Modeling and Optimization of Interpenetrating Polymer Network Process

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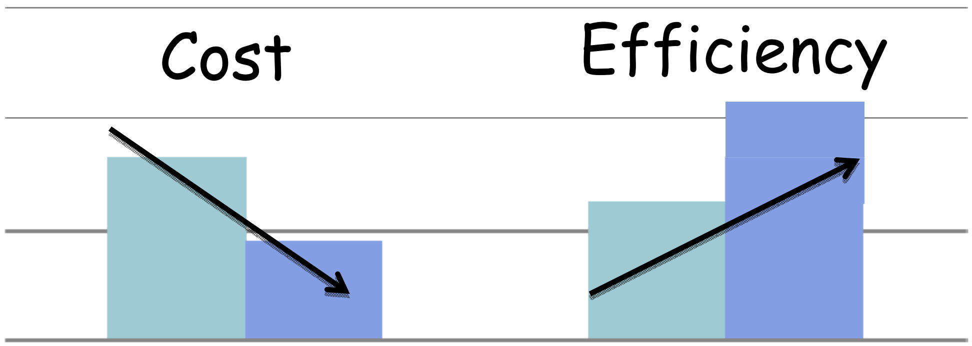
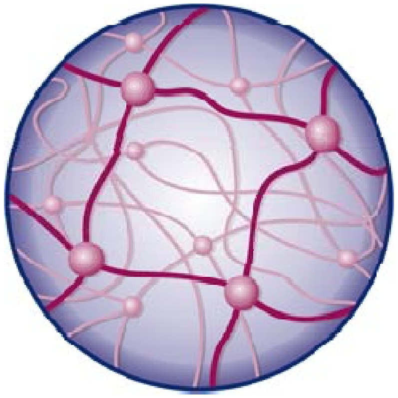
Outline

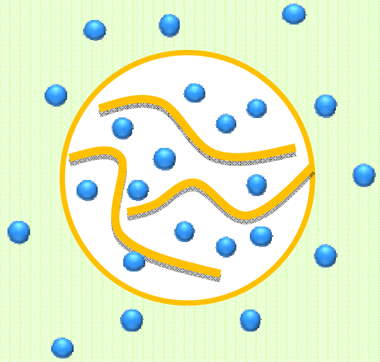
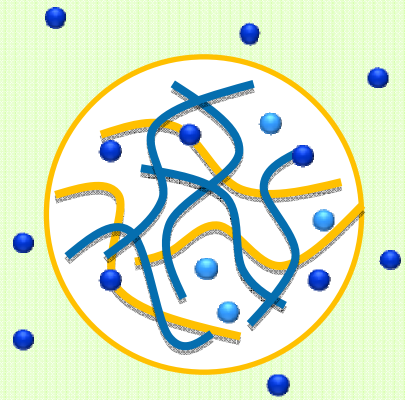
- Project review



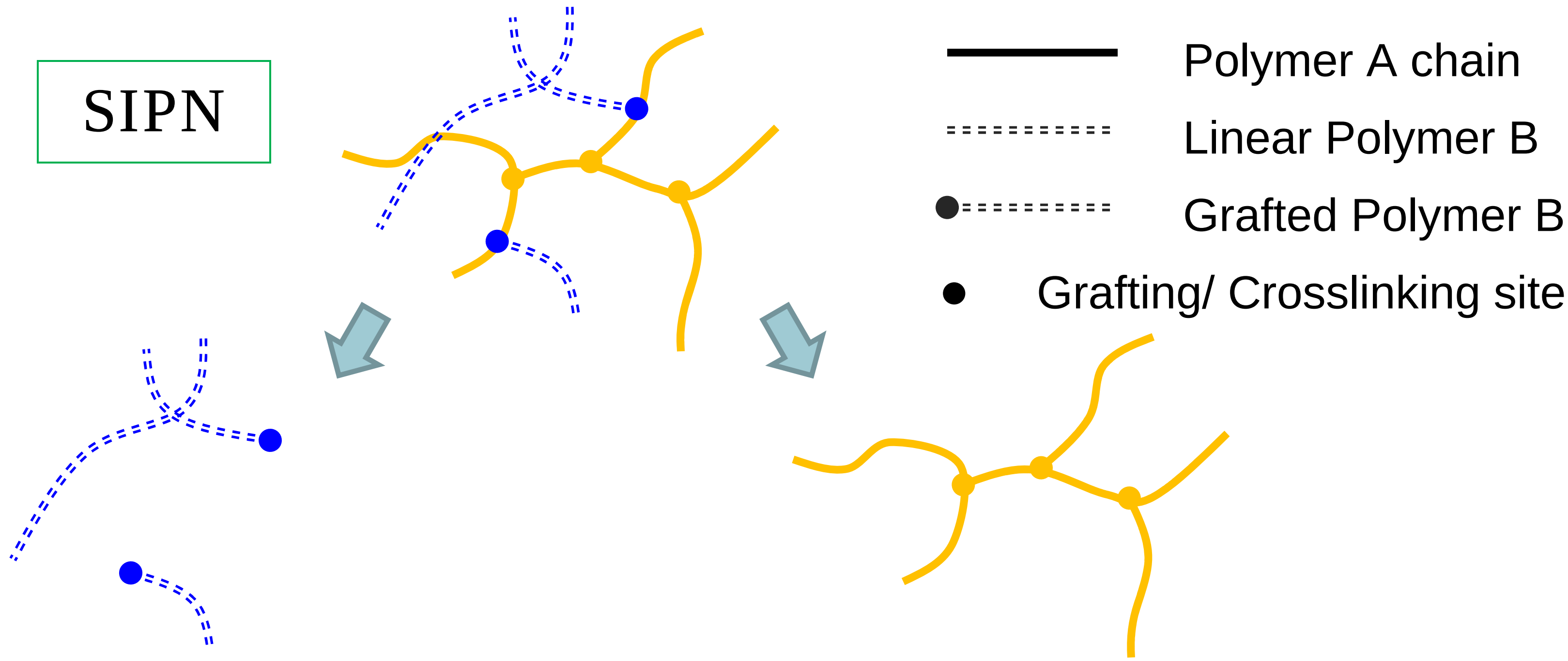


- Progress updates
  - Surrogate model for SIPN kinetics
  - Sub-model Integration
  - New optimal operation strategy
- Future work discussion
- Conclusion

Project Review

Process Stages	  I. Swelling; II. Polymerization	 III. Crosslinking
Features	*Complex diffusion; single component reaction*	*Complex composite networking reaction*
Modeling	**Particle Growth model**	**Semi-IPN kinetic model**
Optimization variables	• Monomer feeding rate • Initiator feeding rate	• Initial polymer • Monomer concentration • Initiator concentration • Holding temperature • Holding duration
Optimization Approach	**Dynamic Optimization**	

Review of the SIPN Model (1)



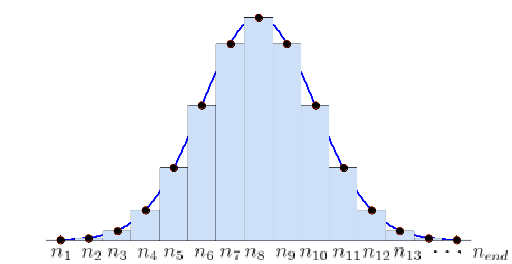
- **Polymer B**

Continuous variable approximation

$$p^{(i)}(t) = \int_0^\infty x^i p(x,t)\,dx$$

- **Polymer A**

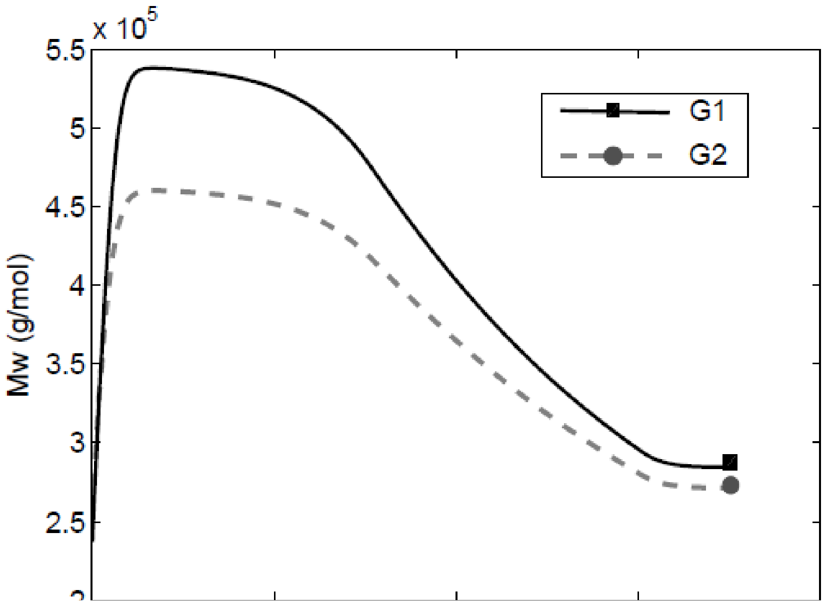
Sectional grid approach



Review of the SIPN Model (2)

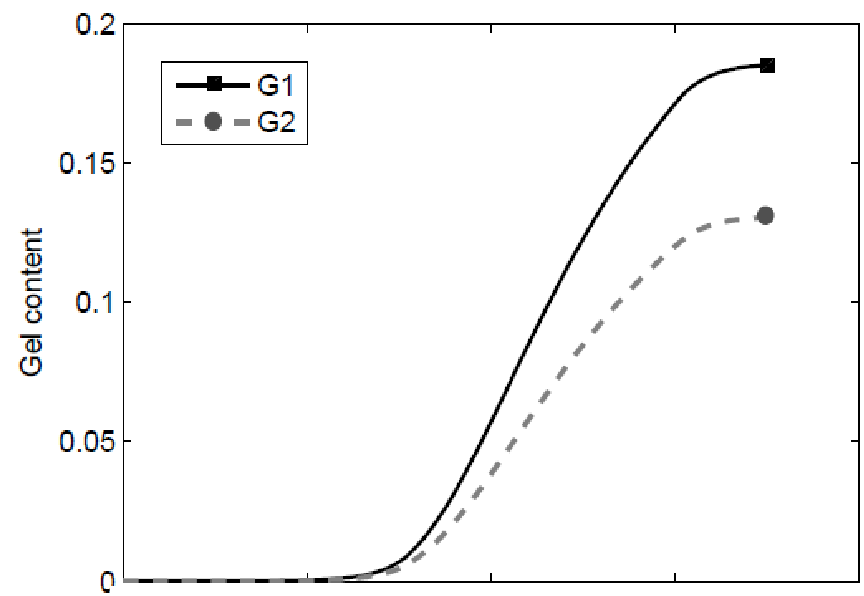
Product property simulation

(a) Polymer B Mw development



Time (scaled)

(b) SIPN Gel Content development



Time (scaled)

Figure 1. Simulation of different grades of SIPN products

Computational Challenges for Optimization

- SIPN kinetic model
  - Large set of stiff DAEs → Large scale nonlinear eqns.

    (small discretization steps are required for the gel grids)

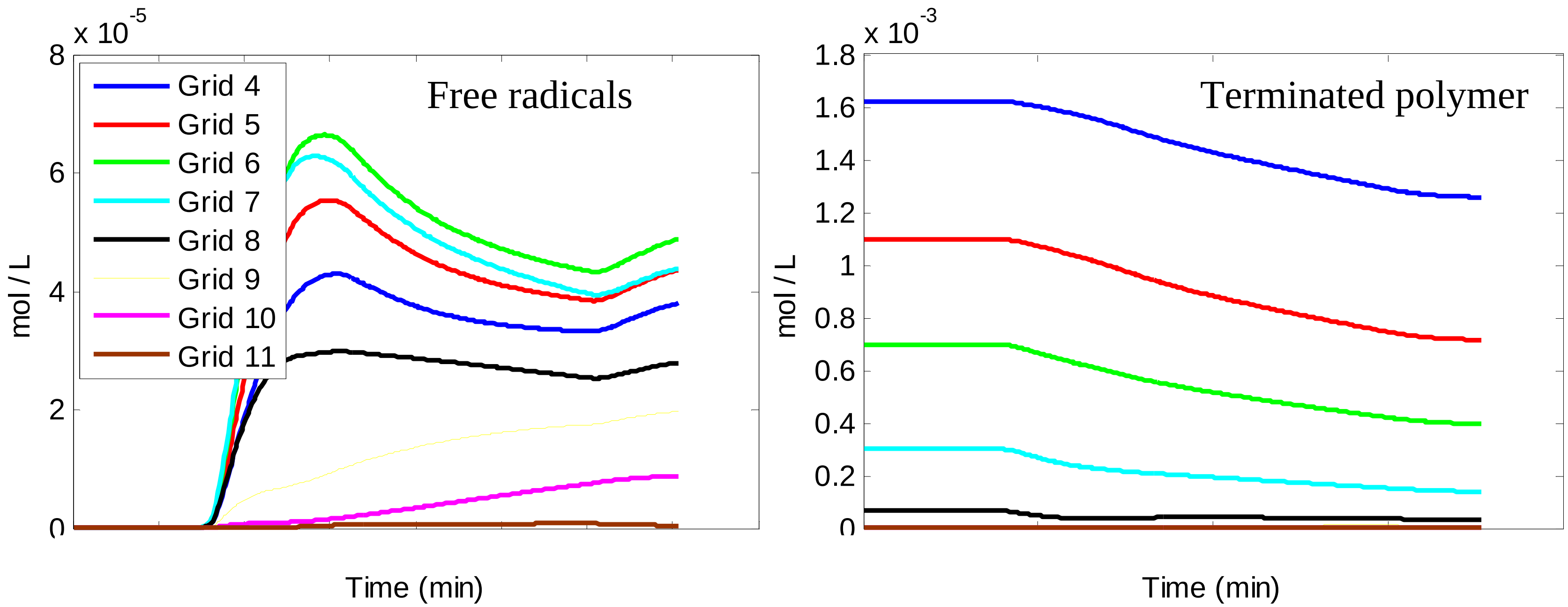


Figure 2. Dynamics of representative sectional grids

Proposed Approach for Optimization

- Surrogate model for SIPN kinetics

Full mechanistic model

$$y = \mathcal{F}(x, p, V_c)$$

Reduced to a correlation between a set of controls and the output where the inputs and parameters are fixed.

$$y|_{x,p} \approx f(V_c^*)$$

- Surrogate-based approaches
  - Kriging model
  - Response surface model
  - Linear Regression

Kriging Interpolation

Kriging method origins from geostatistical application to interpolate the value of a random field

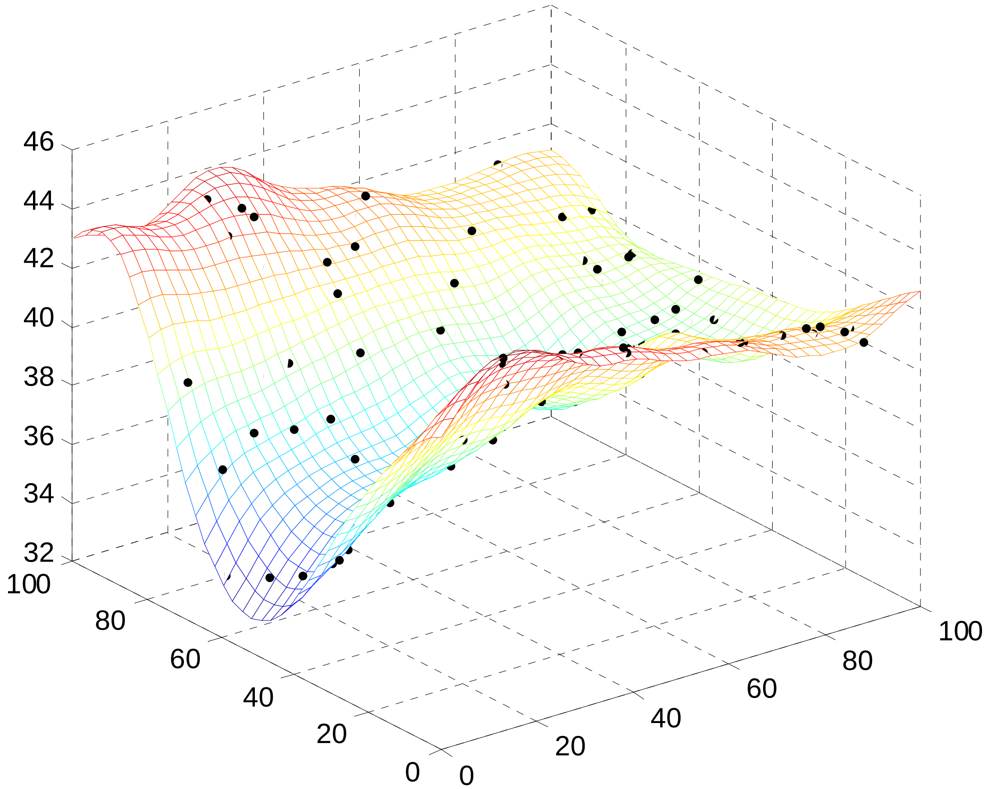


Figure 3. An example of Kriging

A Kriging estimator

$$\hat{f}(x^*) = \sum_{i=1}^{n} \lambda_i(x^*) f(x_i)$$

$$\epsilon(x) = F(x) - \sum_{i=1}^{n} \lambda_i(x) f(x_i)$$

Matlab toolbox : "DACE"

$$F\beta \simeq Y$$

$$\hat{y}(x) = f(x)^T \beta^* + r(x)^T \gamma^*$$

Kriging Model Construction

- *Input*:
  - Control variables:

    Initial condition, Temperature, processing time, monomer/initiator concentration, etc.
- *Output* :
  - SIPN properties:

    Molecular weight, Gel content

  - Computer experiment design

  Latin Hypercube Sampling

Observations: Small correlation; Monotone dependence;
Linear behavior in the constraint range

Linear Regression

$$\hat{y} = \beta \cdot x + k \quad \text{(with regression variable selection)}$$

$$y1 : \mathrm{Gel}_{end} \quad (wt\%)$$

$$y2 : M_{w\,end} \quad (1 \times 10^{6} g/mol)$$

$$x : xs_m, N_{I_1}, N_{I_2}, Mw_{\mathrm{II}}, t, T$$

Estimation Error for "Testing Data" is within 10% range

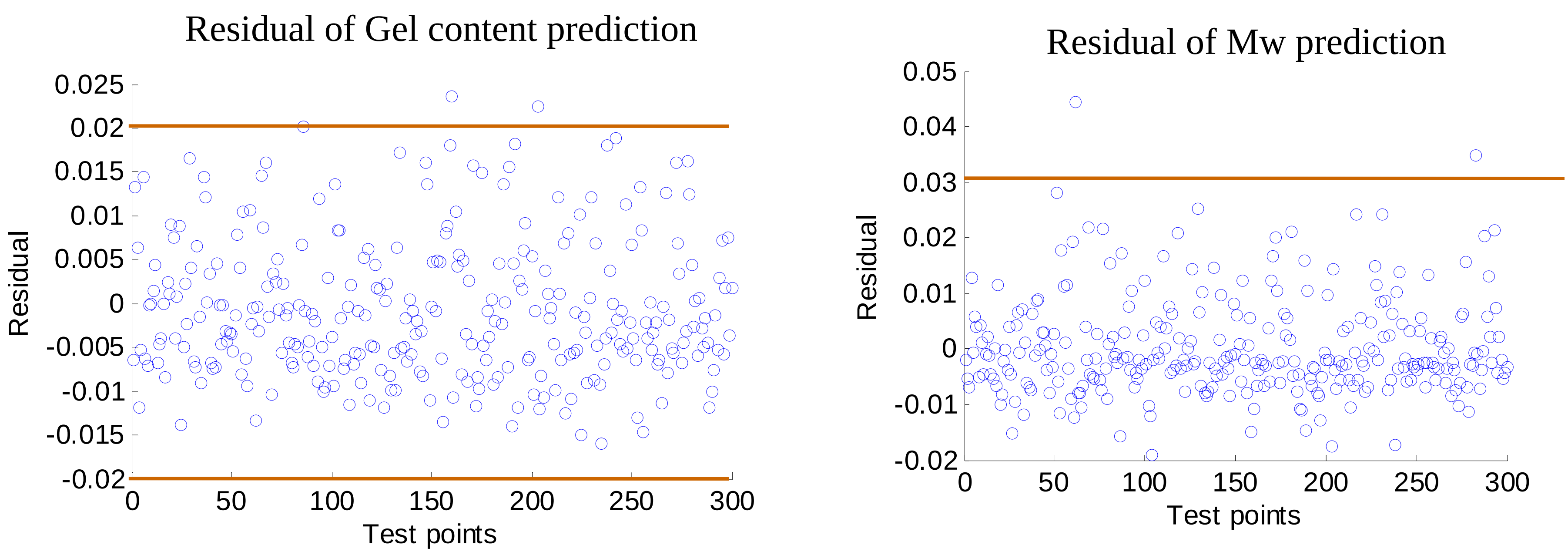


Figure 4. Prediction error of the linear regression model

Discussion on SIPN Surrogate Model

- Linear regression model for approximation
  - Within the interesting range, a linear approximation can have a sufficient accuracy on the final output compared to the full model

- Connection to Stage II
  - Initial condition of Stage II (the end of Stage II) has important effect on SIPN final properties
  - An integrated optimization framework will take full advantage of the understanding from sub-models

Sub-model Integration

Including all sub-process models into optimization

New optimization problem formulation

$$\min \quad t_{II} + t_{III}$$

s.t. Stage II model

Surrogate Stage III model

$$\text{Gel}_{\text{end}} >= \text{Tar}_{gel}$$

$$\text{Mw}_{PS_{\text{end}}} >= \text{Tar}_{M_w}$$

$$\text{Cov}_{\text{II}} >= \text{Cov}^*_{\text{II}}$$

$$M_{wPS_{\text{II}}} >= M_{w\text{II}^*}$$

Dynamic Optimization

→ To minimize the overall reaction time

→ Subjected to the full Stage II model & reduced Stage III model

→ Considering the final property constraints

→ Validated range for the reduced model

Integrated Model Solution Comparison

A better solution is obtained with the integrated model

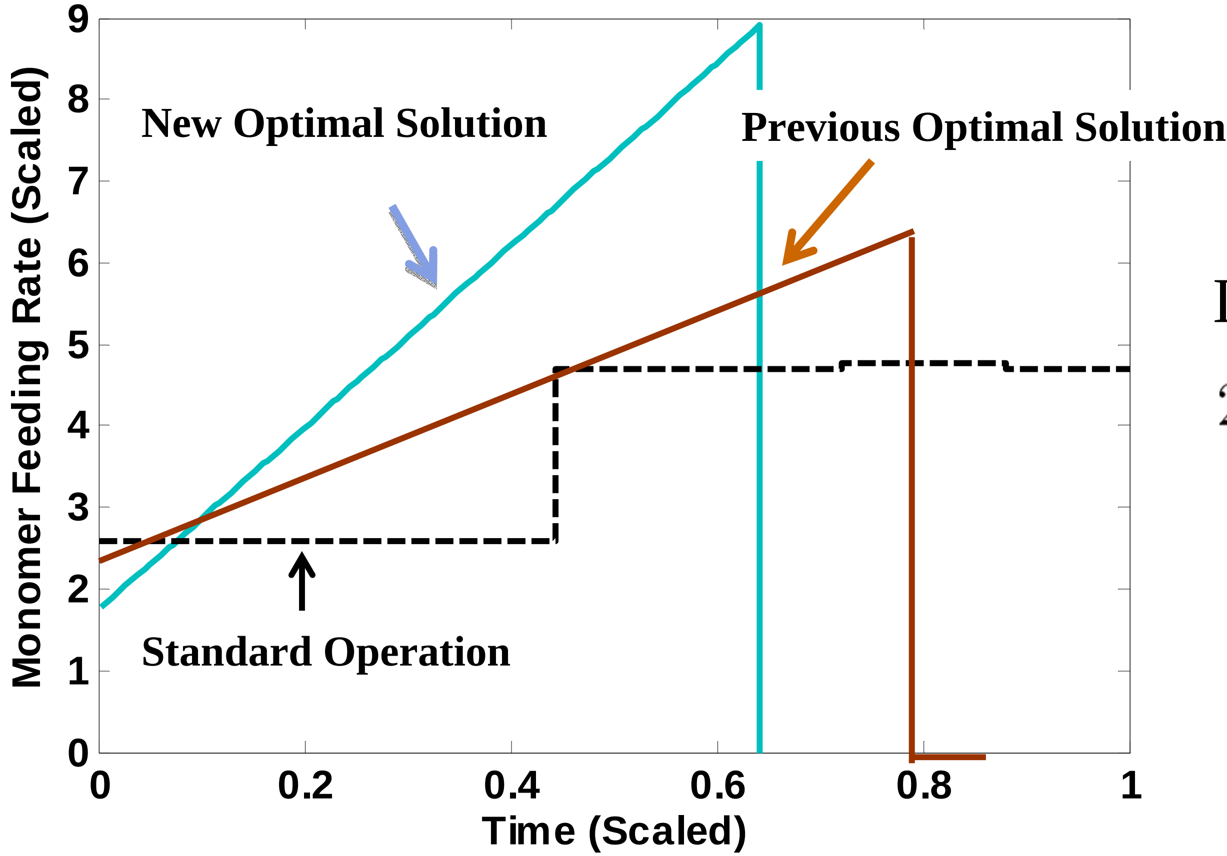


Figure 5. A new optimal solution of monomer feeding rate for the integrated model

Improved efficiency

$20\%^{+}$ time saving

Solution Analysis

- Sensitivity study
  - Solution sensitivity to the quality constraints
- Operational issues
  - Feasibility of the feeding operation
  - Reactor safety issues
- Model uncertainty
  - Prediction variance
  - Uncertain initial conditions

Future Work Discussion

- Refining optimization solution
  - To meet operation and safety standard
- Optimal solution validation
  - Lab experiment
  - Pilot plant trial
- Optimization under uncertainty
  - New solution decomposition algorithm
  - Parallel computation

Summary

- An integrated modeling framework has been built for the SIPN process optimization
- Surrogate-based optimization approach is applied for the complex kinetic system
- An improved new optimal solution is obtained through dynamic optimization
- Further experiments are planned for model validation
- New algorithm is investigated for optimization under uncertainty