Integrated dynamic optimization and control applied to industrial processes: b) Bayer process

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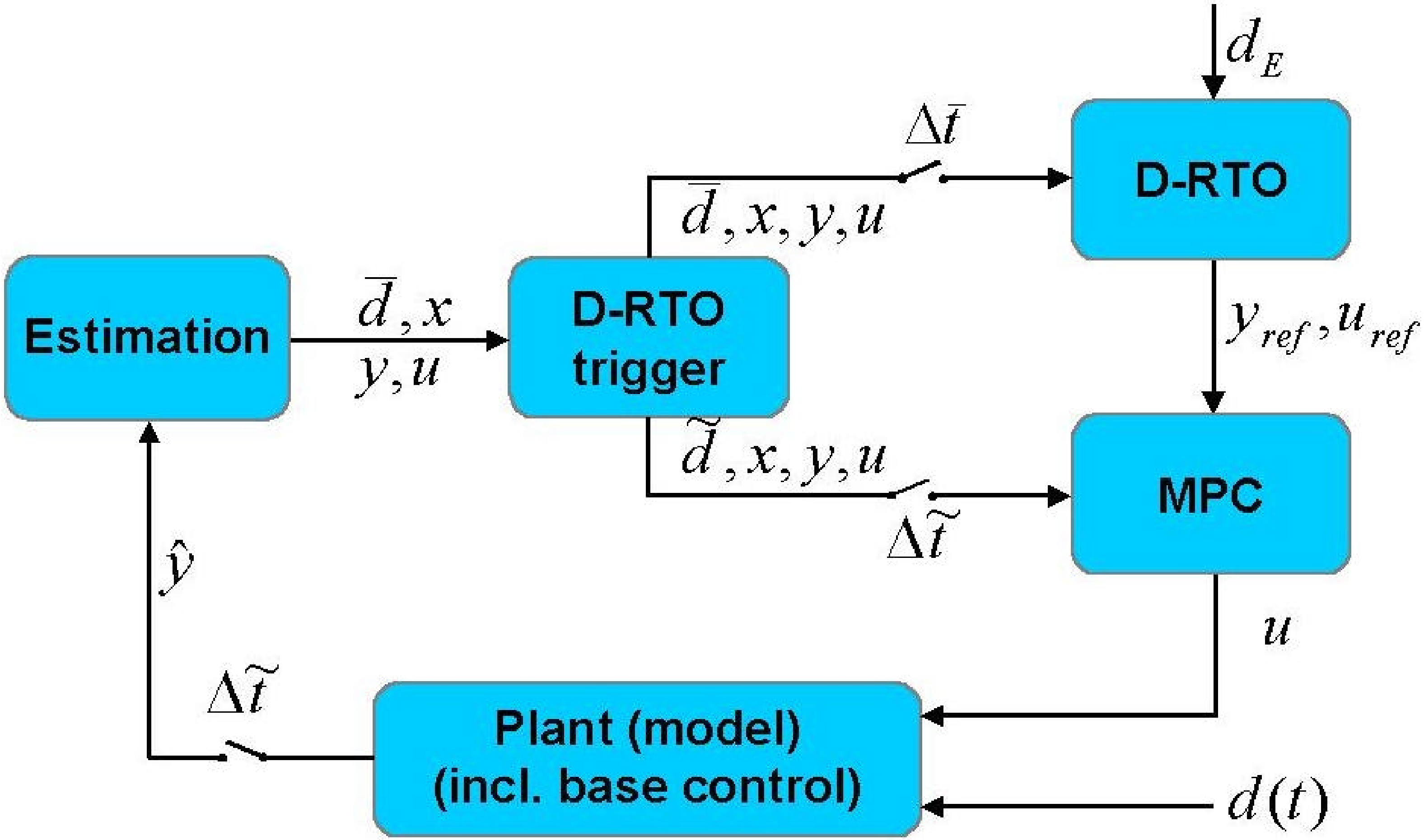
integrated optimization and control

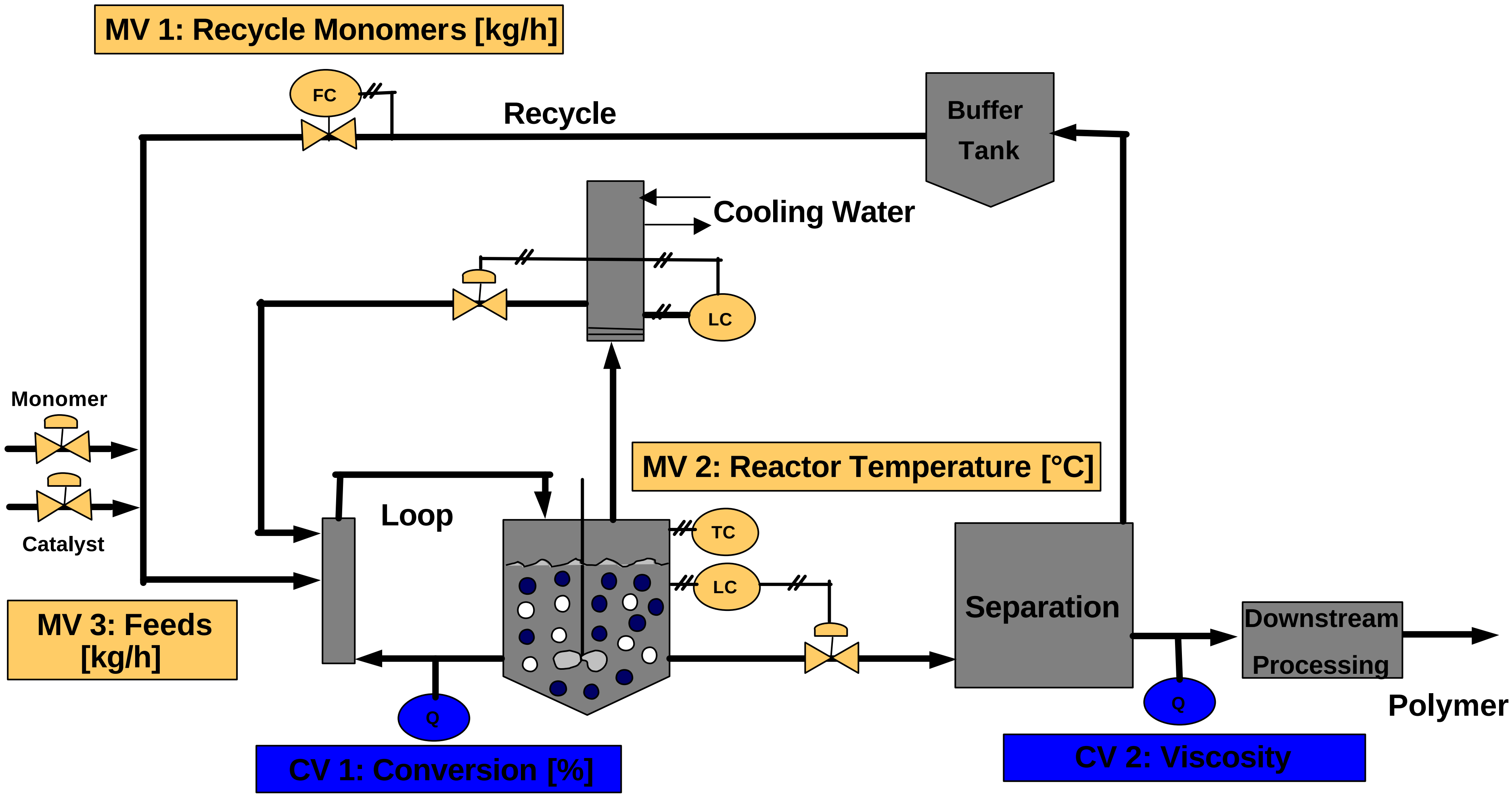


Bayer process

- continuous polymerization process with a subsequent separation unit and monomer recycle
  - monomers,catalyst and solvent used for producing a specialty polymer
  - complex reaction mechanism with more than 80 reactions
  - operated at an open loop unstable operating point due to runaway reaction
  - various polymer grades are in production
  - frequent load changes due to fluctuating polymer demand

- external disturbances due to sudden load changes, scheduled grade changes along with nominal process disturbances associated with any polymerization process

⇒ *a challenging process for on-line optimization and control*


MV 1: Recycle Monomers [kg/h]
FC
Recycle
Buffer
Tank
Cooling Water
LC
Monomer
Catalyst
Loop
MV 2: Reactor Temperature [°C]
TC
LC
Separation
Downstream
Processing
Polymer
MV 3: Feeds
[kg/h]
Q
Q
CV 1: Conversion [%]
CV 2: Viscosity

Bayer process: the INCOOP perspective

- measurements:
  - reactor temperature and holdup (online, with fast sampling time without delay)
  - polymer quality in terms of viscosity (online and with lab samples, approximately 5 minutes sampling time with 30 minute delay)
  - reactor conversion (online, fast sampling time without delay)
  - inlet monomer flowrate (online), recycle and outlet flowrates (online, but with uncertainty and bias)
  - *most of the flow measurements are measured with noise and gross error*

- process model with approximately 2500 DAEs
- uncertainties:
  - plant-model (structural/parametric) mismatch, ...

unscheduled optimal load change problem

- objective: quick transition without off-spec polymer production
- path constraints on monomer inlet and recycle flowrates, reactor temperature and recycle buffer vessel holdup
- transition endpoint constraint in terms of a subsequent steady-state after the transition
- manipulated variables:
  - monomer inlet and recycle flowrates, initiator flowrate
  - reactor temperature is controlled by a base-level controller

optimization problem II

scheduled optimal grade change

- objective: minimum grade transition time with a subsequent steady-state
- path constraints and manipulated variable are same!
- uncertain reaction rate parameters and major process disturbances such as solvent concentration, unreliable flow-measurements

⇒ *a smooth and flexible optimal operation is desired*

a polymer process model

- process model
  - empirical model with rigorous reactor model and an approximate model for the cooling unit
  - 2500 DAE model with embedded base-level controllers
  - disturbance model
  - a steady state filter for checking if a steady-state is achieved

- Is the process too complex or not for on-line optimization and control?
  - depends not on size of the model but on the number of inputs, outputs and constraints
  - depends also on quality of feedback information such as measurements

optimal load change problem

decomposed optimization-control problem

D-RTO

$$\min_{\mathbf{u},t_f} J = \int_{t_0}^{t_f} [s_t + s_{MW}(MW - MW^{ref})^2]\,dt + \dot{\bar{x}}_{tf}^{\,T} P \dot{\bar{x}}_{tf}$$

$$s.t.\ \ 0 = \bar{f}(\dot{\bar{x}}, \bar{x}, u^{ref}, \bar{d}, \bar{t}),\ \bar{x}(t_{0_i}) = \bar{x}_{0_i}$$

$$y^{ref} = \bar{g}(\bar{x}, u^{ref}, \bar{d}, \bar{t})$$

$$0 \geq \bar{h}(\bar{x}, u^{ref}, \bar{d})$$

$$\bar{t} \in [\bar{t}_{0_i}, \bar{t}_{f_i}];$$

$$\bar{t}_{0_{i+1}} = \bar{t}_{0_i} + \Delta\bar{t},\ \bar{t}_{f_{i+1}} = \bar{t}_{f_i} + \Delta\bar{t}$$

MPC

$$\min_{u} \int_{\tilde{t}_{0j}}^{\tilde{t}_{fj}} [\Delta y^T Q \Delta y + \Delta u^T R \Delta u]dt + (\tilde{x}_N - \bar{x}_N)^T P (\tilde{x}_N - \bar{x}_N)$$

$$s.t.\ \dot{\tilde{x}} = A(\tilde{t})\Delta\tilde{x} + B(\tilde{t})\Delta\tilde{u}$$

$$\Delta y = C(\tilde{t})\Delta\tilde{x} + D(\tilde{t})\Delta u$$

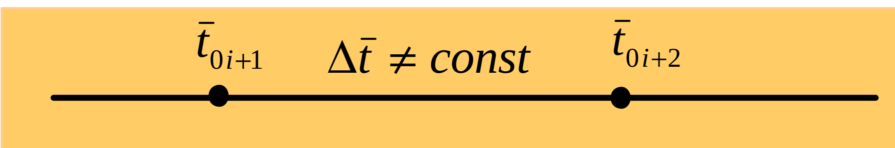
$$\Delta y \leq \Delta y^U$$

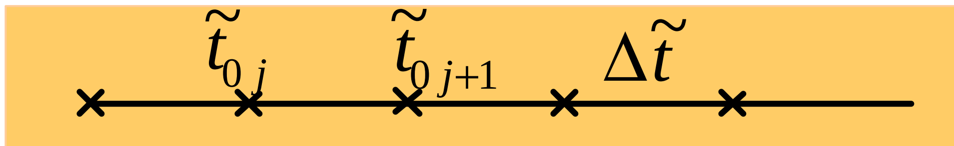
$$\Delta u \leq \Delta u^U; \frac{d}{d\tilde{t}}\Delta u \leq du^U$$

$$\Delta y = y - y^{ref}; \Delta u = u - u^{ref}$$

$$\tilde{t} \in [\tilde{t}_{0_j}, \tilde{t}_{f_j}];$$

$$\tilde{t}_{0_{j+1}} = \tilde{t}_{0_j} + \Delta\tilde{t},\ \tilde{t}_{f_{j+1}} = \tilde{t}_{f_j} + \Delta\tilde{t}$$





- disturbances during on-line control
  - 6 samples delay in viscosity measurement
  - all measurements with high level of noise
  - 5% bias in output flowrate measurement

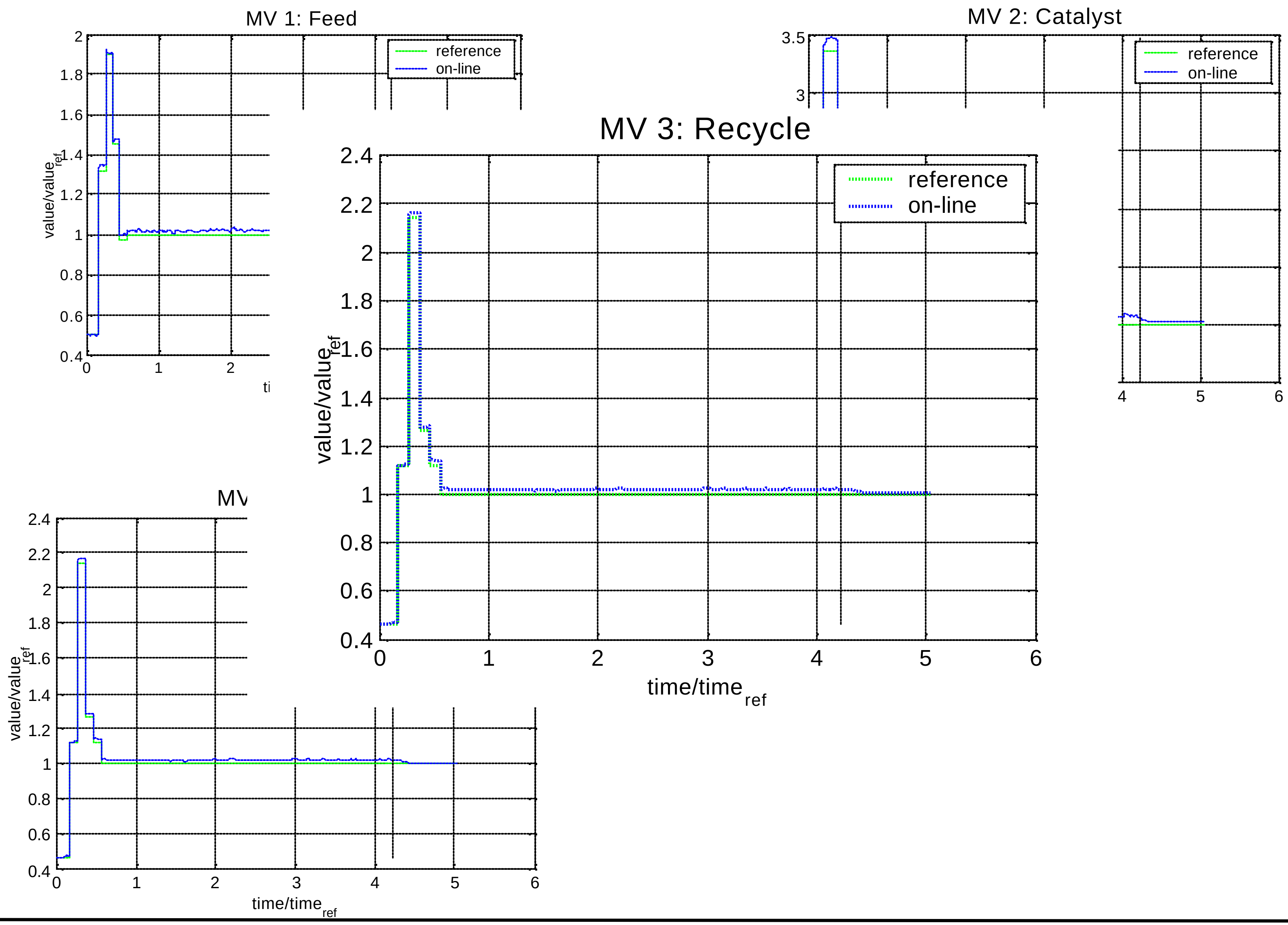
- difficulties
  - unstable control system when we track reference trajectories due to level control being switched off
  - ill-conditioned problem

- solution techniques
  - ADOPT (sequential approach) for solving dynamic optimization problems
  - EKF for estimation problems and LTVMPC for MPC problems

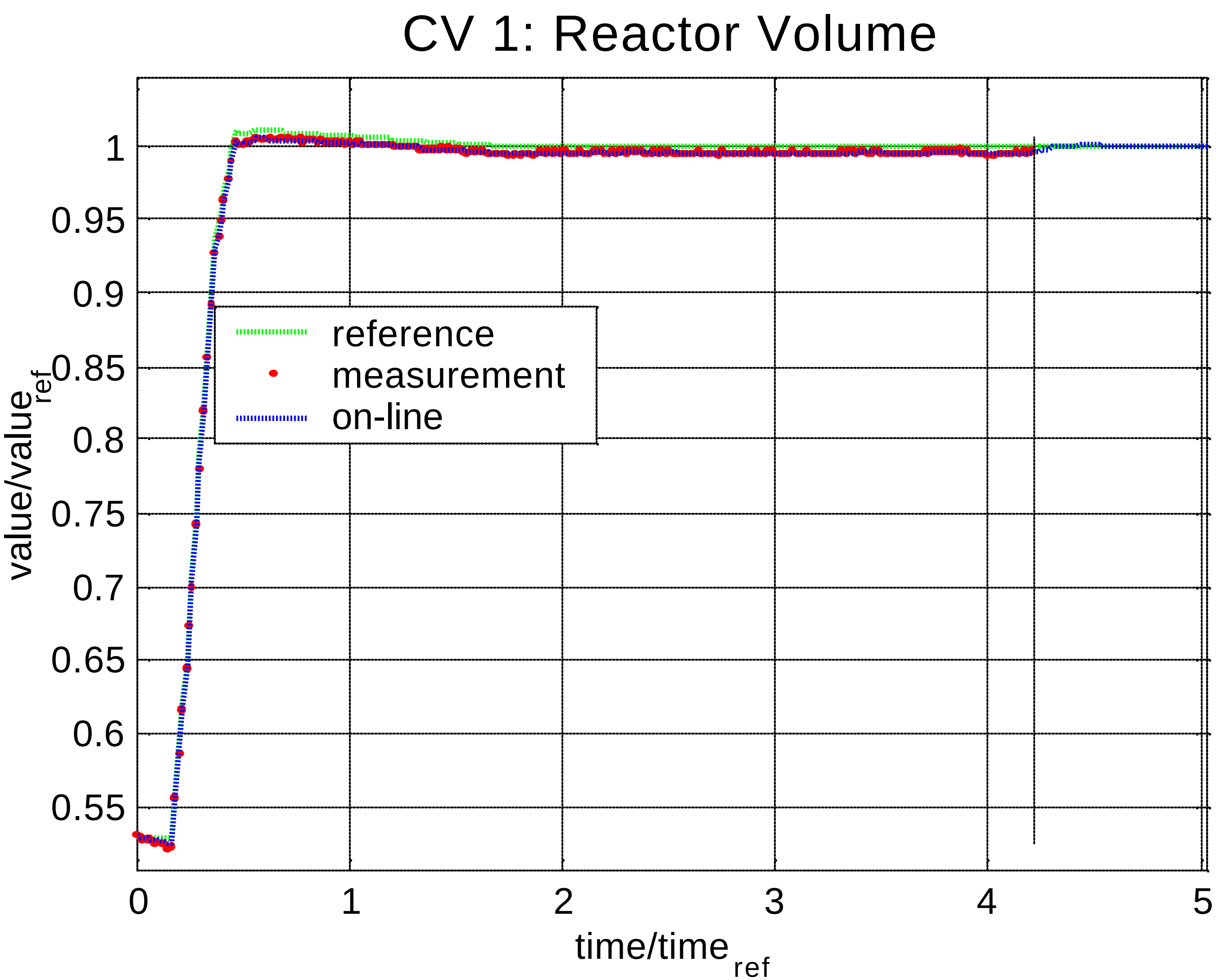
re-optimization for optimal load change problem

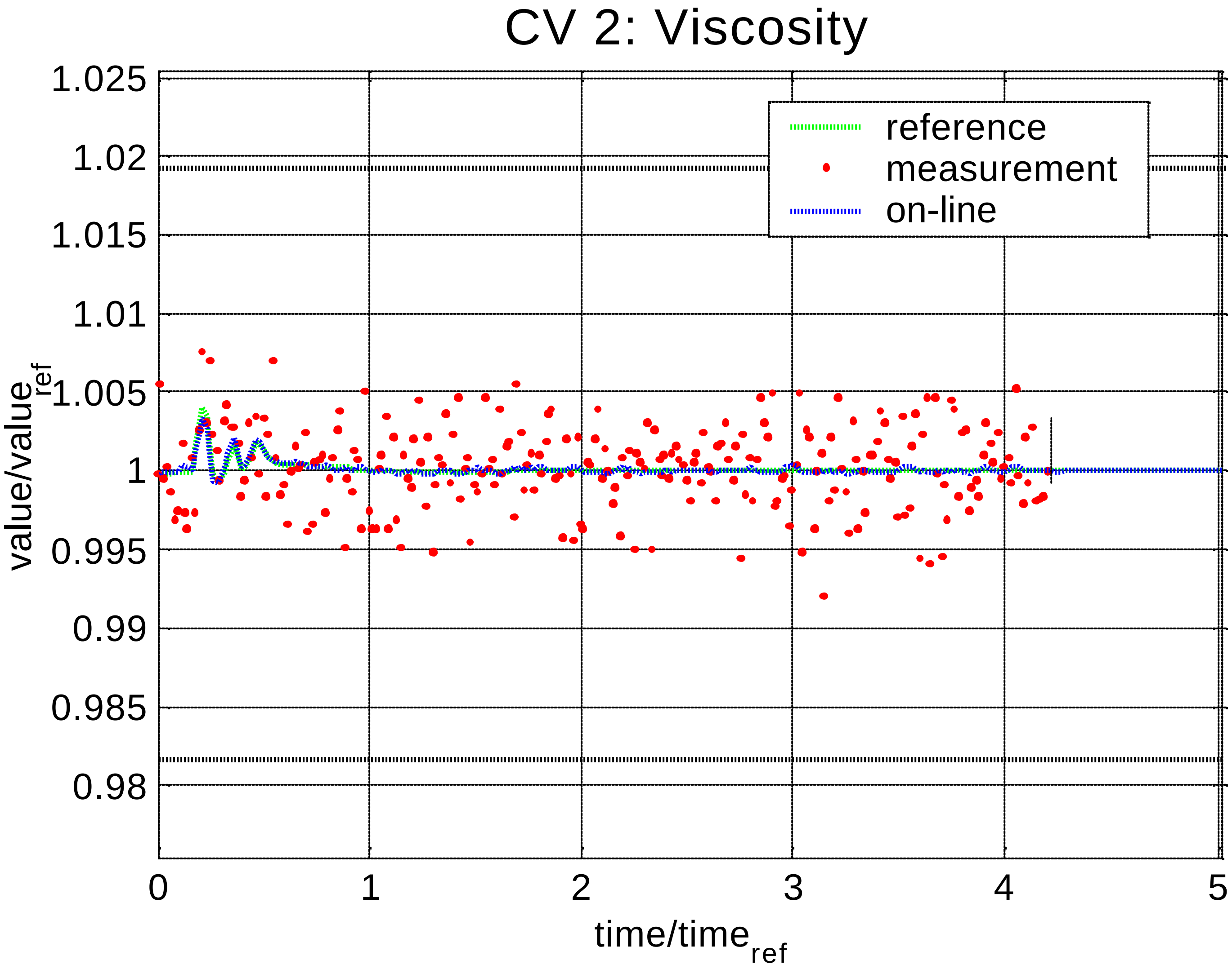
- motivation
  - trajectories for all possible combinations of desired loads and grades need to be pre-optimized ⇒ not always possible
  - unknown initial state and solvent concentration
- re-optimization approach
  - apply off-line computed optimal trajectory corresponding to the closely related load change
  - trigger a re-optimization problem
  - apply the re-optimized results as soon as available
- scenario
  - optimal load change from 50% to 90%
  - catalyst concentration of 95% of nominal value

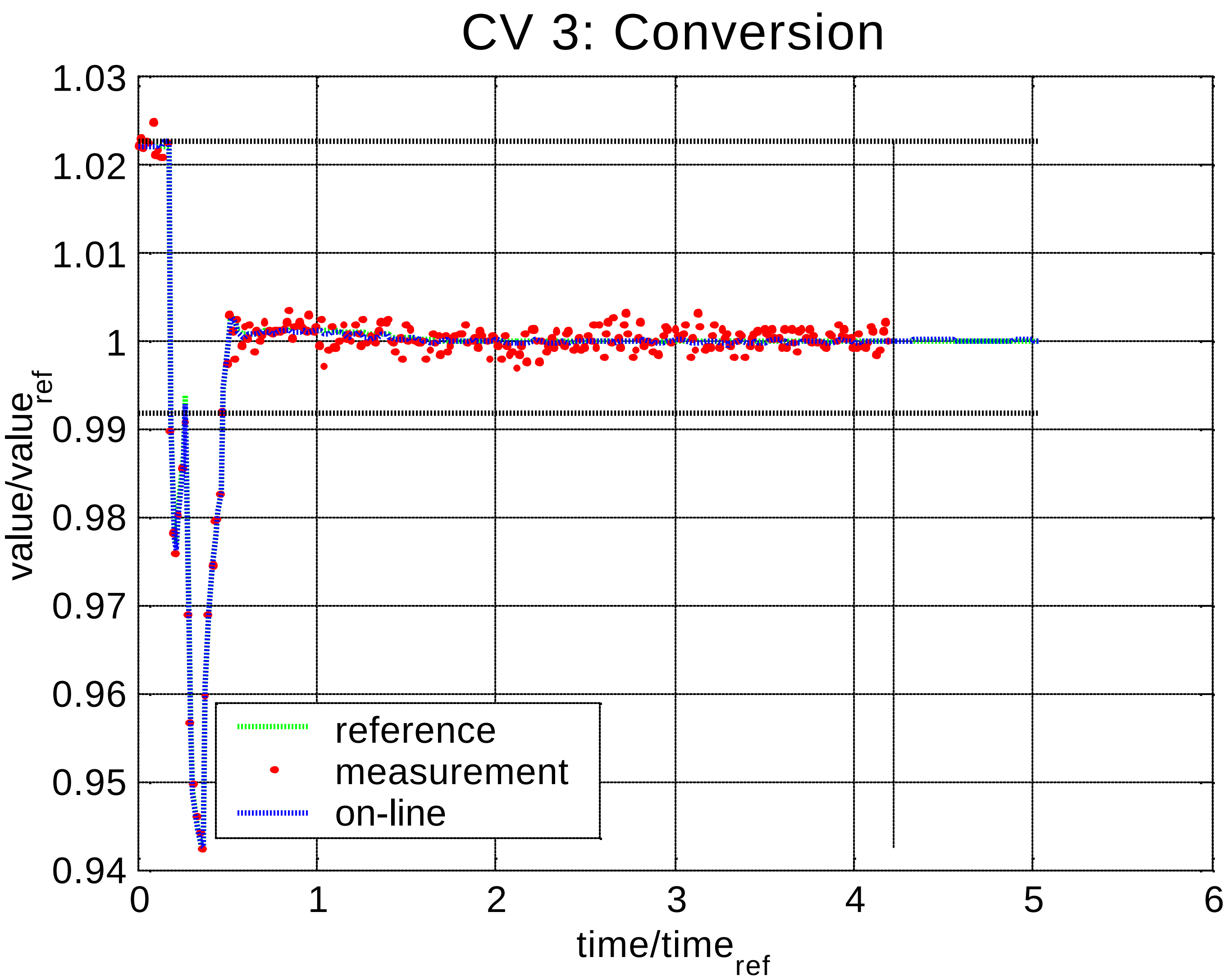
real-time solution (1)



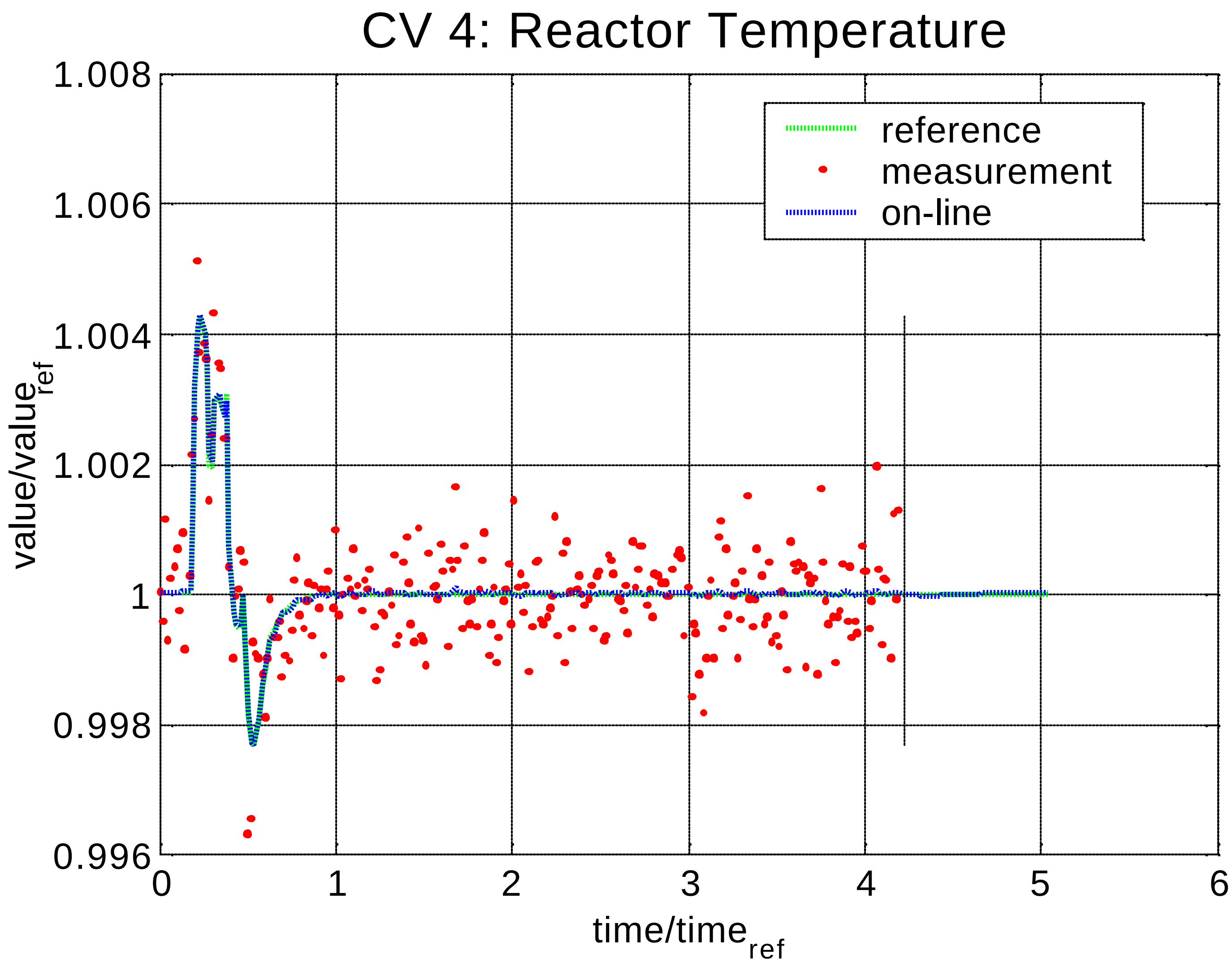
real-time solution (2)




CV 2: Viscosity
1.025
1.02
1.015
1.01
1.005
1
0.995
0.99
0.985
0.98
value/value_ref
0
1
2
3
4
5
time/time_ref
reference
measurement
on-line


CV 3: Conversion
1.03
1.02
1.01
1
0.99
0.98
0.97
0.96
0.95
0.94
value/value$_{ref}$
0
1
2
3
4
5
6
time/time$_{ref}$
reference
measurement
on-line

real-time solution (5)



optimal grade change problem

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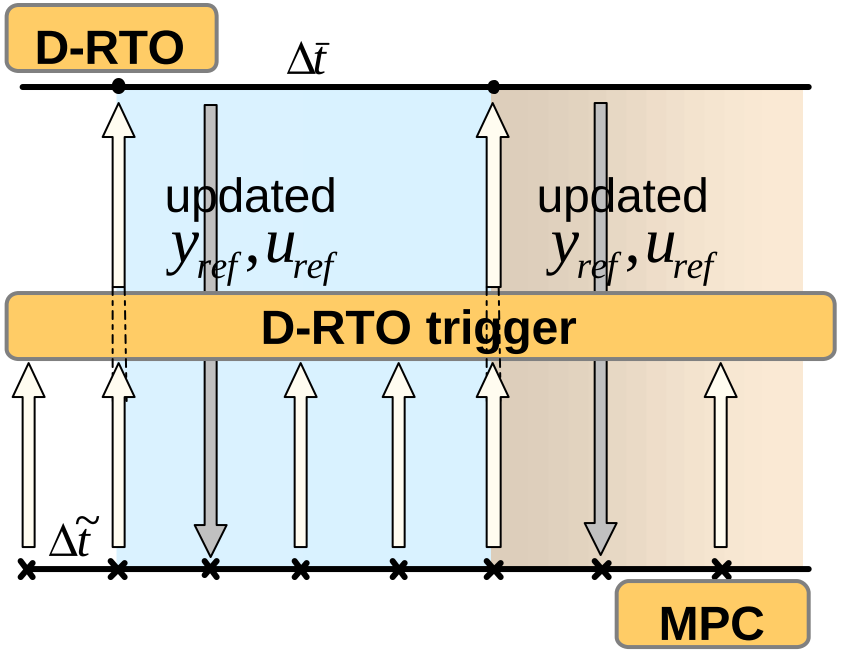
- two uncertain reaction parameters and open-loop unstable operation

  ⇒ re-optimization may be necessary



- D-RTO trigger
  - analyze reference optimal solution in real-time
  - trigger a potential re-optimize; otherwise provide quick updates
  - make changes to problem formulation

- *current state of process and disturbance prediction are necessary*

Lagrange function sensitivities w.r.t. all estimated disturbances

$$\text{compute} \quad S_j = dL_j / d\hat{d}_j \Big|_{\tilde{t}_{0j}} ;$$

$$L_j = \overline{\Phi}(u_i^{ref}, \hat{d}_j) + m_i^T h(u_i^{ref}, \hat{d}_j)$$

- one sensitivity integration of process model at each sampling time $\bar{t}_{0i}$ using previous D-RTO results (and active constraint set) at $\tilde{t}_{0j}$ is required
- compute change in sensitivities ($\Delta S_j = S_j - S_i$) and Lagrange function ($\Delta L_j = L_j - L_i$) can be then calculated

D-RTO trigger (III)

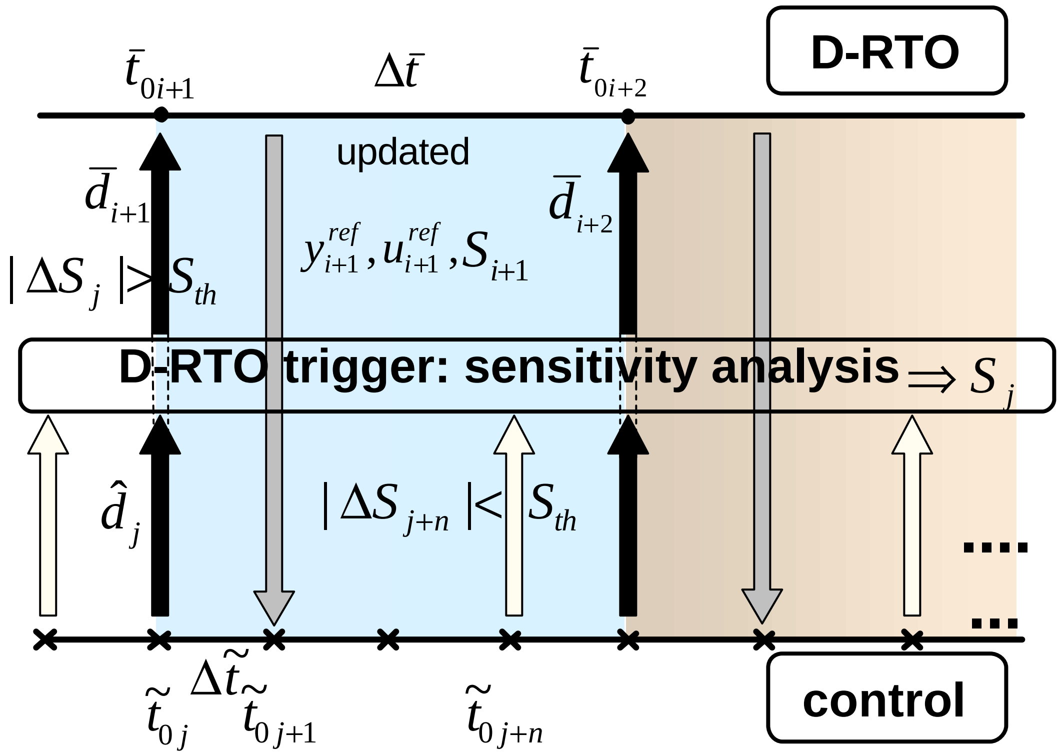
optimal solution sensitivities w.r.t. all estimated disturbances

compute $U_j = du_j^{ref}{}_j \Big/ d\hat{d}_j \Big|_{\tilde{t}_{0\,j}}$

and changed active constraint set

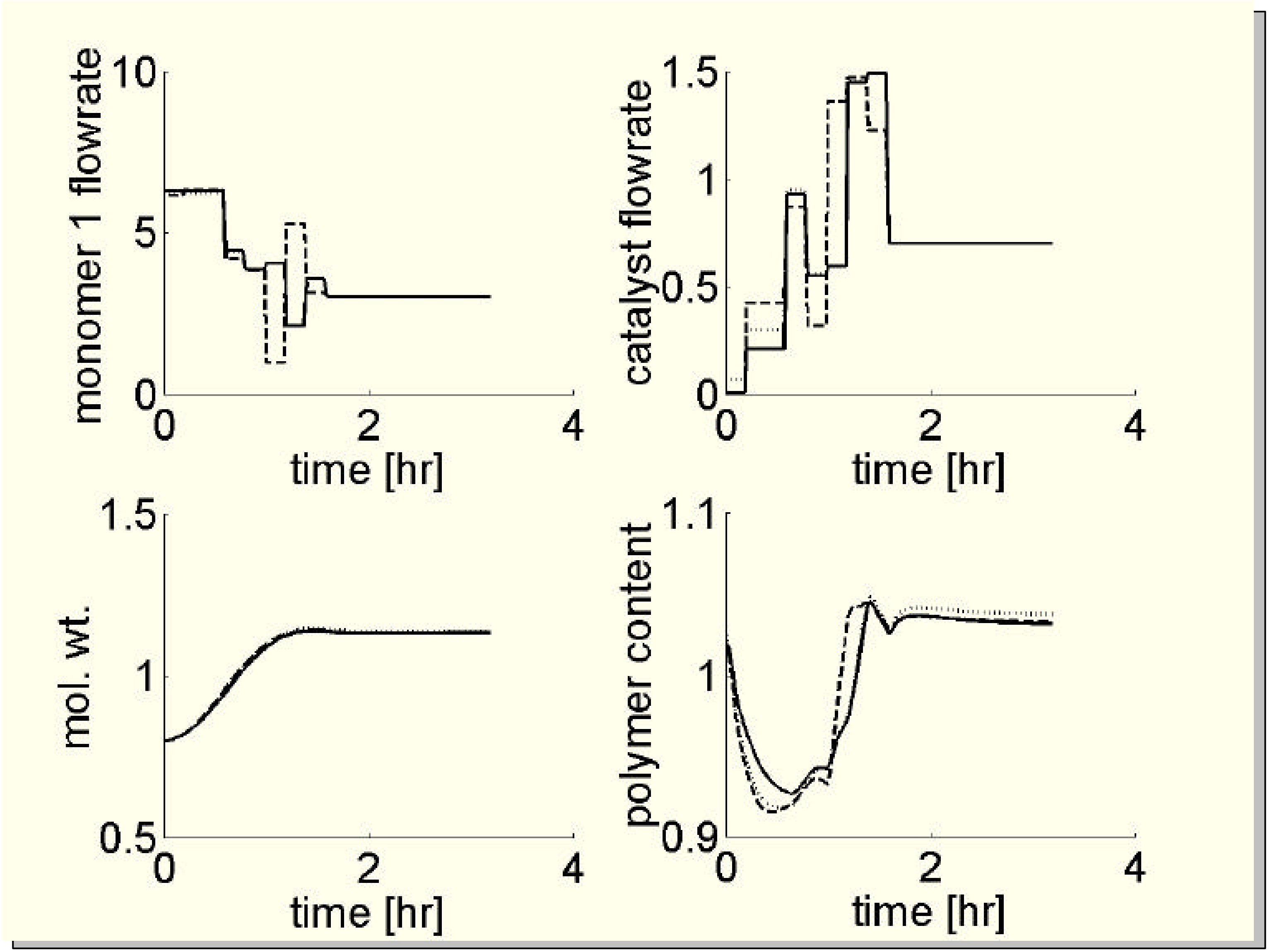
- solution to QP problem:
  - using second order information (Hessian of Lagrange function)
    $\Rightarrow$ *optimal sensitivities*
  - using first order information
    $\Rightarrow$ *feasible only sensitivities*
- updates as $u_j^{ref} = u_i^{ref} + U_i^T(\hat{d}_j - \bar{d}_i)$

D-RTO trigger (IV)



- if ΔS_j and ΔL_j are larger than a threshold value S_{th} and changed active constraint set is predicted, a re-optimization should be done
- else linear updates based on optimal solution sensitivities U_j are sufficient

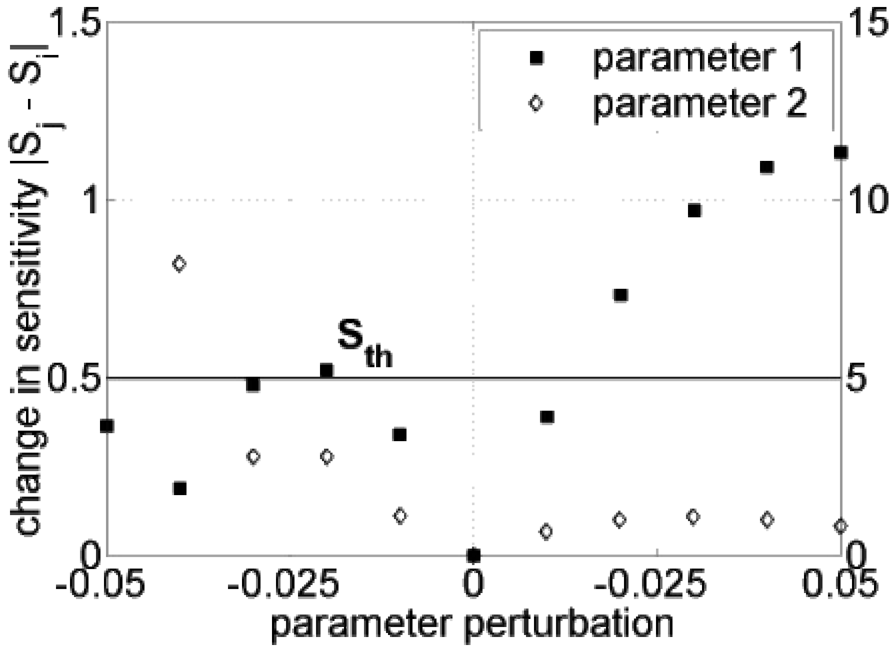
results with re-optimization and feasible updates



re-optimization results (2)

- reaction parameters randomly perturbed between their bounds
- re-optimization done only when necessary

  ⇒ steer to desired grade
- feasible updates only possible up to +4% change in parameter 1



- D-RTO problem needs to be solved only when necessary
- the hybrid integrated D-RTO and control with embedded sensitivity analysis is well suited for large-scale industrial process operation

comparison to conventional approach

- Present benefits of the INCOOP strategy.

conclusion and future perspective

- Present some concluding remarks
- give future perspective