Modeling and Optimization for Interpenetrating polymer network process

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**Project Overview**

- **IPN** *Interpenetrating polymer network*
  - A combination of two polymers in a network form

\[
\text{Network A} \\ 
\text{Network B} \\ 
\text{IPN} = A + B
\]

Fig. 1  IPN network structure

- **Typical Sequential Type of Process**

  **Monomer A**  
  *Initiator Cross-linker*

  **Network A**

  **Monomer B**  
  *Initiator Cross-linker*

  **IPN**

Fig. 2  An IPN process example
• **Goal:** To predict, control and optimize polymer quality & productivity

• **Proposed plan**
  - Construct prototype process model
  - Obtain model parameters through parameter estimation
  - Implement off-line /on-line optimization
Macro-Scale
- Macro-mixing
- Heat removal

Meso-Scale
- Mass transport
- Internal diffusion
- Particle morphology

Micro-scale
- Formation of chains
- Intrinsic kinetics

Fig. 3 Multi-scale model structure

Single Particle Modeling
- Particle growth mechanism
- Heterogeneous properties

IPN kinetic model
- Finite moment method
- Statistical assumption

Progress Update
Major Challenges in the modeling

- Particle growth mechanism
  - Non-ideal mixing behavior
- Intra-particle diffusion
  - Non-constant particle density
- Dynamics of the kinetic
  - Position-dependent reaction rate
Previous Model Description (2008.3)

Classical Reaction Diffusion Equation

\[
\frac{\partial C_i}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( D_{eff}^i r^2 \frac{\partial C_i}{\partial r} \right) - R_i
\]

- Initial condition

\[C_i(r, t = 0) = C_{i0}, \quad R_s(t = 0) = R_{s0}\]

- Boundary condition

\[
\left. \frac{\partial C_i}{\partial t} \right|_{(r=0,t)} = 0
\]

\[
D_{eff}^i \frac{\partial C_i}{\partial r} (r = R_s(t), t) = k_s(C_{ie} - C_i)
\]

Limitation: Particle sizing modeling
Progress update

Modeling Improvement

New model structure

Generalized Reaction Diffusion Model

\[
\frac{dN[i]}{dt} = N[i]^{In} - N[i]^{Out} + N[i]^{R}
\]

Hypothetical shells  ➔ Reaction Zone

- **Particle growth:** Collision absorption mechanism
- **Intra-particle diffusion:** Discrete approximation
- **Dynamic kinetics:** reaction zone dependent reaction rate

Fig. 5 Reaction-Zone-Divided model structure

\( i \) th Zone

\( N_{in} \rightarrow N_{out} \rightarrow r_{i+1} \rightarrow r_{i} \rightarrow \)
Progress update

Model Parameters

- Large Scale Nonlinear Parameter estimation

\[
\min_{p_k} \sum_{k=1}^{N_s} \sum_{i=1}^{Nm_k} (y_k(t_i) - y_{k,i}^M)^T V_y^{-1} (y_k(t_i) - y_{k,i}^M) \\
\text{s.t. } F_k \left[ \frac{dz_k(t)}{dt}, z_k(t), y_k(t), p_k \right] = 0 \\
G_k \left[ z_k(t), y_k(t), p_k \right] = 0 \\
H_k \left[ z_k(t), y_k(t), p_k \right] \leq 0 \\
k = 1, \ldots, N_s
\]

\begin{align*}
N_s & : \text{Number of scenario} \\
Nm_k & : \text{Number of measurements in scenario } k \\
p_k & : \text{Model parameters} \\
V_y^{-1} & : \text{Weight matrix} \\
F_k & : \text{Differential equations} \\
G_k & : \text{Algebraic equations}
\end{align*}
Progress update

Fitting Results (1)

Single process

Fig. 6. Single process fitting result
Combine Two processes. Part 1: Fitting Results (2)

Fig. 7. Fitting result for Two data sets, process A
Combine Two processes. Part 2: **Fitting Results (3)**

**Conversion Ratio**

**Radius**

Fig. 8. Fitting result for Two data sets, process B
Fitting results (4)

Test data

Conversion Ratio

Radius

Mw

Mz

Fig. 9. Testing result for process C
Optimal Control Problem

➢ Connect single particle model to process control

\[
\min_{z(t), u(t)} \varphi(z(t_f))
\]

\[
s.t. \quad \frac{dz(t)}{dt} = f(z(t), u(t))
\]

\[
\begin{align*}
z(t0) &= z0 \\
\text{Molecular weight} &\subset Q \\
\text{Conversion} &\subset C \\
\text{Composition} &= P
\end{align*}
\]

Fig. 10. One example of optimal feeding policy
Future Work Plan

• Integrated process model development
• Multi-scenario parameter estimation
• Optimization of process systems under uncertainty

Fig. 11. Optimal feeding policy changes with uncertain parameters
Summary

• Improved single particle model reveals the heterogeneity of the particle evolution
• Simulation and measurements have consistent agreement on the particle growth
• Further optimization strategies will be incorporated to consider the process uncertainty