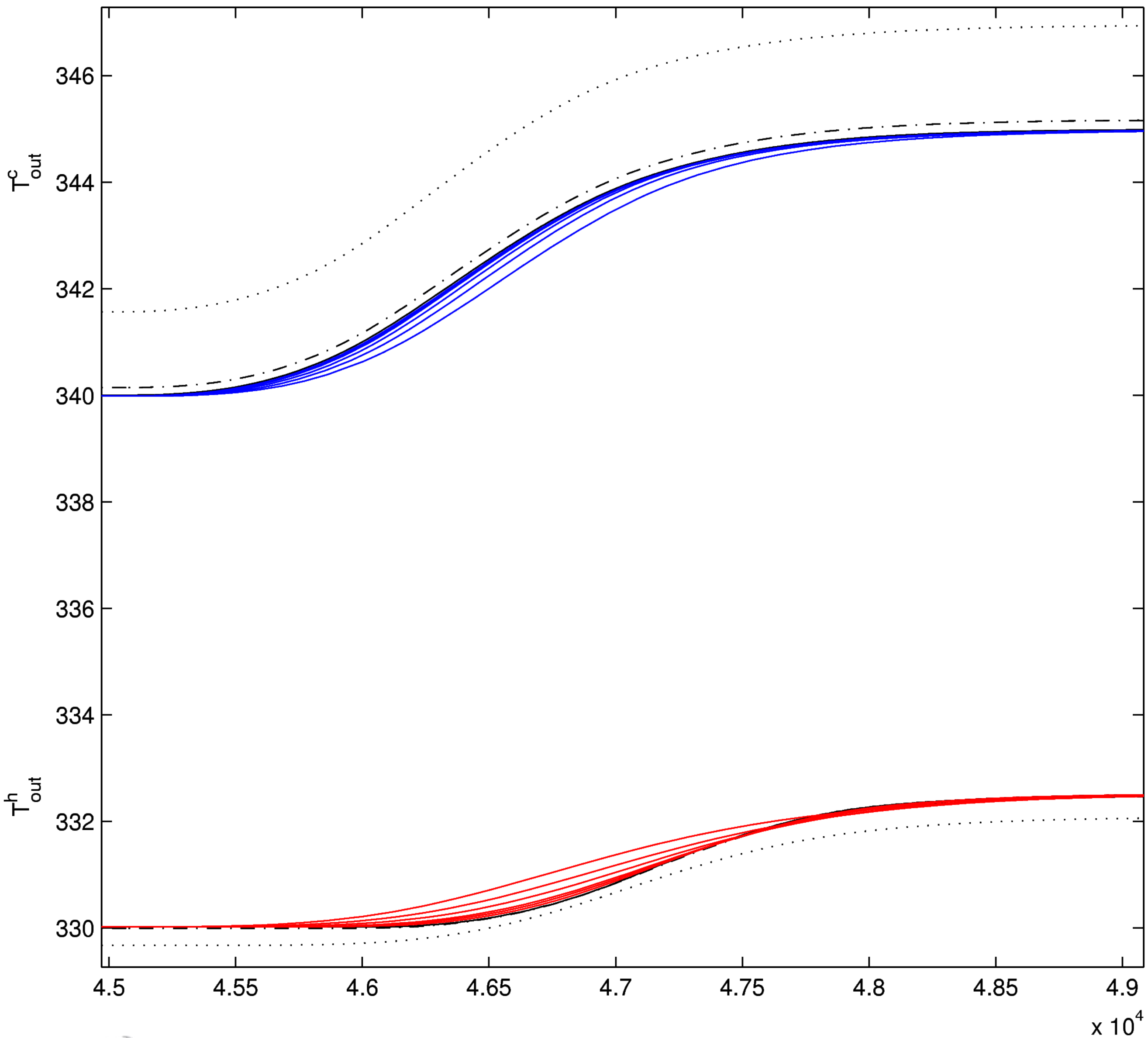


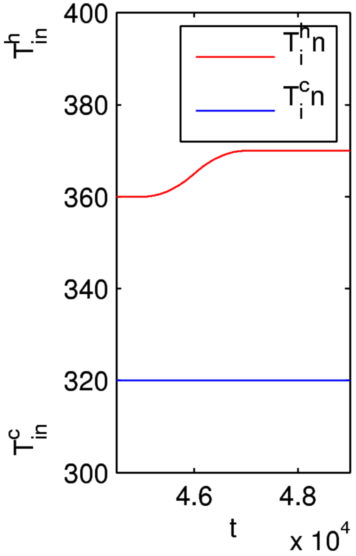


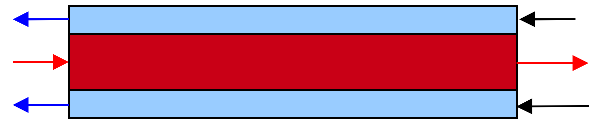
Step change in hot inflow temperature



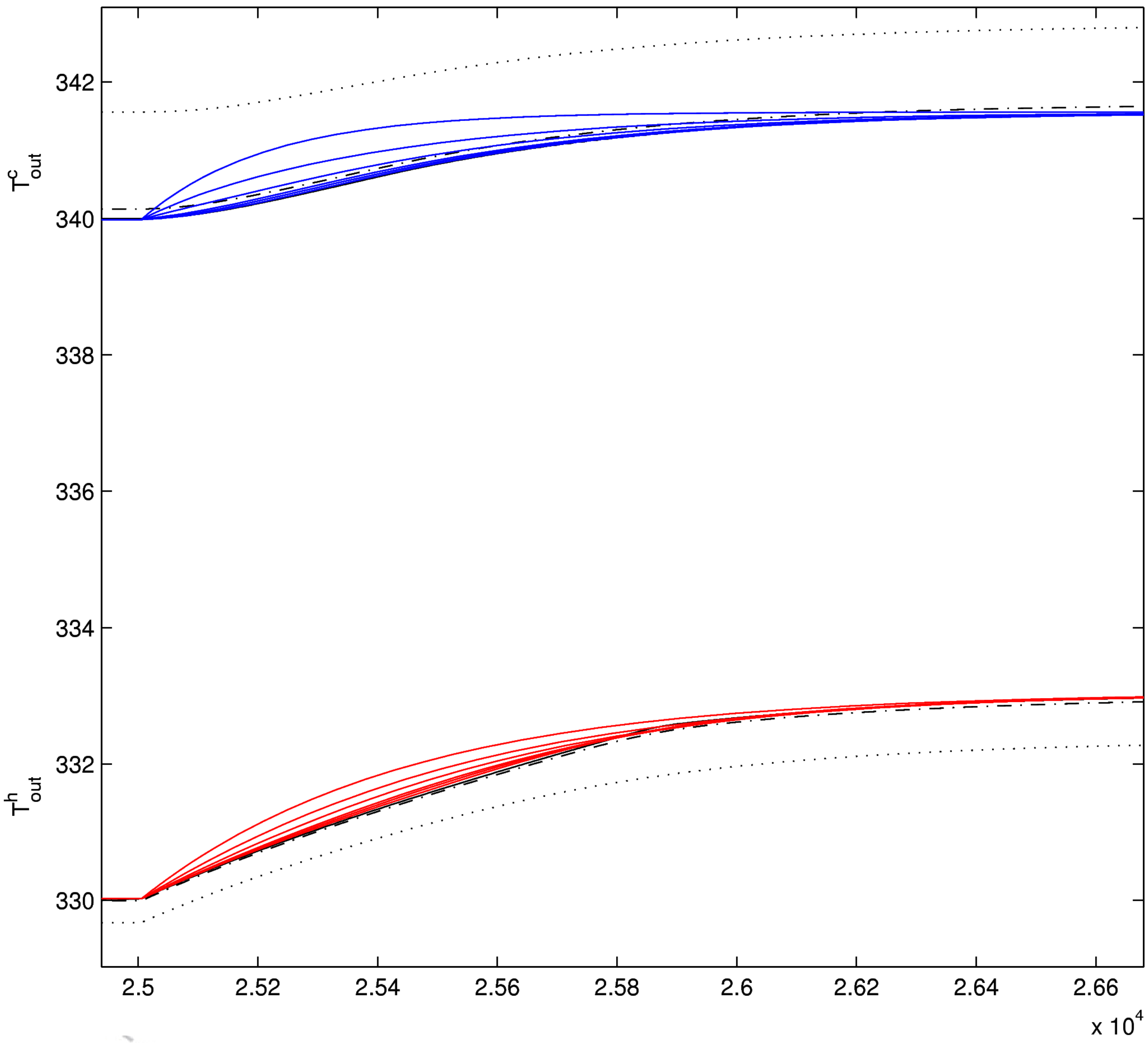
Response of hot and cold outputs to slow change in hot inflow temperature

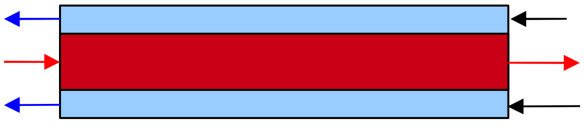


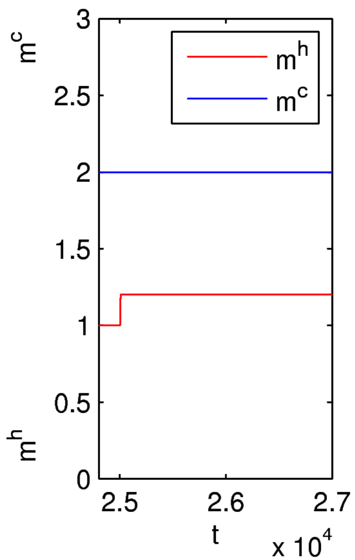




Response of hot and cold outputs to step change in hot inflow rate







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, applying only first step 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)

A. Linhart, S. Skogestad: Computational performance of aggregated distillation models. Computers & Chemical Engineering 31, 296-308 (2009)

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Model stage equations for component mass and energy:

Full model: (stage i)

$$\dot{M}_{i,k} = L^{out}_{i-1} x_{i-1,k} + V^{in}_{i} y_{i+1,k} - L^{out}_{i} x_{i,k} - V^{in}_{i-1} y_{i,k}, \;\; k = \{1,2\}$$

$$\dot{U}^{tot}_{i} = L^{out}_{i-1} h^{liq}_{i-1} + V^{in}_{i} h^{vap}_{i+1} - L^{out}_{i} h^{liq}_{i} - V^{in}_{i-1} h^{vap}_{i}$$

Reduced model: (aggregation stage j with index s_j)

$$H_j \dot{M}_{s_j,k} = L^{out}_{s_j-1} x_{s_j-1,k} + V^{in}_{s_j} y_{s_j+1,k} - L^{out}_{s_j} x_{s_j,k} - V^{in}_{s_j-1} y_{s_j,k}, \quad k = \{1,2\}$$

$$H_j \dot{U}^{tot}_{s_j} = L^{out}_{s_j-1} h^{liq}_{s_j-1} + V^{in}_{s_j} h^{vap}_{s_j+1} - L^{out}_{s_j} h^{liq}_{s_j} - V^{in}_{s_j-1} h^{vap}_{s_j}$$

Reduced model: (steady-state stages)

$$0 = L^{out}_{i-1} x_{i-1,k} + V^{in}_{i} y_{i+1,k} - L^{out}_{i} x_{i,k} - V^{in}_{i-1} y_{i,k}, \;\; k = \{1,2\}$$

$$0 = L^{out}_{i-1} h^{liq}_{i-1} + V^{in}_{i} h^{vap}_{i+1} - L^{out}_{i} h^{liq}_{i} - V^{in}_{i-1} h^{vap}_{i}, \quad i = 1...N, i \neq s_j \;\; (j = 1...n)$$

Performance test:

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

Feed flow rate

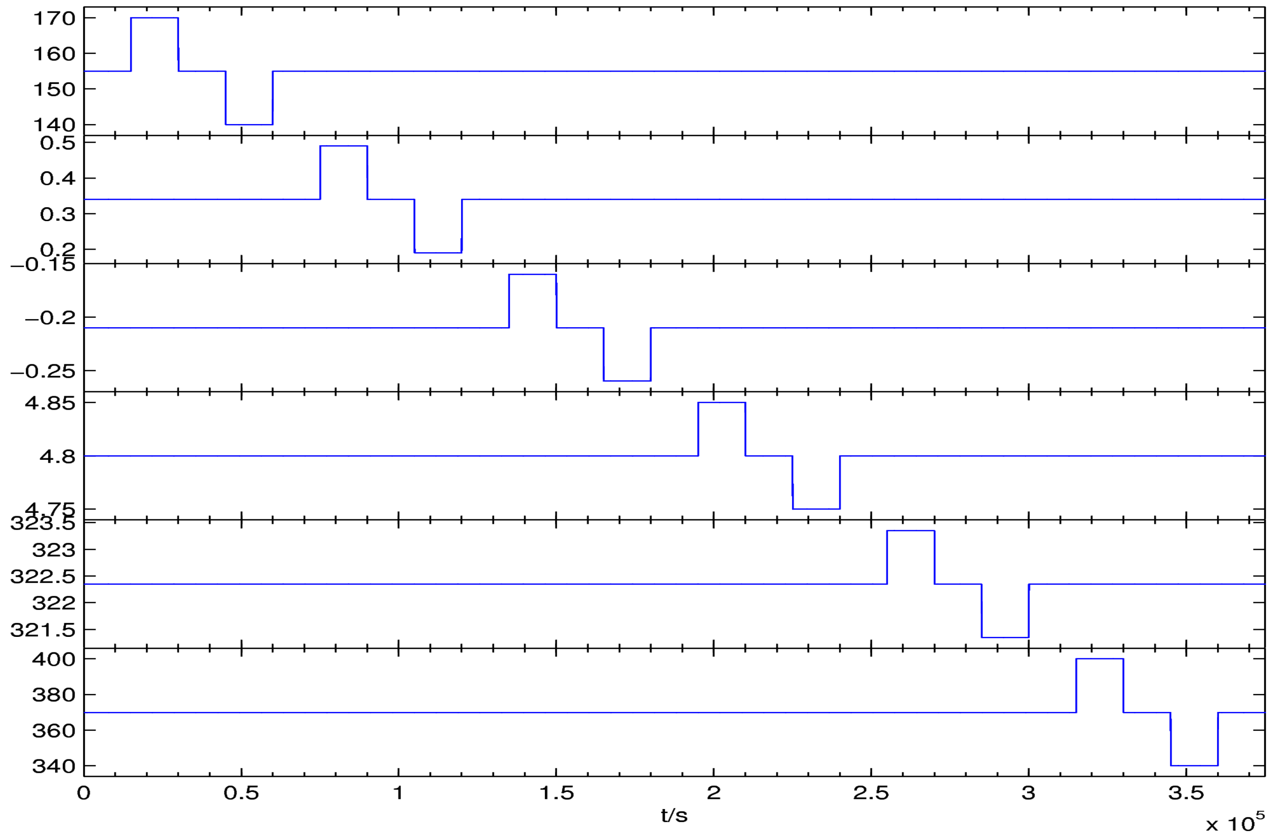
Feed concentration

Feed enthalpy

Pressure setpoint

Temperature setpoint

Reflux flow rate



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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.

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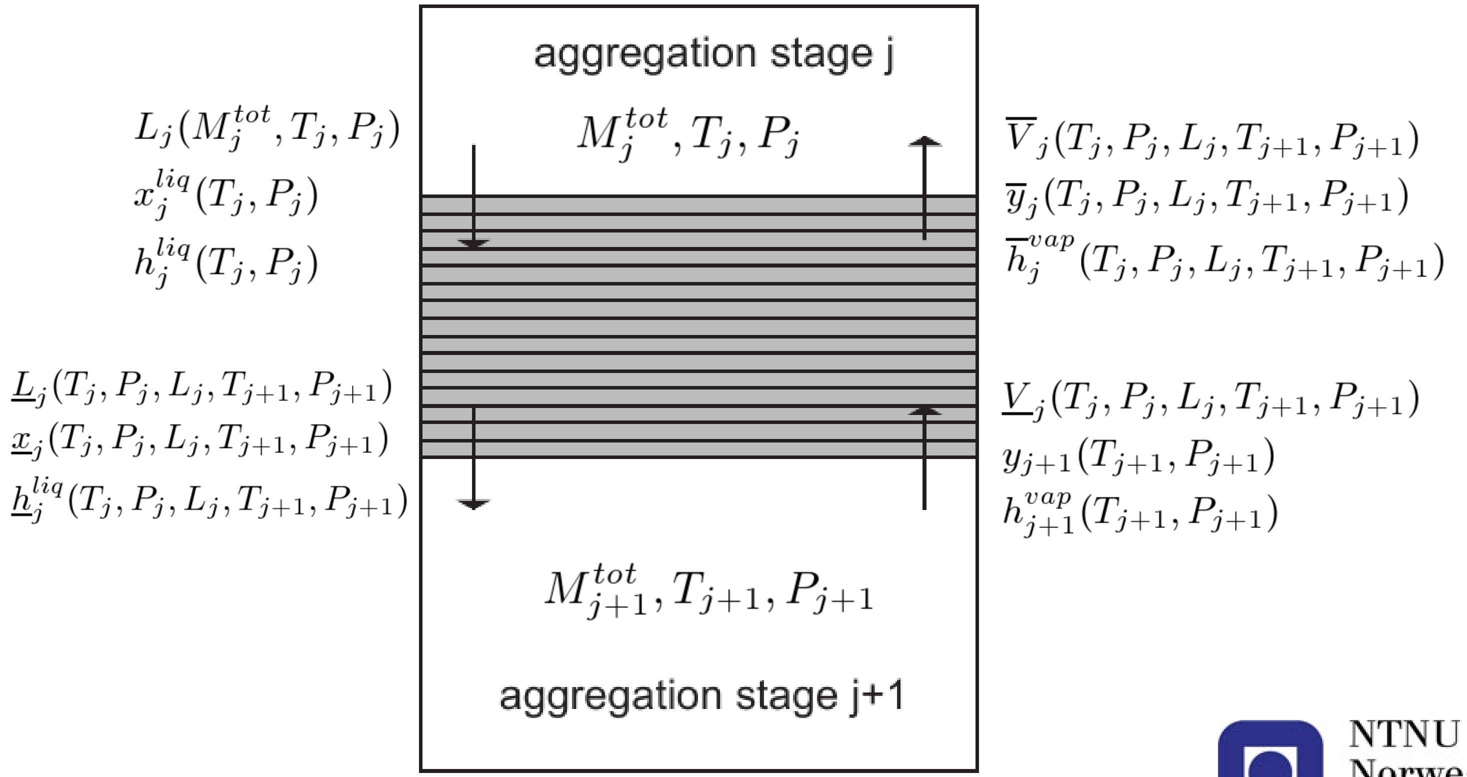
Elimination of steady-state tray equations:

- Equations for consecutive steady-state stages between two aggregation stages can be solved off-line in dependence of states of neighbouring aggregation stages
- 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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Representation of function values:

1) **Tabulation** and retrieval with suitable interpolation scheme

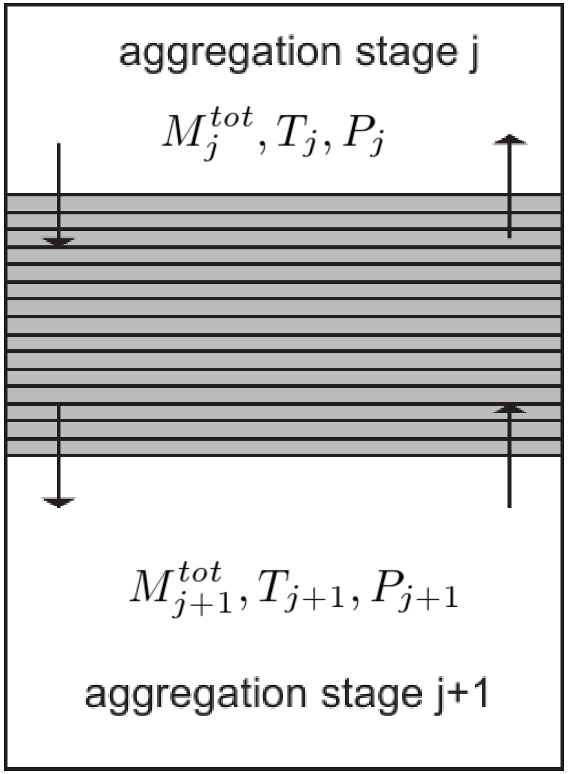
- Can handle the nonlinearities of the function
- Gives rise to very large tables
- Number of independent variables restricted

2) **Polynomial approximation** using linear regression

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

3) **Analytical solution**

- Available only for simple systems



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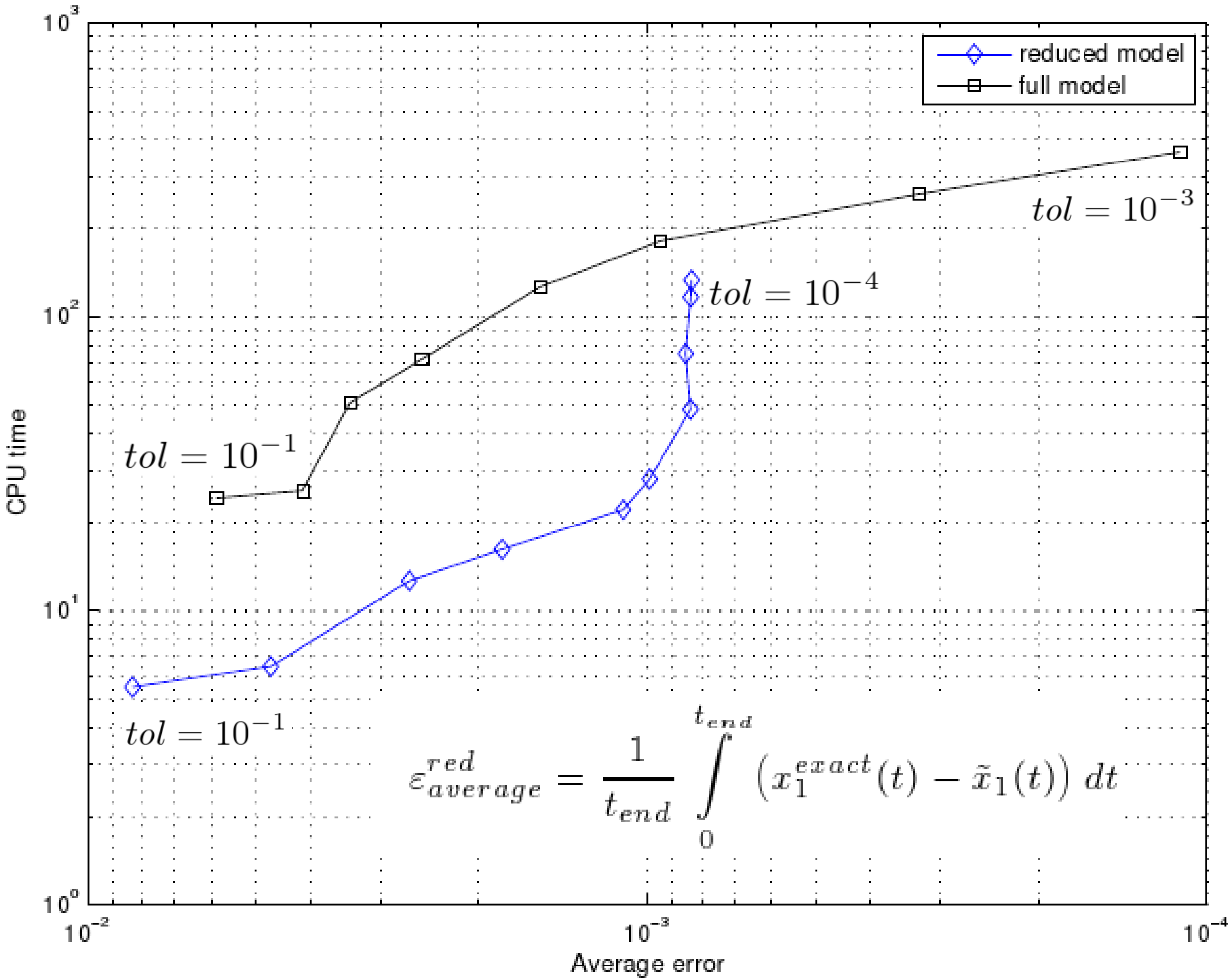
Reduced model equations:

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

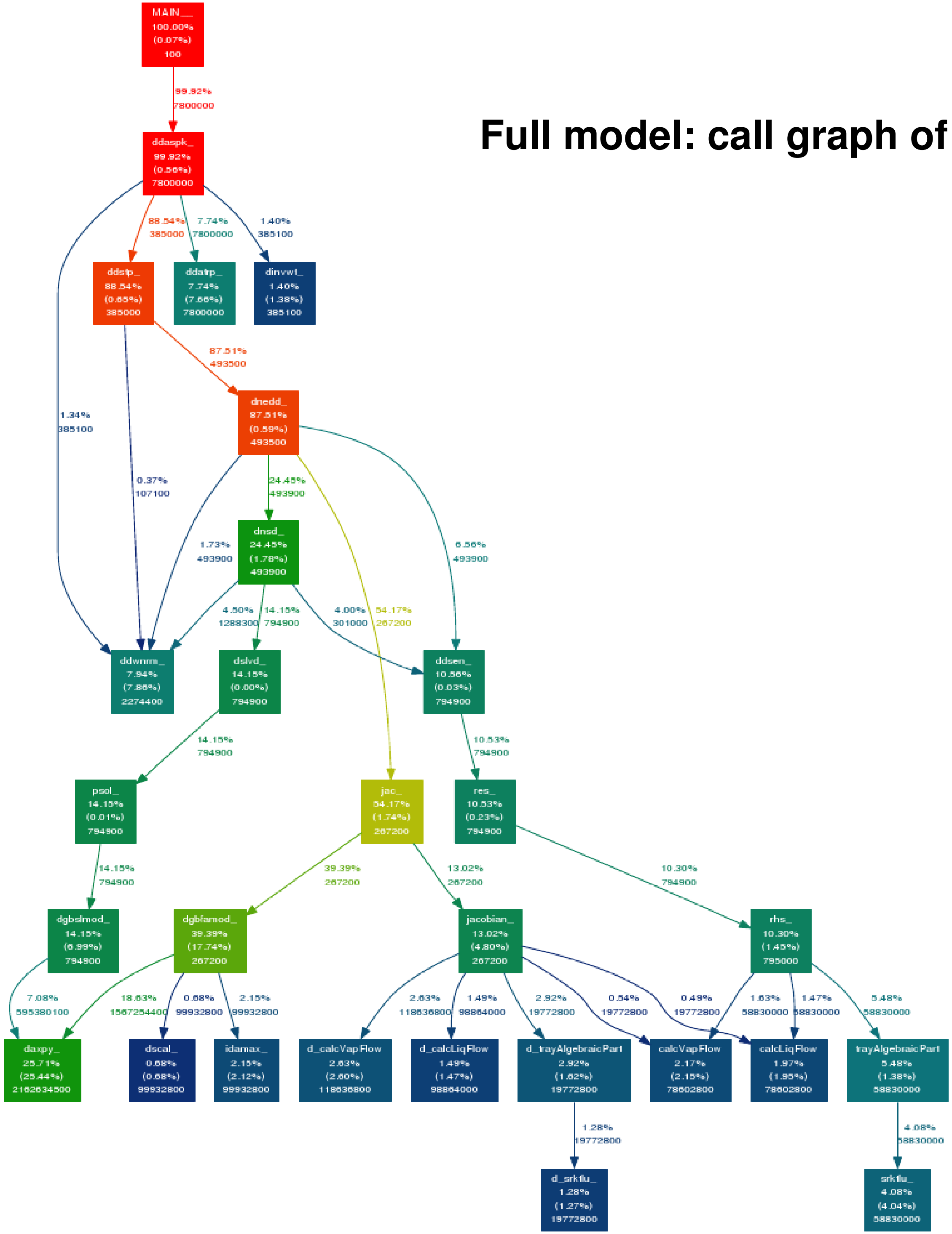
Solutions of steady-state trays:

$$
\begin{array}{ll}
\underline{L}_j (T_j, P_j, L_j, T_{j+1}, P_{j+1}) & \overline{V}_j (T_j, P_j, L_j, T_{j+1}, P_{j+1}) \\
\underline{x}_j (T_j, P_j, L_j, T_{j+1}, P_{j+1}) & \overline{y}_j (T_j, P_j, L_j, T_{j+1}, P_{j+1}) \\
\underline{h}_j^{liq} (T_j, P_j, L_j, T_{j+1}, P_{j+1}) & \overline{h}_j^{vap} (T_j, P_j, L_j, T_{j+1}, P_{j+1})
\end{array}
$$

Performance comparison



Full model: call graph of DASPK simulation



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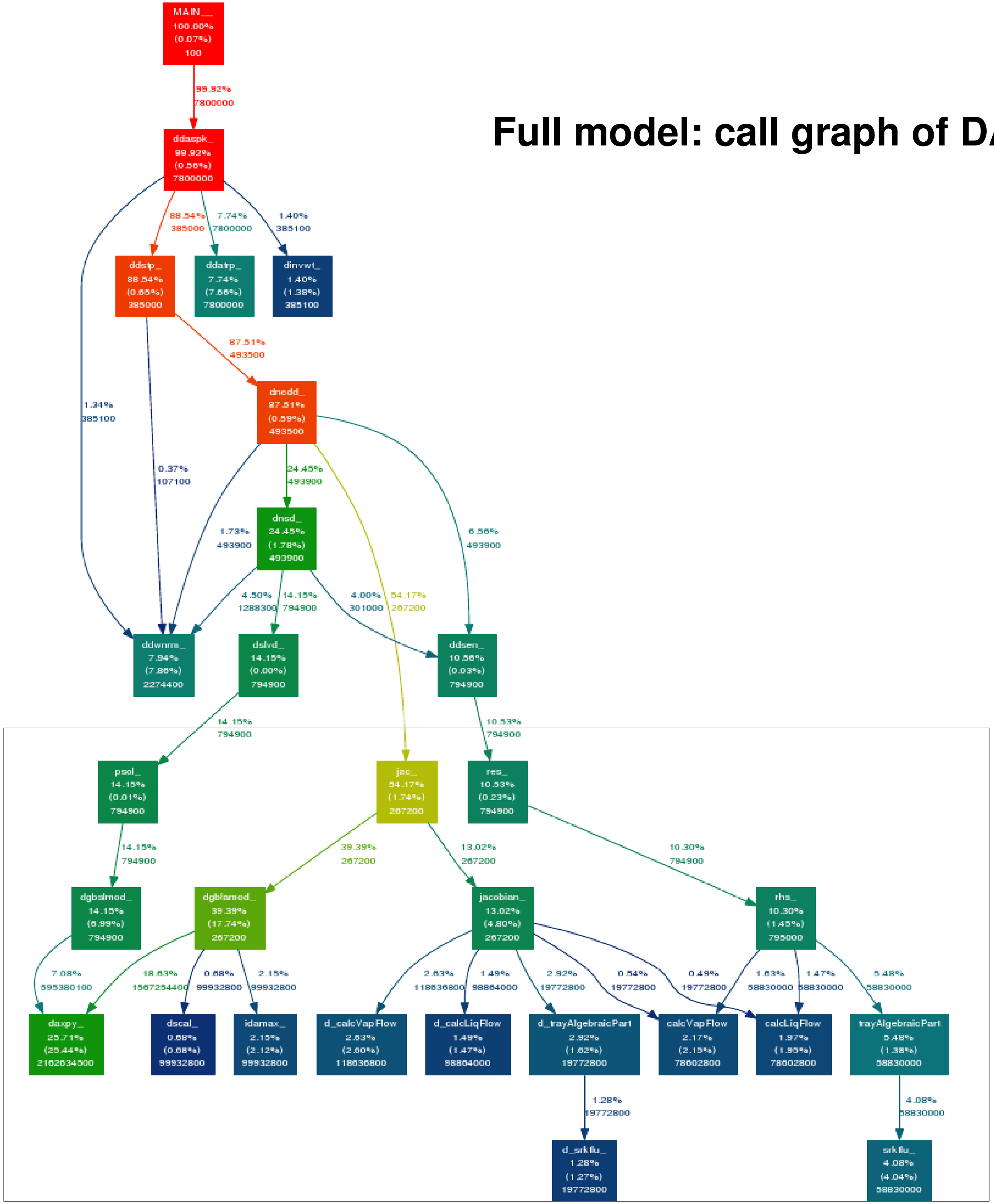
Full model: call graph of DASPK simulation



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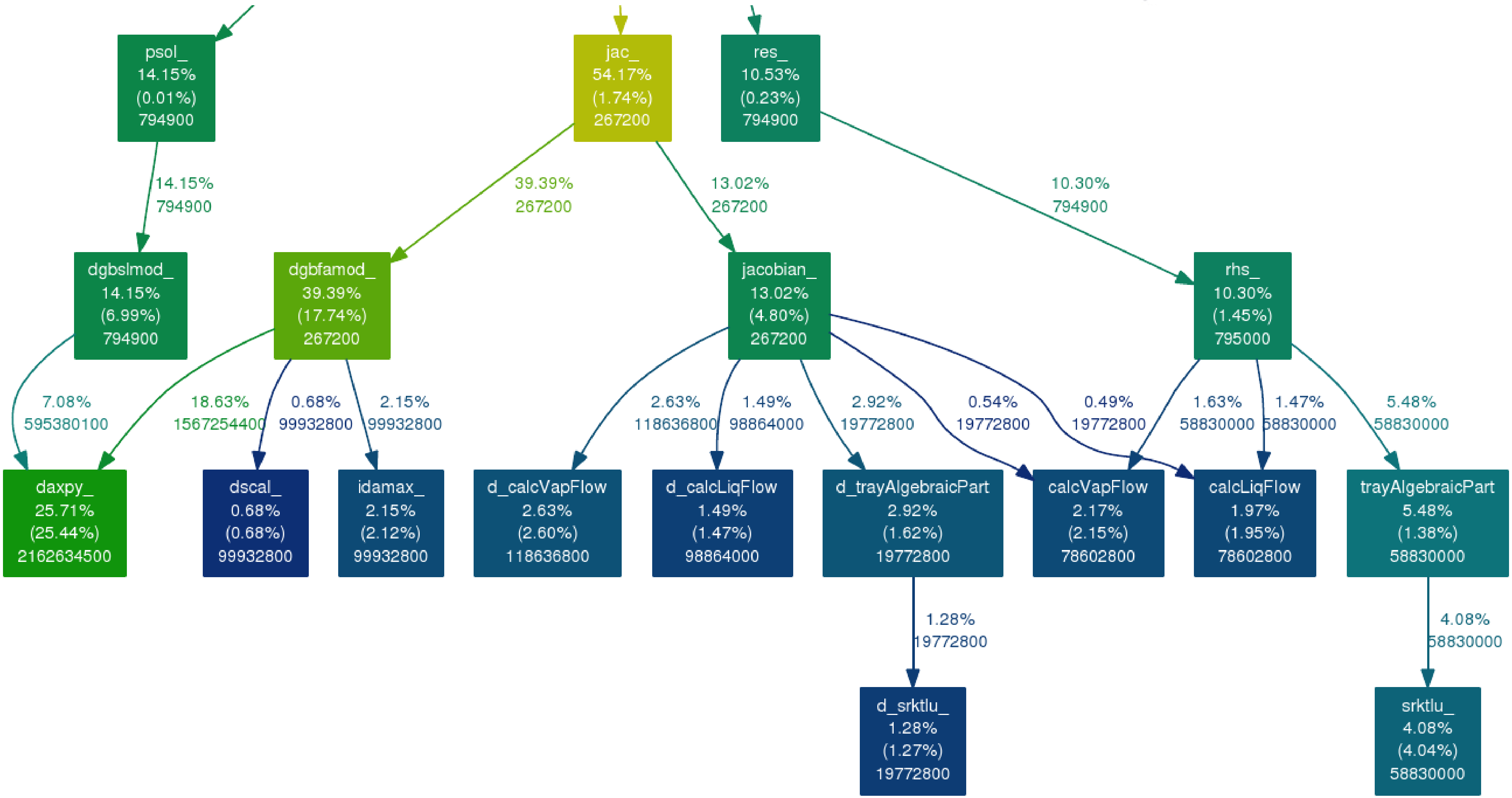
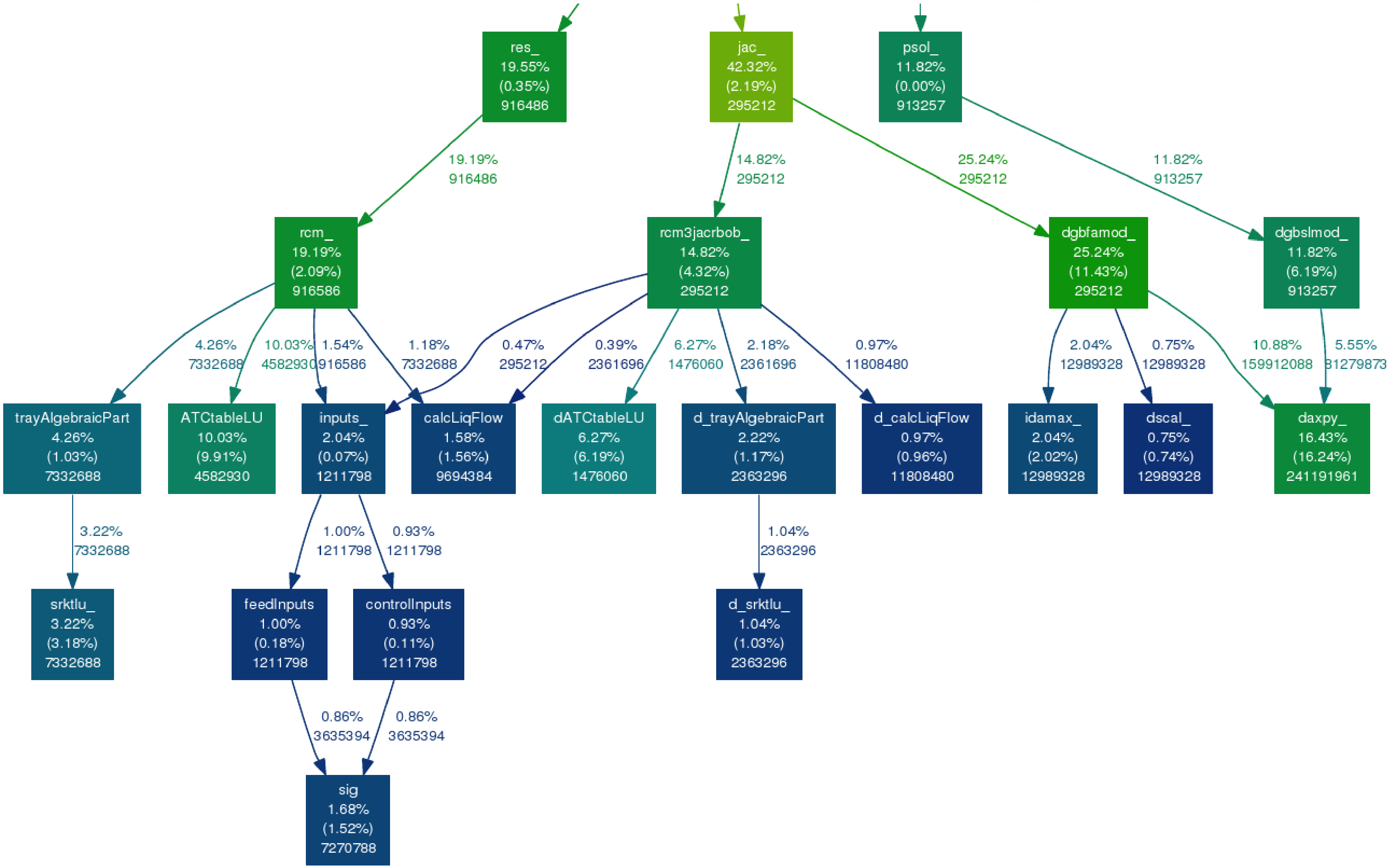
Full model: call graph of DASPK simulation



Reduced model: call graph of DASPK simulation



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

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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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