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# Model Predictive Control of Free Surfactant Concentration in Emulsion Polymerization

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## Context of the study

- The Particle Size Distribution (PSD) affects:
  - The polymer rheology
  - Adhesion
  - Optical properties
- Automatic control of PSD involves:
  - Nonlinear infinite dimensional system
  - Few measurements are available on line

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The main objective is to apply MPC to emulsion polymerization processes modeled by nonlinear Partial Differential Equations to control the PSD shape (monomodal or bimodal)

# Outline

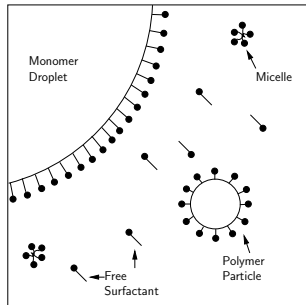
- 1 Polymerization process
  - Emulsion polymerization
  - Aqueous phase reactions
  - Population Balance Equation
- 2 PSD control
  - Measurement
  - Control objective
  - Model Predictive Control
- 3 Conclusion

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# Emulsion polymerization

Heterogeneous medium:

- Monomer droplets
- Polymer particles
- Excess surfactant creates micelles ( $[S]_{aq} > CMC$ )  
→ Micellar nucleation



# Aqueous phase reactions

- Monomer material balance ( $N_m(t), n(r, t), \bar{n}(r, t)$ )
  - Surfactant material balance  
 ( $[S](t), [S]_{aq}(t), Q_S(t), n(r, t), \bar{n}(r, t)$ )
  - Initiator décomposition ( $[I](t)$ )
  - Oligomeric radicals balance  
 ( $[IM_1](t), [IM_i](t)$  avec  $i \in [1, j_{crit} - 1], n(r, t), \bar{n}(r, t)$ )
- 9 nonlinear ordinary differential equations

$$\dot{\underline{x}} = f(N_m, [S], [S]_{aq}, [I], [IM]_i, n(r), \bar{n}(r), Q_S)$$

- coupled with a Population Balance Equation



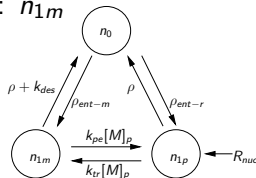
# Available models

PSD can be describe by two type of models:

- The pseudo-bulk model available for large particles
- The “0-1” model available for small particles, 0 or 1 radical per particle

The “0-1” considered for the styrene distinguishes particles who have:

- A polymeric radical:  $n_{1p}$
- No radical:  $n_0$
- A monomeric radical:  $n_{1m}$



## “0-1” model

Model describing the process kinetics and particle evolution for the “0-1” [Crowley et al. 2000]

$$\left\{ \begin{array}{l} \frac{\partial n_0(r, t)}{\partial t} = \rho(r, t)[n_{1p}(r, t) + n_{1m}(r, t) - n_0(r, t)] + k_{des}n_{1m}(r, t) \\ \frac{\partial n_{1p}(r, t)}{\partial t} = \rho_{entr}(r, t)n_0(r, t) - [\rho(r, t) + k_{tr}[M]_p]n_{1p}(r, t) + k_{pe}[M]_pn_{1m}(r, t) \\ \quad - \frac{\partial [G(r)n_{1p}(r, t)]}{\partial r} + \Re_{nuc}\delta(r - r_{nuc}) \\ \frac{\partial n_{1m}}{\partial t} = \rho_{entm}(r, t)n_0(r, t) + k_{tr}[M]_pn_{1p}(r, t) - n_{1m}(r, t)[\rho(r, t) + k_{pe}[M]_p + k_{des}(r)] \end{array} \right.$$

## “Bulk-like” model for the “Zero-one” [Edouard et al. 2005]

The state represents the total number of particles of size  $r$  ( $n(r)$ )

- Change of variable ( $n(r, t) = n_0(r, t) + n_{1m}(r, t) + n_{1p}(r, t)$ )  
→ Process output becomes a part of the state if a sensor is used to measure the PSD
- Quasi-steady assumption for  $n_{1m}(r, t)$
- The following equations represent the PSD of a 0-1 system:

$$\begin{cases} \frac{\partial n(r, t)}{\partial t} = - \frac{\partial [G(r) \bar{n}(r) n(r)]}{\partial r} \\ \frac{\partial \bar{n}(r, t)}{\partial t} = \rho(r)(1 - 2\bar{n}(r)) - k_0(r) \frac{n_{1m}(r)}{n(r)^2} + \frac{\partial [G(r) \bar{n}(r) n(r)]}{\partial r} \left( \frac{\bar{n}(r)-1}{n(r)} \right) \end{cases} \quad (1)$$

with the boundary conditions:

$$\begin{cases} n(r_{nuc}, t) = \frac{\Re_{nuc}(t)}{G(r_{nuc})} \\ \bar{n}(r_{nuc}, t) = 1 \end{cases} \quad (2)$$

- The nonlinear PDE model is discretized using the finite differences

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## On line data available for feedback

- Sensors used to measure the PSD usually require sampling, dilution and analysis. Due to this difficult and time consuming analysis, usually soft sensors or open loop model based observers were employed
- The conductivity measurements and ion-selective electrodes to monitor the free surfactant concentration [Santos et al. 2007]. This information provides information about the particle stabilization and the rate of nucleation which gives an alternative measurement to control the PSD

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The free surfactant concentration in the aqueous phase measurement is used for the closed-loop control

## Control objective

Latex products have enhanced properties due to the dispersity of the PSD.

→ Objective: obtain a prescribed monomodal or bimodal PSD

In the literature, many solutions:

- Open loop model optimization to attain a final target PSD
- Batch-to-batch control of PSD
- MPC strategy

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We consider an inferential closed-loop control of the final PSD using MPC of the free surfactant concentration in the aqueous phase, with surfactant flow rate as input



# Model Predictive Control

## Advantages:

- Constraints (such as manipulated variables physical limitations, constraints due to operating procedures or safety reasons) may be specified
- A model aims to predict the future behavior of the process and the best one is chosen by a correct optimal control of the manipulated variables

## Drawbacks:

- Computational time needed may limit on line use
- Suboptimal solutions

# Model Predictive Control strategy

Developed for nonlinear PDE model control

Main idea [Dufour et al. 2003]:

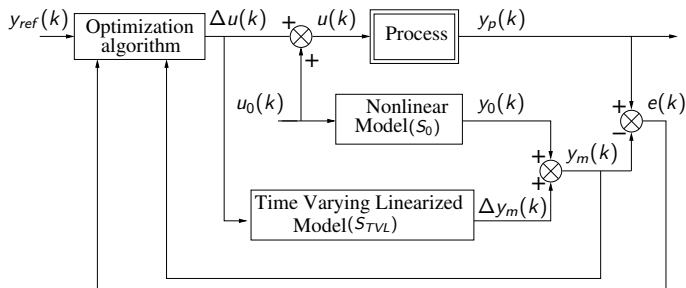
- Decrease the on line time needed to compute the PDE model based control

Approach:

- Input constraints: hyperbolic transformation
- Linearization + sensitivities computed off line
- On line use of a time varying linear model
- On line resolution of a penalized (and so unconstrained) optimization control problem: a modified Levenberg Marquardt Algorithm
- MPC@CB software developed

# General linearized IMC-MPC

- Nonlinear differential equations ( $S_0$ ) are solved off line
- The time varying linearized system ( $S_{TVL}$ ) is solved on line



# Optimization problem

$J$  is the cost function according to the desired objective, trajectory tracking in this study:

$$J(p) = \sum_{j=k+1}^{k+N_p} g(y_{ref}(j), y_m(j), u(j-1), e(k)) \quad (3)$$

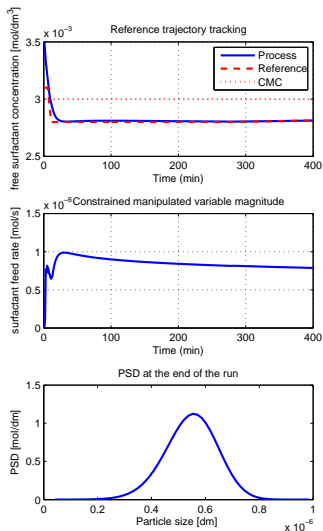
Constraints on the manipulated variable:

$$\begin{cases} u_{min} \leq u(j) \leq u_{max} & \forall j \in [k+1, k+N_p] \\ \Delta u_{min} \leq u(j) - u(j-1) \leq \Delta u_{max} & \forall j \in [k+1, k+N_p] \end{cases} \quad (4)$$

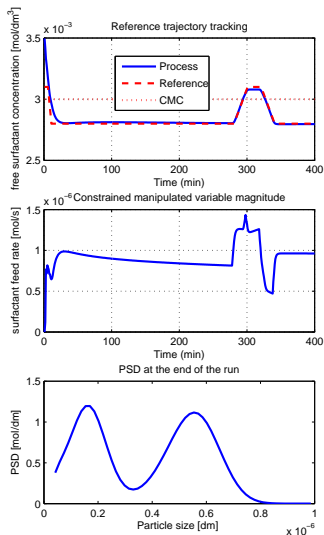
## Simulation results

- The choice of the free surfactant concentration reference directly affects the final PSD
- To create a new population, the output free surfactant concentration must be above the CMC
- To ensure the latex stability without creating new particles, the output must be below the CMC but close to the CMC

# Monomodal PSD



# Bimodal PSD



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## Conclusion

- Controlling the free surfactant concentration is efficient for PSD dispersity on line control
- The proposed MPC strategy allows decreasing the computational burden during on line control
- A turnkey MPC@CB software is used with Matlab

## Perspectives

- Controlling the whole PSD (nucleation and growth), measuring both the PSD and the surfactant in the aqueous phase
- MIMO control problem
- Experimental validation of this approach

Paper WeA25.1

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Thank you  
Any questions ?