# A multiscale method for separation processes in chemical engineering

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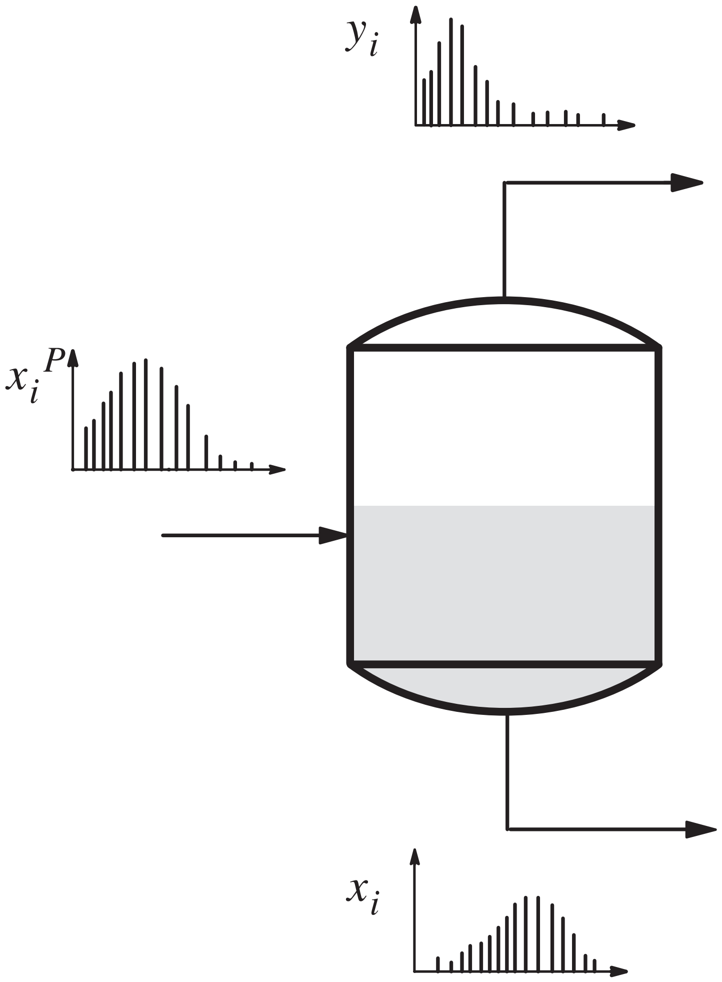
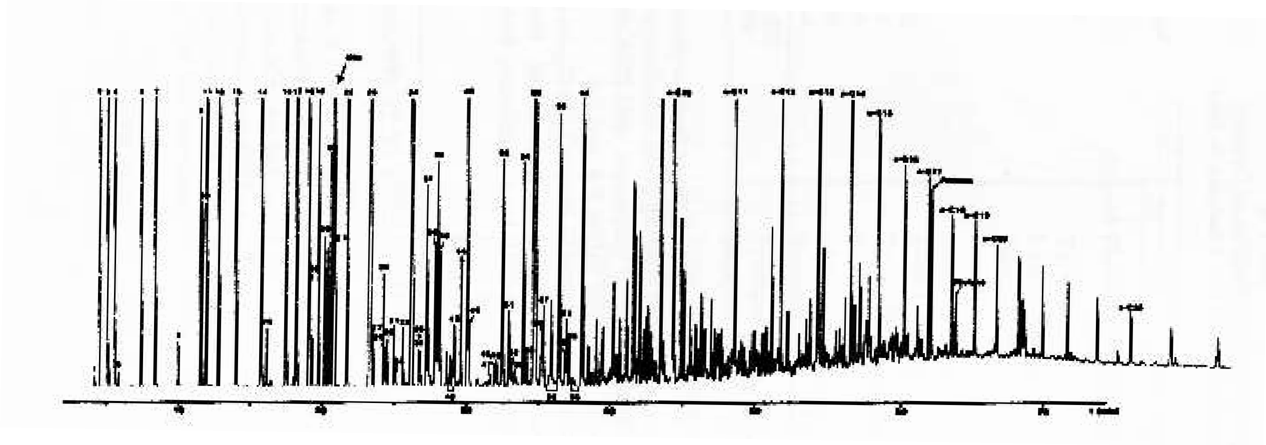
## A separation process – single equilibrium flash unit




- the feed is separated by the unit into the vapour and the liquid stream
- generic submodel of a separation process
- example: oil tanks in a harbour

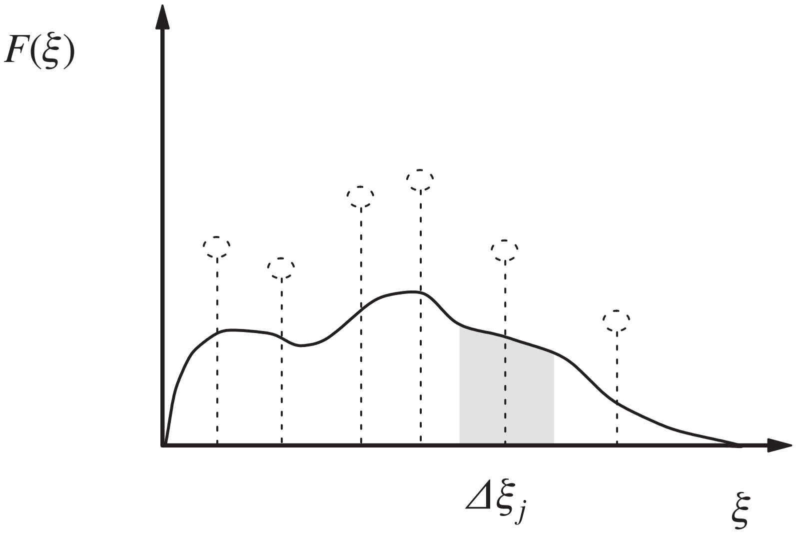
## An example – A north sea oil



- nearly no separation between species possible
  $\rightsquigarrow$ no exact thermodynamic modelling
- very strong scattering
- no knowledge of redundancy

- high reduction of the system
  $\rightsquigarrow$ reproduce curvature with global functions
- high local approximation order
  $\rightsquigarrow$ reproduce local scatter by local functions
- after reduction all components should be reproducable

## Continuous modelling

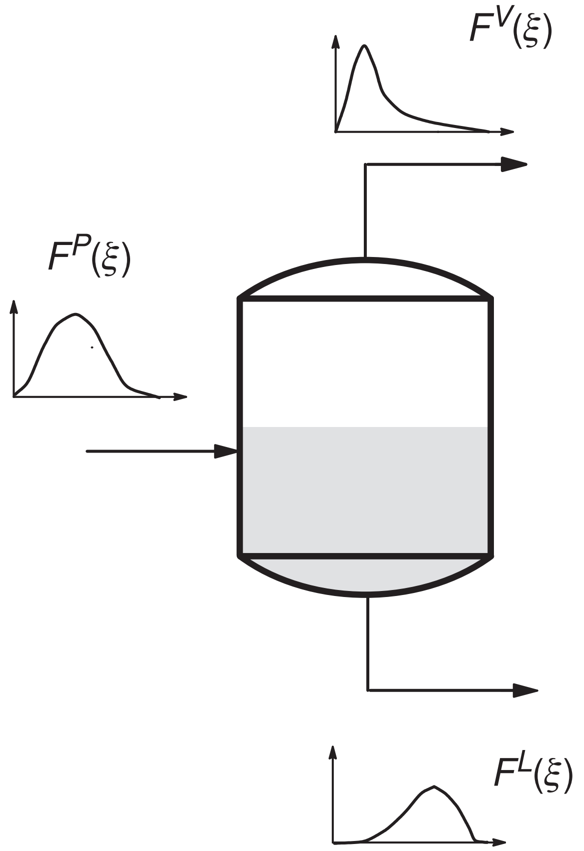



- histogram is approximated by a distribution function
- given: $x_i(t)$, $i = 1, \ldots, N$
- find: a distribution function $F(\xi, t)$ such that

$$x_i(t) = \int_{\Delta\xi_i} F(\xi, t)\, d\xi, \quad i = 1, \ldots, N$$

$\rightsquigarrow$ consistent framework in thermodynamic

## Governing equations




| | | |
|---|---|---|
| **Given:** | $P,\ F^P$ | Feed |
| | $\alpha$ | evapouration rate |
| | $K(\cdot,\cdot,\cdot)$ | phase equilibrium coefficient |
| | $n$ | holdup constant |
| **Seek for:** | $V,\ F^V$ | Vapour stream |
| | $L,\ F^L$ | Liquid stream |
| | $T$ | Temperature |

$$
\begin{aligned}
n\,\frac{\partial}{\partial t}F^L(\xi,t) + L\,F^L(\xi,t) + V\,F^V(\xi,t) &= P\,F^P(\xi,t) && (1)\\
F^V(\xi,t) - K(F^L,F^V,T)\,F^L(\xi,t) &= 0 && (2)\\
\int_\xi F^V(\xi,t)\,d\xi &= 1 && (3)\\
V &= \alpha\,P && (4)\\
L + V &= P && (5)\\
F^L(\xi,0) &= F_0^L(\xi) && (6)
\end{aligned}
$$

- (1): component mass balance
  (2): equlibrium relation
  (5): overall mass balance
- $\rightsquigarrow$ (highly) nonlinear DAE system

## Mathematical Modelling

- $\tilde{\varphi} = \chi_{[0,1]}$,
  choose $\varphi$ as a dual function according to $\tilde{\varphi}$, i. e.

  $$(\varphi_{j,k}, \tilde{\varphi}_{j,k'})_{L^2([0,1])} \;=\; \delta_{k,k'}$$

  $\rightsquigarrow$ arbitrary high approximation order
  (Cohen, Daubechies, Feauveau; Dahmen, Kunoth, U.)

- $N = 2^j$, $\Delta\xi_i = [(i-1)2^{-j}, i2^{-j}]$, $i = 1, \ldots, N$
  $\rightsquigarrow F^P(\xi, t) := \sum\limits_{k=1}^{N} c_k^P(t)\,\varphi_{j,k}$

- $\rightsquigarrow$

  $$\begin{aligned} c_k^P(t) \;&=\; \sum_{i=1}^{N} c_i^P(t)\,(\varphi_{j,i}, \tilde{\varphi}_{j,k})_{L^2([0,1])} \;=\; \sum_{i=1}^{N} c_i^P(t) \int_{\Delta\xi_k} \varphi_{j,i}(\xi)\,d\xi \\ &=\; \int_{\Delta\xi_k} F^P(\xi, t)\,d\xi \;=\; x_i^P(t) \end{aligned}$$

- $\psi$, $\tilde{\psi}$ biorthogonal wavelets according to $\varphi$, $\tilde{\varphi}$

- $\rightsquigarrow$ for $X \in \{P, L, V\}$:

  $$\begin{aligned} F^X(\xi, t) \;&= \sum_k c_k^X(t)\,\varphi_{j,k}(\xi) && \text{single scale representation} \\ &= \sum_{m=-1}^{j-1} \sum_k d_{m,k}^X(t)\,\psi_{m,k}(\xi) && \text{multiscale representation} \end{aligned}$$

- combination of global curvature and local details

## Biorthogonal spline wavelets

(Cohen, Daubechies, Feauveau)

## Multiscale methods

- treat nonlinear system by a Petrov–Galerkin method
- trial spaces: $S_j = \operatorname{span}\{\varphi_{j,k} : k \in I_j\}$ (multiresolution on an interval)
- wavelet spaces: $W_j = \operatorname{span}\{\psi_{j,k} : k \in J_j\}$

$$S_{j+1} = S_j \oplus W_j$$

- for $X \in \{P, L, V\}$:

$$\begin{aligned} F^X(\xi,t) &= \sum_k c_k^X(t)\,\varphi_{j,k}(\xi) && \text{single scale representation} \\ &= \sum_{m=-1}^{j-1} \sum_k d_{m,k}^X(t)\,\psi_{m,k}(\xi) && \text{multiscale representation} \end{aligned}$$

- single scale representation:
  - efficient evaluation of integrals
  - sparse matrices
  - reproducability of all components
- multiscale representation:
  - preconditioners
  - adaptivity
  - reduction of the size of the system
- $T_j : \boldsymbol{c}^j \mapsto \boldsymbol{d}^j$ *Multiscale transformation*

## Model size reduction

- consider multiscale representation

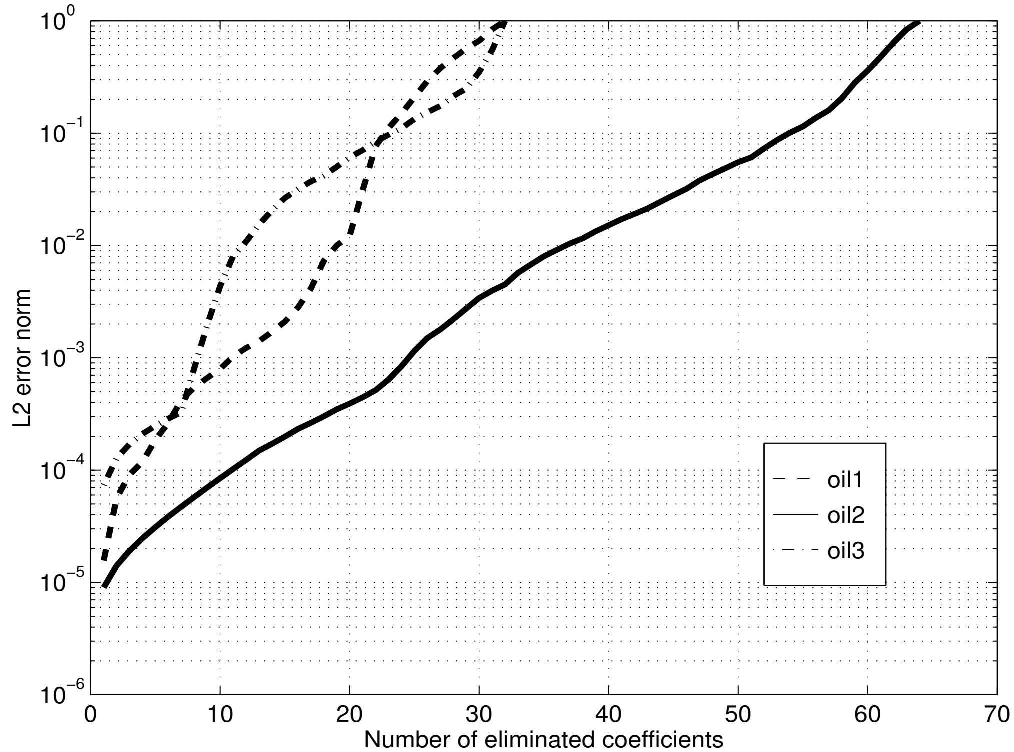
$$F^P(\xi, t) = \sum_{m=-1}^{j-1} \sum_k d_{m,k}^P(t)\, \psi_{m,k}(\xi)$$

- build approximation by thresholding:

$$F^P(\xi, t) \approx \sum_{m=-1}^{j-1} \sum_k \hat{d}_{m,k}^P(t)\, \psi_{m,k}(\xi)$$

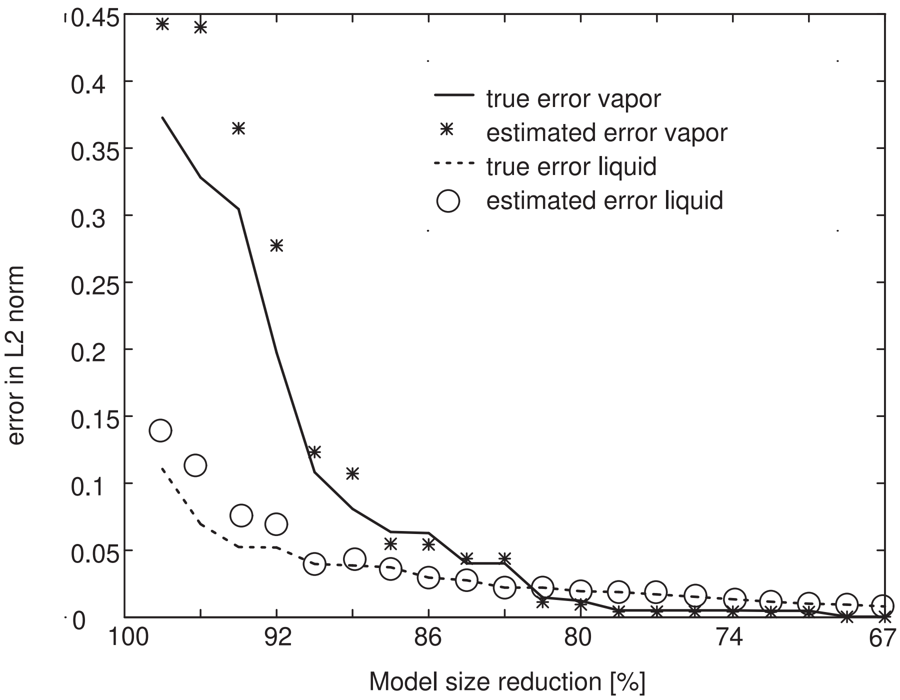
$$\hat{d}_{m,k}^P(t) := \begin{cases} d_{m,k}^P(t), & \text{if } |d_{m,k}^P(t)| > \varepsilon, \\ 0, & \text{else,} \end{cases}$$

for a given tolerance $\varepsilon$.



## Adaptive techniques

- represent residual of the system in multiscale representation
- start on a very coarse level
- construct estimator for the error of the unconsidered multiscale coefficients
- add those equations according to coefficients needed for a given accuracy



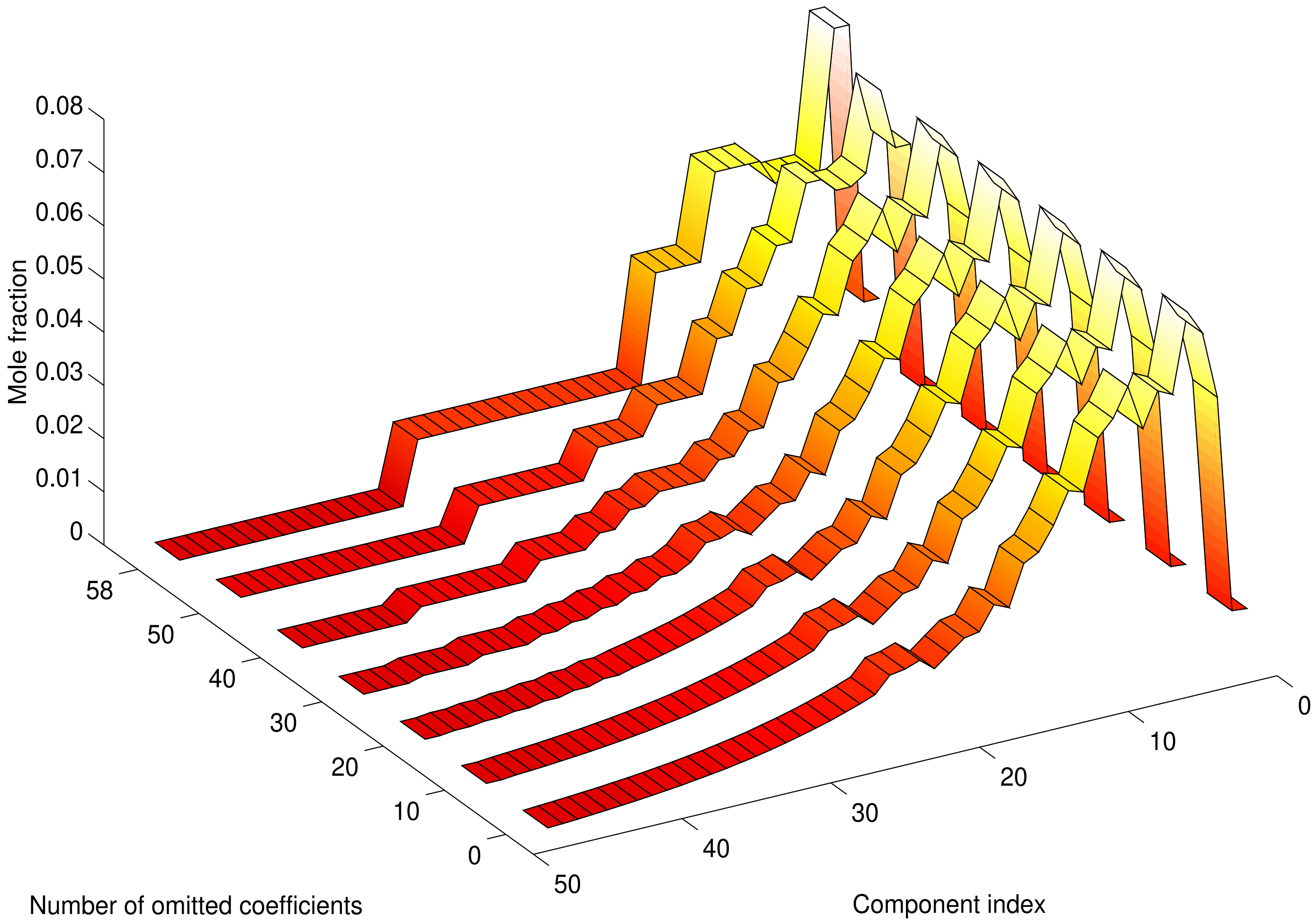
## First results

- implicit Euler for time discretization
- Newton-type method for the nonlinear system (IMSL)
- numerical evaluation of Jacobi matrices
- Haar wavelets

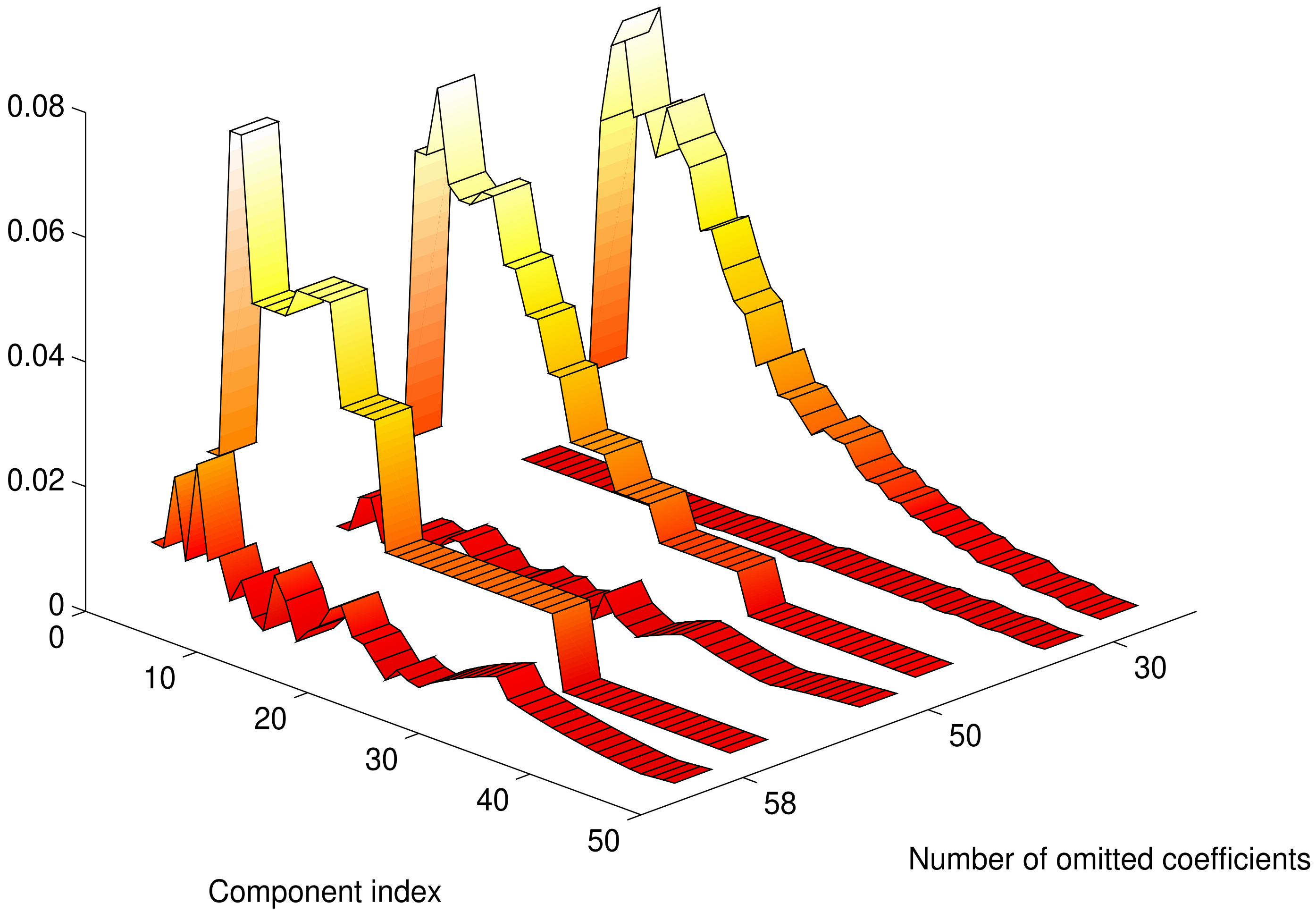
## Outlook

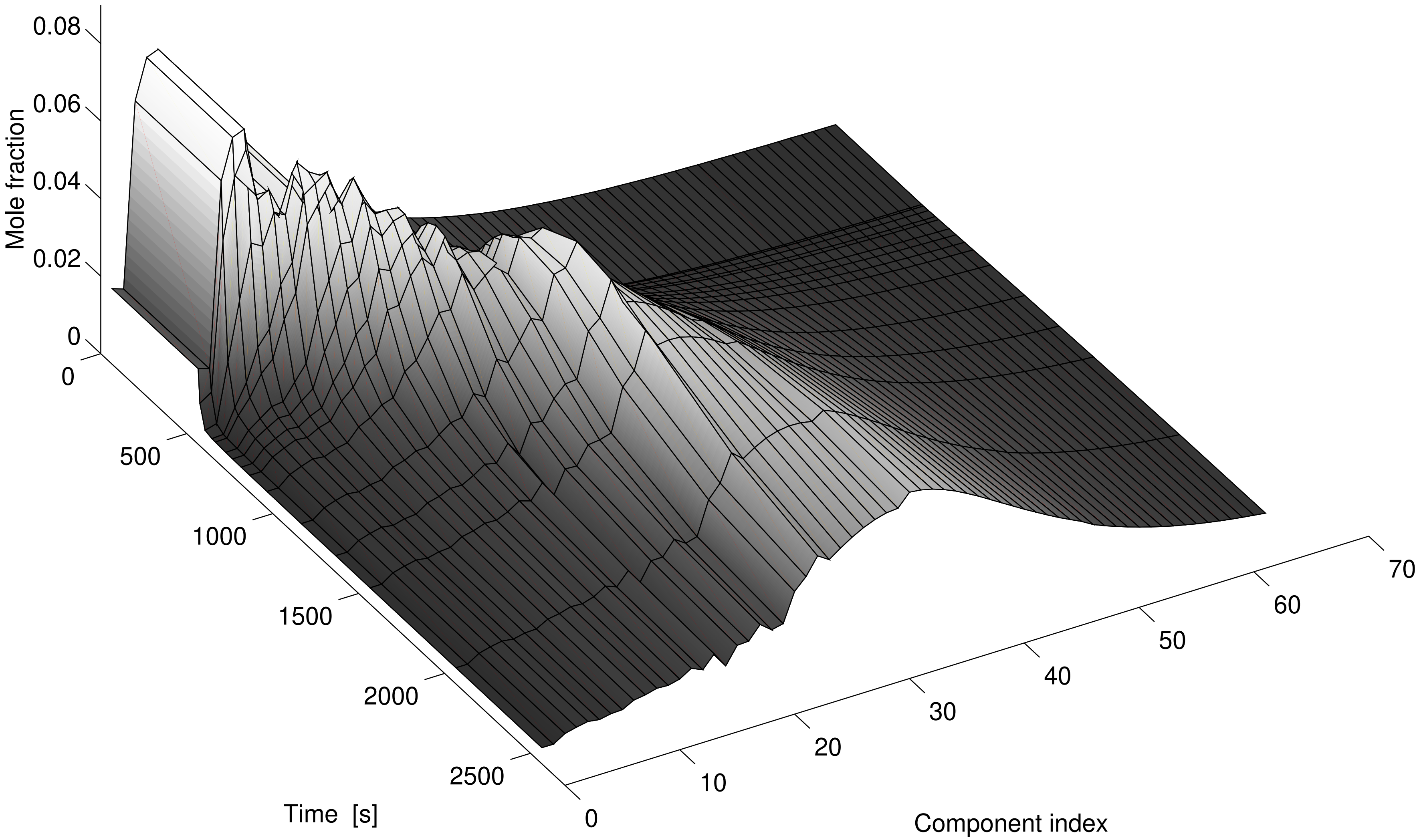
- construction of error estimators
- implement multilevel preconditioners
- wavelet systems of higher approximation order
- exact evaluation of Jacobi matrices (Dahmen/Micchelli)
- ...

# Model Reduction: Adjustable Accuracy



# Model Reduction: Error Distribution




Mole fraction
0.08
0.06
0.04
0.02
0
Time [s]
0
500
1000
1500
2000
2500
Component index
0
10
20
30
40
50
60
70