Dynamic optimization of a plate reactor start-up

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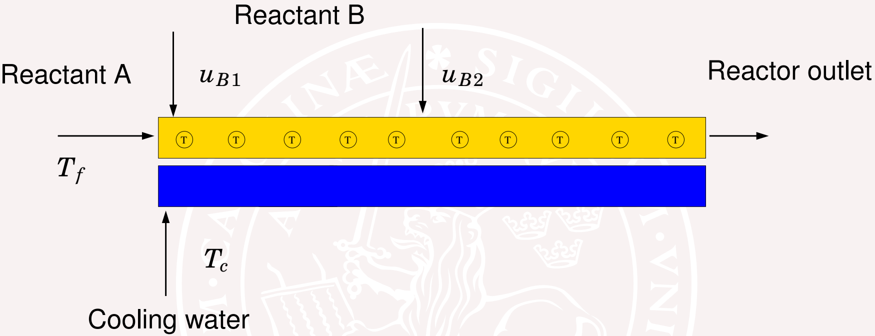
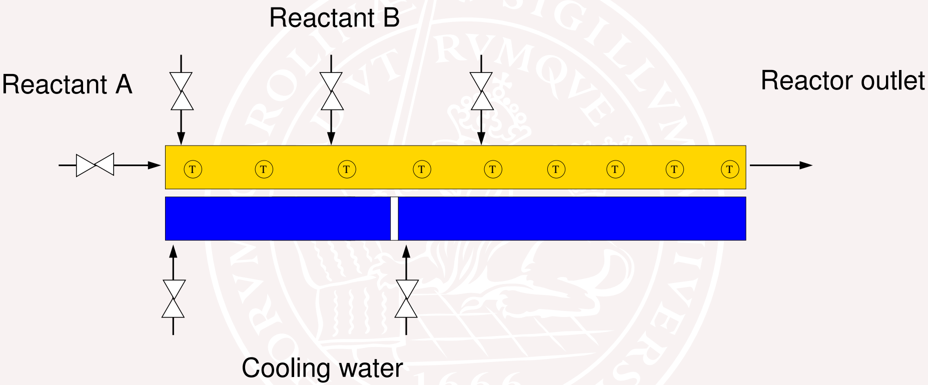
Process configurations : 2 inj. / 1 cool zone

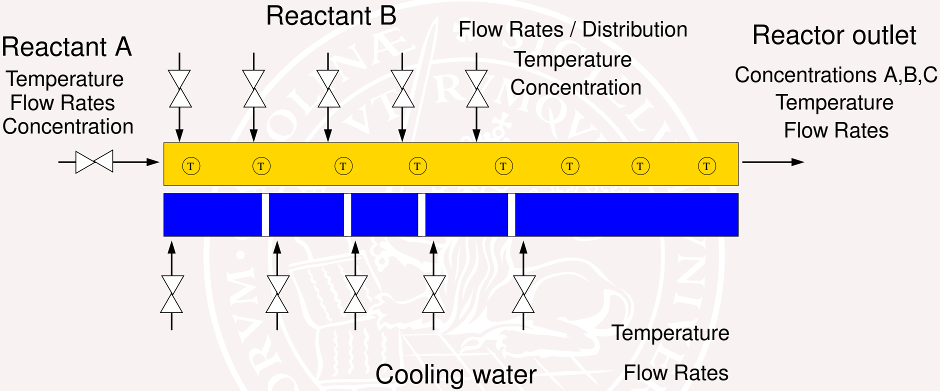


- Large flexibility in injection points and cooling zones.
- More actuators lead to better performance, but more expensive and complex process.
- Four control variables: $u_{T_{feed}}$, $u_{T_{cool}}$, u_{B1} and u_{B2}
- PDE model is discretized to a system of ODEs

Process configurations : 3 inj. / 2 cool zones

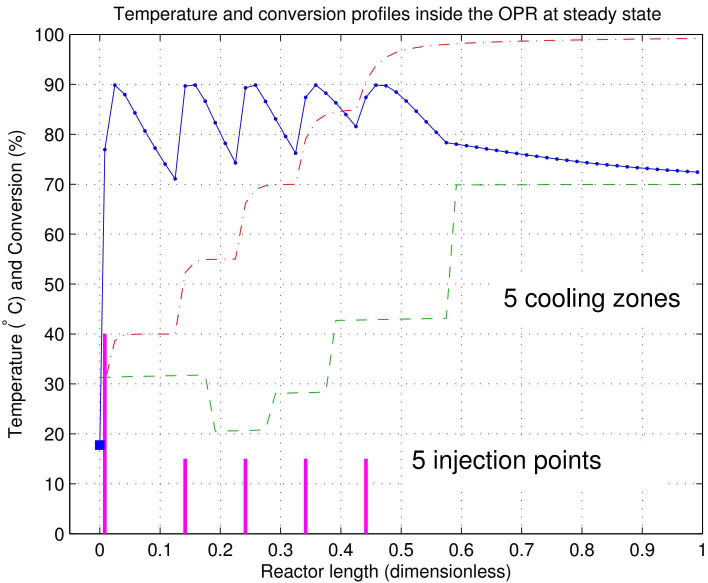


Process configurations : 5 inj. / 5 cool zone



Large flexibility: 18 input varibles available for control !

Process design choices



Start-up objectives & challenges

- Bring the process *safely* from initial cold state to optimal operating point with full heat release
- Minimize minimize off-spec product, amount of outflowing unreacted chemicals or minimize start-up time

- Highly nonlinear dynamics with multiple steady states
- Limiting actuator dynamics
- Process uncertainties

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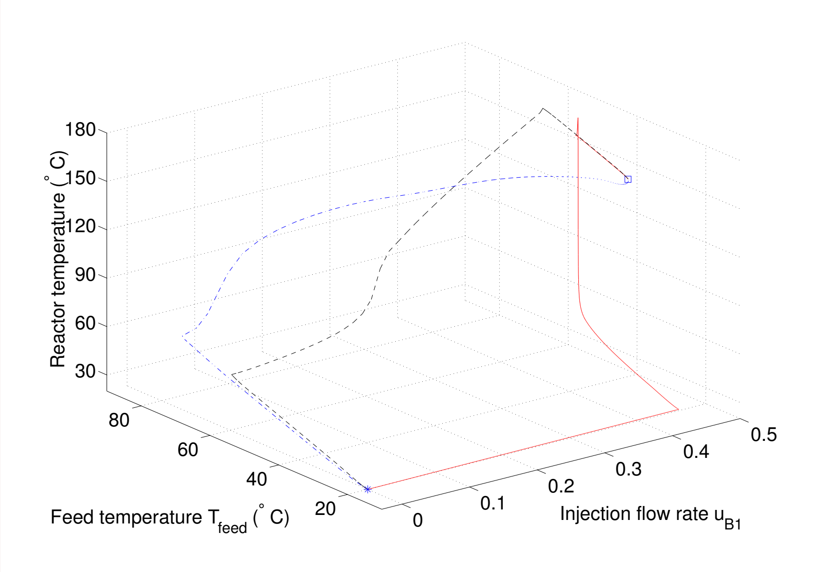
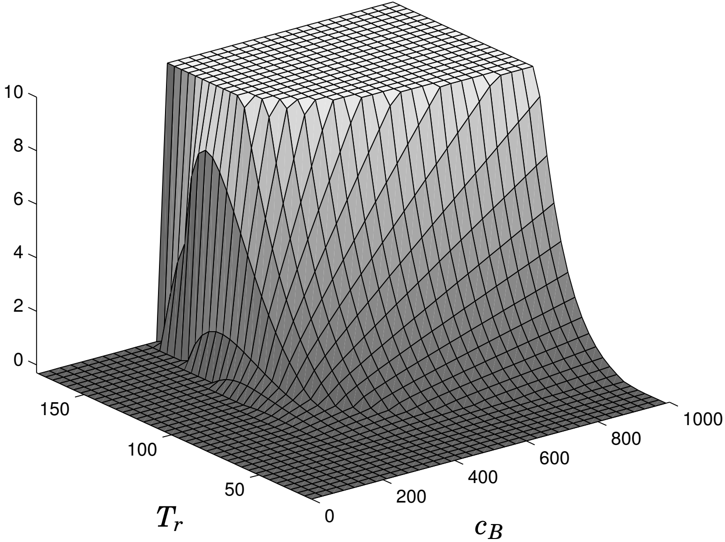
Motivating examples



Motivating examples cont'd



Safety conditions for ignition and conversion

Avoid regions in the state-space, where there are fast and dangerous dynamics

1. The reactor temperature should be driven to a required initial temperature at which reactant B can be fed into the reactor safely
2. Before the next downstream injection starts, it is necessary to check that almost all reactants injected upstream has converted

Nonlinear Model Predictive Control

Components in the controller

- Nonlinear model is available, derived from first principles (120 states), PDEs discretized to a system of ODEs.
- Dynamic optimization by a single-shooting, using ESDIRK methods for integration and sensitivity computation
- Extended Kalman filter
- NMPC needed primarily for start-up, but also for optimization of productivity, finding operating points for parallel reactions...

Details of the NMPC implementation

Cost function

$$\phi = \underbrace{\int_{t_0}^{t_p} g(x(t), u(t), \bar{u}(t), r(t))dt}_{=\phi_1} + \underbrace{\frac{1}{2}\sum_{k=0}^{N-1} \|\Delta u_k\|_{2,S}^2}_{=\phi_2} \tag{1}$$

where

$$\begin{aligned} g(x(t), u(t), \bar{u}(t), r(t)) = \\ \frac{1}{2}\|C_z x(t) - r(t)\|_{2,Q_z}^2 + \frac{1}{2}\|u(t) - \bar{u}(t)\|_{2,R}^2 \\ + \frac{1}{2}\|s(x(t))\|_{2,Q_{2s}}^2 + \|s(x(t))\|_{1,Q_{1s}} \end{aligned} \tag{2}$$

and $s(\cdot)$ is a soft constraint penalty function

Details of the NMPC implementation

Objective function

$$\psi = \psi(\{u_k\}_{k=0}^{N-1}) = \{\phi : \dot{x}(t) = f(x(t), u(t), d(t)), x(t_0) = x_0\} \tag{3}$$

The optimization problem is then

$$\min_{\{u_k\}_{k=0}^{N-1}} \quad \psi = \psi(\{u_k\}_{k=0}^{N-1}) \tag{4}$$

- **Compute ψ by integrating forward, given guess on $\{u_k\}_{k=0}^{N-1}$**
- **Compute $\nabla_{u_k}\psi$ by integrating backwards**
- **Compute new control trajectories by solving NLP**

The Alfa Laval plate reactor