# 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

**Network A**
**Network B**
**IPN = A + B**

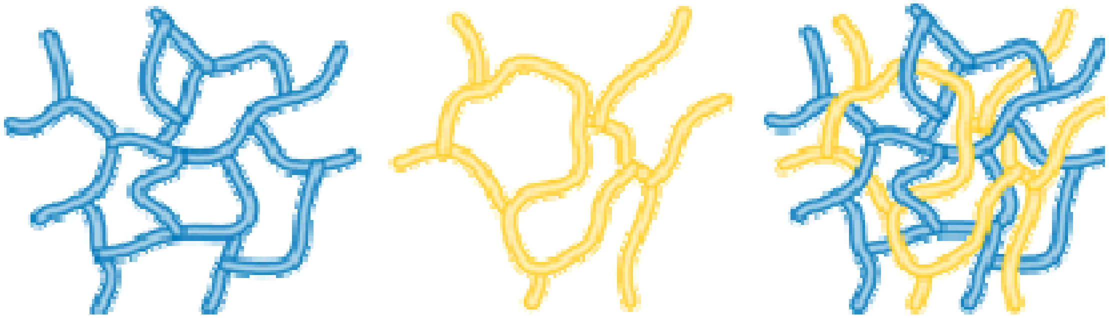
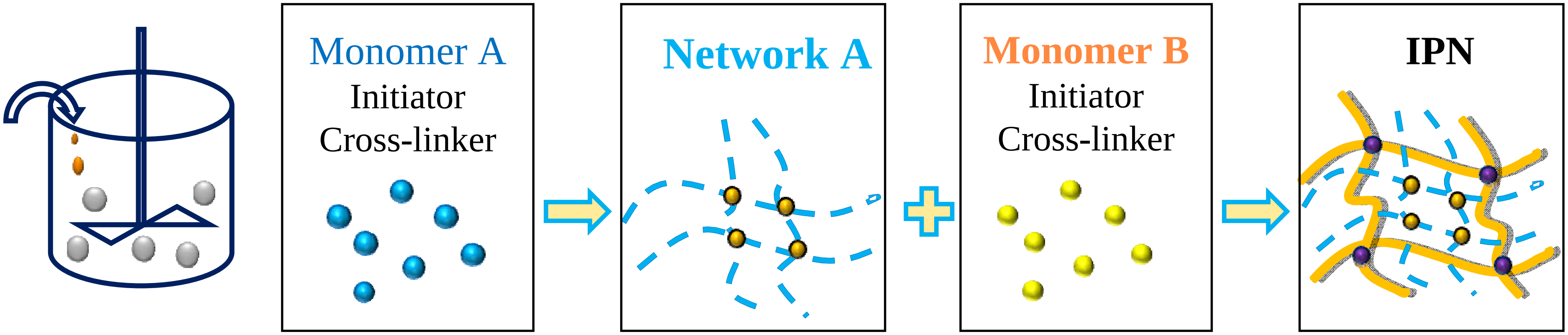


Fig. 1 IPN network structure

- Typical Sequential Type of Process



Monomer A
Initiator
Cross-linker

**Network A**

**Monomer B**
Initiator
Cross-linker

**IPN**

Fig. 2 An IPN process example

# Project Overview

- **Goal:** To predict, control and optimize polymer quality & productivity
- **Proposed plan**

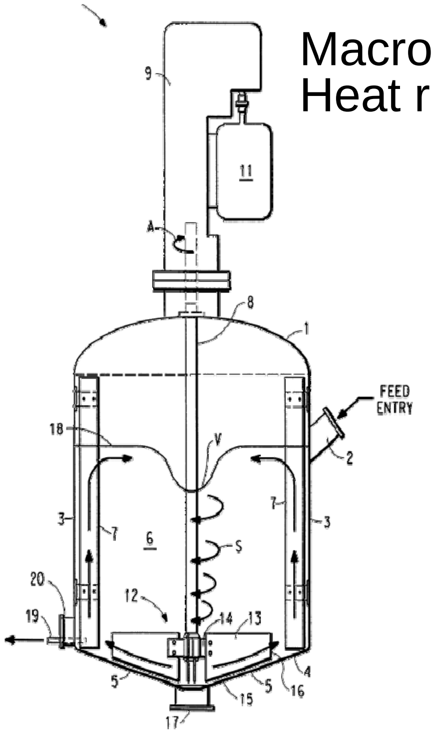
  → Construct prototype process model

  → Obtain model parameters through parameter estimation

  → Implement off-line /on-line optimization

# Multi Scale Modeling

## Macro- Scale

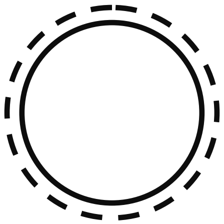


Macro-mixing
Heat removal

**Relationship ?**

## Meso-Scale

- Mass transport
- Internal diffusion
- Particle morphology



Suspended particles

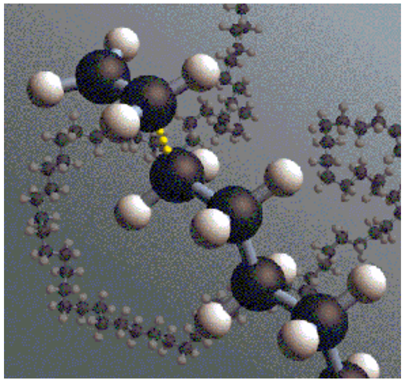
### Single Particle Modeling

※ Particle growth mechanism
※ Heterogeneous properties

**11/2007 - 9/2008**

## Micro-scale

- Formation of chains
- Intrinsic kinetics



### IPN kinetic model

✓ Finite moment method
✓ Statistical assumption

**10/2006 - 10/2007**

Fig. 3 Multi-scale model structure

# Single Particle Modeling

- 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

# Modeling Improvement

## Previous Model Description (2008.3)

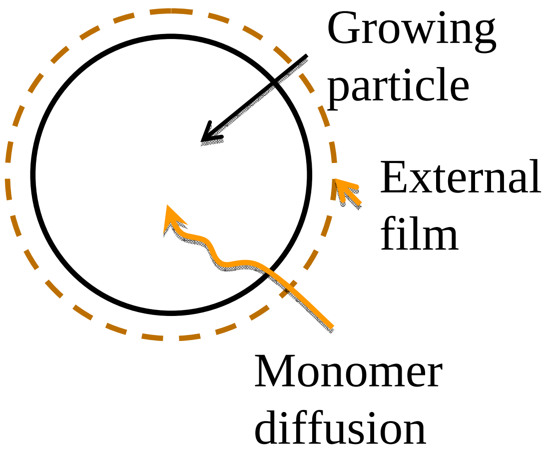


Fig.4 Moving Boundary Model Structure

### Classical Reaction Diffusion Equation

$$\frac{\partial C_i}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D^i_{eff} r^2 \frac{\partial C_i}{\partial r}\right) - r_i$$

- Initial condition

$$C_i(r, t=0) = C_{i0} \qquad R_s(t=0) = R_{s0}$$

- Boundary condition

$$\frac{\partial C_i}{\partial t}|_{(r=0,t)} = 0$$

$$D_{eff_i}\frac{\partial C_i}{\partial r}(r = R_s(t), t) = k_s(C_{ie} - C_i)$$

*Limitation: Particle sizing modeling*

# Modeling Improvement

## New model structure

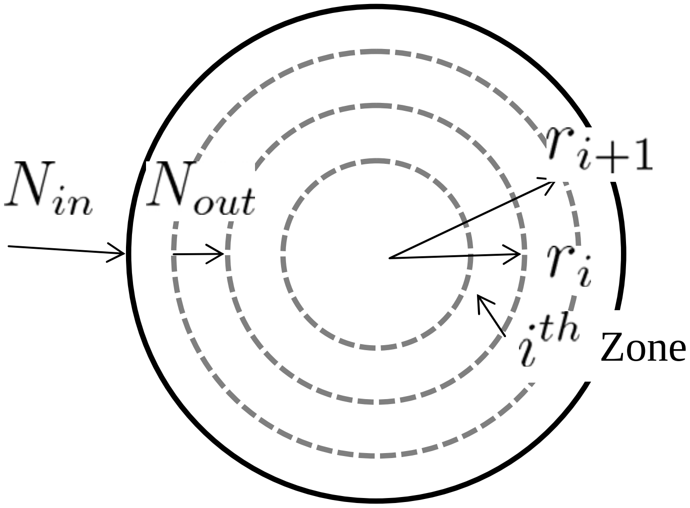


Fig. 5 Reaction-Zone-Divided model structure

### 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

# Model Parameters

- Large Scale Nonlinear Parameter estimation

$$\min_{p_k} \sum_{k=1}^{Ns} \sum_{i=1}^{Nm_k} (y_k(t_i) - y_{k,i}^M)^T V_y^{-1} (y_k(t_i) - y_{k,i}^M)$$

$$s.t. \quad F_k[\frac{dz_k(t)}{dt}, z_k(t), y_k(t), p_k] = 0$$

$$G_k[z_k(t), y_k(t), p_k] = 0$$

$$H_k[z_k(t), y_k(t), p_k] \leq 0$$

$$k = 1, ..., Ns$$

$Ns$ : Number of scenario

$Nm_k$ : Number of measurements in scenario k

$p_k$ : Model parameters

$V_y^{-1}$ : Weight matrix

$F_k$ : Differential equations

$G_k$ : Algebraic equations

Progress update

# Fitting Results (1)

Single process

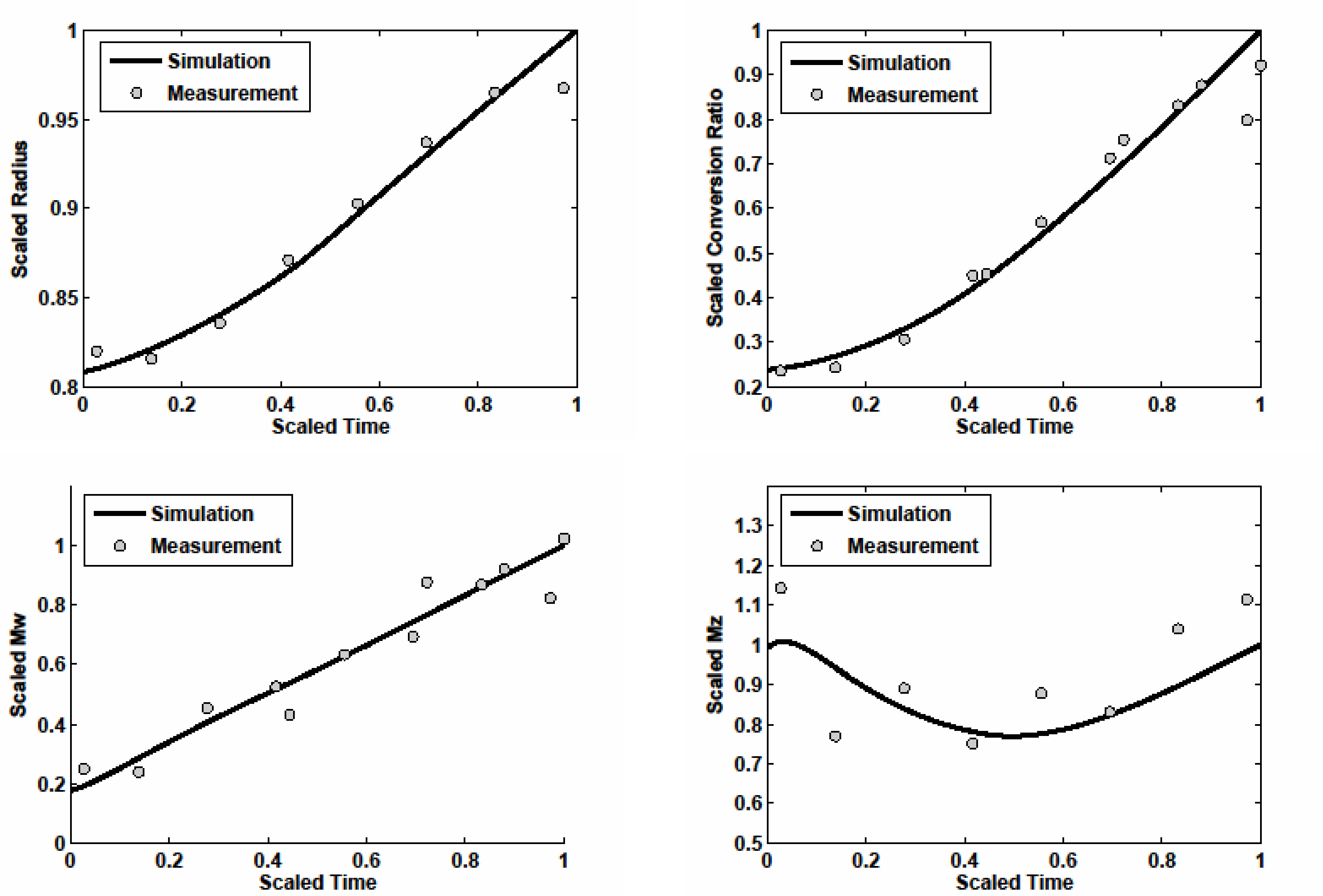
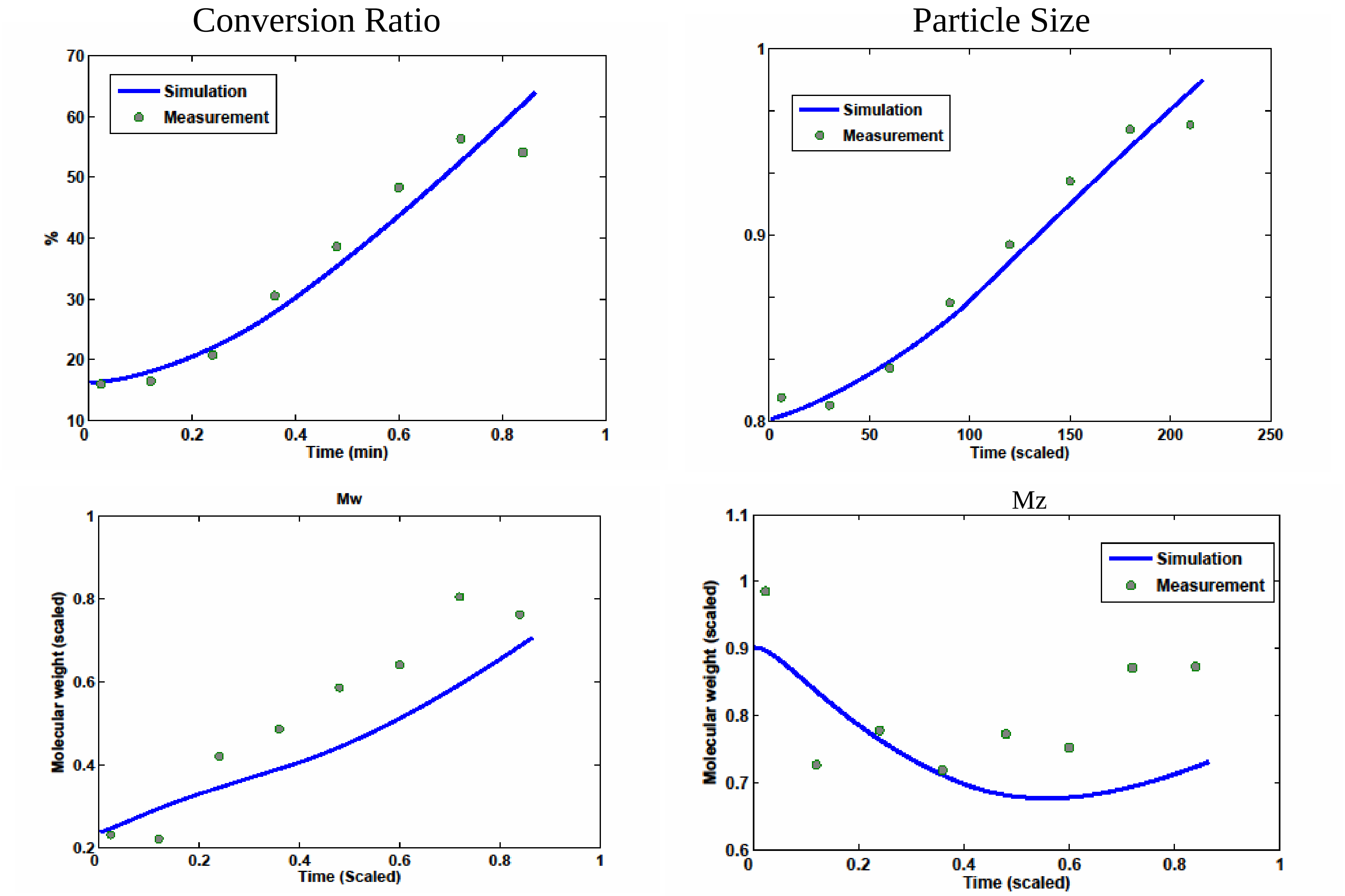


Fig. 6. Single process fitting result

# Combine Two processes. Part 1: **Fitting Results (2)**



Conversion Ratio

Particle Size

Mw

Mz

Fig. 7. Fitting result for Two data sets, process A

# Combine Two processes. Part 2: **Fitting Results (3)**

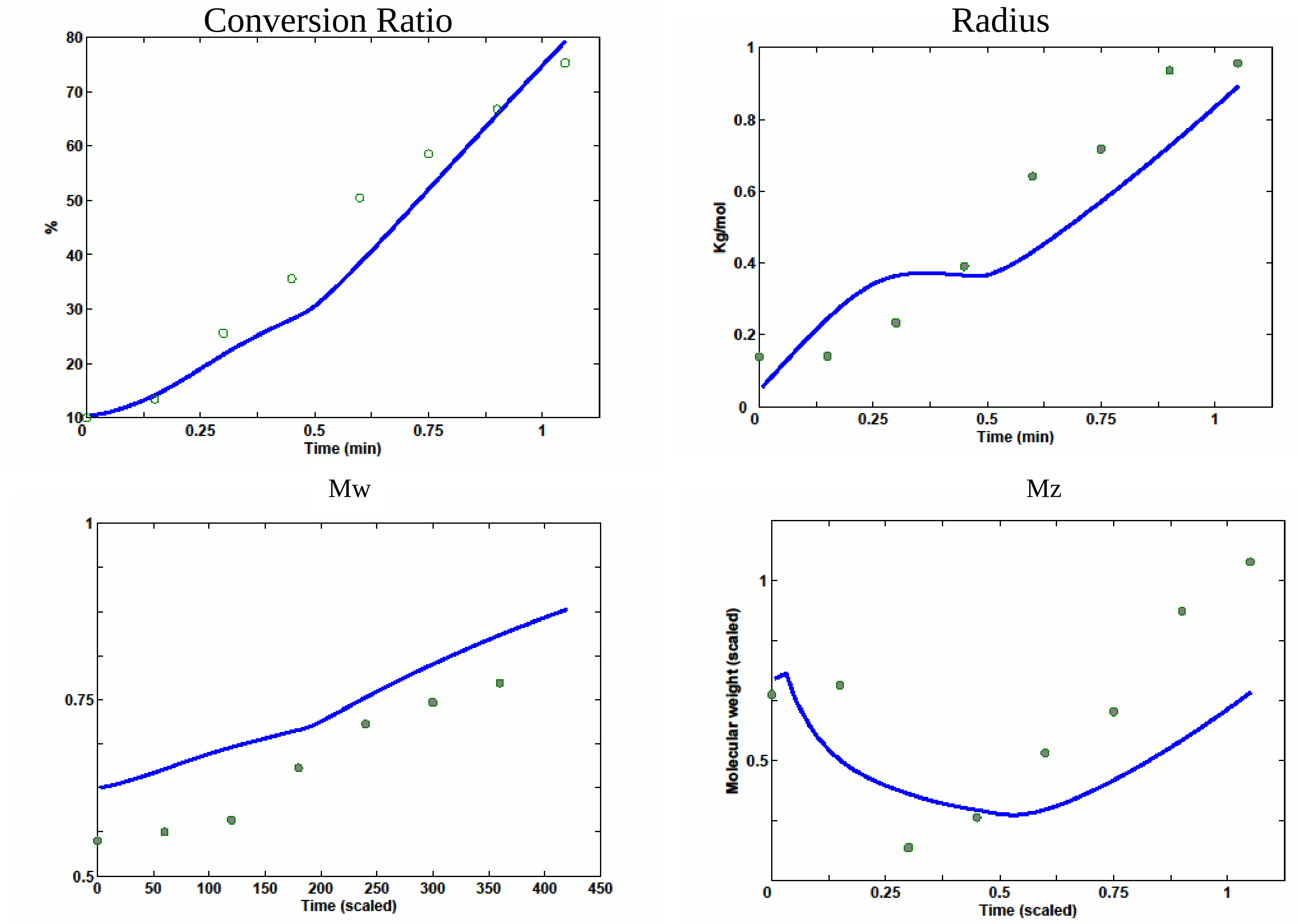
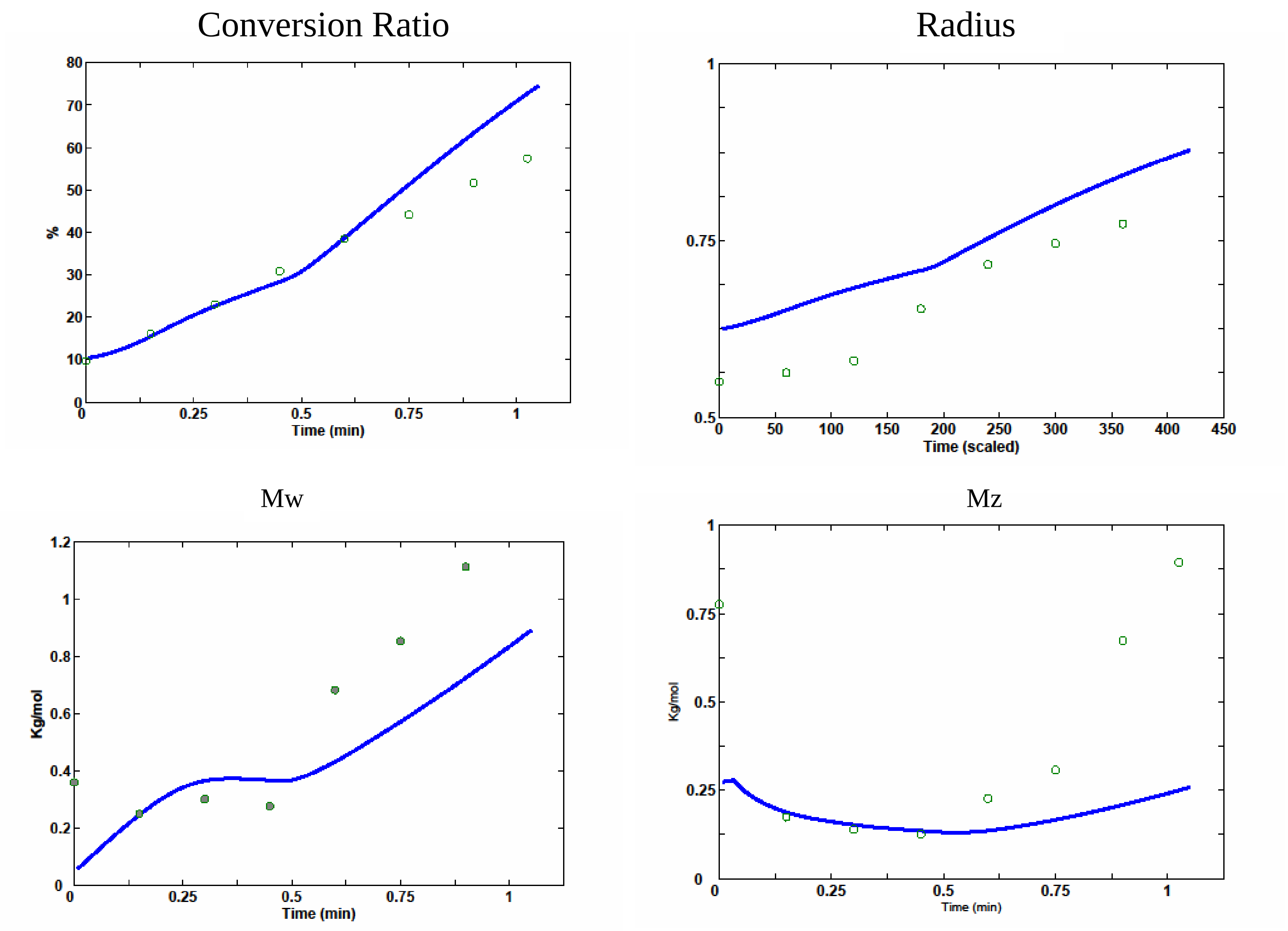


Fig. 8. Fitting result for Two data sets, process B

Progress update

# Fitting results (4)

Test data


Conversion Ratio

Radius

Mw

Mz

Fig. 9. Testing result for process C

Progress update

# Optimal Control Problem

- Connect single particle model to process control

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

$$\left.\begin{aligned} s.t.\ \frac{dz(t)}{dt} &= f(z(t),u(t)) \\ z(t0) &= z0 \end{aligned}\right\} \text{Kinetic model}$$

$$\left.\begin{aligned} \text{Molecular weight} &\subset Q \\ \text{Conversion} &\subset C \\ \text{Composition} &= P \end{aligned}\right\} \text{Quality constraint}$$

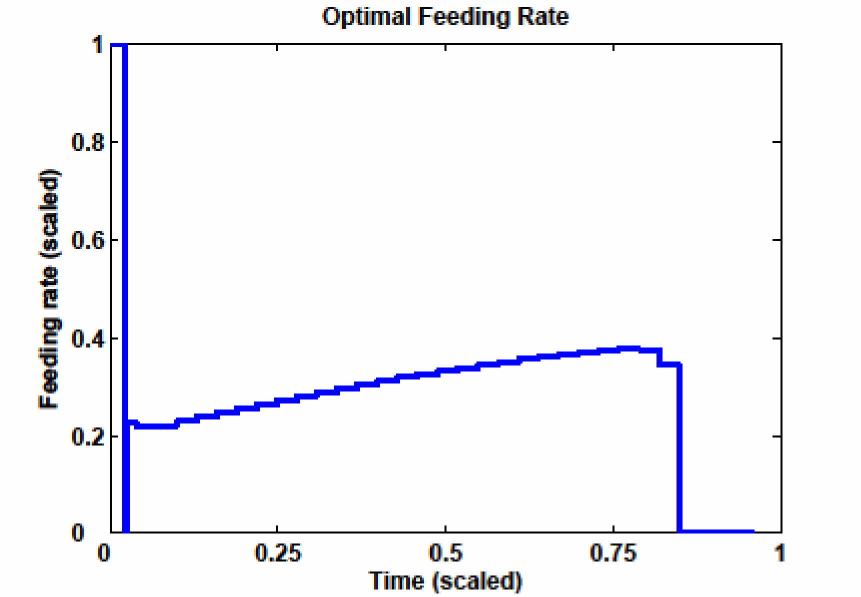


Fig. 10. One example of optimal feeding policy

# Future Work Plan

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

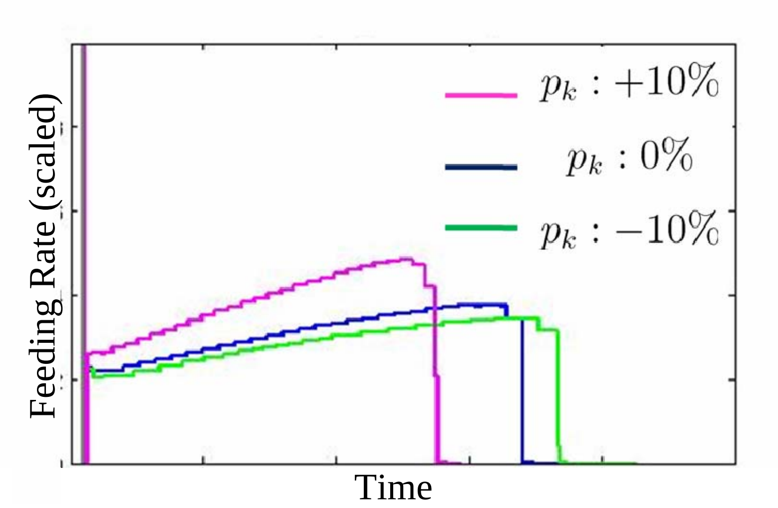


Fig. 11. Optimal feeding policy changes with uncertain parameters

# 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