# Industrial Challenges and Requirements for Optimisation and Control of Polymerisation Processes

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# Polymer production at Bayer


- **Annual sales of approx. 11 billion € (2001)**
- **over 100 sites throughout the world**
- **Product portfolio:**

**Plastics**

- Polycarbonates
- Styrenics
- Polyamides and Polyesters
- Thermoplastic Polyurethanes

**Polyurethane raw materials**

- Isocyanates
- Polyols

**Rubber**

- Solid Rubber
- Rubber chemicals
- Modifiers

**Coating Raw Materials**

- Coatings
- Colorants

**Fibers**

## Why is optimisation and control important in this business?

**Product quality**

- ◊ Product specifications for high value products become tighter and tighter

**Speciality polymers becoming commodities**

- ◊ Lower margins
- ◊ Bigger production units
- ◊ High pressure for efficient production
  - ◊ Automation
  - ◊ Flexible production
  - ◊ Less off-spec production by quality control

**Higher flexibility**

- ◊ Marked demands cause frequent changes in polymer grade, production load and product quality

# Technical problem formulation

## 1. The quality control problem

- Keep product quality (e.g. viscosity) at desired setpoint despite disturbances
- Control problem relies either on frequent lab samples or ideally on online analytics
- Problem frequently described in academic literature as application for MPC technology

## 2. The grade change problem

- Continuous polymerisation plant produces different grades of the same polymer with frequent changeovers
- Trajectories need to be optimised to minimise production of „intermediate“ grade during transition
- Problem frequently described in academic literature as application for dynamic optimisation

## 3. The load change problem

- Production rate of polymer needs to be adjusted spontaneously due to planned or unplanned throughput changes of downstream processing unit(s)
- Trajectories need to be optimised to avoid production of offspec material at all
- Problem has practical relevance and is related to grade change problem, but is not described in academic literature

# Practical questions and problems I

**MPC is a mature technology also for polymerisation processes but ....**

**quality control problems are not yet frequently solved by MPC approaches because of**

**Nonlinearity**

- Polymerisation processes tend to be highly nonlinear

**Quality measurements**

- Online analytics are often available, but their reliability is not always high enough for closed loop control
- Replacement of online measurements by lab samples must be possible to ensure best operation at all times

**Modelling issues**

- How can I obtain a good model and maintain it?

Existing industrial applications are concentrated on Polyolefines where the above issues are nearly solved

**Offline dynamic optimisation of changeovers is "state of the art" but ....**

**integration into daily production has proven to be difficult because of**

**Combinatorial explosion**

- Trajectories for all possible combinations of desired loads and grades need to be pre-optimised

**Unknown initial states**

- The start of the trajectory is not the nominal steady state

**Handling of disturbances**

- How do disturbances affect the optimality and feasibility of the trajectories?

**Model accuracy**

- Is the model good enough for the trajectories being applied without feedback?

**Regulatory control**

- Can the regulatory control handle the fast changes as desired?

# Practical questions and problems III

## Potential benefits of the integration of optimisation and control ....

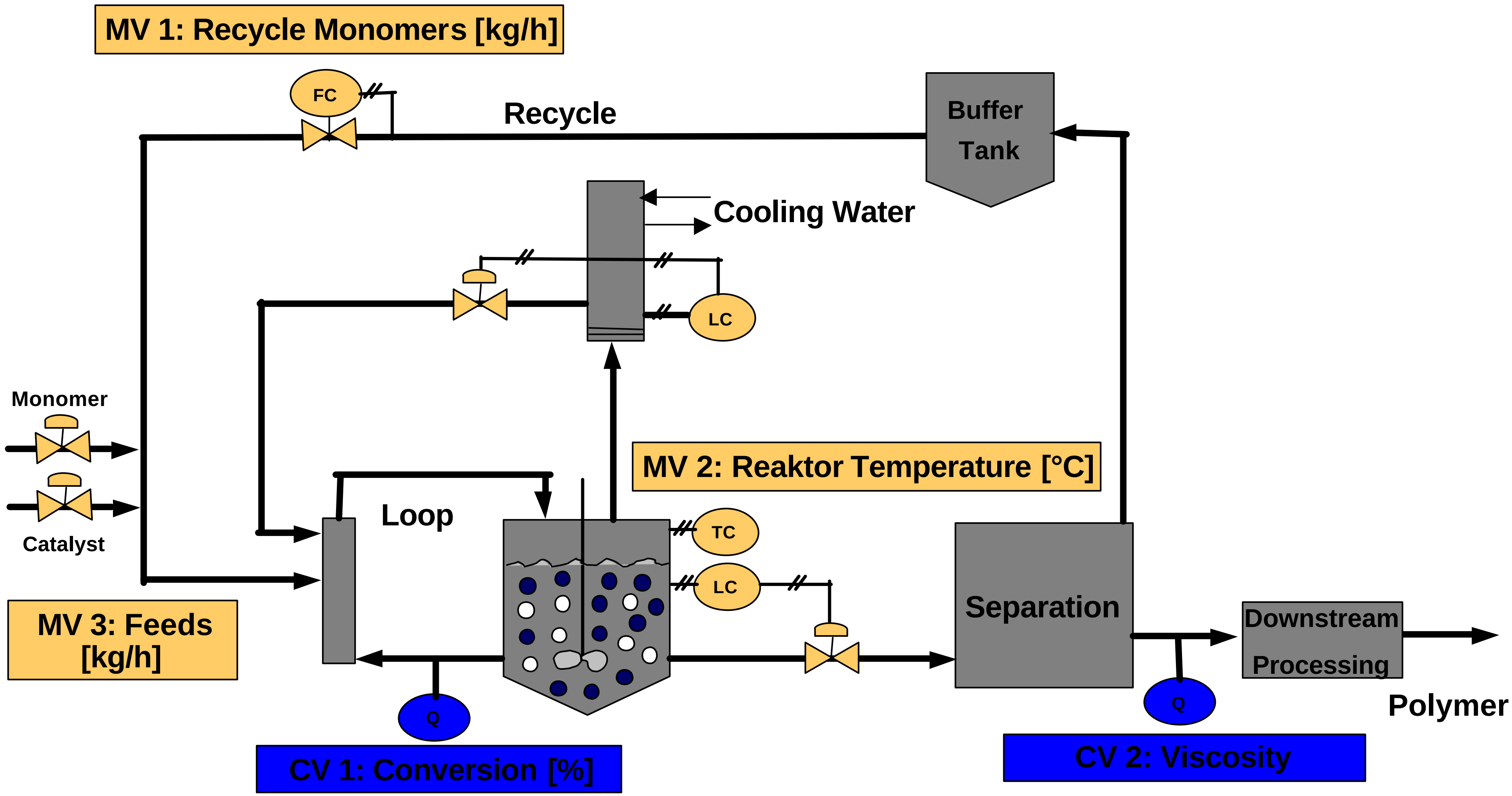
**I Most of the problems associated with offline dynamic optimisation can be avoided**

- Disturbances
- Initial States
- Combinatorial Explosion

**II Fast and frequent changeovers (planned and unplanned) would be possible to**

- Allow flexible production
- Avoid off-spec production and therefore
- Significantly improve the economic operation of the plant

# Process scheme



# Current situation



**I Quality control is currently manual based on lab samples of the final product**

**II Frequent changeovers are necessary**

- Grade changes
- Load changes to compensate for planned or unplanned throughput changes of downstream processing

**and currently result in offspec production during transition due to suboptimal trajectories**

**III Open loop dynamics of reactor are unstable and are stabilised by cascaded temperature control thus limiting the maximum speed of transitions**

# Special problems and disturbances

I Load changes need to be performed instantaneously since polymer melt can not be stored

II Outlet flow of the reactor can only be measured (and controlled) with low precision due to polymer properties

III Important polymer property viscosity is not observable from any other available measurement

IV Online viscosity measurement is located downstream after the separation and therefore has a significant time delay

V In case of failure of online viscosity measurement, it needs to be replaced in the control strategy by less frequent and delayed lab samples

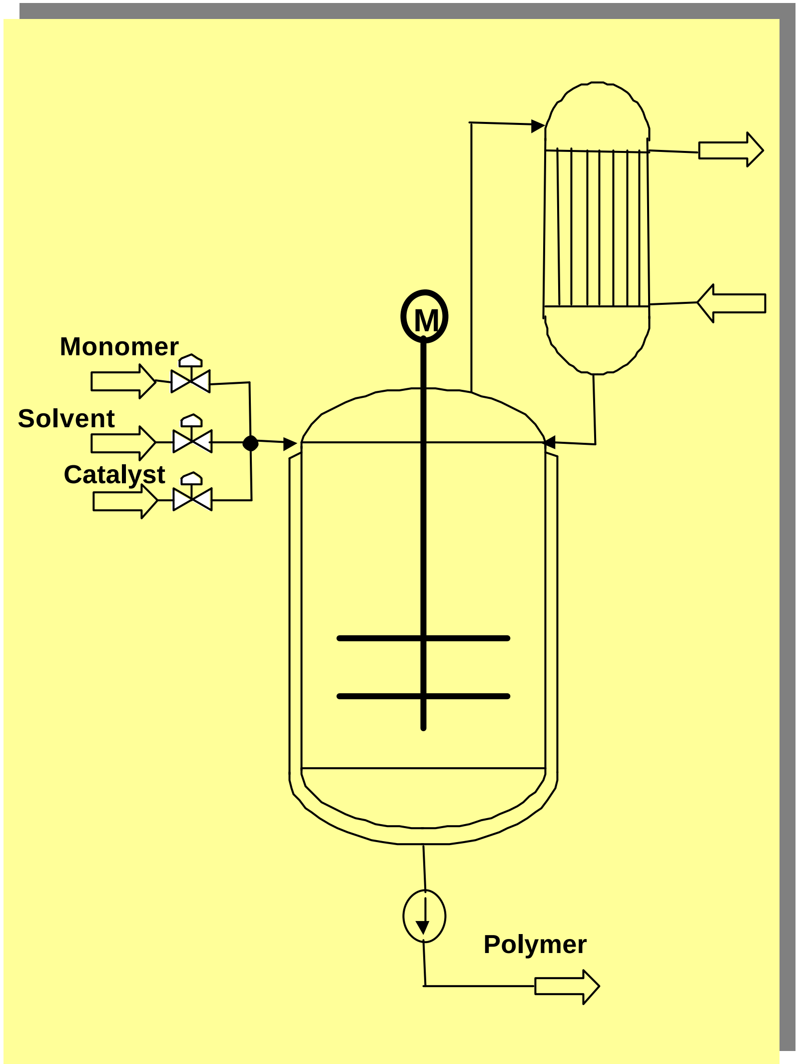
VI Long term accumulation of unknowns affect the reaction and are compensated by purging

VII Effect of unknowns to reaction can not be modelled exactly and therefore leads to time variant plant-model mismatch

# The load change optimisation problem

## Problem:

- Optimisation of planned or spontaneous load change due to throughput change in downstream processing unit
- Spontaneous reduction of reactor outlet to new setpoint
- Reactor level / residence time should reach new setpoint as soon as possible
- Product quality (Molecular weight / viscosity) should not leave product specification




## Controls:

- Monomer feed (fresh and recycled)
- Catalyst dosing

# Problem formulation for dynamic optimisation

## Solution strategy

- Implementation of the process model in gPROMS (PSE Ltd.)
- Stabilisation of reactor dynamics by subsidiary temperature control.
- Use of the dynamic optimisation tool ADOPT (*Lehrstuhl für Prozesstechnik*, RWTH Aachen) linked to gPROMS via ESO interface.

## Results:

- Load changes can be realised fast and with no off-spec product.
- Methodology can be applied to grade change problem as well.

### Optimisation formulation

$$\min_{\mathbf{u},t_f} J = \int_{t_0}^{t_f} [s_t + s_{MW}(MW - MW_{sp})^2]\,\mathrm{d}t$$

$$\text{u.B.v.} \quad \mathbf{g}(\dot{\mathbf{x}},\mathbf{x},\mathbf{z},\mathbf{u},t) = \mathbf{0}$$

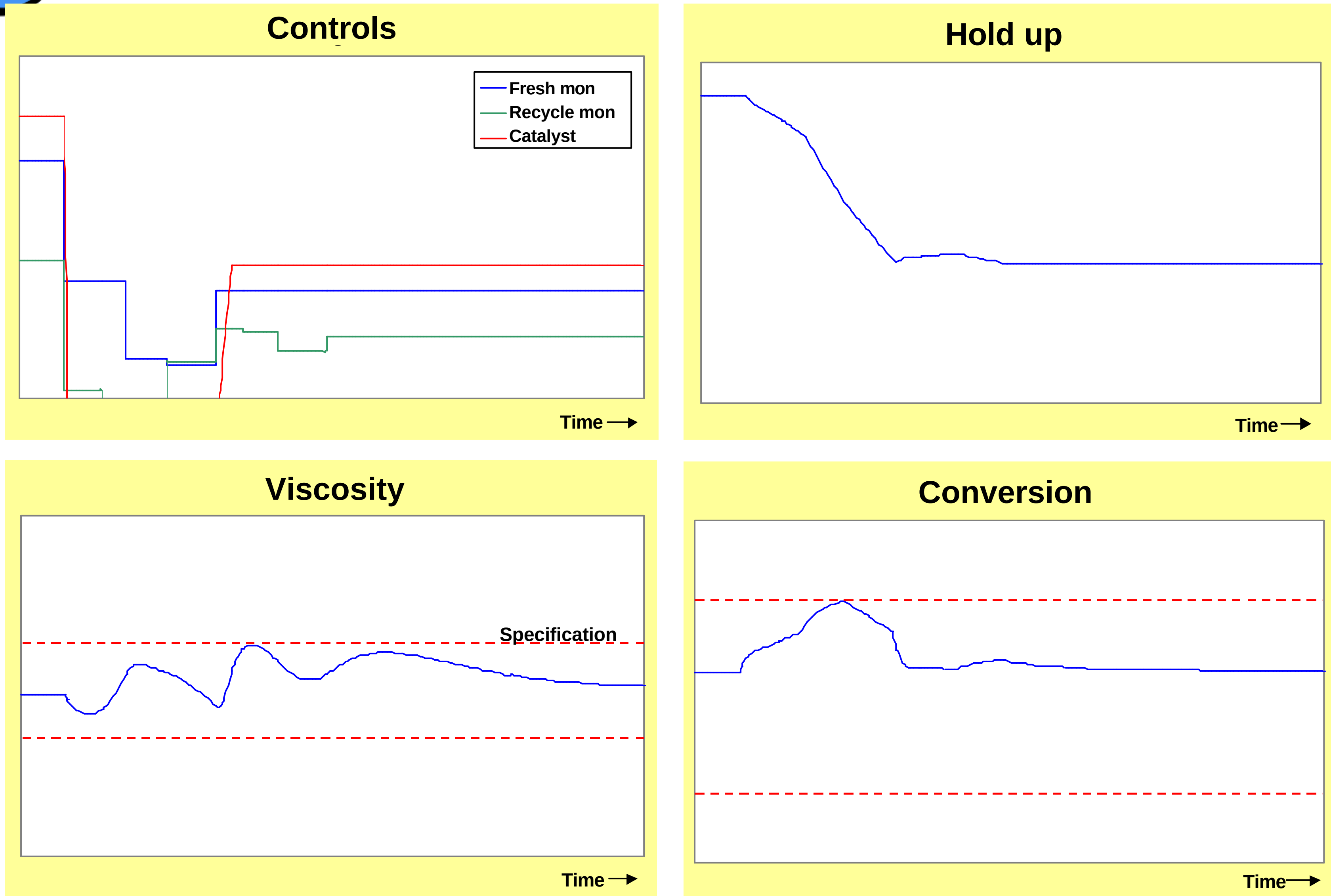
$$\mathbf{h}(\mathbf{x},\mathbf{z},\mathbf{u},t) \le \mathbf{0}$$

$$\mathbf{x}(t=0) = \mathbf{x}_0$$

### Model properties

- Complex reaction kinetics
- approx. 200 states
- approx. 2500 algebraic variables
- thermally unstable operating point

# Example: Optimal trajectory



## Dynamic optimisation results applied to the plant show ...

- Optimised profiles are significantly different from conventional operating procedure
- Somewhat more agressive changes in setpoint could only be realised with improved regulatory control
- Optimisation results for several scenarios investigated predict that load changes can be realised with no offspec material (compared to several hours of off-spec production in conventional (manual) operation)
- First validation of prediction: „Optimised“ trajectories have been applied manually, model predictions could be verified