Modeling of Polyvinyl Acetate Polymerization Process for Control Purposes

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Introduction

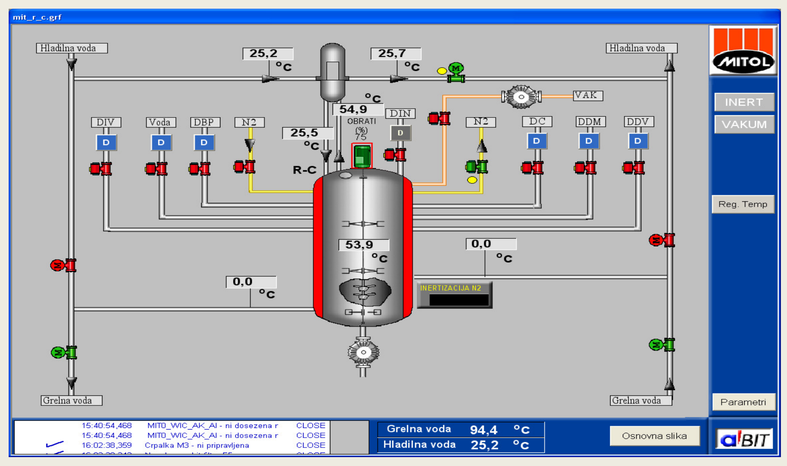
The presented research work considers polymerization process of a semi-batch operation in MITOL, chemical factory in Sežana, Slovenia. The goal is to increase the production rate and decrease the batch time. The model presented hereby will be used for a batch optimization with a purpose to achieve the mentioned goal.

In our work we present a model that predicts conversion and product quality parameters. The work of Aller et al. is used as a base model. By using first principles modeling (energy balance) the dynamics of the temperature is derived as a function of the concentration of the reacting chemicals. Preliminary simulation results based on real plant data are presented.

gPROMS modeling environment is used for modeling, simulations, estimations and optimization of the model.

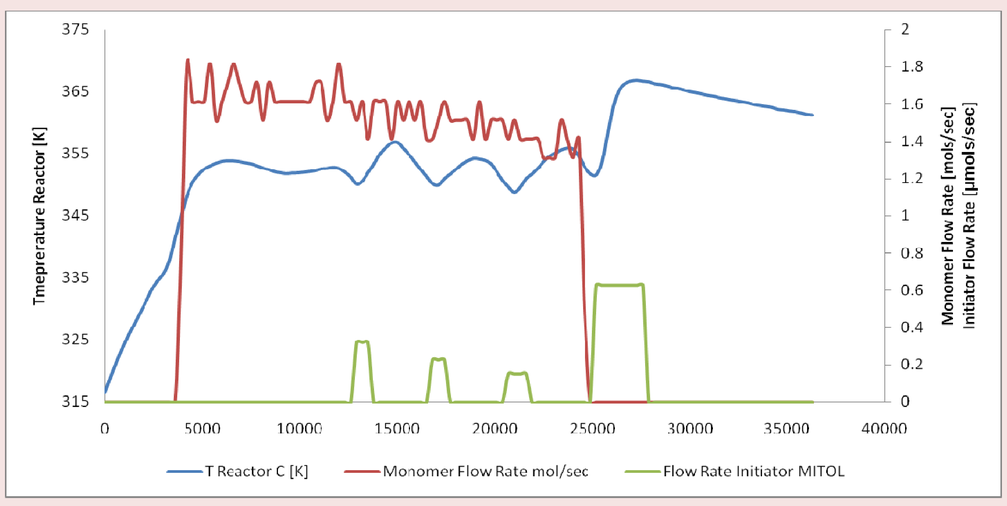
Process Description

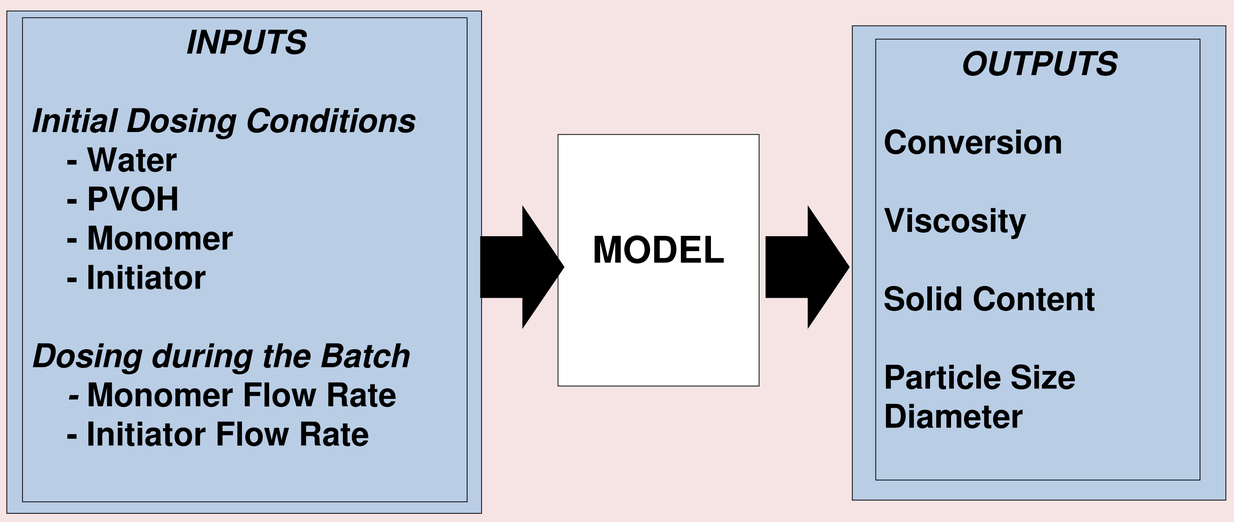
- **Vinyl Acetate – modeled compound**
- **Semi-Batch polymerization process**
- **Continuous addition of Monomer**
- **Addition of Initiator every time the temperature drops off**



Model

The overall model uses the initial polymerization compounds and the dosing during the batch to observe the changes due to the reactions and predicts the four output parameters. During the reaction the temperature should be kept between 350-355K, which is achieved by adding a certain amount of initiator whenever the temperature decreases. Temperature in the reactor (T_R) is modeled using the energy balance model. The flow of the added monomer during the batch is measured while the addition of initiator is calculated from the weight change of the initiator dozing tank.

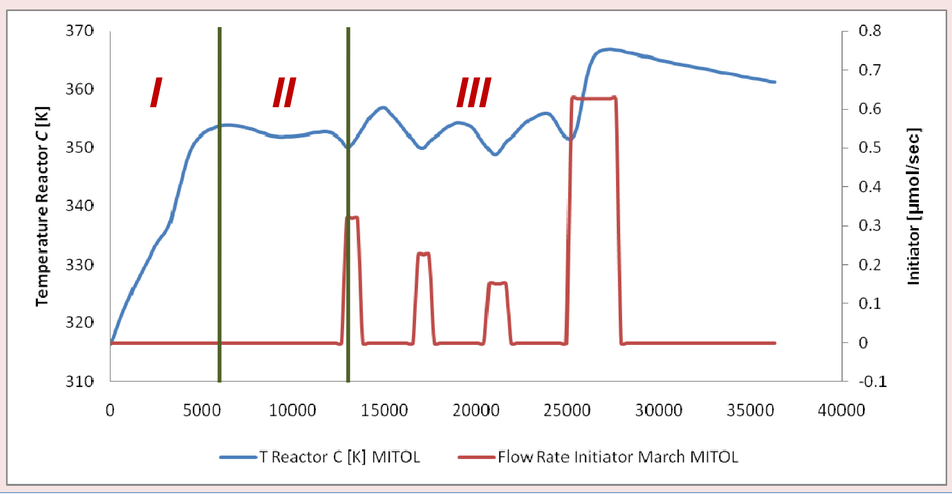




The energy balance model is based on reaction heat capacity (K_R), and the energy produced and consumed during the reaction. The latter include the following:

- **heating of the reactor through the heating jacket (ΔH_{jacket})**
- **producing the heat in the exothermic reaction ($\Delta H_r r_{pol}$)**
- **heating the incoming monomer to the reactor temperature ($Q_m MW_m Cp_m T_{mon}$)**
- **cooling of the reactor by the reflux (Q_{cond})**
- **heat losses to the surrounding (Q_{loss})**

The temperature model is split into three parts depending on the stage of the process and the reaction.



$$T_R \frac{dK_R}{dt} + K_R \frac{dT_R}{dt} = Q_m MW_m Cp_m T_{mon} - \triangle H_r r_{pol} - \triangle H_{jacket} \quad \text{I}$$

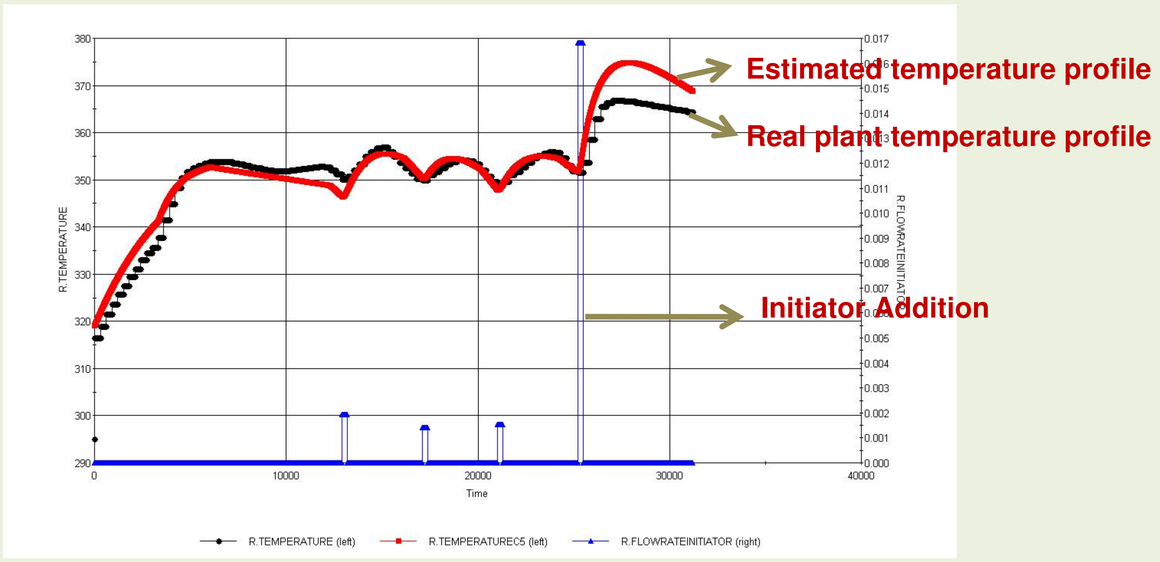
$$T_R \frac{dK_R}{dt} + K_R \frac{dT_R}{dt} = Q_m MW_m Cp_m T_{mon} - \triangle H_r r_{pol} \quad \text{II}$$

$$T_R \frac{dK_R}{dt} + K_R \frac{dT_R}{dt} = Q_m MW_m Cp_m T_{mon} - \triangle H_r r_{pol} - Q_{cond} - Q_{loss} \quad \text{III}$$

Results

The presented model is simulated using gPROMS modeling tool. The overall model has thirteen differential equations and seven adjustable parameters. The adjustable parameters of the temperature model are in the equation for heat losses to the surroundings and in the equation describing the heat production due to the exothermic reaction.

The model was validated on 5 batches from real plant production. The model agreement between real plant and simulated temperature is quite satisfactory. The obtained model still needs fine tuning of parameter values for precise model output predictions.



Conclusion

Having obtained the temperature profile we are able to apply control strategies for decreasing the batch time and increasing the production rate while at the same time keeping the quality parameters at the desired values.

Acknowledgment

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