Product Design in Enterprise Wide Optimization

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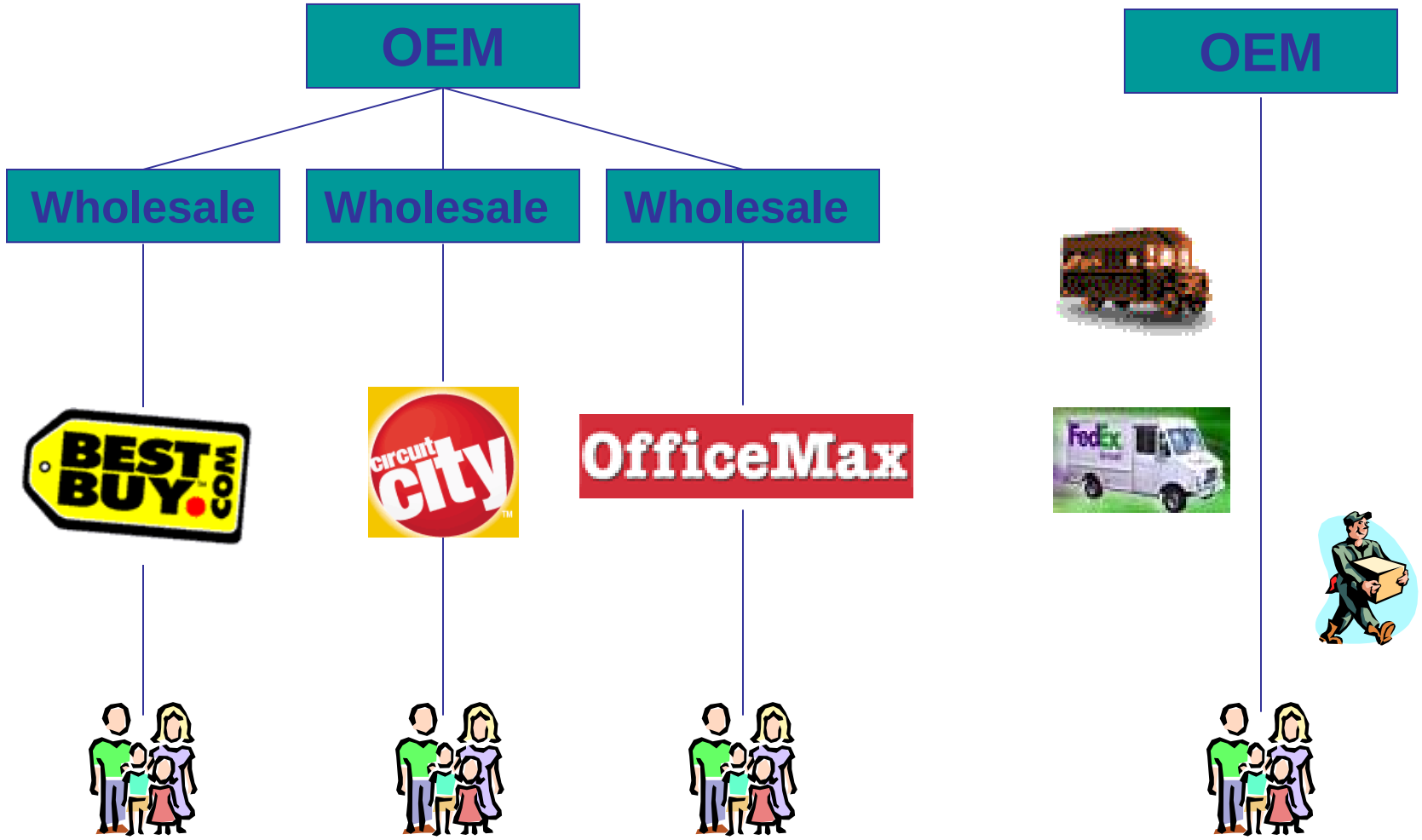
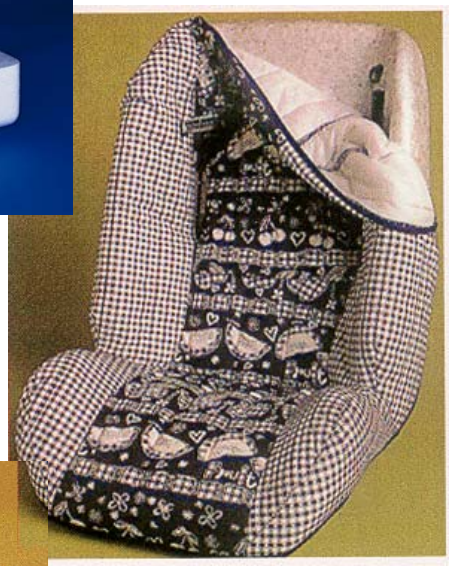
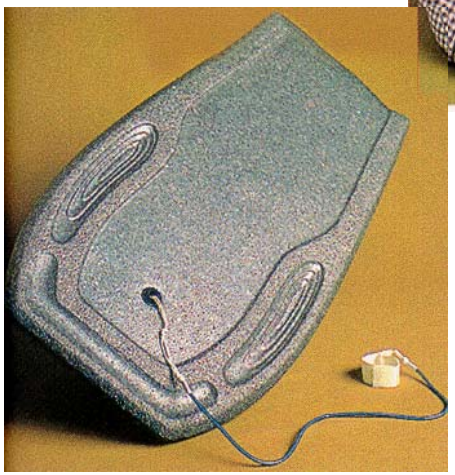
A Changing Distribution Model - Uncontrolled Shipping







The Markets

ARCEL®

- Protective Packaging
- Protective Handling
- Safety
- Recreation

ARCEL® Advantages

PS

- Rigidity
- Processing Ease
- Compressive Strength
- Stability

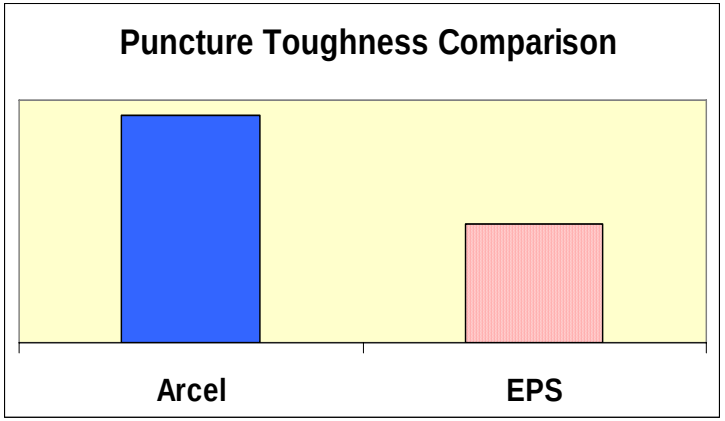
PE

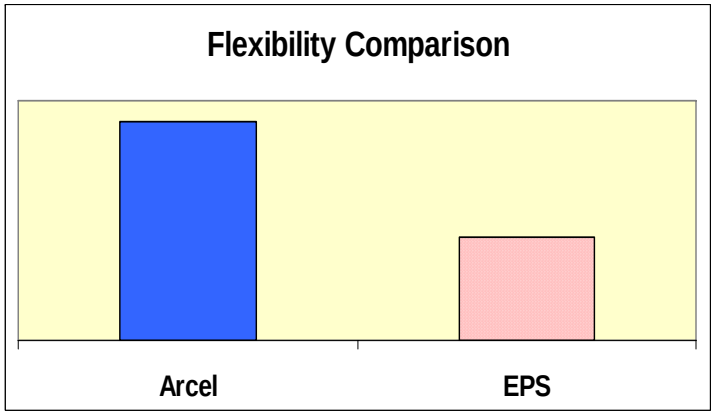
- Durability
- Solvent Resistant
- Flexibility
- Re-usable

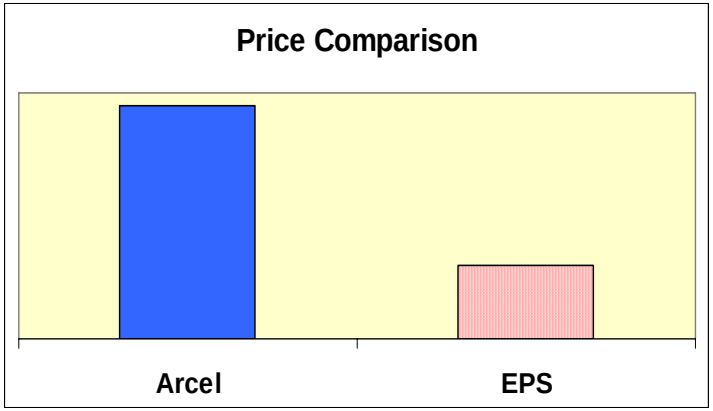
Recyclable

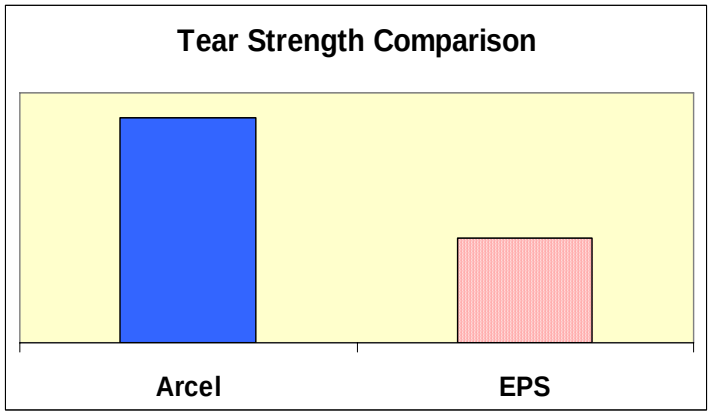
The magical combination = a sum much greater than the parts

ARCEL® Vs EPS

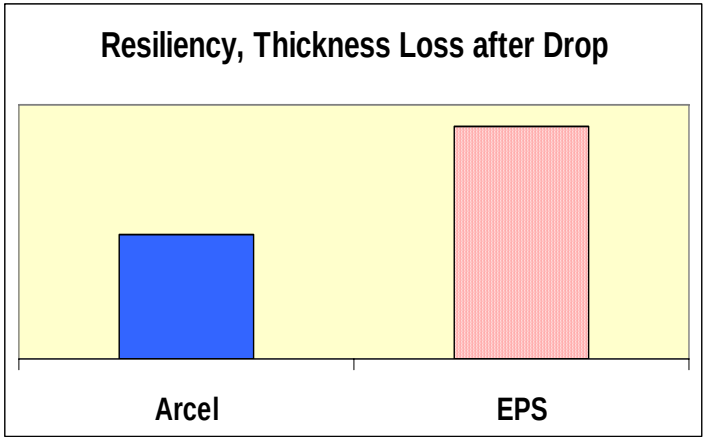

Puncture Toughness Comparison
Arcel
EPS

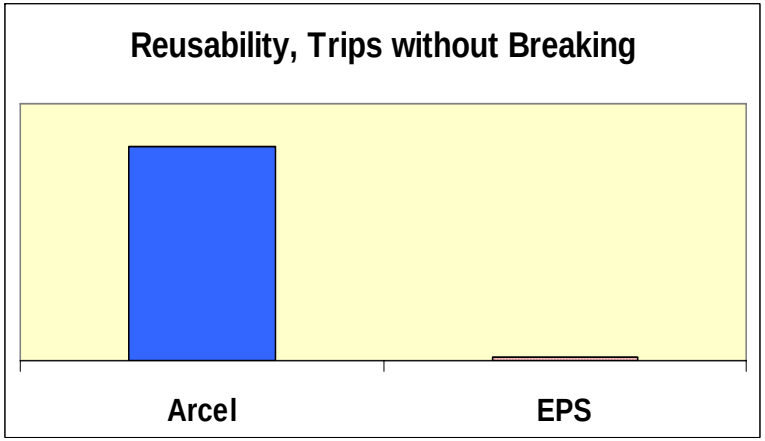

Flexibility Comparison
Arcel
EPS

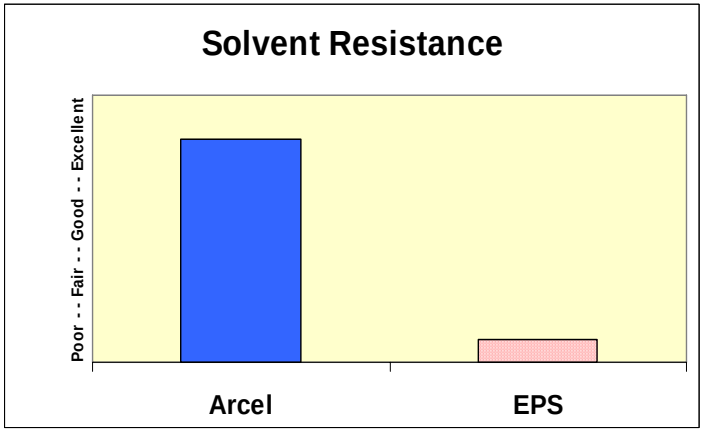

Price Comparison
Arcel
EPS


Tear Strength Comparison
Arcel
EPS

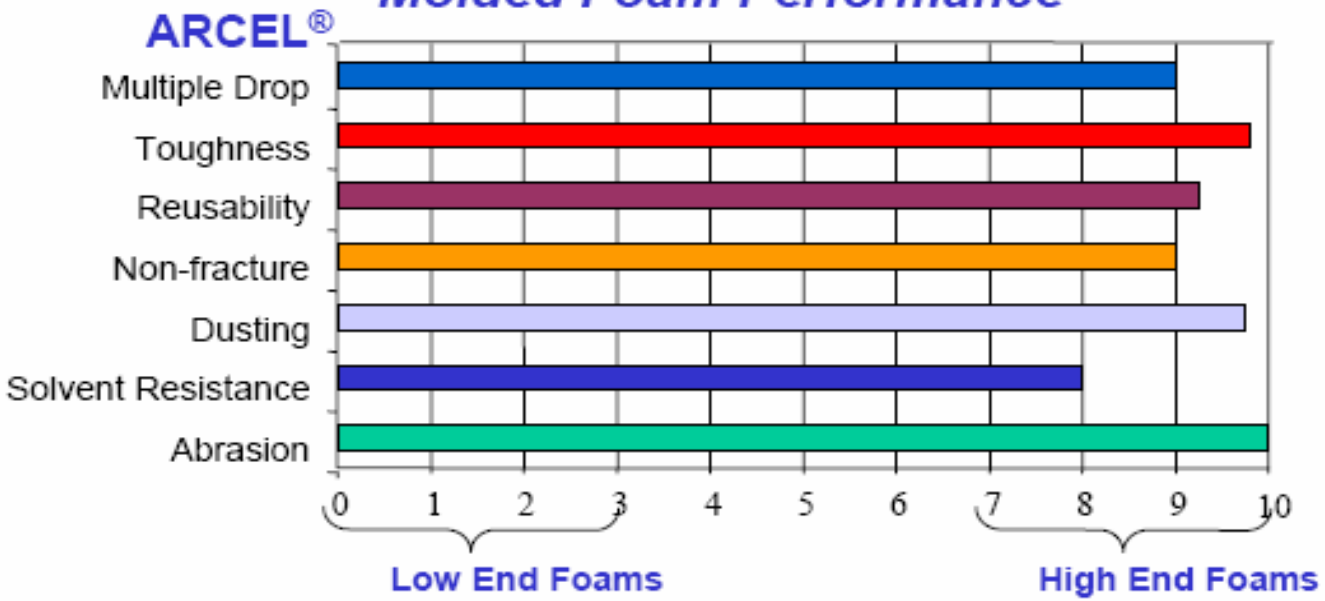
ARCEL® Vs EPS


Resiliency, Thickness Loss after Drop
Arcel
EPS

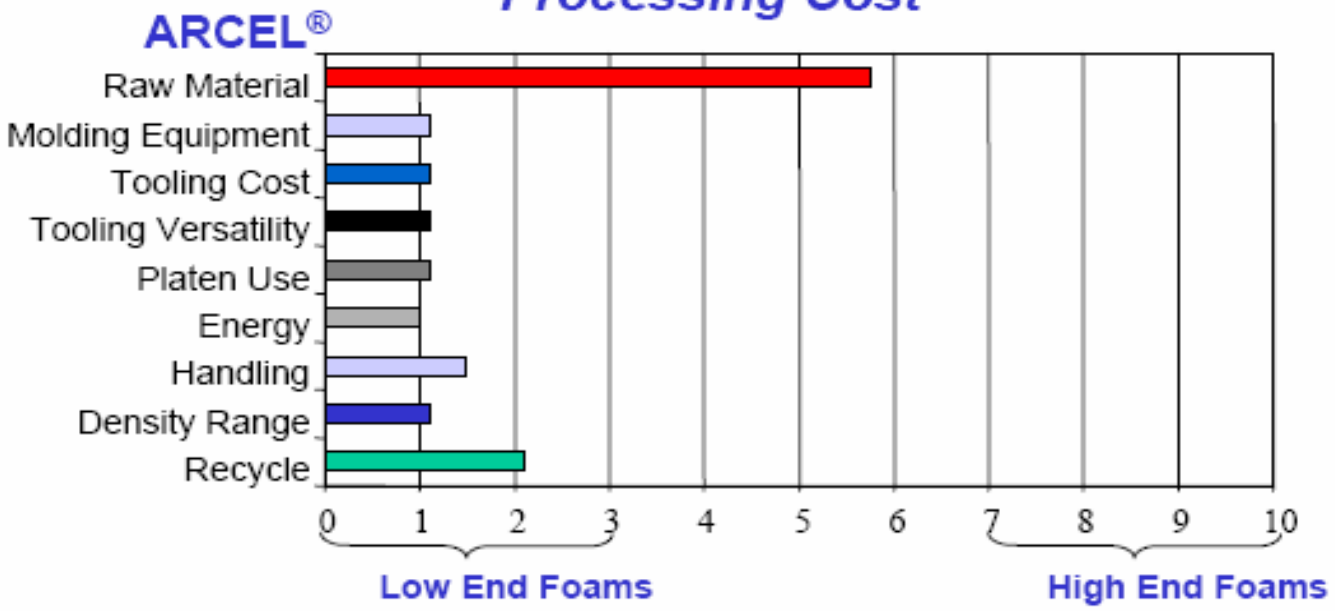

Reusability, Trips without Breaking
Arcel
EPS


Solvent Resistance
Poor -- Fair -- Good -- Excellent
Arcel
EPS

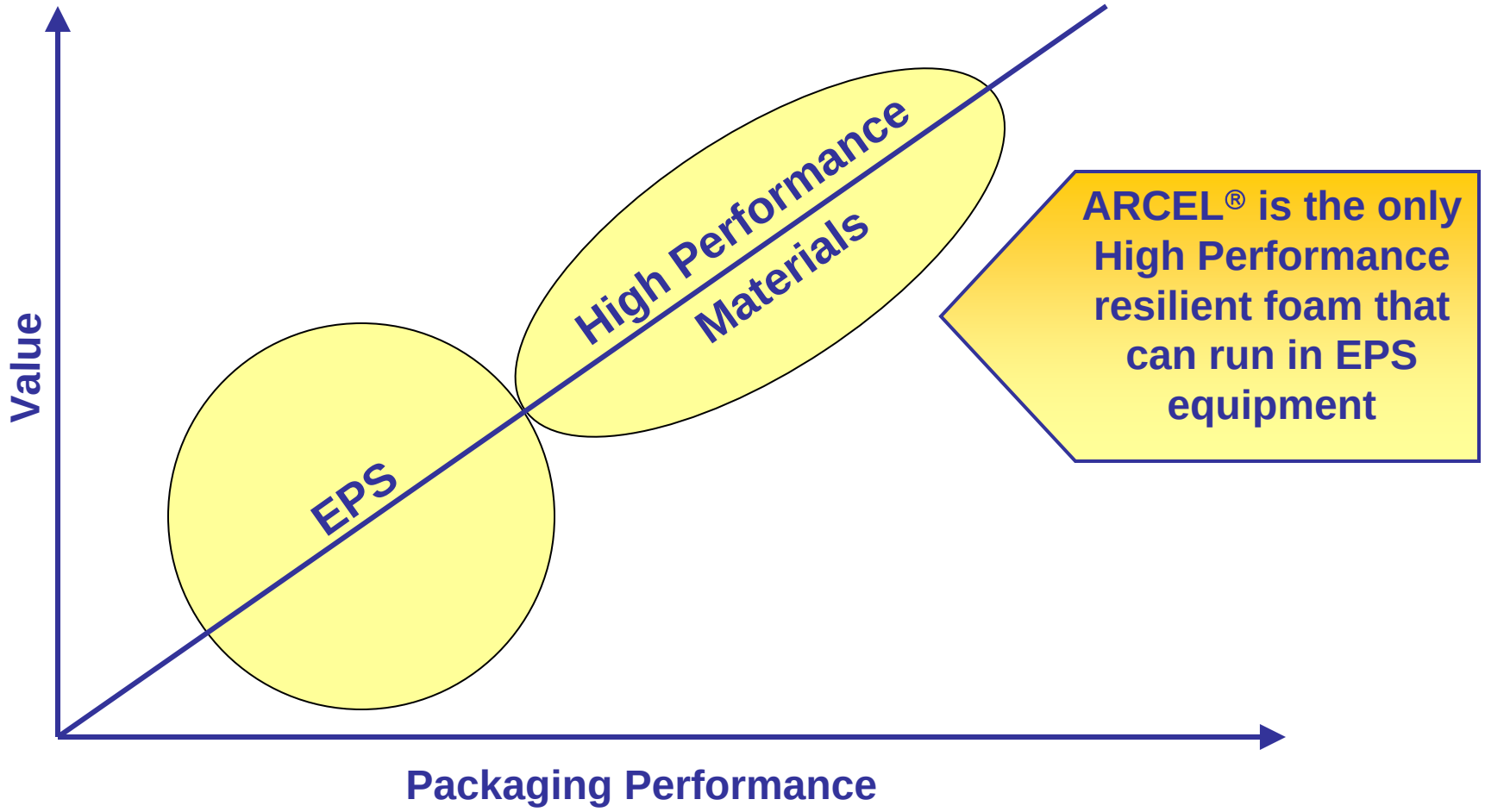
Molded Foam Performance



Processing Cost



Value Performance Migration



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

$$R^{\cdot} + M_1 \xrightarrow{k_{I_1}} P_{1,0}$$

$$R^{\cdot} + M_2 \xrightarrow{k_{I_2}} Q_{0,1}$$

Chain Propagation

$$P_{r,s} + M_1 \xrightarrow{k_{p11}} P_{r+1,s}$$

$$P_{r,s} + M_2 \xrightarrow{k_{p12}} Q_{r,s+1}$$

$$Q_{r,s} + M_1 \xrightarrow{k_{p21}} P_{r+1,s}$$

$$Q_{r,s} + M_2 \xrightarrow{k_{p22}} Q_{r,s+1}$$

Chain Transfer to Monomer

$$P_{r,s} + M_1 \xrightarrow{k_{fm11}} P_{1,0} + M_{r,s}$$

$$P_{r,s} + M_2 \xrightarrow{k_{fm12}} Q_{0,1} + M_{r,s}$$

$$Q_{r,s} + M_1 \xrightarrow{k_{fm21}} P_{1,0} + M_{r,s}$$

$$Q_{r,s} + M_2 \xrightarrow{k_{fm22}} Q_{0,1} + M_{r,s}$$

Chain Transfer to Solvent

$$P_{r,s} + S_i \xrightarrow{k_{si1}} P_{1,0} + M_{r,s}$$

$$Q_{r,s} + S_i \xrightarrow{k_{si2}} Q_{0,1} + M_{r,s}$$

Chain Transfer to Polymer

$$P_{r,s} + M_{x,y} \xrightarrow{k_{fp11}} P_{x,y} + M_{r,s}$$

$$P_{r,s} + M_{x,y} \xrightarrow{k_{fp12}} Q_{x,y} + M_{r,s}$$

$$Q_{r,s} + M_{x,y} \xrightarrow{k_{fp21}} P_{x,y} + M_{r,s}$$

$$Q_{r,s} + M_{x,y} \xrightarrow{k_{fp22}} Q_{x,y} + M_{r,s}$$

Termination by Combination

$$P_{r,s} + P_{x,y} \xrightarrow{k_{tc11}} M_{r+x,s+y}$$

$$P_{r,s} + Q_{x,y} \xrightarrow{k_{tc12}} M_{r+x,s+y}$$

$$Q_{r,s} + Q_{x,y} \xrightarrow{k_{tc22}} M_{r+x,s+y}$$

Termination by Disproportionation

$$P_{r,s} + P_{x,y} \xrightarrow{k_{td11}} M_{r,s} + M_{x,y}$$

$$P_{r,s} + Q_{x,y} \xrightarrow{k_{td12}} M_{r,s} + M_{x,y}$$

$$Q_{r,s} + Q_{x,y} \xrightarrow{k_{td22}} M_{r,s} + M_{x,y}$$

Backbitting

$$P_{r,s} \xrightarrow{k_{b1}} P_{r,s} \; or \; Q_{r,s}$$

$$P_{r,s} \xrightarrow{k_{b2}} Q_{r,s} \; or \; P_{r,s}$$

β-scission

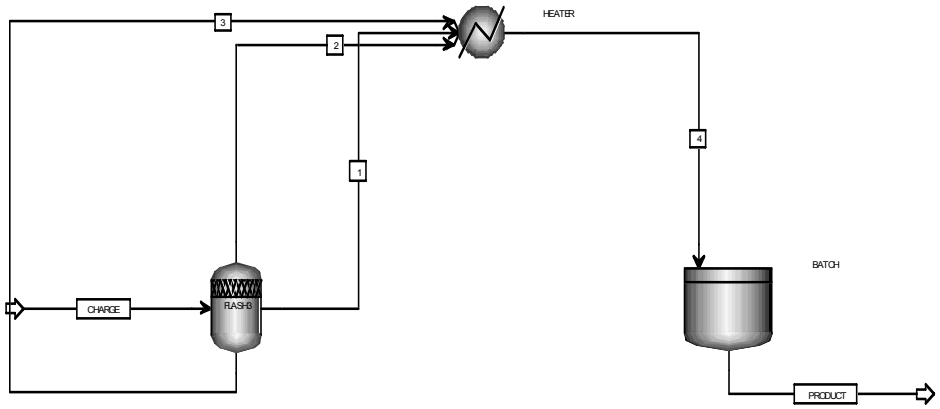
$$P_{r,s} \xrightarrow{k_{\beta 1}} M^{=}_{r,s} + P_{1,0}$$

$$P_{r,s} \xrightarrow{k_{\beta 2}} M^{=}_{r,s} + Q_{0,1}$$

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?