Dynamic Process Models

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Overview

- Ordinary Differential Equations (ODE)
- Boundary Conditions, Objective
- Differential-Algebraic Equations (DAE)
- Multi Stage Processes
- Partial Differential Equations (PDE) and Method of Lines (MOL)

Dynamic Systems and Optimal Control

“Optimal control” = **optimal choice of inputs for a dynamic system**

What type of dynamic system?

- Stochastic or deterministic?
- Discrete or continuous time?
- Discrete or continuous states?

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In this course, treat deterministic differential equation models (ODE/DAE/PDE)

(Some other dynamic system classes)

- Discrete time systems:

$$x_{k+1} = f(x_k, u_k), \quad k = 0, 1, \ldots$$

  system states $x_k \in X$, control inputs $u_k \in U$. State and control sets X, U can be discrete or continuous.
- Games like chess: discrete time and state (chess figure positions), adverse player exists.
- Robust optimal control: like chess, but continuous time and state (adverse player exists in form of worst-case disturbances)
- Control of Markov chains: discrete time, system described by transition probabilities

$$P(x_{k+1} | x_k, u_k), \quad k = 0, 1, \ldots$$

- Stochastic Optimal Control of ODE: like Markov chain, but continuous time and state

Ordinary Differential Equations (ODE)

System dynamics can be manipulated by controls and parameters:

$$\dot{x}(t) = f(t, x(t), u(t), p)$$

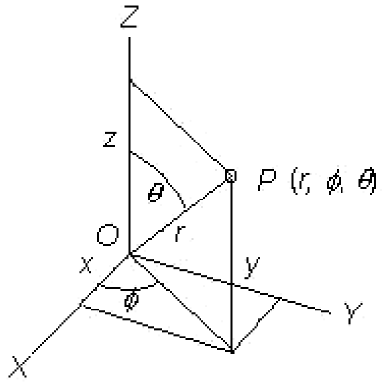
- simulation interval: $[t_0, t_{\mathrm{end}}]$
- time $t \in [t_0, t_{\mathrm{end}}]$
- state $x(t) \in \mathbb{R}^{n_x}$
- controls $u(t) \in \mathbb{R}^{n_u}$ $\longleftarrow$ manipulated
- design parameters $p \in \mathbb{R}^{n_p}$ $\longleftarrow$ manipulated

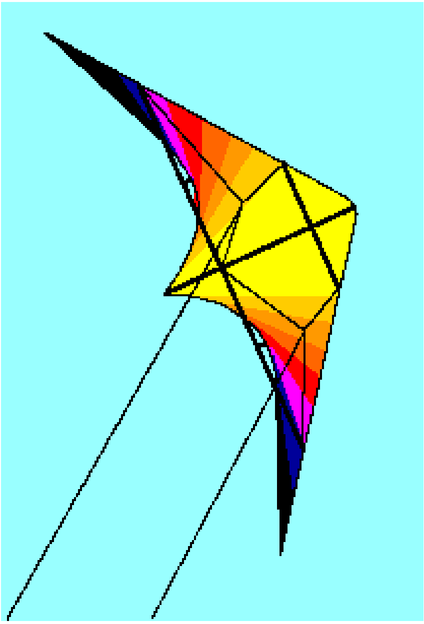
ODE Example: Dual Line Kite Model

- Kite position relative to pilot in spherical polar coordinates r, ϕ, θ. Line length r fixed.
- System states are $x = (\theta, \phi, \dot{\theta}, \dot{\phi})$.
- We can control roll angle $u = \psi$.
- Nonlinear dynamic equations:

$$\begin{aligned}\ddot{\theta} &= \frac{F_\theta(\theta, \phi, \dot{\theta}; \dot{\phi}, \psi)}{rm} + \sin(\theta)\cos(\theta)\dot{\phi}^2 \\ \ddot{\phi} &= \frac{F_\phi(\theta, \phi, \dot{\theta}; \dot{\phi}, \psi)}{rm\sin(\theta)} - 2\cot(\theta)\dot{\phi}\dot{\theta}\end{aligned}$$

- Summarize equations as $\dot{x} = f(x, u)$.





Initial Value Problems (IVP)

THEOREM [Picard 1890, Lindelöf 1894]:
Initial value problem in ODE

$$\begin{aligned} \dot{x}(t) &= f(t, x(t), u(t), p), \quad t \in [t_0, t_{\text{end}}], \\ \dot{x}(t_0) &= x_0 \end{aligned}$$

- with given initial state x_0, design parameters p, and controls $u(t)$,
- and Lipschitz continuous $f(t, x, u(t), p)$

has **unique** solution

$$x(t), \quad t \in [t_0, t_{\text{end}}]$$

NOTE: Existence but not uniqueness guaranteed if $f(t, x, u(t), p)$ only continuous [G. Peano, 1858-1932].
Non-uniqueness example: $\dot{x} = \sqrt{|x|}$

Boundary Conditions

Constraints on initial or intermediate values are important part of dynamic model.

STANDARD FORM:

$$r(x(t_0), x(t_1), \ldots, x(t_{\mathrm{end}}), p) = 0, \quad r \in \mathbb{R}^{n_r}$$

E.g. fixed or parameter dependent initial value x_0:

$$x(t_0) - x_0(p) = 0 \qquad (n_r = n_x)$$

or periodicity:

$$x(t_0) - x(t_{\mathrm{end}}) = 0 \qquad (n_r = n_x)$$

NOTE: Initial values $x(t_0)$ need not always be fixed!

Kite Example: Periodic Solution Desired

- Formulate periodicity as constraint.
- Leave $x(0)$ free.
- Minimize integrated power per cycle

$$\min_{x(\cdot),u(\cdot)} \int_0^T L(x(t),u(t))dt$$

subject to

$$\begin{aligned} x(0) - x(T) &= 0 \\ \dot{x}(t) - f(x(t),u(t)) &= 0, \; t \in [0,T]. \end{aligned}$$

Objective Function Types

Typically, distinguish between

- *Lagrange term* (cost integral, e.g. integrated deviation):

$$\int_0^T L(t, x(t), u(t), p)dt$$

- *Mayer term* (at end of horizon, e.g. maximum amount of product):

$$E(T, x(T), p)$$

- Combination of both is called *Bolza objective*.

Differential-Algebraic Equations (DAE)

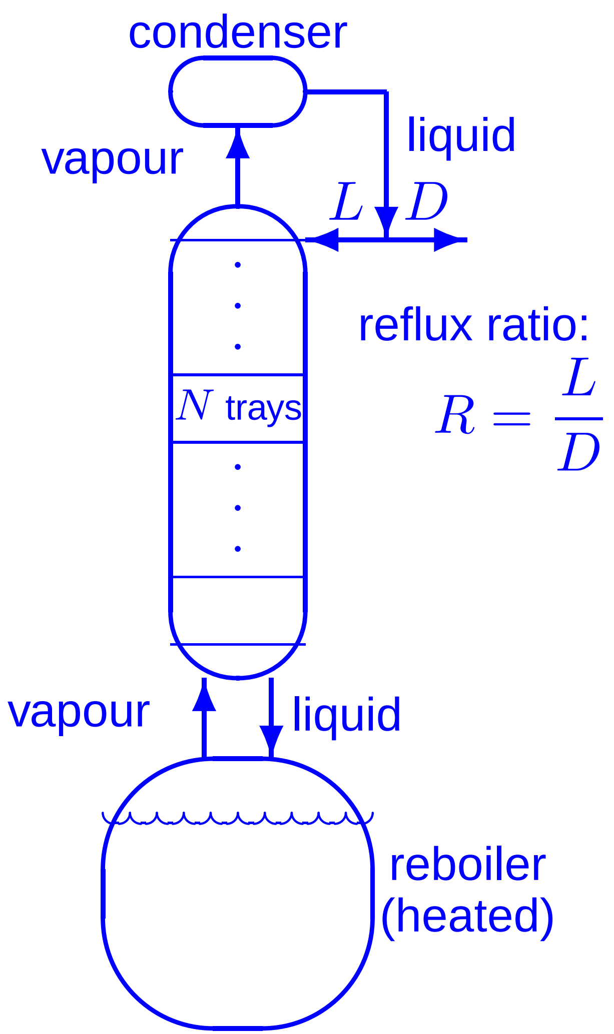
Augment ODE by **algebraic equations** g and **algebraic states** z

$$
\begin{aligned}
\dot{x}(t) &= f(t, x(t), z(t), u(t), p) \\
0 &= g(t, x(t), z(t), u(t), p)
\end{aligned}
$$

- differential states $x(t) \in \mathbb{R}^{n_x}$
- algebraic states $z(t) \in \mathbb{R}^{n_z}$
- algebraic equations $g(\cdot) \in \mathbb{R}^{n_z}$

Standard case: index one $\Leftrightarrow$ matrix $\frac{\partial g}{\partial z} \in \mathbb{R}^{n_z \times n_z}$ invertible.
Existence and uniqueness of initial value problems similar as for ODE.

DAE Example: Batch Distillation



- concentrations $X_{k,\ell}$ as differential states x
- tray temperatures T_ℓ as algebraic states z
- T_ℓ implicitly determined by algebraic equations

$$1 - \sum_{k=1}^{3} K_k(T_\ell)\, X_{k,\ell} = 0, \quad \ell = 0, 1, \ldots, N$$

with

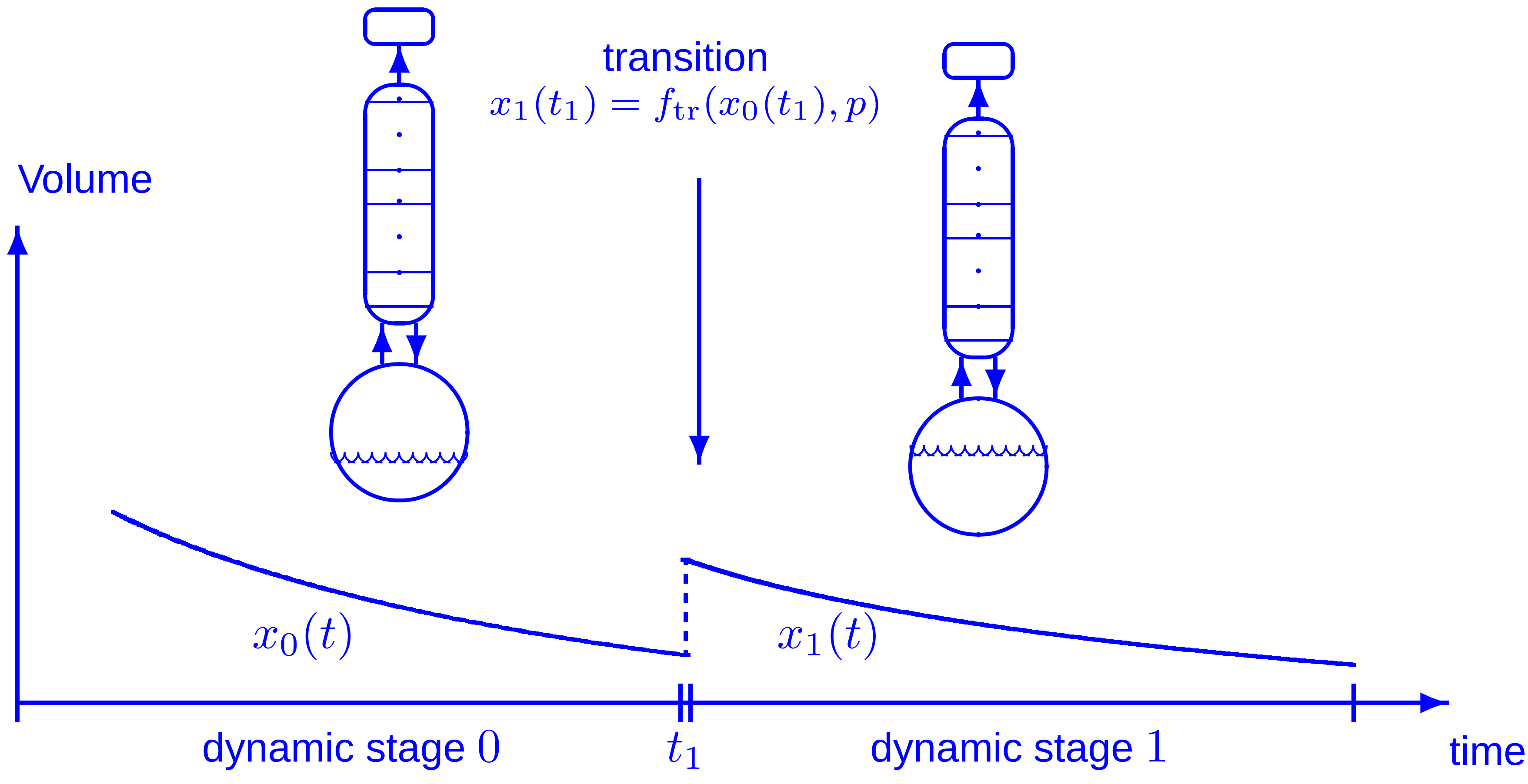
$$K_k(T_\ell) = \exp\left(- \frac{a_k}{b_k + c_k T_\ell} \right)$$

- reflux ratio R as control u

Multi Stage Processes

Two dynamic stages can be connected by a discontinuous “transition”.

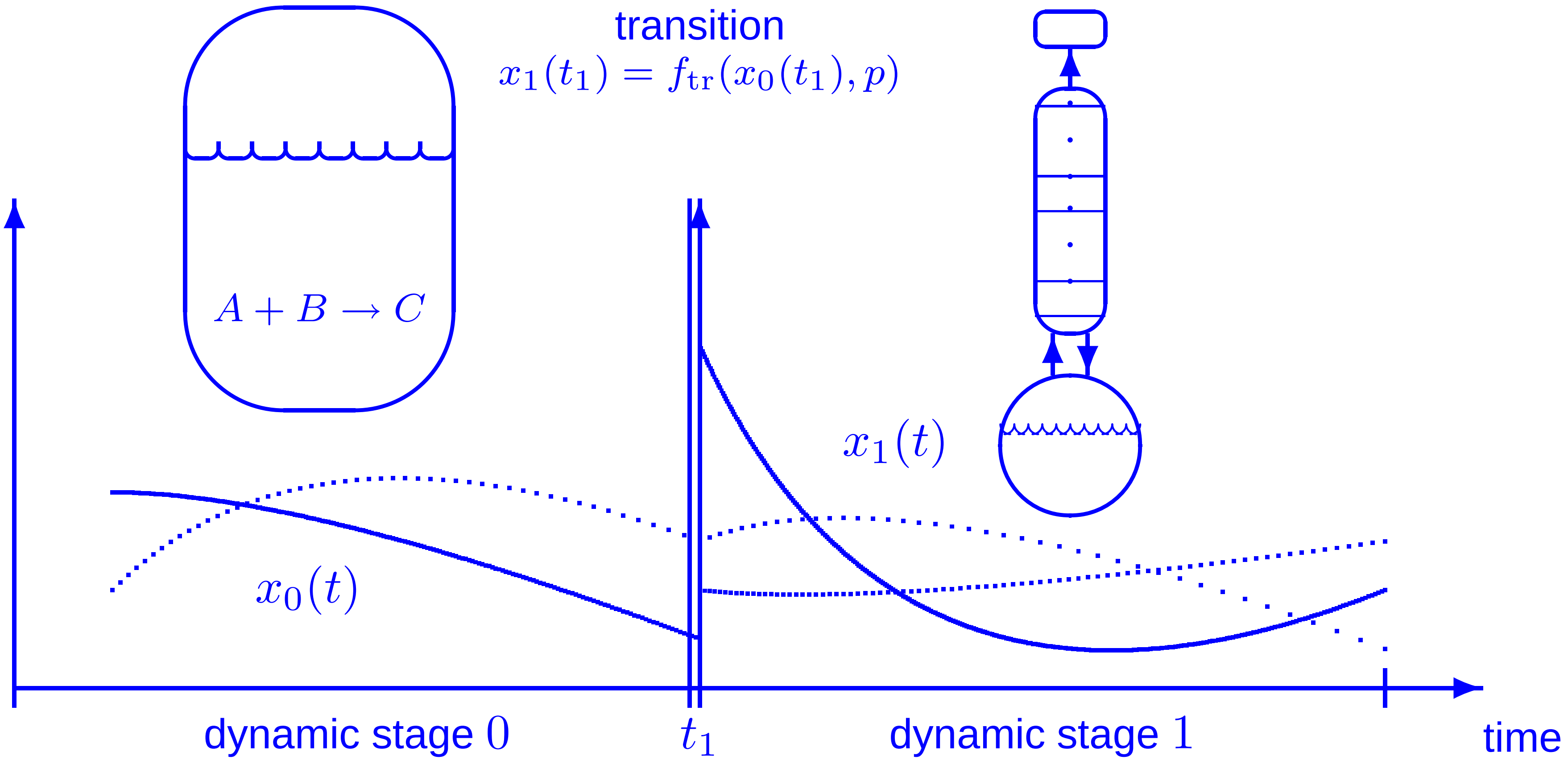
E.g. Intermediate Fill Up in Batch Distillation



Multi Stage Processes II

Also **different** dynamic systems can be coupled.

E.g. batch reactor followed by distillation (different state dimensions)

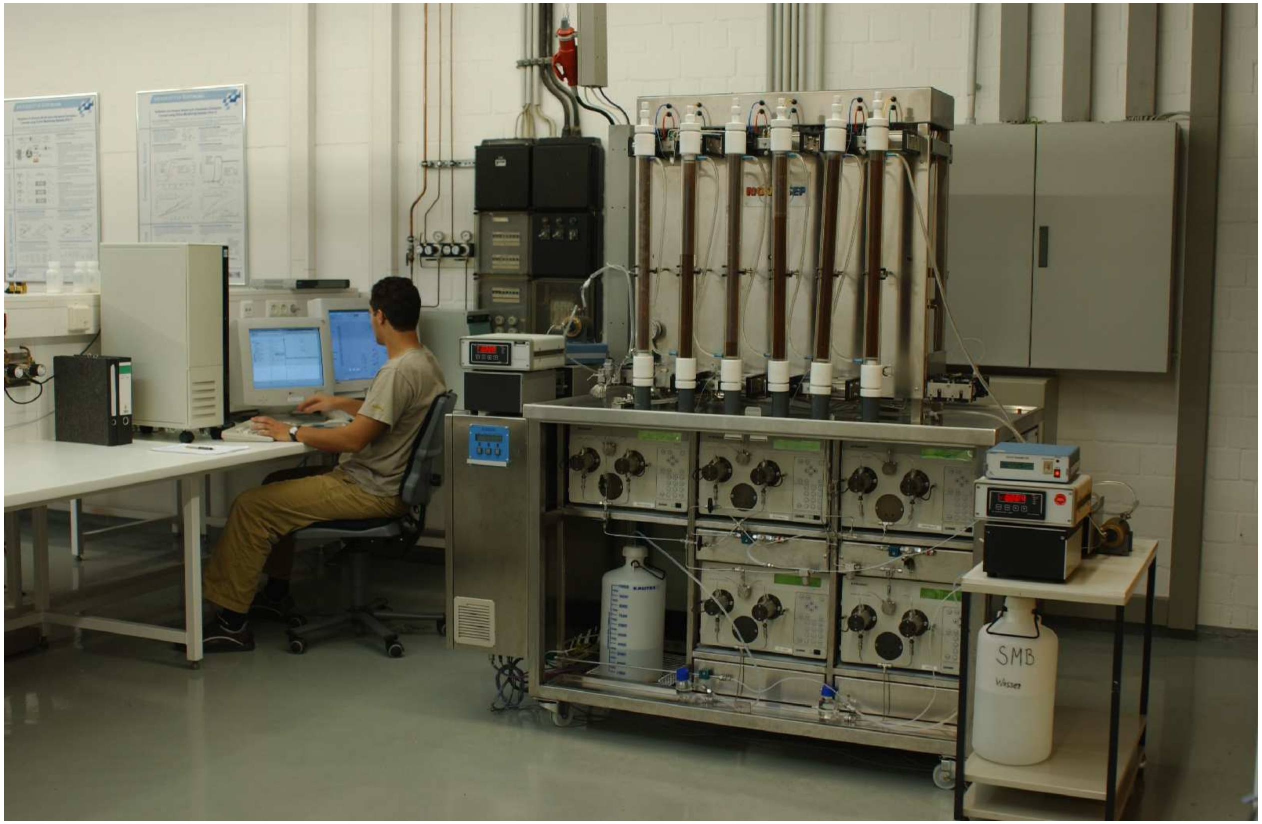


Partial Differential Equations

- Instationary partial differential equations (PDE) arise e.g in transport processes, wave propagation, ...
- Also called “distributed parameter systems”
- Often PDE of subsystems are coupled with each other (e.g. flow connections)
- Method of Lines (MOL): discretize PDE in space to yield ODE or DAE system.
- Often MOL can be interpreted in terms of compartment models.
- Best seen at example.

Simulated Moving Bed (SMB) Process

(with A. Toumi and S. Engell, Dortmund)



Chromatographic separation of fine chemicals.

Method of Lines (MOL)

E.g. transport equations in each SMB column:

$$\frac{\partial c_{\mathrm{b}}}{\partial t} = -K(c_{\mathrm{b}} - c_{\mathrm{p}}) + D_{\mathrm{ax}} \frac{\partial^2 c_{\mathrm{b}}}{\partial x^2} + u \frac{\partial c_{\mathrm{b}}}{\partial x},$$

- introduce spatial grid points $x_0, \ldots, x_N$
- approximate spatial derivatives, e.g. by finite differences

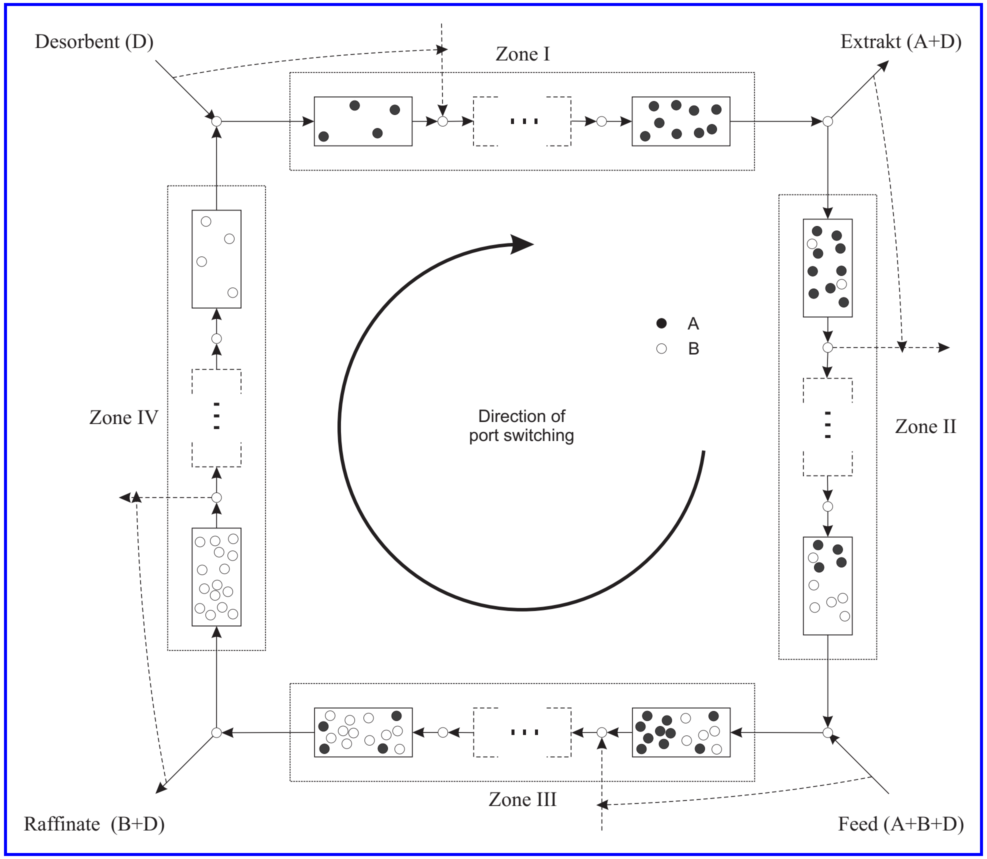
$$\frac{\partial c_{\mathrm{b}}}{\partial x} \approx \frac{\partial c_{\mathrm{b}}(x_{i+1}) - c_{\mathrm{b}}(x_i)}{x_{i+1} - x_i}, \quad \text{etc.}$$

- define state vector $x_{\mathrm{col}} := (c_{\mathrm{b}}(x_0), \ldots, c_{\mathrm{b}}(x_N))$,
- obtain ODE

$$\dot{x}_{\mathrm{col}}(t) = f_{\mathrm{col}}(x_{\mathrm{col}}(t), u(t), p)$$

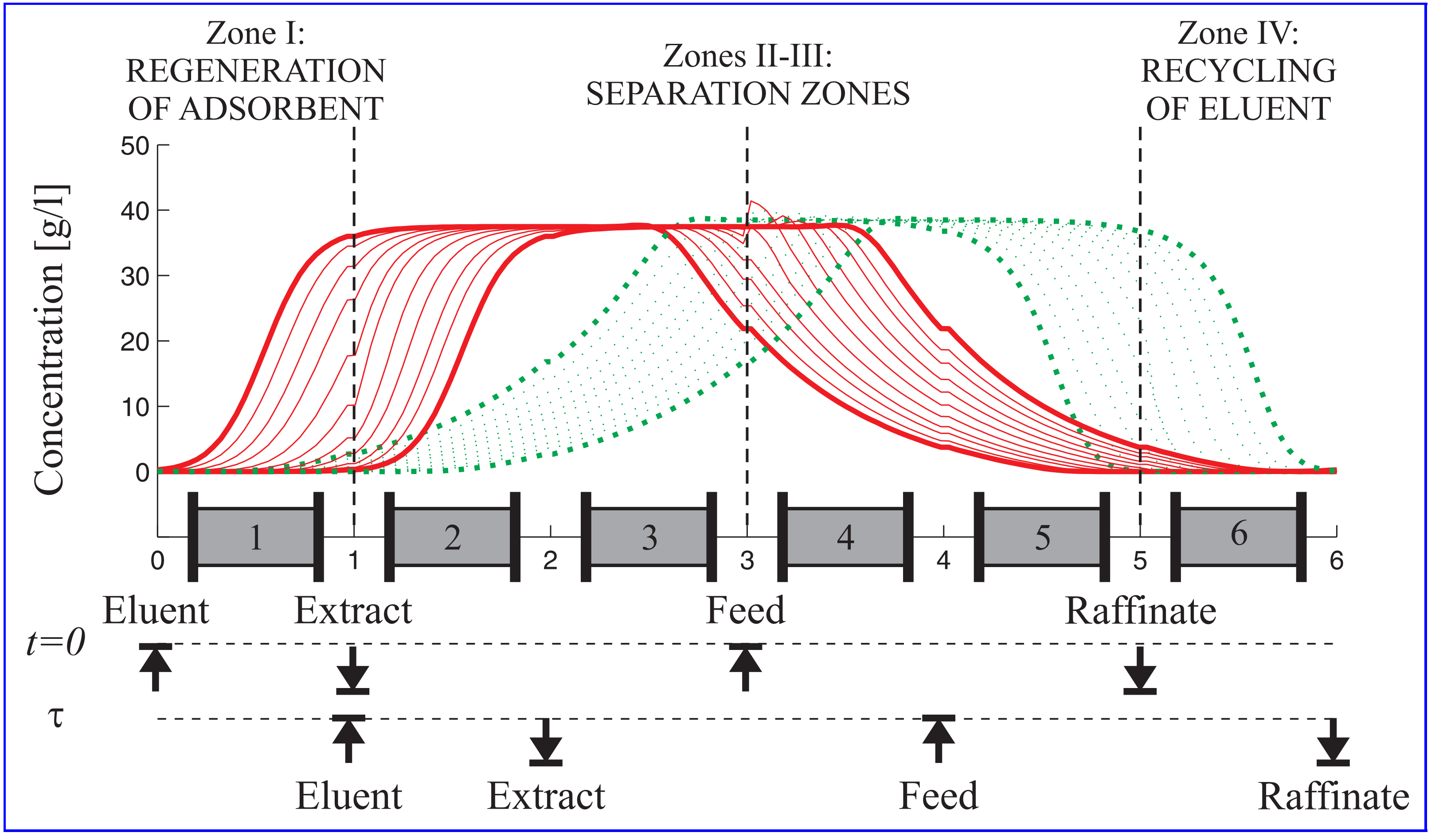
Simulated Moving Bed Principle

Columns coupled in loop, plus in- and outlet ports.



Periodic switching simulates countercurrent, leads to **cyclic steady state**.

SMB: Cyclic Steady State



After one cycle system state is simply shifted in space. Continuous and discrete dynamics of one cycle can be summarized in a map Γ.

Representation of PDE in gPROMS

Some Equations from a catalytic tube reactor model

```
     # --- MASS BALANCE FOR REACTOR: [mol/(mR3*s)] ---
       FOR i := 1 TO NoComp DO
        FOR z := 0|+ TO TubeLength DO
          FOR r := 0|+ TO TubeRadius|- DO
            Void*$C(i,z,r) = - us*PARTIAL(C(i,z,r),Axial)
                  + Dez*PARTIAL(C(i,z,r),Axial,Axial)
                  ...
          END # For r
        END # For z
      END # For i
...
     # --- Discretisation method ---
      Axial  := [ BFDM, 1, 50 ] ;
      Radial := [ OCFEM, 2, 5 ] ;
```

PDE is automatically discretized by MOL and transformed into DAE

Summary

Dynamic models for optimal control consist of

- differential equations (ODE/DAE/PDE)
- boundary conditions, e.g. initial/final values, periodicity
- objective in Lagrange and/or Mayer form
- transition stages in case of multi stage processes

PDE often transformed into DAE by Method of Lines (MOL)

DAE standard form:

$$\begin{aligned} \dot{x}(t) &= f(t, x(t), z(t), u(t), p) \\ 0 &= g(t, x(t), z(t), u(t), p) \end{aligned}$$

References

- K.E. Brenan, S.L. Campbell, and L.R. Petzold: The Numerical Solution of Initial Value Problems in Differential-Algebraic Equations, SIAM Classics Series, 1996.
- U.M. Ascher and L.R. Petzold: Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations. SIAM, 1998.