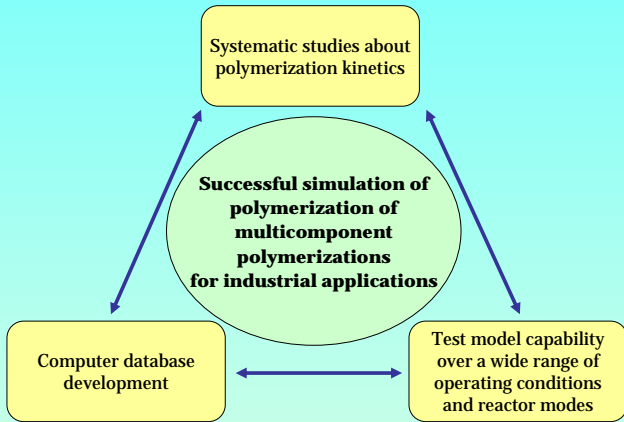
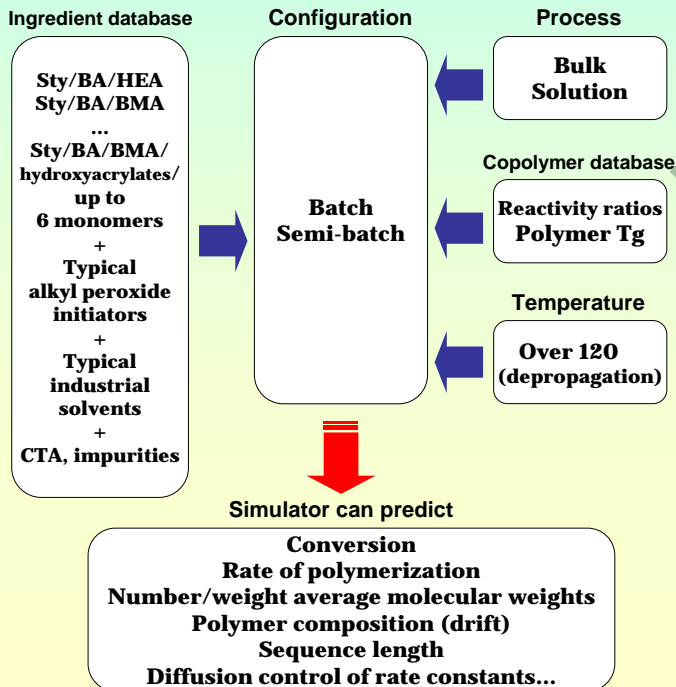


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1. Introduction



2. Objectives



3. Model development (sample)

Reaction	Chemical equation	Rate equation	Pseudo rate expression
Initiation	$I \xrightarrow{k_d} 2R_{in}^*$ $R_{in}^* + M_j \xrightarrow{k_{tj}} R_j^*$	$R_i = 2fk_d[I]$	
Propagation	$R_i^* + M_j \xrightarrow{k_{pj}} R_j^*$	$R_p = -\sum_i \frac{d(M_i)}{dt} = \sum_i \sum_j k_{pj} [R_i^*][M_j]$ $= k_{p,i} [R^*][M]$	$k_p = \sum_i \sum_j k_{p,ij} \phi_i^* f_j$
Termination	$R_i^* + R_j^* \xrightarrow{k_{td}} \text{Dead polymer}$	$R_t = \sum_i \sum_j k_{td,ij} [R_i^*][R_j^*]$ $= k_t [R^*]^2$	$k_t = \sum_i \sum_j k_{t,ij} \phi_i^* \phi_j^*$
Radical transfer (Monomer)	$R_i^* + M_j \xrightarrow{k_{tmj}} P + R_j^*$	$R_{tm} = \sum_i \sum_j k_{tm,ij} [R_i^*][M_j]$ $= k_{tm} [R^*][M]$	$k_{tm} = \sum_i \sum_j k_{tm,ij} \phi_i^* f_j$
Radical transfer (CTA)	$R_i^* + T \xrightarrow{k_{CTA}} P + T^*$	$R_{CTA} = \sum_i k_{CTA,i} [R_i^*][T]$ $= k_{CTA} [R^*][T]$	$k_{CTA} = \sum_i k_{CTA,i} \phi_i^*$
Radical transfer (Solvent)	$R_i^* + S \xrightarrow{k_{Sj}} P + S^*$	$R_{Sj} = \sum_i k_{Sj,i} [R_i^*][T]$ $= k_{Sj} [R^*][T]$	$k_{Sj} = \sum_i k_{Sj,i} \phi_i^*$
Inhibition (Impurity)	$R_i^* + Z \xrightarrow{k_{Zj}} P$	$R_{Zj} = \sum_i k_{Zj,i} [R_i^*][Z]$ $= k_{Zj} [R^*][Z]$	$k_{Zj} = \sum_i k_{Zj,i} \phi_i^*$

* Branching reactions to be added later

Monomer balances

$$\frac{d(V_R[M_i])}{dt} = F_{M_i,in} - k_{p,ij} [R^*][M_j]V_R - F_{M_i,out}$$

Initiator balance

$$\frac{d(V_R[I])}{dt} = F_{I,in} - k_d[I]V_R - F_{I,out}$$

Polymer balances

$$\frac{d(V_R[P_i])}{dt} = F_{P_i,in} + k_{p,ij} [R^*][M_j]V_R - F_{P_i,out}$$

Radical balances

$$\frac{d(V_R[R^*])}{dt} = 2fk_d[I]V_R - k_z[Z][R^*]V_R - k_t[R^*]^2V_R$$

Energy balances

$$\frac{d(V_R H)}{dt} = F_{H,in} + k_p[M][R^*]V_R(-\Delta H_p) - UA(T_R - T_{jacket}) - F_{H,out}$$

4. Typical simulation examples

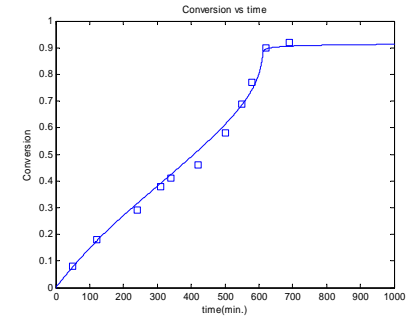


Figure 1. Simulation of conversion vs time of Styrene bulk homopolymerization (60 °C, [AIBN] = 0.09992 M, Data of Arai and Saito, 1976)

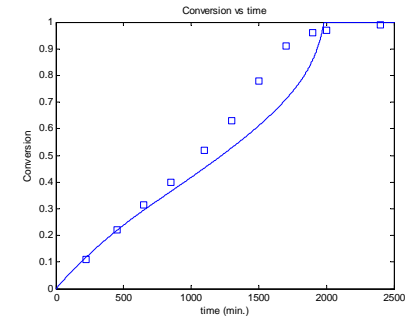


Figure 2. Simulation of conversion vs time of Styrene/BA bulk copolymerization (50 °C, [AIBN] = 0.05 M, $f_{Sty} = 0.600$, Data of Dube et al., 1990)

5. Future work plan

- MAsC project started in **September, 2006**.
- Background work is based on **WATPOLY®** simulator developed by Penlidis group.
- Extensive literature search for kinetic parameters and building mathematical concepts for multicomponent modeling are currently under progress.