Finite state estimation and control of a multi-input CSTR benchmark

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TOULOUSE IFAC 2017

IFAC 2017 World Congress, Toulouse, France

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Outline:

- **MDP and state estimation**
  - **MDP & state estimation**
  - **FADP (finite ADP)**
- **VDV benchmark simulations**
  - **System set-up**
  - **Simulations**
- **Conclusions & Future works**

Finite state and action optimal control design I

- **Markov decision processes (MDP)**
  - Discrete time finite state and action Markov chains
  - Dynamic programming
- **Discretization**
  - irregular grid $s = \lfloor \arg\min_{s \in \mathcal{S}} \|\mathbf{x} - \mathbf{x}_s^c\|_{\mathbf{W}} \rfloor$
  - modeling (simulation + counting => **P**'s & **L**)

$$\begin{aligned} \mathbf{x}(k+1) &= f(\mathbf{x}(k), \mathbf{u}(k), \mathbf{w}(k)) \\ \mathbf{y}(k) &= h(\mathbf{x}(k), \mathbf{v}(k)) \end{aligned} \qquad \begin{aligned} \mathbf{q}(k+1) &= \mathbf{q}(k)\mathbf{P}^{a(k)} \\ \mathbf{o}(k) &= \mathbf{q}(k)\mathbf{L}(k), \end{aligned}$$

- **Optimal control**
  - minimize sum of immediate costs in future horizon

$$J = \sum_{k'=0,1,\ldots,K} \lambda^{k'} c(\mathbf{x}(k+k'), \mathbf{u}(k+k'))$$

  - value iteration => control table
- **Cell filter**
  - Bayesian state estimation

$$\begin{aligned} \mathbf{q}(k|k-1) &= \mathbf{q}(k-1|k-1)\mathbf{P}^{a(k-1)} \\ \mathbf{q}(k|k) &\sim \mathbf{1}^{\top}{}_{m(k)} \cdot \mathbf{q}(k|k-1) \end{aligned}$$

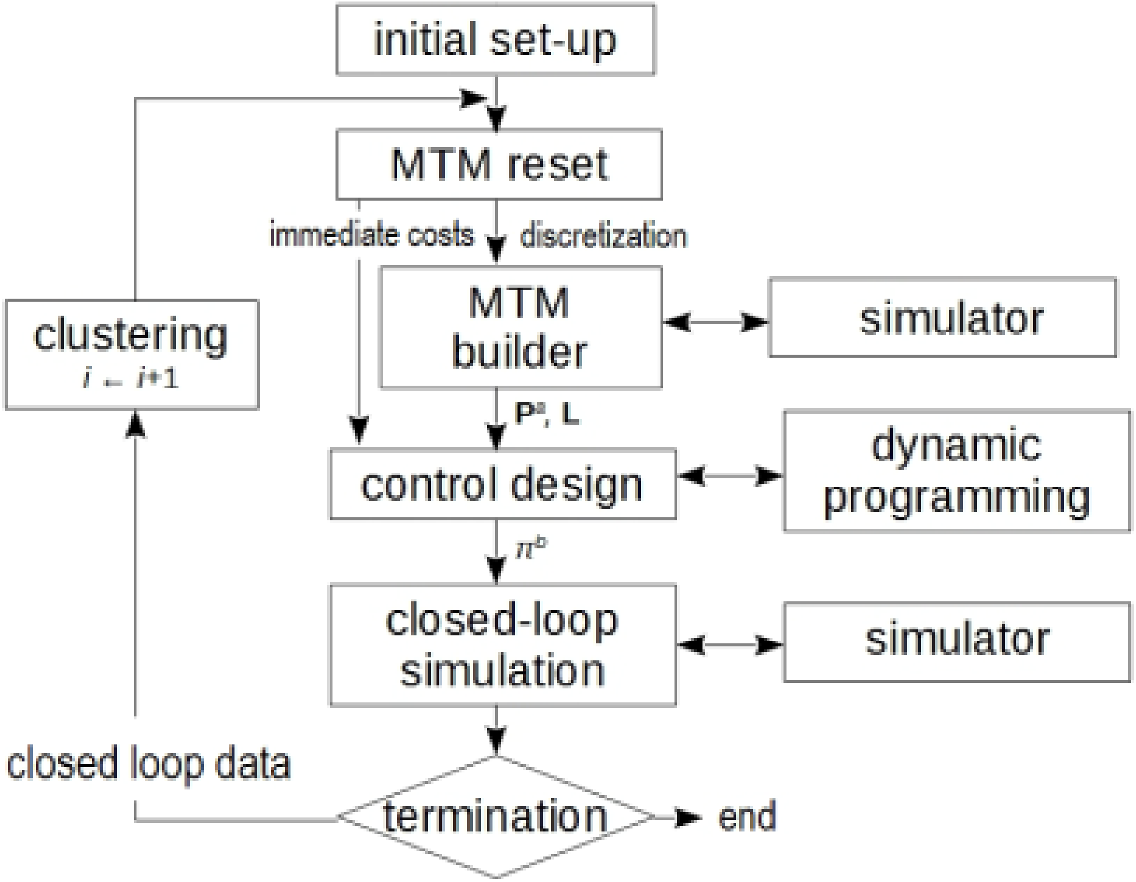
  - ML estimate for control

Finite state and action optimal control design II

FADP

– **Finite Approximate Dynamic Programming**

- iterative re-discretization of closed-loop data
- hierarchical k-means clustering



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Process control using finite Markov chains with iterative clustering

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Process control using finite Markov chains with iterative clustering

– FADP

- Finite approximate dynamic programming
- An approach to tackle the curse of dimensionality problem
  yet retaining the benefits of the finite state MDP in control and estimator design
- iterative re-discretization based on clustering of closed-loop data.
- hierarchical k-means clustering

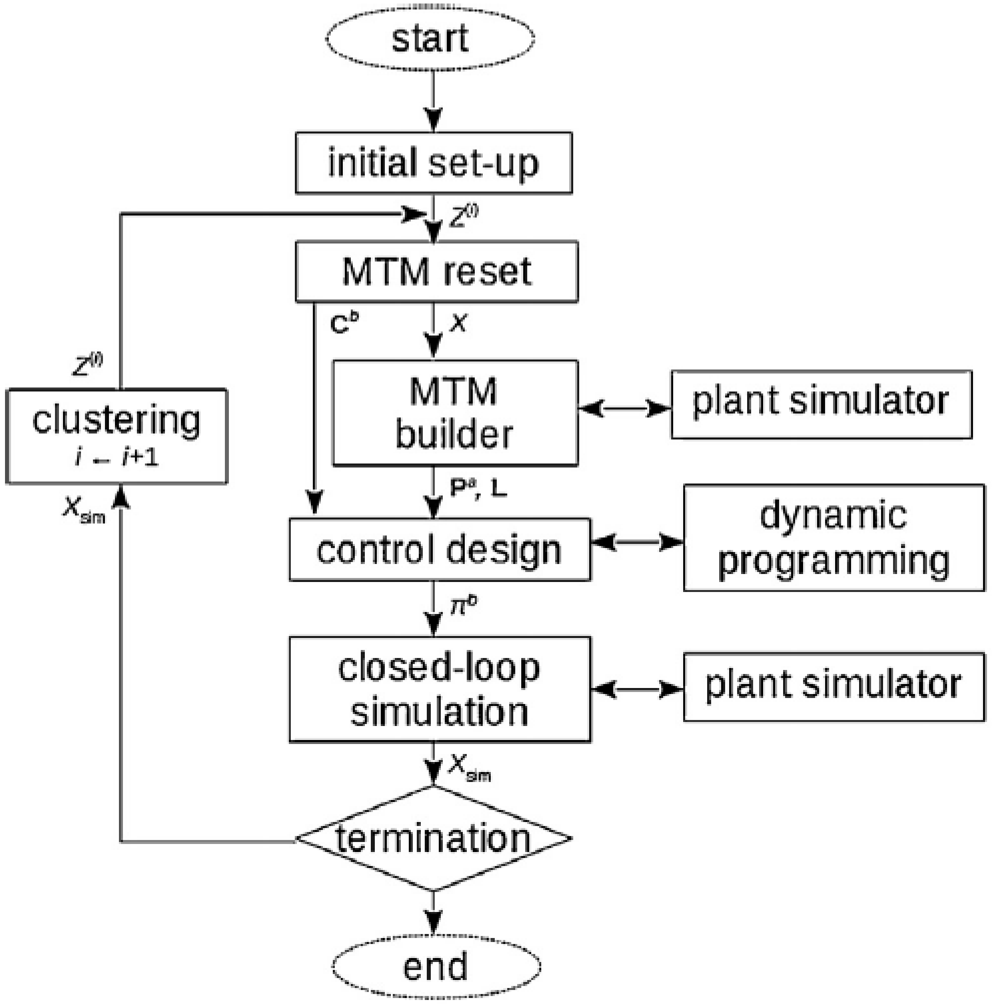

Fig. 1. FADP algorithm.

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FADP

steps

- **Clustering** of the data in X_{sim} is conducted using hierarchical k-means to find N new cluster centroids $Z^{(i+1)}$. Clustering at first few iterations may not provide a proper description of the space occupied by the closed-loop system, and to avoid unnecessary simulations the number of model evaluations E and clusters N can be gradually increased as a function of iterations: $E_{i+1} = E_i + \Delta E$, $N_{i+1} = N_i + \Delta N$.

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- **Initial set-up** includes the MTM discretization of input and measurement spaces into A and M finite sets(defined by $Y = \{\mathbf{y}_m\}$ and $U = \{\mathbf{u}_a\}$, with weighing matrices if used) and the initial clustering $Z^{(0)}$ of $\mathcal{X}$ with weighing matrix $\mathbf{W}$. The design specifications fo… c(…

- **MTM reset** constructs the state discretization $X = \{\mathbf{x}_s^c\}$ based on the clustering $Z^{(i)}$. The immediate cost matrix $\mathbf{C}^b = [c_{s,a}^b]$ corresponding to the discretization and control designs specifications is… o… d…

- **MTM builder** constructs the probability transition matrices $\mathbf{P}^a$, as well as the likelihood matrix $\mathbf{L}$. The building of MTM is based on simulating the system one sample time ahead E times, drawing th… e… acts… requ…

- **Control design** solves for the optimal controllers, based on the matrices $\mathbf{P}^a$ and $\mathbf{C}^b$. Simple value iteration can be used.

- **Closed-loop simulations** are conducted using the designed controllers and the plant simulator. The simulations should result in a sufficient number of state trajectory data X_{sim} in order to describe t… t… f… i… … considered as starting points. Since the plant is simulated, the states can be assumed to be fully known.

- **Termination** of the algorithm can be based on convergence of the clustering (e.g., mean distance between data point and its closest cluster centroid), satisfactory control performance (observed from closed-loop simulations), or simply on a predefined number of iterations or alike.

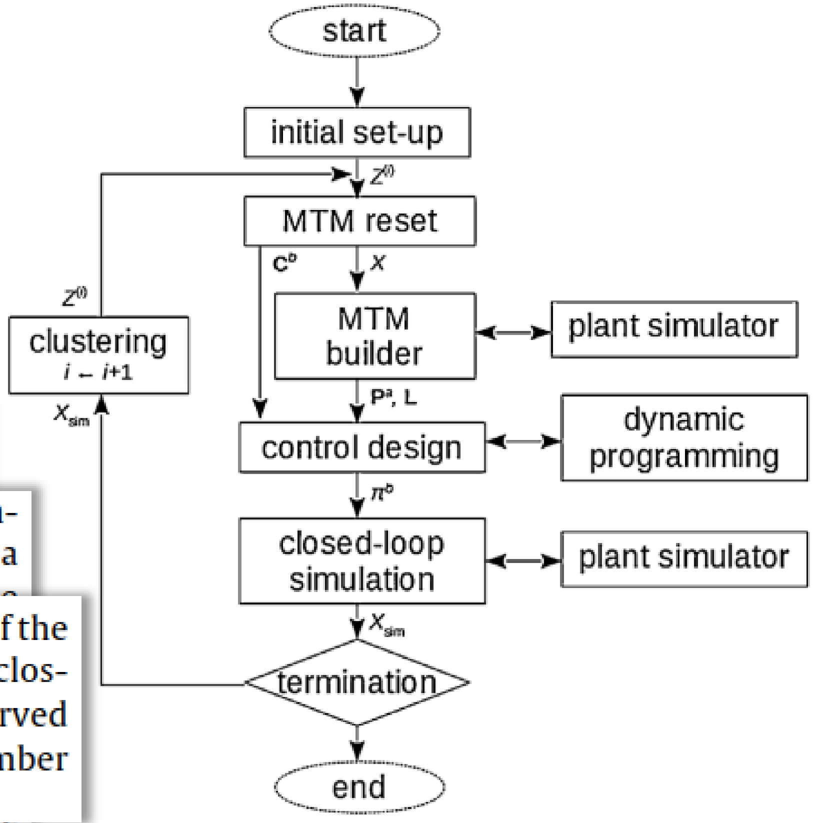

Fig. 1. FADP algorithm.

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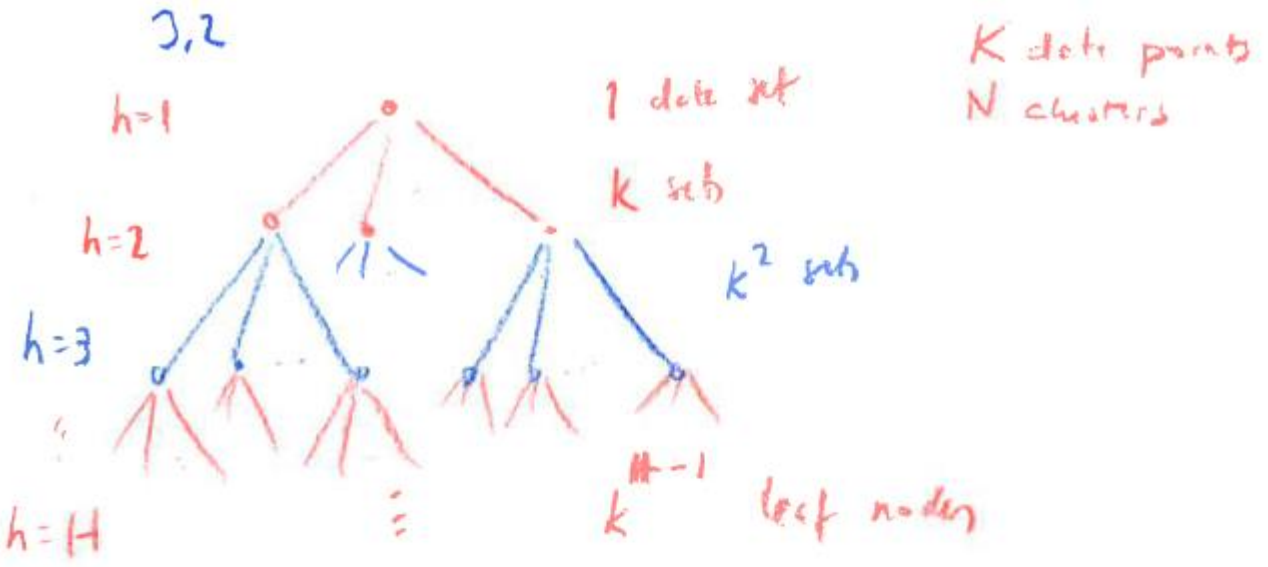
FADP

clustering with hierarchical k-means

Algorithm 1. The hierarchical k-means algorithm.

```
function [Z,D] = hkmeans(X,W,k,H,h,Z,D)
if nargin<4,
  N = k; H=ceil(log10(N)); k = ceil(N^(1/H)); h=1; Z=[]; D=[];
end
if h<H
  [~,~,w]=k_means(X,W,k);
  for c=1:k
    x = X(w==c,:);
    [Z,D] = hkmeans(x,W,k,H,h+1,Z,D);
  end
else
  [z,d]=k_means(X,W,k);
  Z = [Z;z]; D = [D;d];
end
```



Choose $k = \lceil N^{\frac{1}{H}} \rceil$ and $H = \lceil \log N \rceil$

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FADP
properties

- **FADP:**
  - based on iteratively enhanced clustering of state space, occupied by the plant in closed-loop.
  - scales well (*S* can be set)
  - preserves **P**^{a}'s and **L**
  - enables use of finite state & action MDP tools
    - DP, cell filter, analysis
  - model can be reinforced with data
  - off-line design procedure

- **Irrespective of the method used for discretizion:**
  - difficult to know *a priori* the state space covered by the plant in closed-loop
  - FADP provides an automated means to find a discretization suitable for control
- **Increased computational load**
  - re-building of transition matrices
  - simulation of closed-loop trajectories

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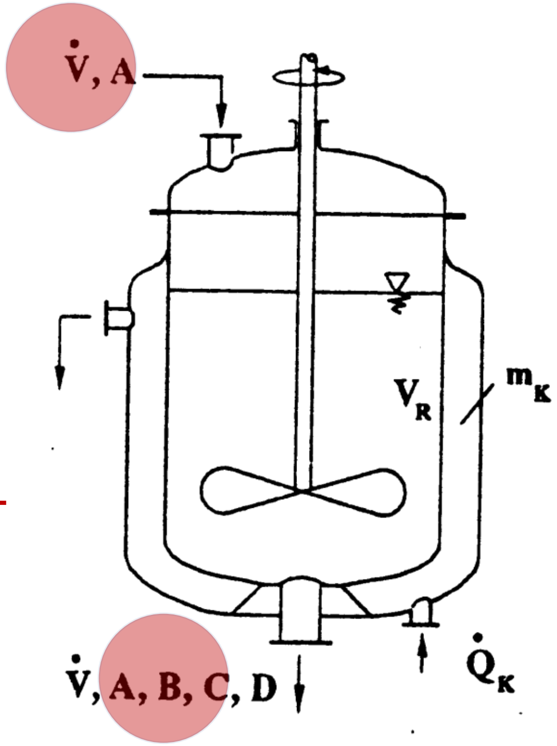
FADP

non-linear non-minimum phase CSTR

- van der Vusse benchmark
  (Chen et al. 1995)

$$
\begin{array}{ccccc}
A & \xrightarrow{k_1} & B & \xrightarrow{k_2} & C \\
2A & \xrightarrow{k_3} & D\ . & &
\end{array}
$$

By use of control we want to guarantee the production of cyclopentenol with desired purity $c_{B|s}$ despite variations in the feed temperature ϑ_0. We distinguish two control problems: A multi-input problem and a (more demanding) single-input problem.



NONLINEAR PREDICTIVE CONTROL OF A BENCHMARK CSTR

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The dynamics of the reactor can be described by the following nonlinear differential equations that are derived from component balances for substances A and B and from energy balances for the reactor and cooling jacket:

$$
\begin{aligned}
\dot{c}_A &= \frac{\dot{V}}{V_R}(c_{A0} - c_A) - k_1(\vartheta)c_A - k_3(\vartheta)c_A{}^2 && \text{(2a)}\\
\dot{c}_B &= -\frac{\dot{V}}{V_R}c_B + k_1(\vartheta)\,c_A - k_2(\vartheta)c_B && \text{(2b)}\\
\dot{\vartheta} &= \frac{\dot{V}}{V_R}(\vartheta_0 - \vartheta) - \frac{1}{\rho C_p}\Big(k_1(\vartheta)c_A \Delta H_{R_{AB}} \\
&\quad + k_2(\vartheta)c_B \Delta H_{R_{BC}} + k_3(\vartheta)c_A{}^2 \Delta H_{R_{AD}}\Big) \\
&\quad + \frac{k_w A_R}{\rho C_p V_R}(\vartheta_K - \vartheta) && \text{(2c)}\\
\dot{\vartheta}_K &= \frac{1}{m_K C_{PK}}\Big(\dot{Q}_K + k_w A_R(\vartheta - \vartheta_K)\Big)\,, && \text{(2d)}\\
& c_A \geq 0,\ c_B \geq 0\,.
\end{aligned}
$$

The concentrations of substances A and B are c_A and c_B respectively. The temperature in the reactor is denoted by ϑ, while the temperature in the cooling jacket is given by ϑ_K. The reaction velocities k_i are assumed to depend on the temperature via the Arrhenius law

$$
k_i(\vartheta) = k_{i0}\cdot\exp\left(\frac{E_i}{\vartheta/{}^oC + 273.15}\right), \ i = 1,2,3\,. \qquad \text{(2e)}
$$

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FADP (single-input)

non-linear non-minimum phase CSTR

Discretization (initial)

4.2.1. Algorithm set-up

The manipulated variable $\dot{V}/V_R$ was discretized into $A = 31$ values in the range [3, 35]1/h: {3, 4, 4.5, . . ., 9.5, 10, 11, 12, . . ., 21, 22, 24, 26, 28, 30, 35}, based on the static gain characteristics of the system. The measurement space was discretized into $M = 38 \times 23 = 874$ values using {0.20, 0.30, 0.40, 0.50, 0.54, 0.58, 0.60, . . ., 1.06, 1.08, 1.09, 1.10, 1.12, . . ., 1.18, 1.20, 1.24, . . ., 1.36, 1.40} for the product concentration c_B and {80, 90, 92, . . ., 128, 130, 140} for the reactor temperature ν. Following the benchmark (Chen et al., 1995), the cost function was defined as the squared error between the product concentration and its set point; the discount factor λ was set to 0.995 (*cf.* MPC prediction horizon of 200 samples). Two controllers with set points at 1.09 and 0.95 mol/l were designed, *i.e.*, $B = 2$.

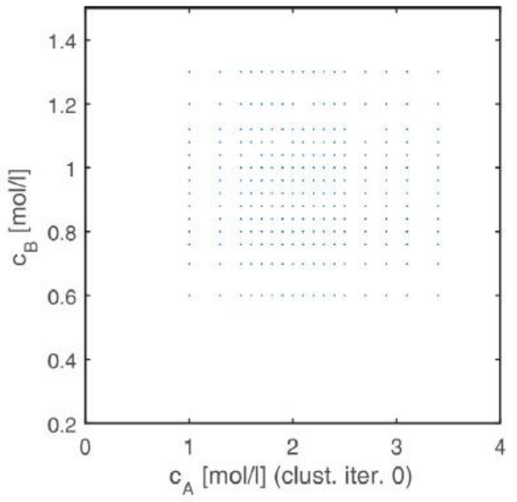

Fig. 2. Clustering of initial reactant and product concentrations.

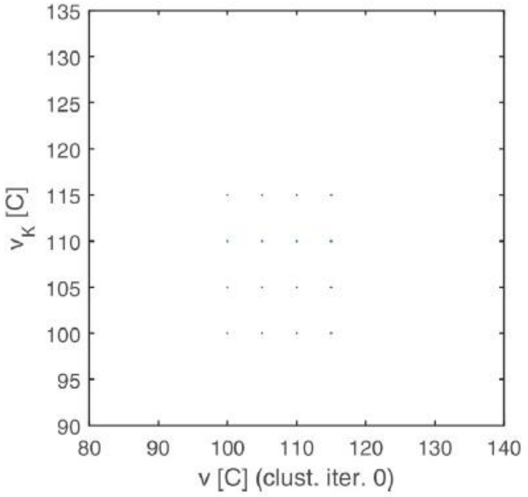

Fig. 3. Clustering of reactor and coolant temperatures.

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FADP (single-input)

non-linear non-minimum phase CSTR

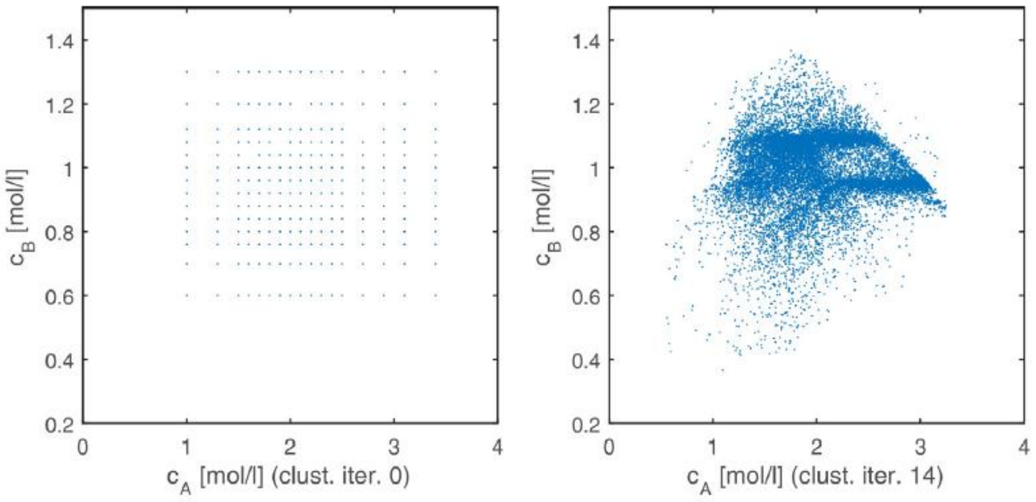
Discretization (iterative FADP steps)

Table 1
Simulation set-up and root-mean-square errors (RMSE) on controlled variable. N is the number of cluster centers (resolution of discretization), E is the number of one-step ahead simulations for each state cell.

N	E	Iteration	RMSE	RMSE ($E = 200$)
1000	5	0	0.051	–
2358	10	1	0.045	–
4060	20	3	0.028	0.026
6514	25	4	0.029	0.027
9976	50	9	0.025	0.027
16,716	75	14	0.021	0.022
15,232	200	Ref.	–	0.031

reference case (grid)

number of clusters | number of model evaluations per cell | iteration count | RMSE at the end if FADP | RMSE when completed to E=200



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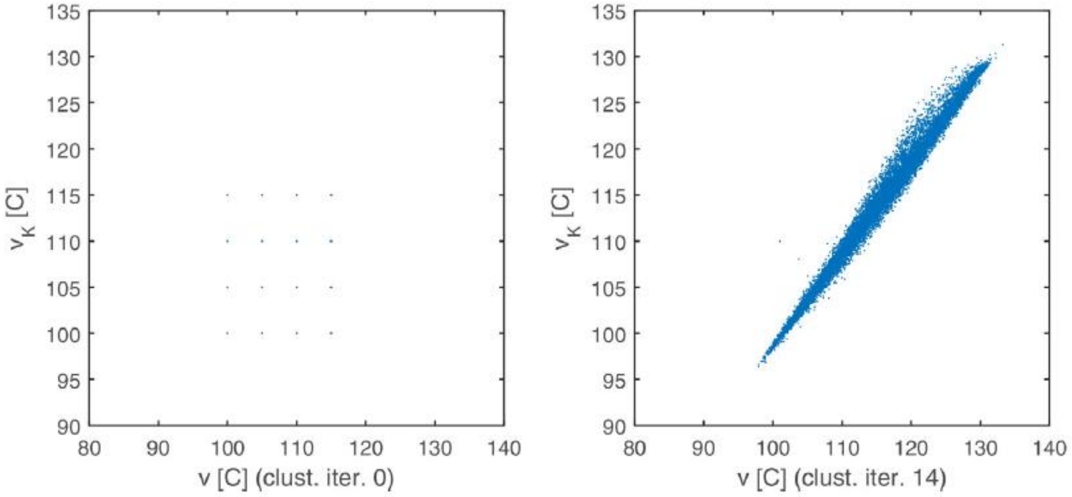

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measurement + prediction
= state distribution
-> inferred ML estimate s
-> controller output $a = \pi(s)$

state estimate distributions

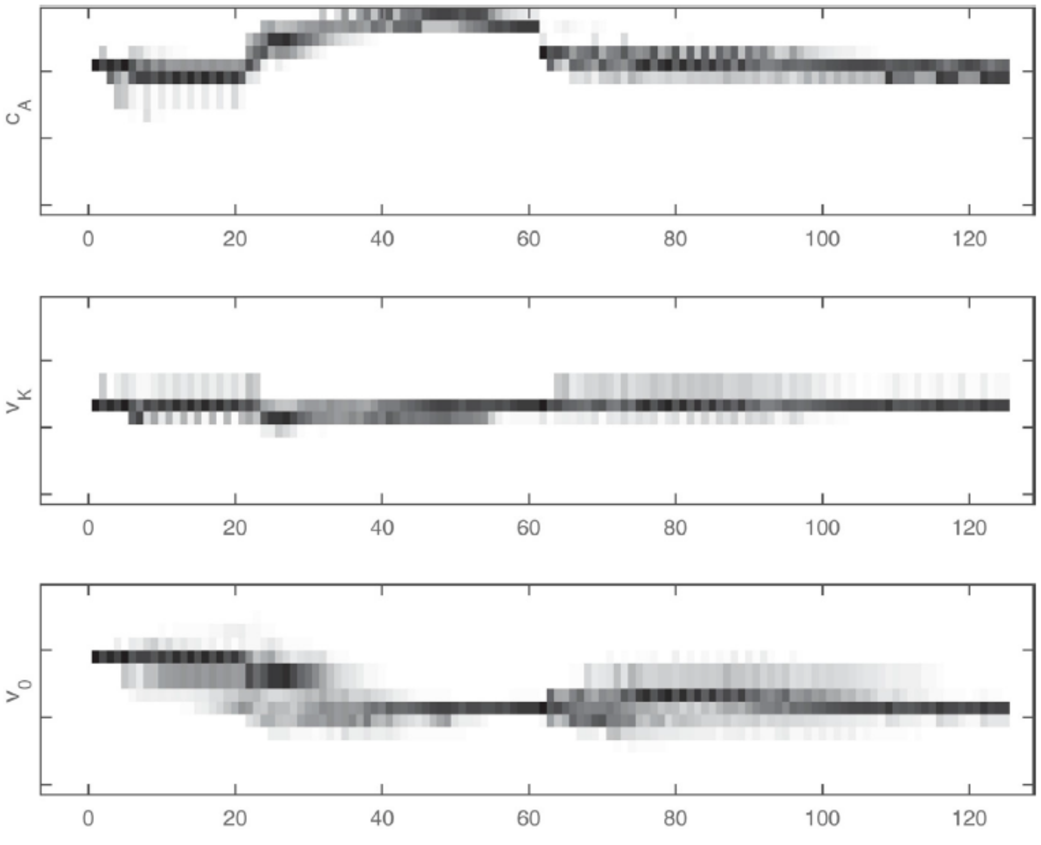

Fig. 6. State and disturbance estimation distributions for set point tracking.

true and inferred (ML) estimates

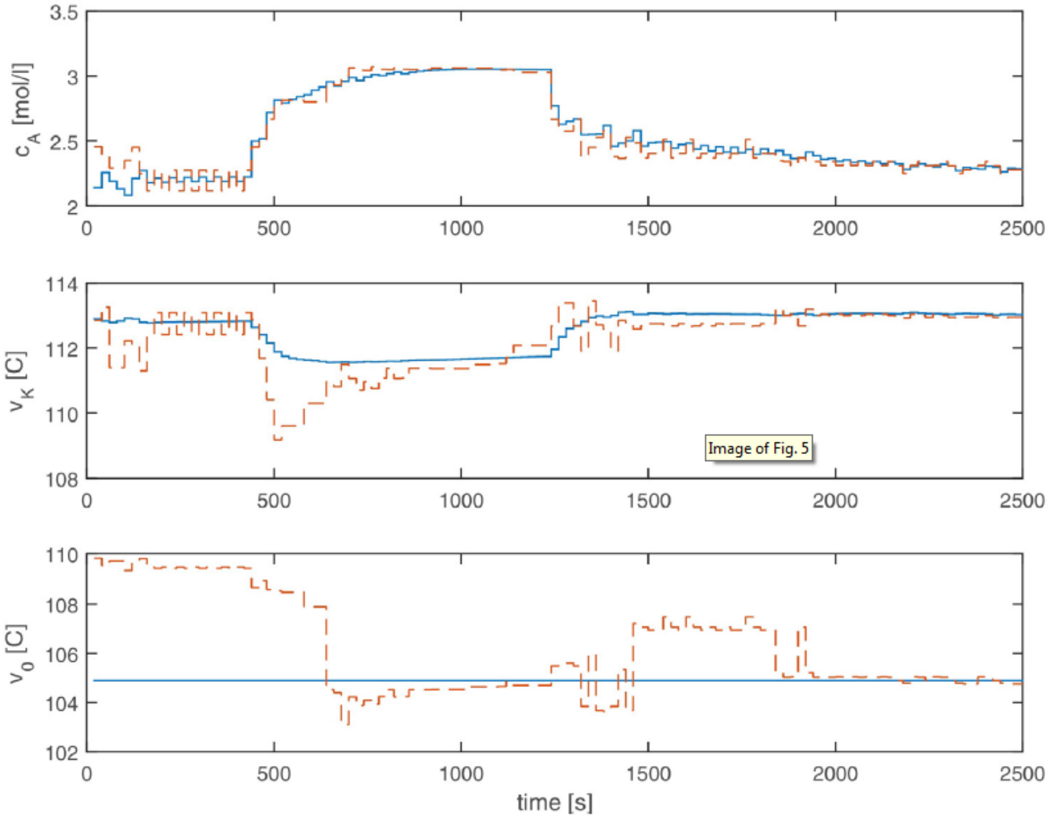

Fig. 5. State and disturbance estimation for set point tracking. Solid line: true state, dashed line: inferred ML estimate.

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FADP (single-input)

non-linear non-minimum phase CSTR

For the evaluation of the controller performance, the following tests are suggested in Chen et al. (1995):

- i) step changes in the set point from maximal to minimal values and back. The simulation starts with a large initial error in the state estimator ($\hat{\mathbf{x}}$ = [2.50 mol/l, 1.09 mol/l, 114.2 °C, 114 °C, 110 °C]), the set point is decreased at 400 s, and returns back at 1200 s.
- ii) step changes in the feed temperature to maximal and minimal values. Starting from nominal optimal, the feed temperature changes to 115 °C at 0 s, and to 100 °C at 1500 s.
- iii) robustness can be tested by considering two extreme cases (in the sense of worst-case deviation from nominal values) for parameter uncertainty (see (Chen et al., 1995) for numerical details). Starting with the first worst-case setting (ν_0 = 104.9 °C), set point is decreased at 400 s and ν_0 is decreased to 100 °C at 1100. An abrupt mismatch to the other worst-case parameter setting occurs at 1800 s, followed by a set point change at 2300 s and a step in ν_0 to 115 °C at 3000 s.

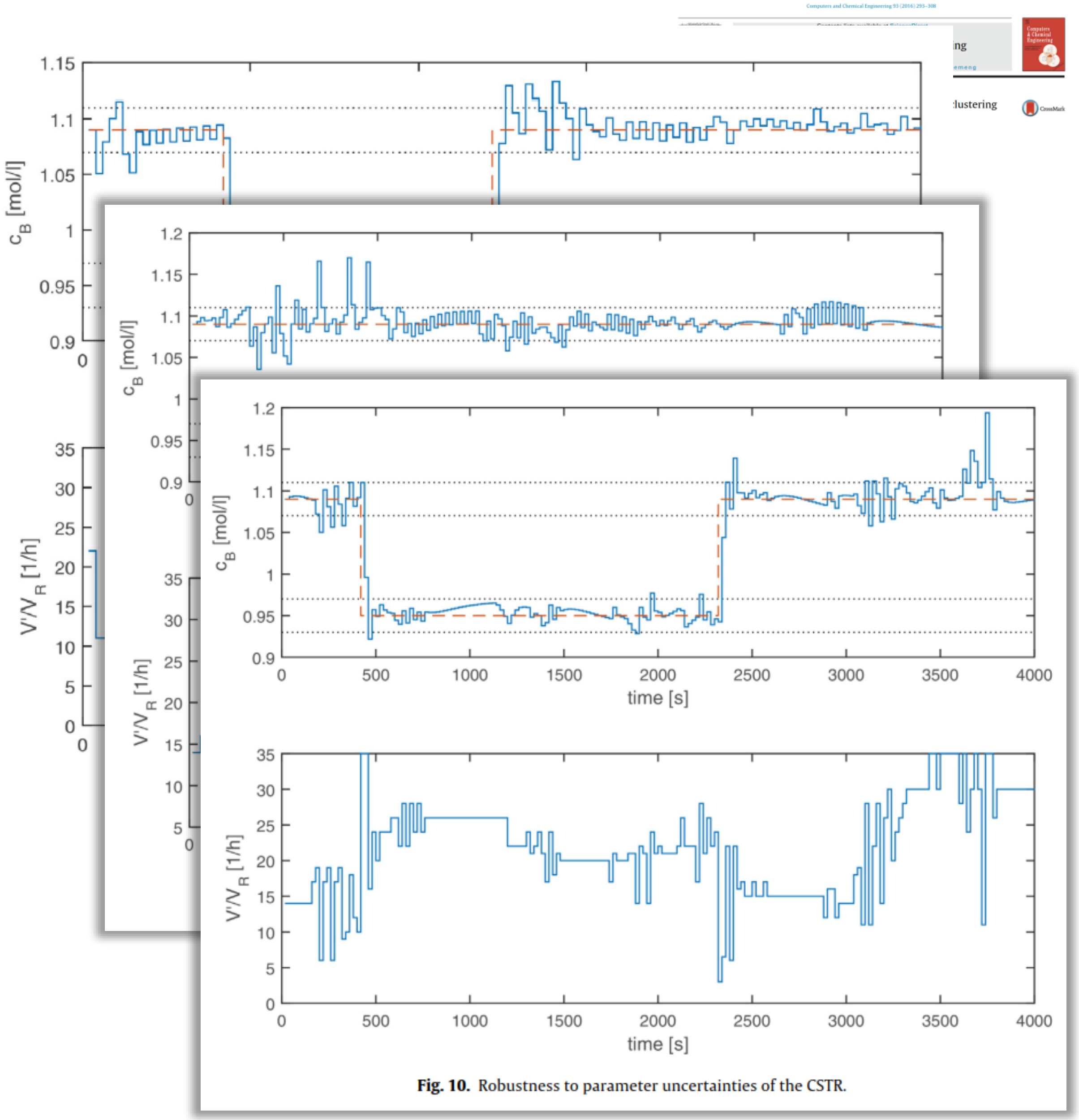

Fig. 10. Robustness to parameter uncertainties of the CSTR.

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noise in product concentration and reactor temperature + random walk in feed temperature
(not in the benchmark)

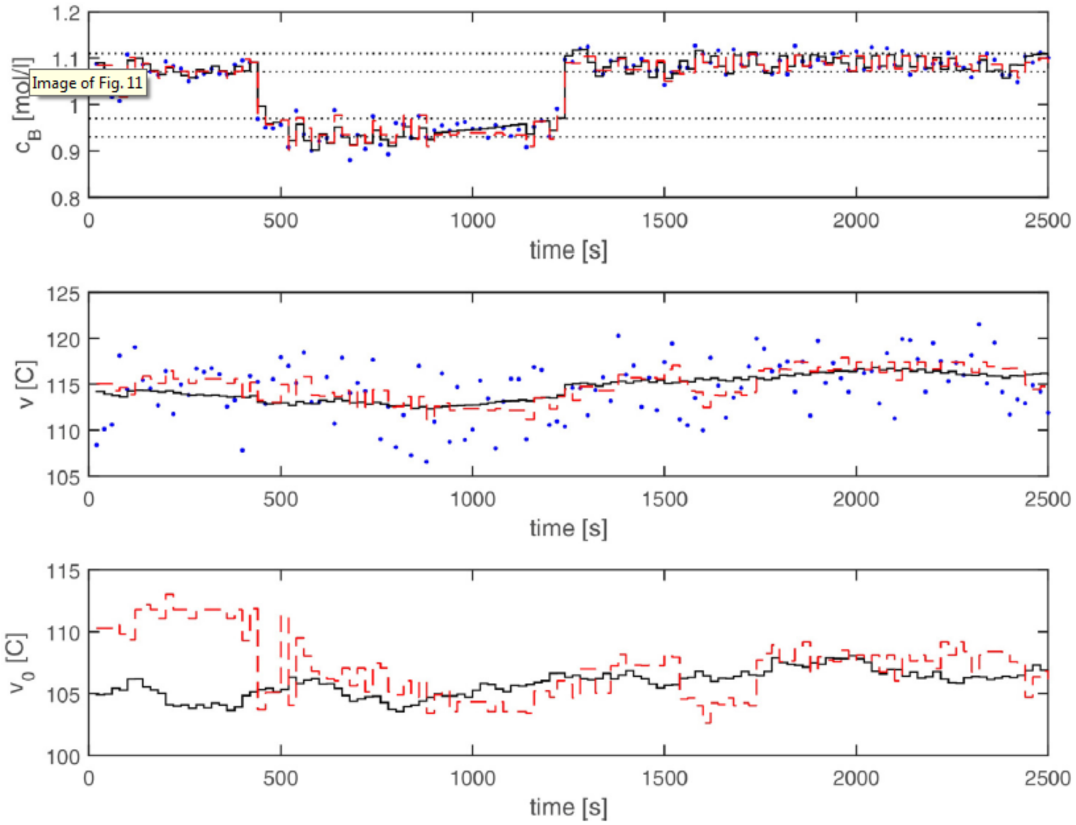

Fig. 11. Set point tracking in the presence of stochastic state and measurement noise. Solid line: true state, dashed line: inferred ML estimate, dots: measurements.

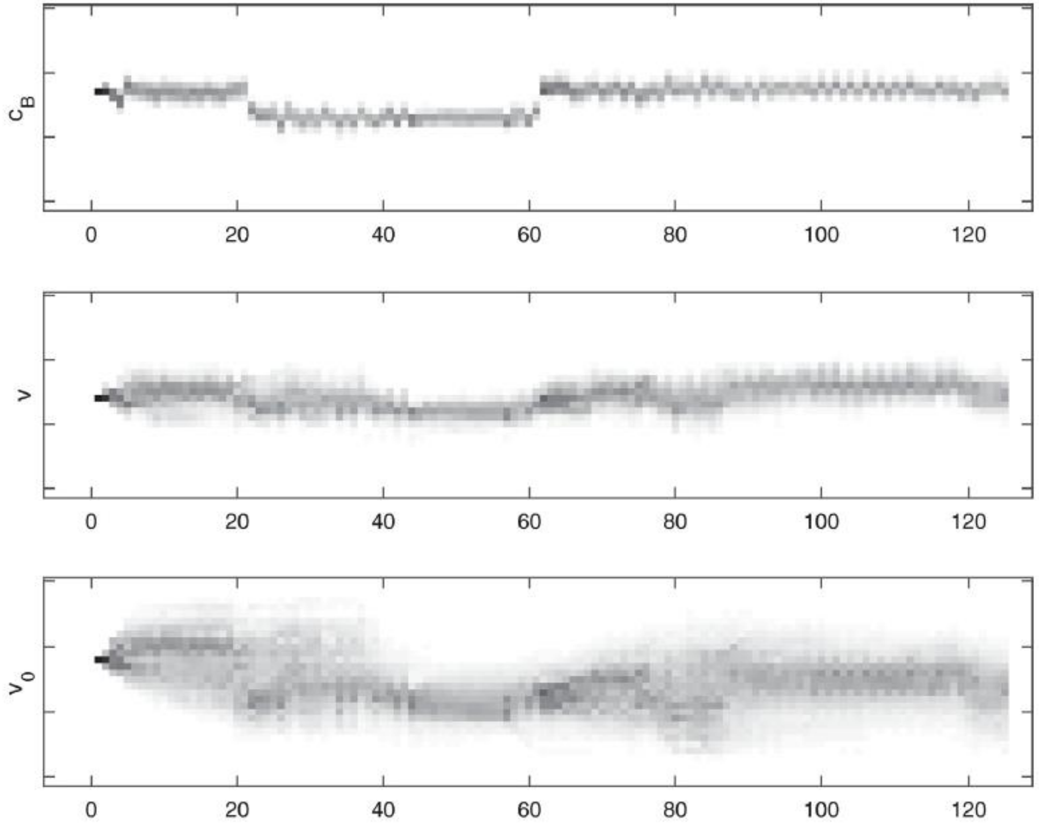

Fig. 12. Estimated state distributions in the presence of stochastic state and measurement noise.

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FADP

non-linear non-minimum phase CSTR

- van der Vusse benchmark (Chen et al. 1995)

$$
\begin{array}{ccccc}
A & \xrightarrow{k_1} & B & \xrightarrow{k_2} & C \\
2A & \xrightarrow{k_3} & D\,. & &
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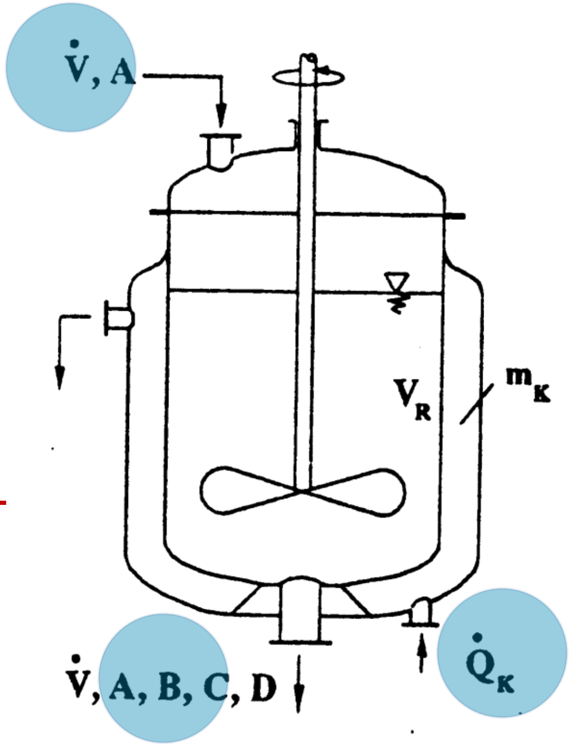

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&\quad + \frac{k_w A_R}{\rho C_p V_R}(\vartheta_K - \vartheta) && \text{(2c)}\\
\dot{\vartheta}_K &= \frac{1}{m_K C_{PK}}\left(\dot{Q}_K + k_w A_R(\vartheta - \vartheta_K)\right), && \text{(2d)}
\end{aligned}
$$

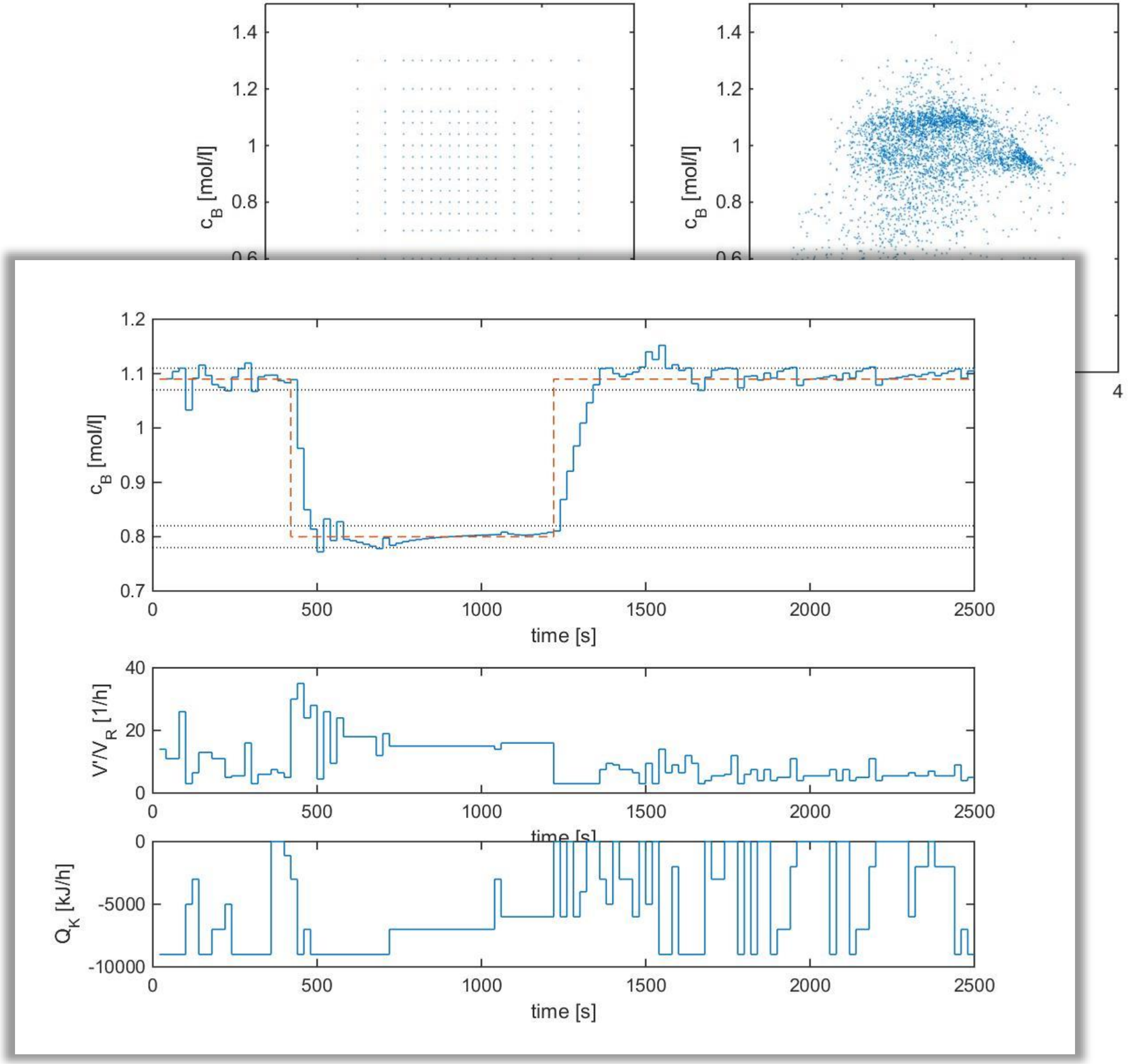
$$c_A \geq 0,\; c_B \geq 0\,.$$

The concentrations of substances A and B are c_A and c_B respectively. The temperature in the reactor is denoted by ϑ, while the temperature in the cooling jacket is given by ϑ_K. The reaction velocities k_i are assumed to depend on the temperature via the Arrhenius law

$$k_i(\vartheta) = k_{i0} \cdot \exp\left(\frac{E_i}{\vartheta/{}^oC + 273.15}\right), \; i = 1, 2, 3\,. \quad \text{(2e)}$$

FADP
(multiple-input)

- benchmark (noiseless)
- clustering using FADP
- system input/output



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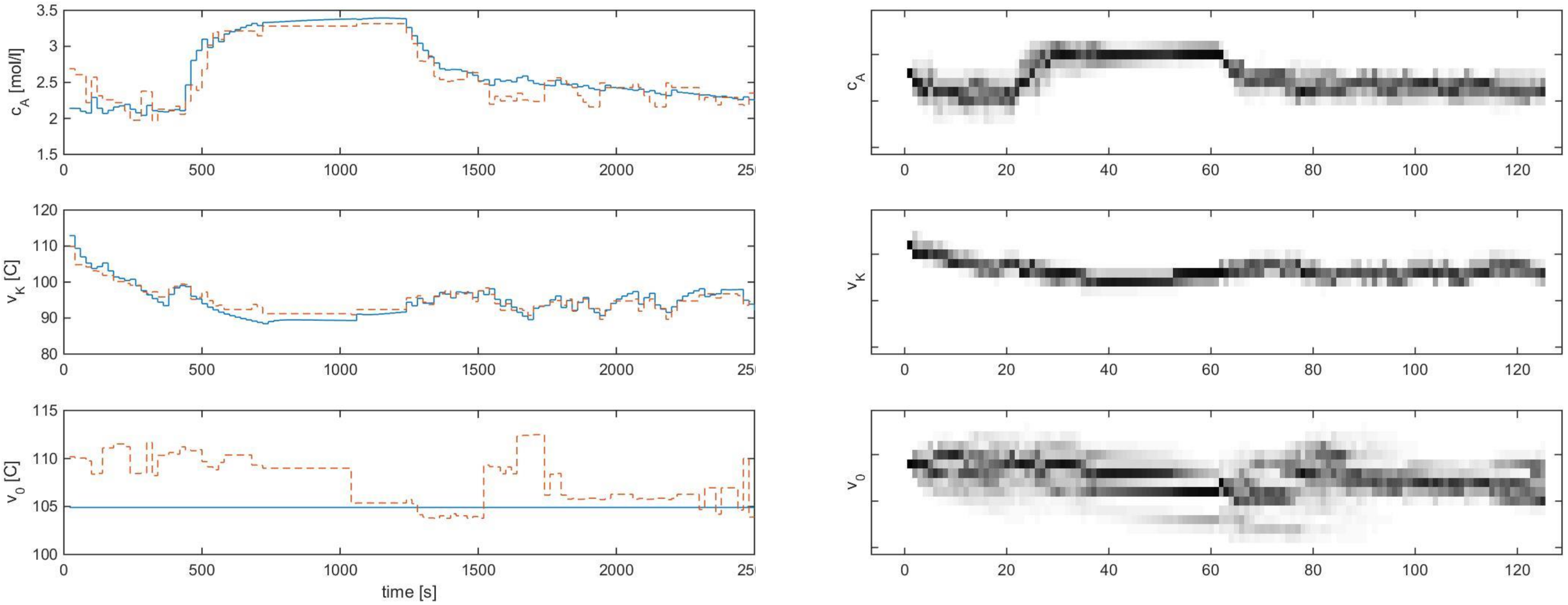
FADP
(multiple-input)

- benchmark (noiseless)
- state estimates: ML & densities



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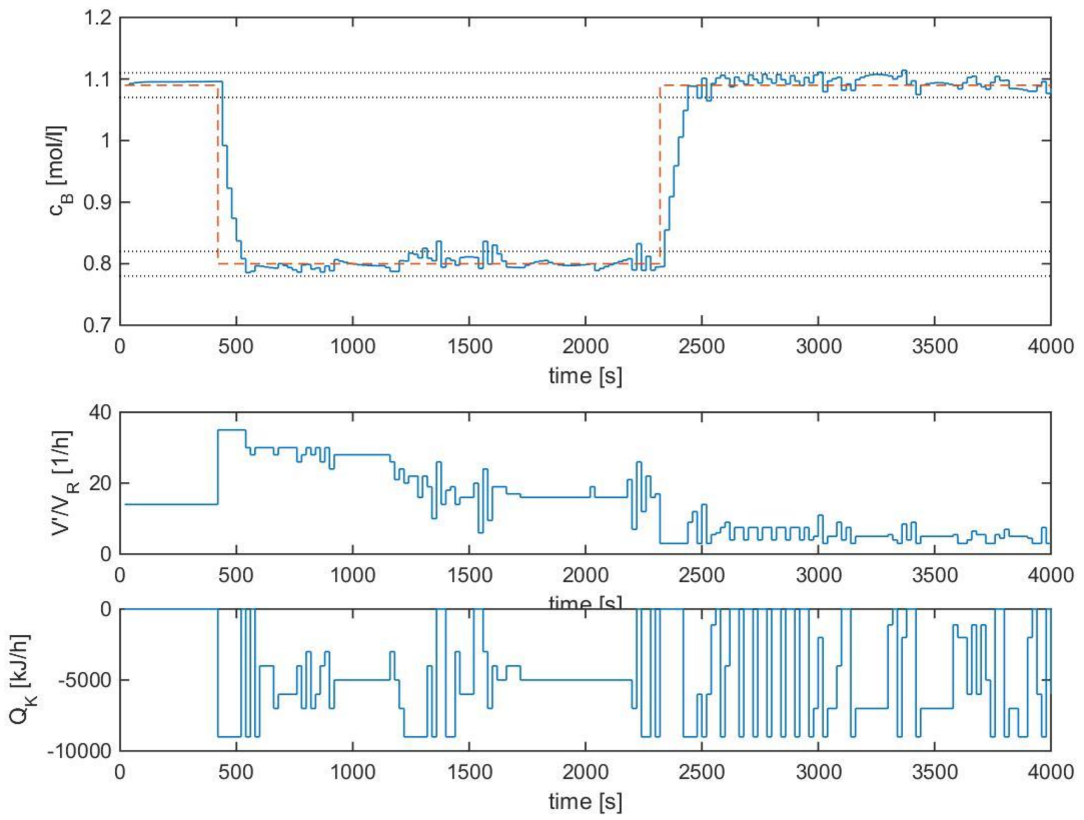
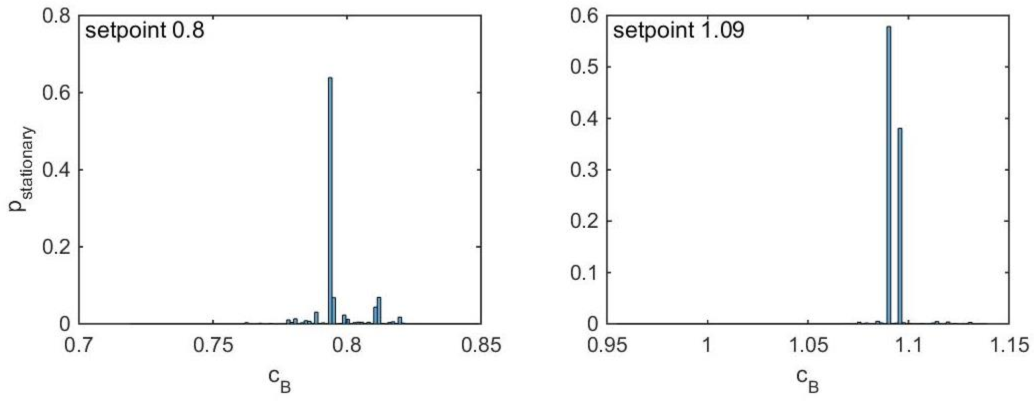
FADP
(multiple-input)

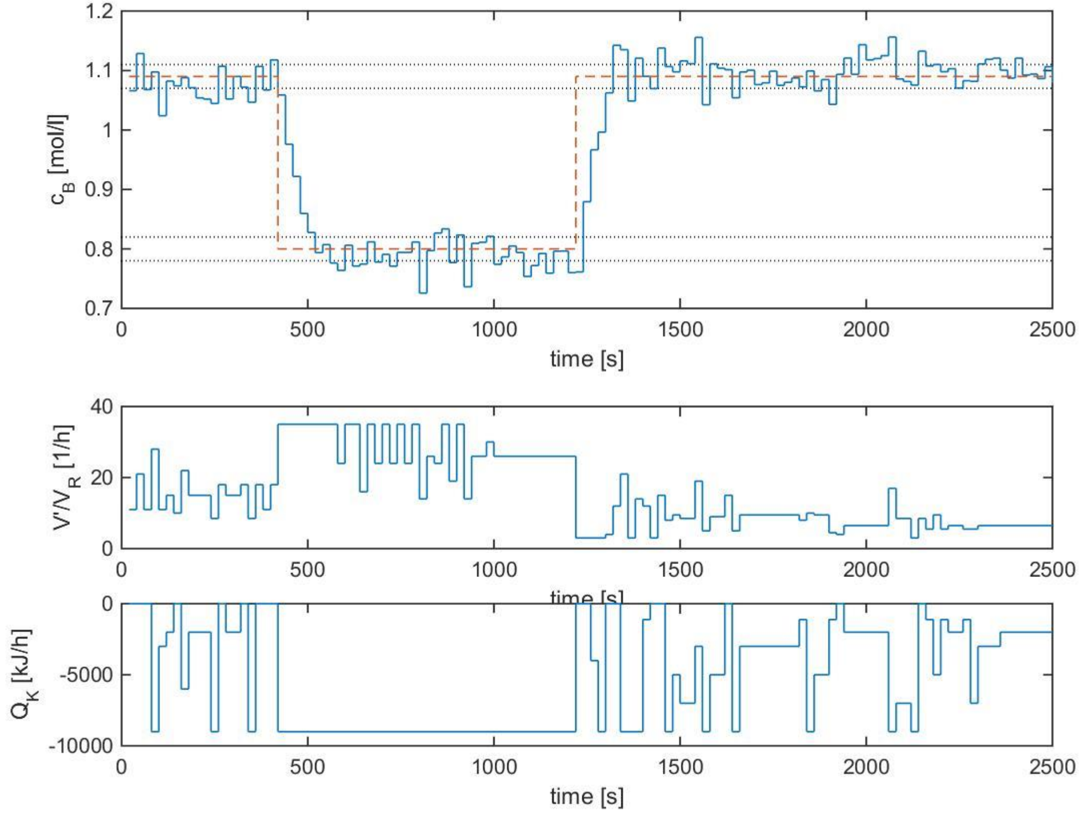
- benchmark (noiseless)
- robustness test



FADP
(multiple-input)

- state & signal noise
- MC analysis of closed-loop behavior





Future works

Conclusions & Future

Process control and state estimation

- optimal control based on finite state and action plant description
  - Bayesian state estimation (cell filter)
  - optimal control (DP)
- FADP
  - attempt to solve the curse-of-dimensionality in ‘ADP style’
- van der Vusse CSTR (SISO & MISO)
  - nonlinear, stochastic, nonminimum-phase dynamics
  - 2 inputs, 5 states => tractable computations on a laptop PC

Future

- experience from industrial application studies
- state estimation for monitoring => how to provide added value from improved uncertainty information to plant operators and automatic control

Finite state estimation and control of a multi-input CSTR benchmark

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THANK YOU

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