Product Design in Enterprise Wide Optimization

Paul Arch, Michel Berghmans, Hany Farag
NOVA Chemicals

Weijie Lin, A. M. Jacobson and L. T. Biegler
Carnegie Mellon University

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A Changing Distribution Model - Uncontrolled Shipping
The Markets

ARCEL®

- Protective Packaging
- Protective Handling
- Safety
- Recreation
ARCEL® Advantages

**PS**
- Rigidity
- Processing Ease
- Compressive Strength
- Stability

**PE**
- Durability
- Solvent Resistant
- Flexibility
- Re-usable

Recyclable

*The magical combination = a sum much greater than the parts*
ARCEL® Vs EPS

- Puncture Toughness Comparison
- Flexibility Comparison
- Price Comparison
- Tear Strength Comparison
ARCEL® Vs EPS

Resiliency, Thickness Loss after Drop

Reusability, Trips without Breaking

Solvent Resistance

Arceil

EPS
ARCEL® is the only High Performance resilient foam that can run in EPS equipment.
Work to Date

• NOVA Research Meeting (2/15/07)
  – Review of Manufacturing Process and tour of plant
  – Tour of research facilities
    • Polymer lab/Pilot Plant/Production
    • Analytical labs
  – Team discussion – along with Alberta counterparts
    • Process development
    • Product characterization
  – Coordination of experiments with modeling questions
  – Modeling strategies and tools
  – Future directions
Modeling Issues

• PS growth models
  – Literature kinetic models (e.g., EPS)
  – Software developed

• PS/PS interactions
  – Characterization of product and morphology
  – Comparison with different experimental results and processing strategies
  – Dominant kinetic mechanisms

• Kinetic Model development
  – Moment models, MWD, link to experimental properties
LDPE Kinetic Mechanisms  
(Kiparissides, et al., 2006)

**Initiator decomposition**

\[ I_i \xrightarrow{k_{d_i}} 2R \quad i = 1, N_I \]

**Chain Initiation**

\[ \begin{align*}
R^* + M_1 & \xrightarrow{k_{t1}} P_{1,0} \\
R^* + M_2 & \xrightarrow{k_{t2}} Q_{0,1}
\end{align*} \]

**Chain Propagation**

\[ \begin{align*}
P_{r,s} + M_1 & \xrightarrow{k_{p11}} P_{r+1,s} \\
P_{r,s} + M_2 & \xrightarrow{k_{p12}} Q_{r,s+1} \\
Q_{r,s} + M_1 & \xrightarrow{k_{p21}} P_{r+1,s} \\
Q_{r,s} + M_2 & \xrightarrow{k_{p22}} Q_{r,s+1}
\end{align*} \]

**Chain Transfer to Monomer**

\[ \begin{align*}
P_{r,s} + M_1 & \xrightarrow{k_{m11}} P_{1,0} + M_{r,s} \\
P_{r,s} + M_2 & \xrightarrow{k_{m12}} Q_{0,1} + M_{r,s} \\
Q_{r,s} + M_1 & \xrightarrow{k_{m21}} P_{1,0} + M_{r,s} \\
Q_{r,s} + M_2 & \xrightarrow{k_{m22}} Q_{0,1} + M_{r,s}
\end{align*} \]

**Chain Transfer to Solvent**

\[ \begin{align*}
P_{r,s} + S_i & \xrightarrow{k_{s1}} P_{1,0} + M_{r,s} \\
Q_{r,s} + S_i & \xrightarrow{k_{s2}} Q_{0,1} + M_{r,s}
\end{align*} \]

**Chain Transfer to Polymer**

\[ \begin{align*}
P_{r,s} + M_{x,y} & \xrightarrow{k_{f11}} P_{x,y} + M_{r,s} \\
P_{r,s} + M_{x,y} & \xrightarrow{k_{f12}} Q_{x,y} + M_{r,s} \\
Q_{r,s} + M_{x,y} & \xrightarrow{k_{f21}} P_{x,y} + M_{r,s} \\
Q_{r,s} + M_{x,y} & \xrightarrow{k_{f22}} Q_{x,y} + M_{r,s}
\end{align*} \]

**Termination by Combination**

\[ \begin{align*}
P_{r,s} + P_{x,y} & \xrightarrow{k_{t11}} M_{r+x,s+y} \\
P_{r,s} + Q_{x,y} & \xrightarrow{k_{t12}} M_{r+x,s+y} \\
Q_{r,s} + Q_{x,y} & \xrightarrow{k_{t22}} M_{r+x,s+y}
\end{align*} \]

**Termination by Disproportionation**

\[ \begin{align*}
P_{r,s} + P_{x,y} & \xrightarrow{k_{td11}} M_{r,s} + M_{x,y} \\
P_{r,s} + Q_{x,y} & \xrightarrow{k_{td12}} M_{r,s} + M_{x,y} \\
Q_{r,s} + Q_{x,y} & \xrightarrow{k_{td22}} M_{r,s} + M_{x,y}
\end{align*} \]

**Backbiting**

\[ \begin{align*}
P_{r,s} & \xrightarrow{k_{b1}} P_{r,s} \text{ or } Q_{r,s} \\
P_{r,s} & \xrightarrow{k_{b2}} Q_{r,s} \text{ or } P_{r,s}
\end{align*} \]

**β-scission**

\[ \begin{align*}
P_{r,s} & \xrightarrow{k_{\beta1}} M_{r,s} = P_{1,0} \\
P_{r,s} & \xrightarrow{k_{\beta2}} M_{r,s} = Q_{0,1}
\end{align*} \]
Modeling Resources

• PS models
  – FORTRAN models
  – Literature data

• Simulation tools
  – Polymers/Plus – process modeling
  – Predici – reactor modeling
  – Gap analysis of commercial tools

• Missing information
  – Complete product characterization
  – Kinetic mechanisms and constants
  – Experimental trials to generate data for parameter estimation
ASpEN Polymers Plus - EPS Case Study
(Sunday et al., 2006)

Reaction kinetics and rate laws for suspension EPS are adapted from Villalobos et al. based on the following reactions:

- **Thermal initiation**: $3M \rightarrow 2R$
- **Initiator decomposition**: $I \rightarrow 2R$
- **Chain initiation**: $R + M \rightarrow P_1$
- **Propagation**: $P_n + M \rightarrow P_{n+1}$
- **Chain transfer to monomer**: $P_n + M \rightarrow D_n + P_1$
- **Termination by combination**: $P_n + P_m \rightarrow D_{n+m}$

Reactor model modified to resemble additional characteristics of ARCEL process
Ongoing Work

- Development of kinetic model based on PS growth and PS/PE interactions.
- Identify missing information for parameter estimation.
- Refinement and validation of simulation models with operating and specific property data.

Future Work

- Benchmark model and evaluate process modifications and improvements.
- Extend model to perform economic analysis and process optimization.
- Consider optimal operation under process and model uncertainties.
Questions?