Modelling, Simulation and Control of a Semi-batch Industrial Polymerization Reactor

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Presentation outline:

- ✓Polymerization process description
- ✓Process model
- ✓Simulation using real-plant data
- ✓Reactant dosing control
- ✓Conclusions

1. Problem decription

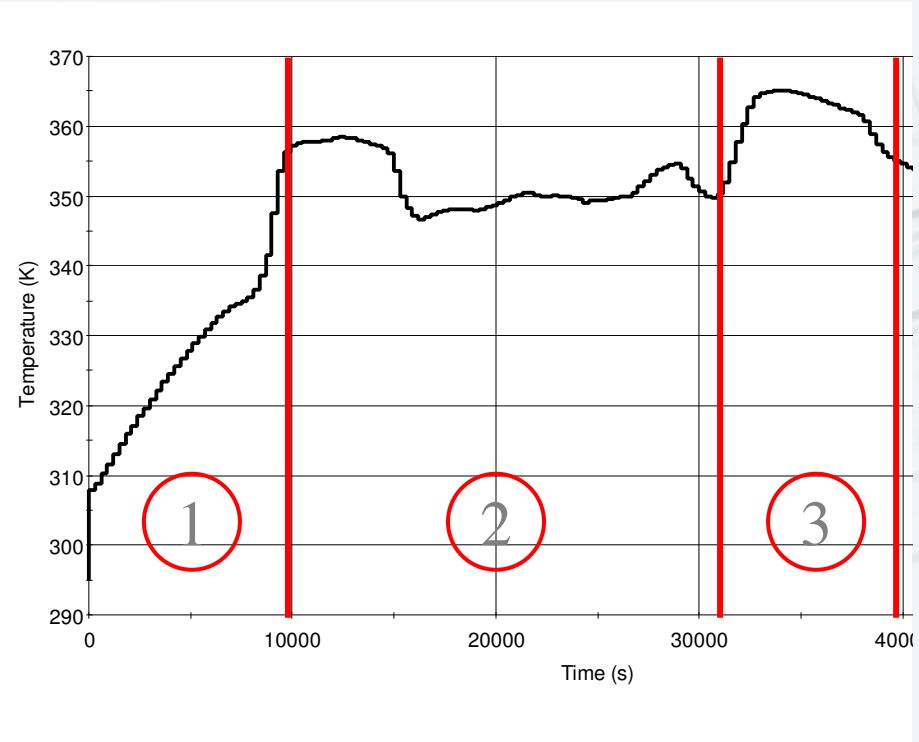
- ✓ Mitol, polymer factory in Sezana, Slovenia
  - Currently using more than 90 % capacity
  - Goal: reduce the time of the reaction

Dynamic model →

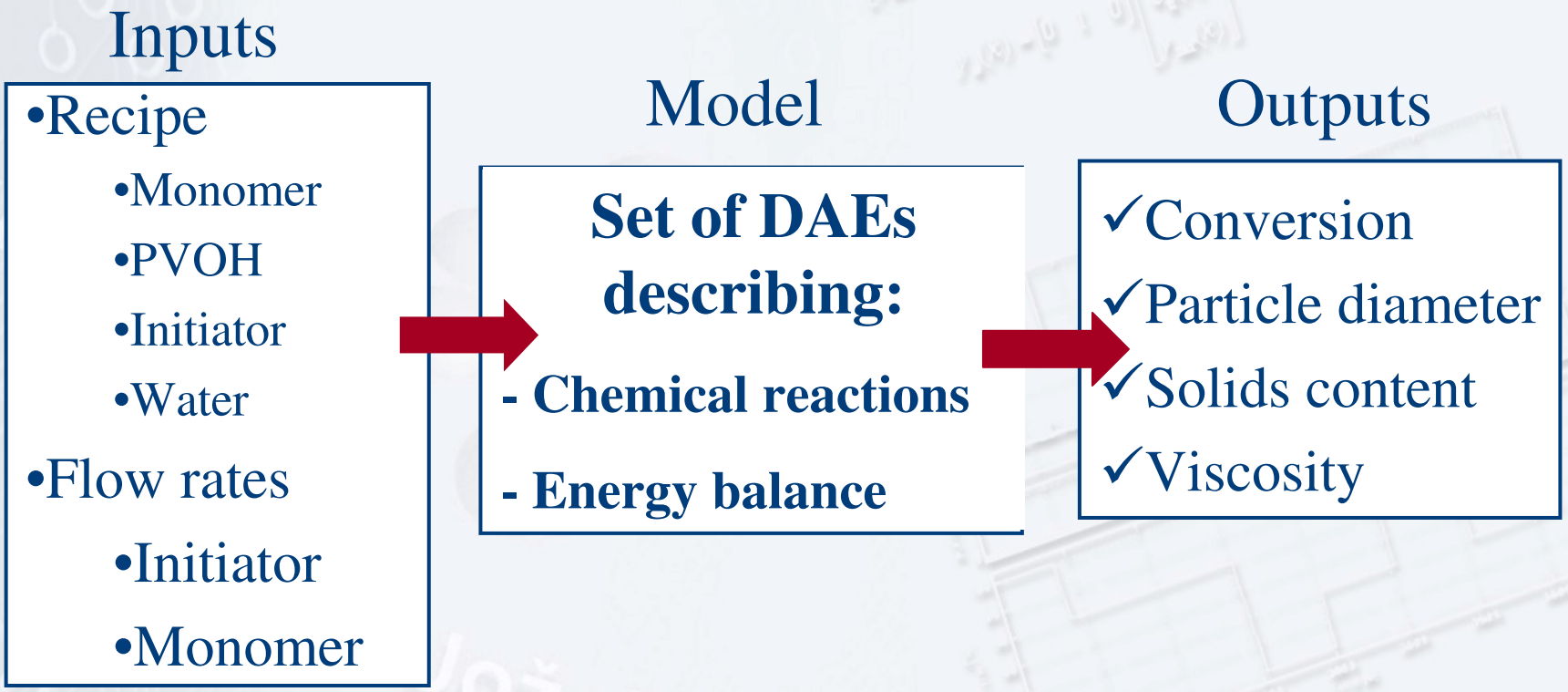
- ✓**Optimization**
- ✓**Control**

The Process

- ✓ Semi-batch emulsion polymerization
- ✓ Three main steps
  1. Initiation
  2. Monomer and initiator addition
  3. Termination



2. Process model



Chemical reactions model

- ✓Detailed modelling of chemical reactions

$$\frac{dI}{dt} = I_e - k_d I$$

$$\frac{dM_m}{dt} = q_m - M_w(k_{iwm}[R\cdot] + k'_{iwm}[M_1\cdot] + k_{pw}([R_w\cdot] - [M_1\cdot]) + k_{trm}([R_w\cdot] - [M_1\cdot])) + k_{pp}[M_p]\overline{n}\sum_{i=1}^{NoC} PSD_i$$

$$V_w[G_w] + K_{gd}[G_w]V_d + \frac{A_{c\infty}K_{ad}[G_w]A_{ps}}{1 + K_{ad}[G_w]} = \frac{G_0}{MW_{PVOH}}$$

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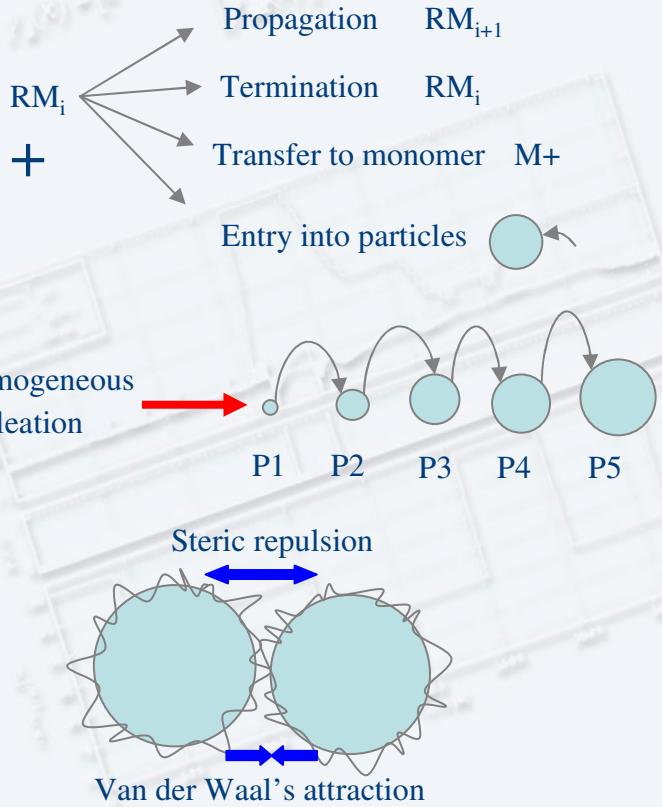


Energy balance model

- ✓ Reaction heat capacity

$$K_R = M_m MW_m Cp_{mon} + M_{conv} MW_m Cp_{pol} + \rho V_w Cp_{water} + G_0 Cp_{pol}$$

- ✓ Heating of the reactor through the heating jacket

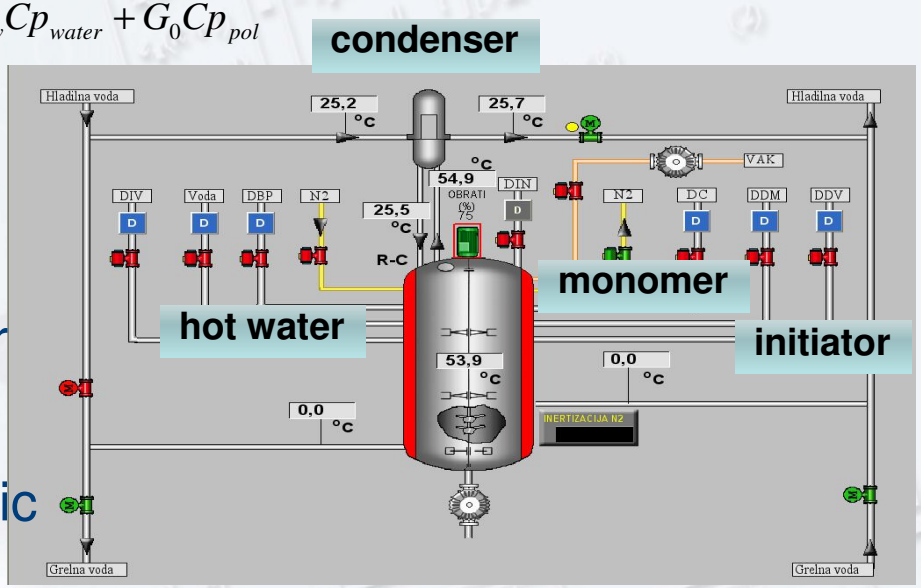
$$\Delta H_{jacket} = UA(T_{jacket} - T)$$

- ✓ Heating the incoming monomer

$$Q_{mon} = q_m MW_m Cp_{mon} T_{mon}$$

- ✓ Heat produced in the exothermic reaction

$$Q_{pol} = -\Delta H_r r_{pol}$$



- ✓ Cooling the reactor by the reflux through the condenser

$$Q_{cond} = q_{FC} Cp_{Cout} (T_{Cout} - T_{Cin}) + q_{FC} \lambda$$

- ✓ Heat losses to the surroundings

$$Q_{loss} = C_{loss} (T - T_{ext})$$

Energy Balance I

Change R temperature
Change Heat capacity

Monomer Enthalpy

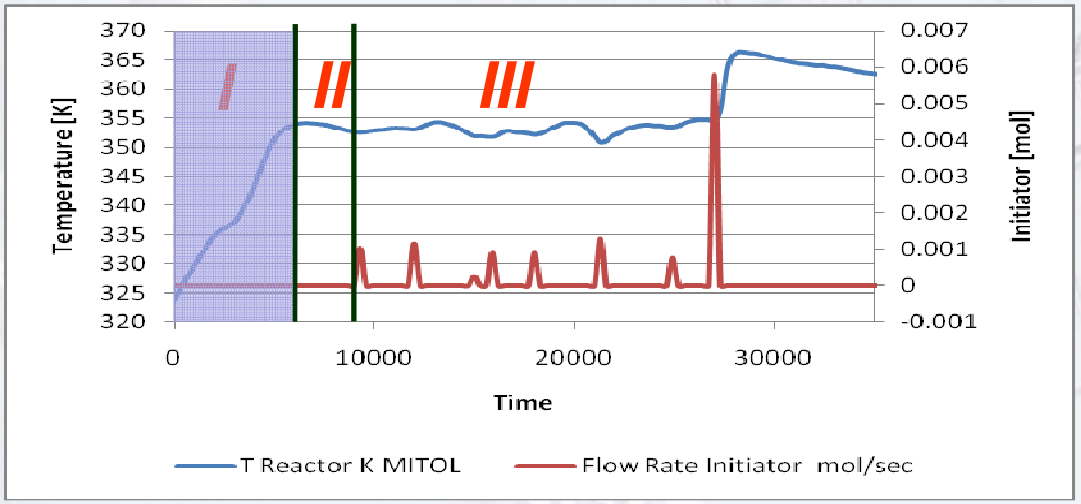
Reaction Heat

Heating Jacket

$$K_R \frac{dT}{dt} + T \frac{dK_R}{dt} = q_m MW_m Cp_{mon} T_{mon} - C_{pol,1} \Delta H_r r_{pol} - \Delta H_{jacket}$$

$$\frac{dT_{jacket}}{dt} = 0$$

Q_{cond} Q_{loss}



Energy Balance II

Change R temperature
Change Heat capacity

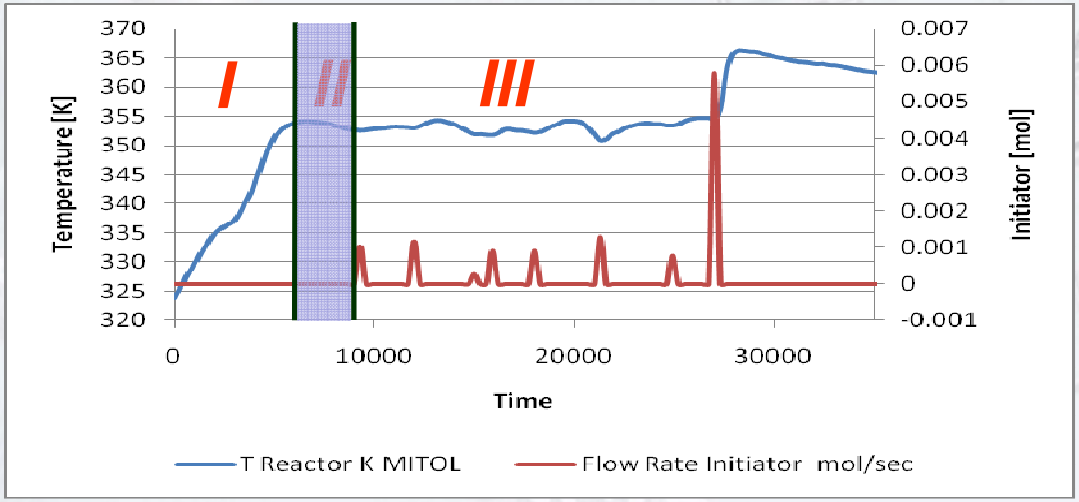
Monomer Enthalpy

Reaction Heat

$$K_R \frac{dT}{dt} + T \frac{dK_R}{dt} = q_m MW_m Cp_{mon} T_{mon} - C_{pol,2} \Delta H_r r_{pol}$$

$$\frac{dT_{jacket}}{dt} = 0$$

~~ΔH_{jacket}~~ ~~Q_{cond}~~ ~~Q_{loss}~~



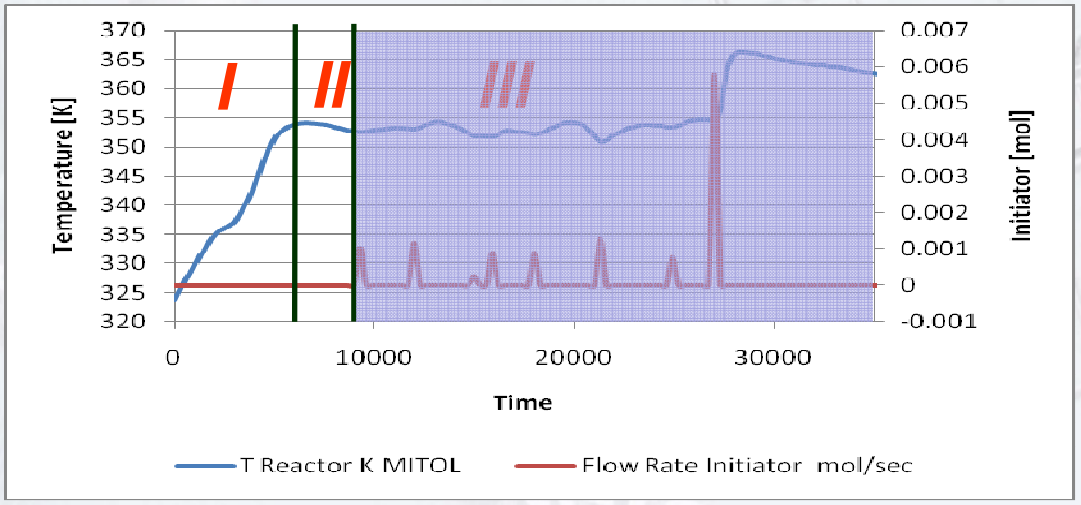
Energy Balance III

Change R temperature Change Heat capacity | *Monomer Enthalpy* | *Reaction Heat* | *Cond. Losses* | *Surround. Losses*

$$K_R \frac{dT}{dt} + T \frac{dK_R}{dt} = q_m MW_m Cp_{mon} T_{mon} - C_{pol,3} \Delta H_r r_{pol} - Q_{cond} - C_{loss,1} Q_{loss}$$

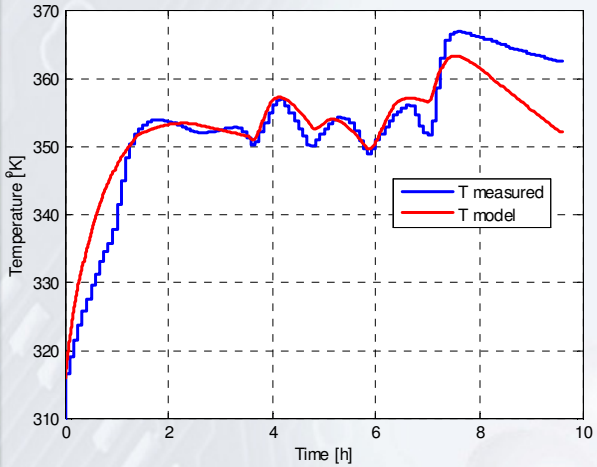
$$dT_{jacket} / dt = -\frac{UA}{m_w Cp_{water}} (T_{jacket} - T)$$

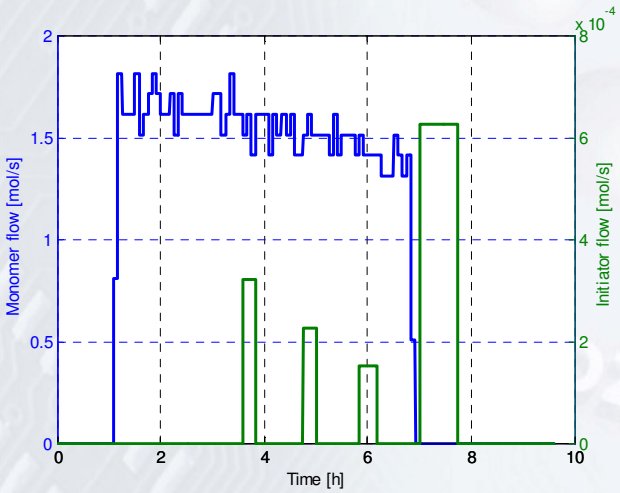
$$\cancel{\Delta H}_{jacket}$$



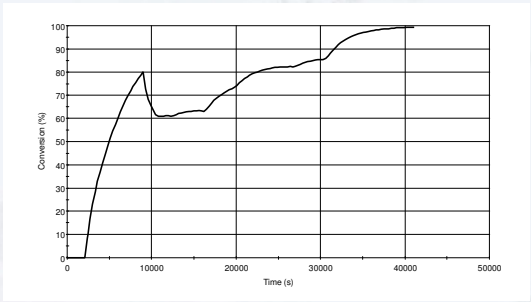
3. Simulation using real-plant data

Temperature

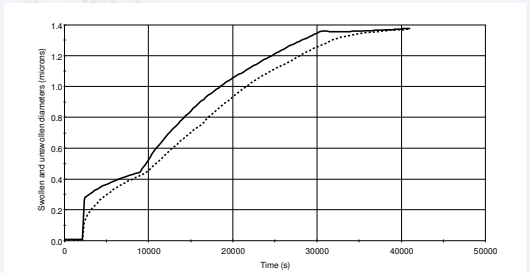




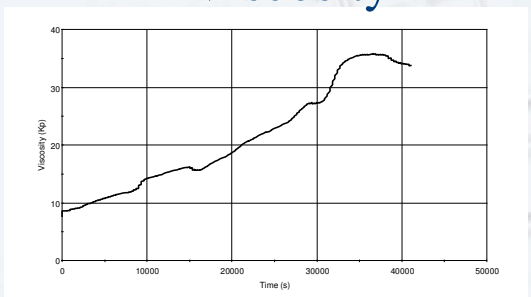
Conversion



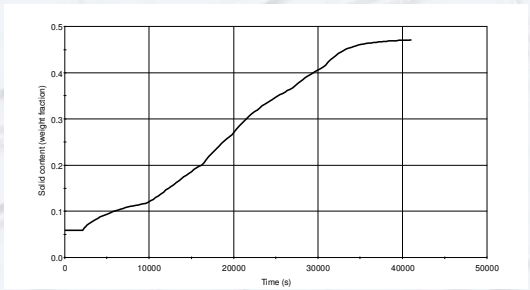
Particle diameter



Viscosity



Solids content



Simulation results

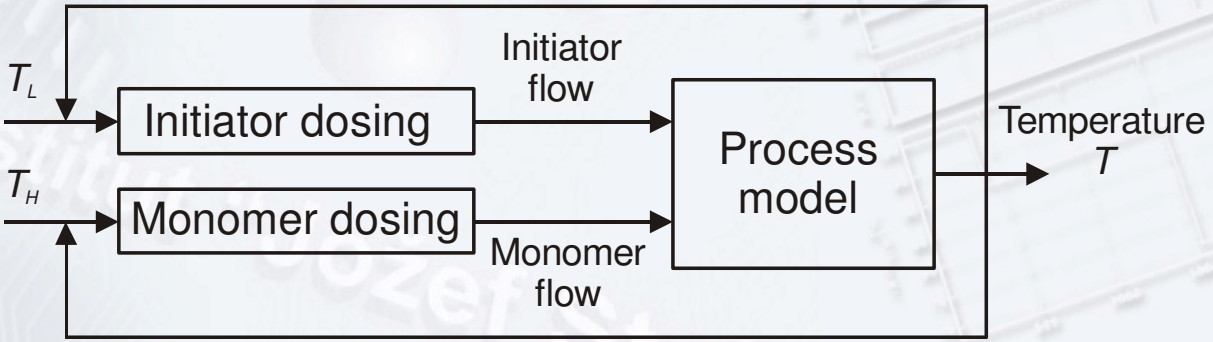
Batch No.	Conversion [%]		Solids Content [%]		Viscosity [mPas]	
	Process	*Model*	*Process*	*Model*	*Process*	*Model*
1192	99.95	99.78	46.4	47.15	37520	33618
1203	99.90	99.15	45.9	46.91	31200	35419
1214	99.89	94.92	45.4	44.59	25040	31879
1253	99.13	98.87	46.9	47.06	34000	35911
1256	99.37	97.07	46.4	45.87	30160	31706

RMSE: 2.5% 1.5% 13%

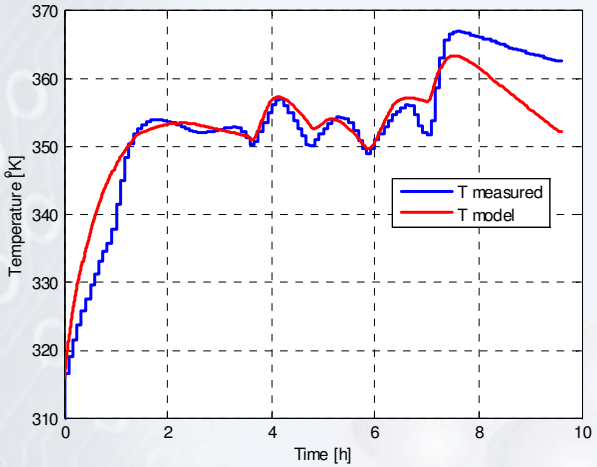
4. Reactant dosing control

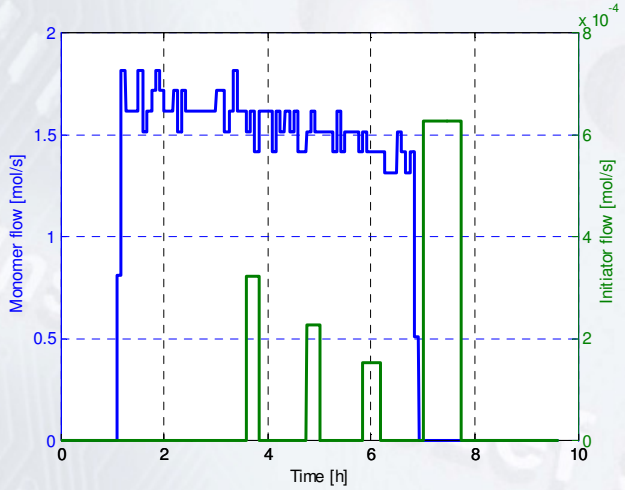
Monomer flow rate

Initiator flow rate

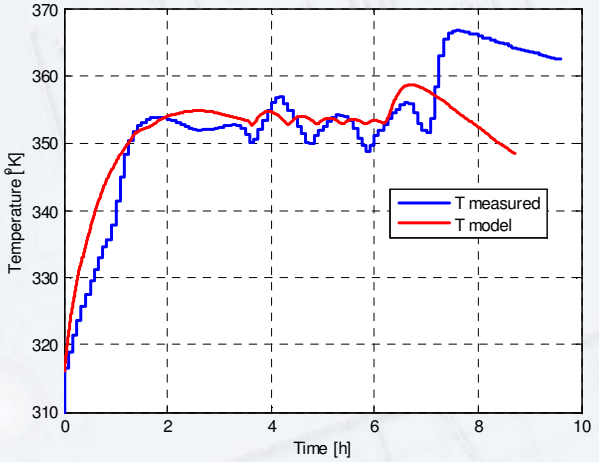


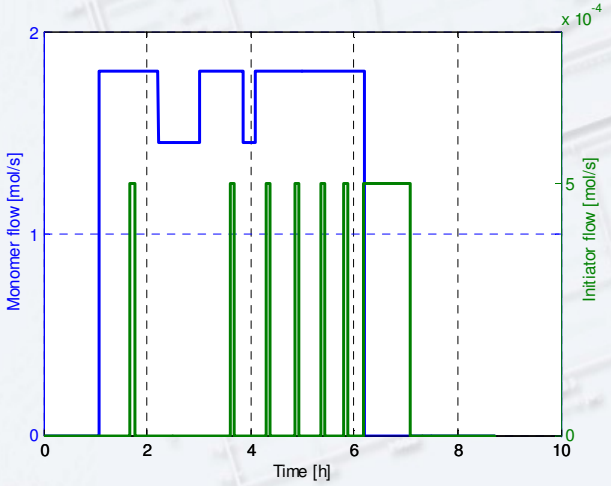
A) Real plant simulation





B) Simulation with control





Control Results

Batch N	Time MITOL [sec]	Time with Control [sec]	Reduced time
1192	34500	30130	1h 13min
1203	31800	29750	34min
1214	33600	30790	46min
1253	35700	30640	1h 24min
1256	35100	30560	1h 15min

6% production increase

5. Conclusions

- ✓ **The Model**
  - With the model we can estimate the four outputs of the reaction
  - The outputs are in the range with the real/plant data
  - With the energy balance we are able to observe the changes in the temperature and design control strategies
- ✓ **Control**
  - With the proposed control the temperature could be kept in a narrower region
  - This allows the increase of monomer flow and consequently the shortening of batch time
  - The results need to be confirmed by real plant experiments