

# Commercial Applications of a Dynamic Model for the Production of Styrene/Maleic Anhydride Copolymers

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# Presentation Outline

- Model purpose and objectives
- The SMA model
- Polymer mechanical properties
- Grade transition case
- Conclusions

# Model Purpose and Objectives

- Predict reactor performance during unsteady state operating conditions
- Optimize reactor steady state operating conditions
- Optimize grade transitions strategies to minimize off-grade products
- A training tool off-line for engineers and technicians at the plant site

# Model Purpose and Objectives (cont.)

- Use of the model will help reduce risks especially going to plant trials (i.e. to ease scale-up of new commercial product formulations) by:
  - Targeting conditions
  - Predicting overall performance
- Predict Polymer properties
- Test various system configurations, such as dual reactors versus a single CSTR

# The SMA Model

- Model based on fundamental polymerization principles with a full Free-Radical polymerization kinetic scheme for the system Styrene, MA, and Rubber
- Aspen Plus was used to generate the properties file
- Aspen Dynamics and Aspen Custom Modeler were used for the dynamic simulation
- Polymer Non-Random Two-Liquid (Poly-NRTL) model is used for the calculation of the activity coefficients of the system and the related physical properties

## The SMA Model (cont.)

- The Van Krevelen Thermo–Physical property models are used to calculate segment property parameters (such as heat capacity, molar volume, enthalpy, entropy, Gibbs energy of formation, glass transition and melt transition temperatures), which are in turn used to calculate polymer property parameters.

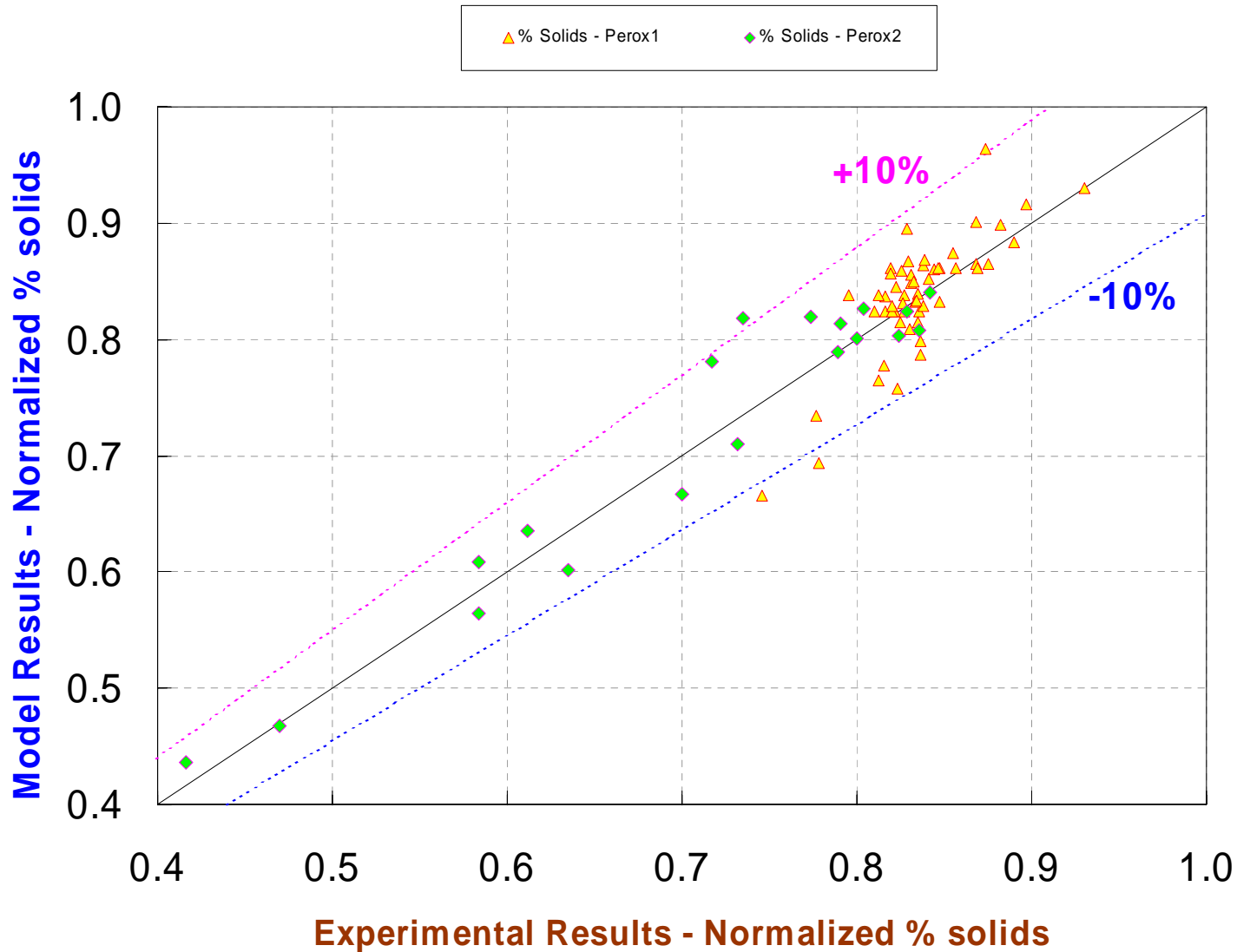
# The SMA Model (cont.)

- Input to the model includes: Feed composition, reactor operating conditions, rubber mix composition and degree of polymerization.
- Output from model includes: Polymer production rate, polymer composition,  $M_w$ ,  $M_n$ , and polymer mechanical properties such as tensile strength, tensile Modulus, flexural Modulus, IZOD, Heat Distortion Temperature Under Load ( DTUL), and melt index .

# The SMA Model (cont.)

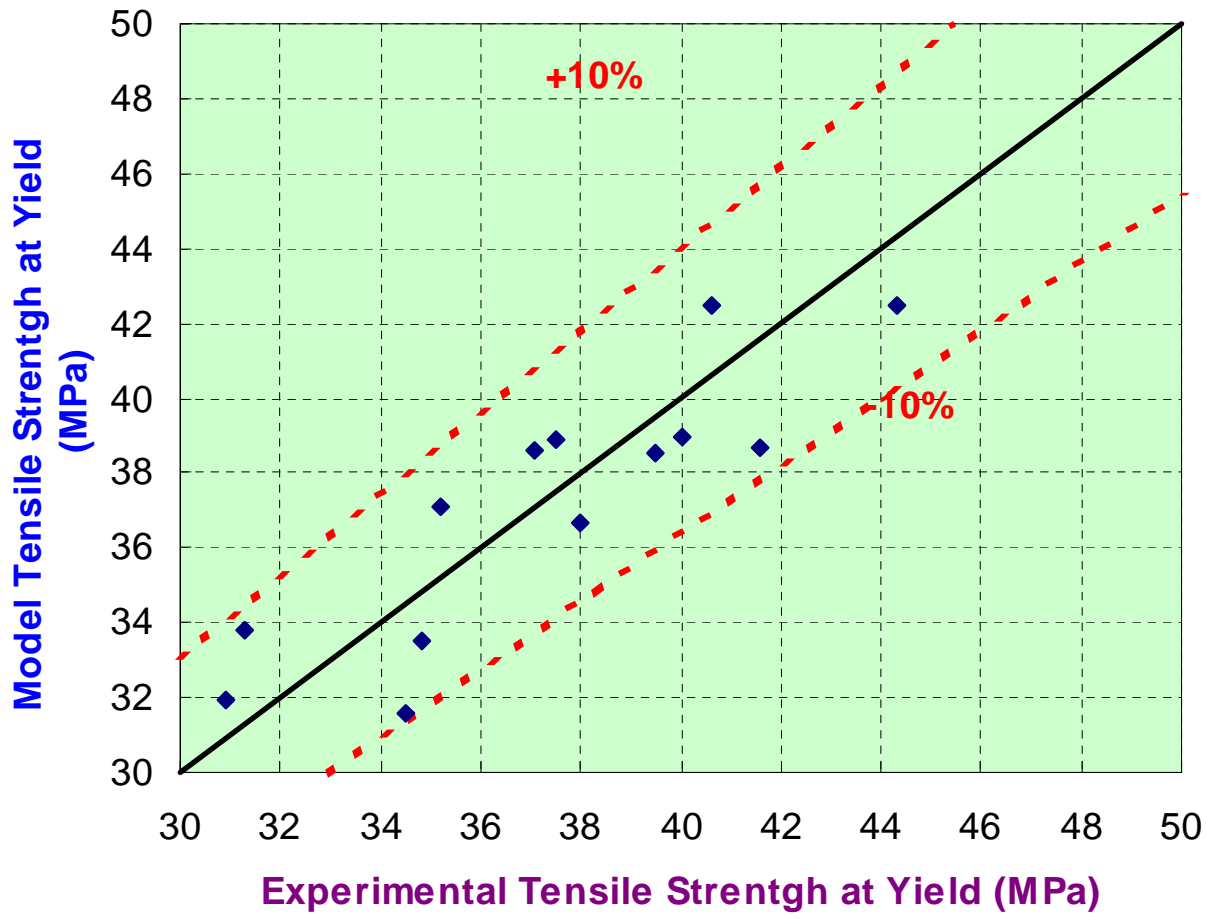
## The SMA Kinetic Scheme

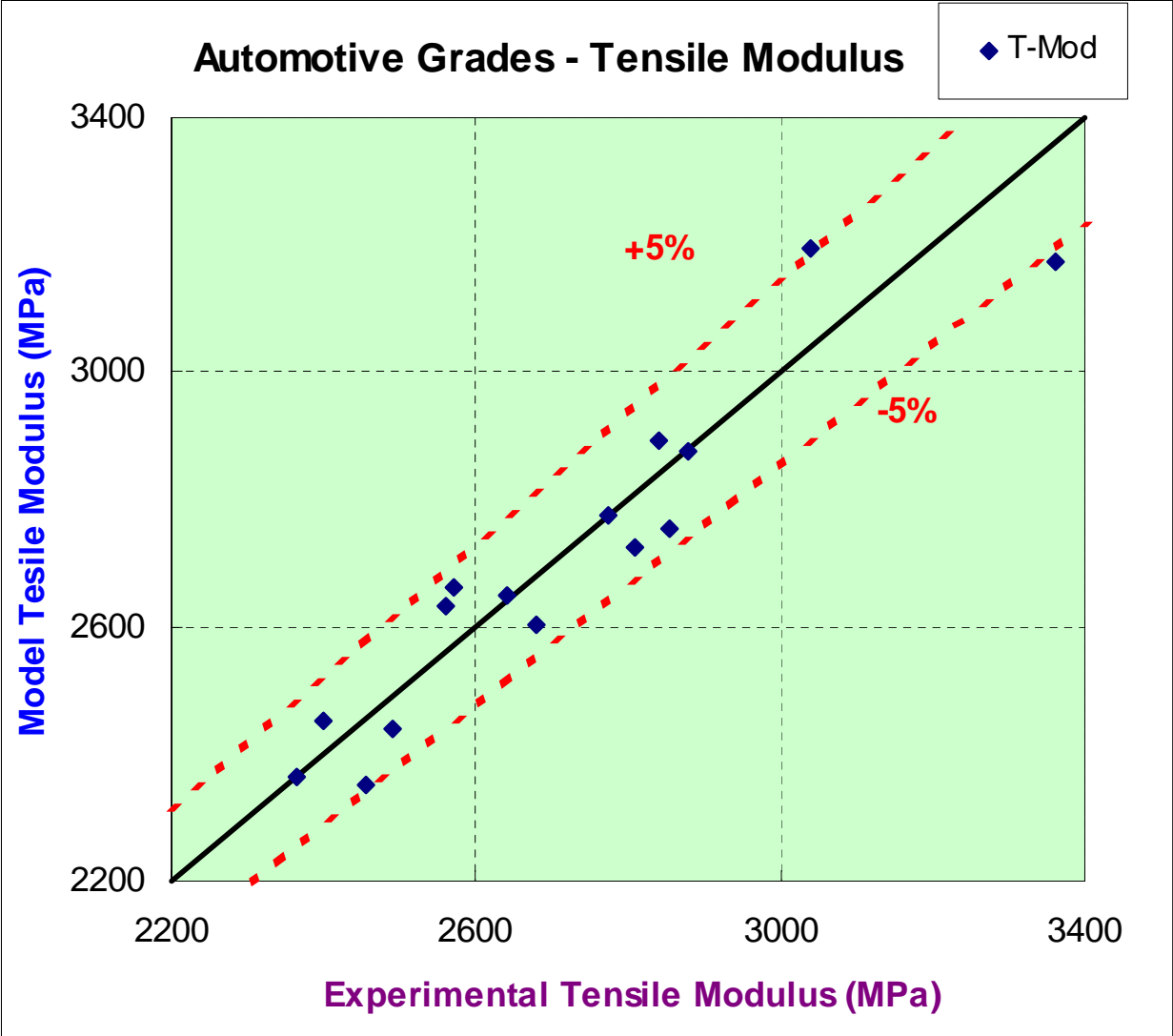
- Peroxide Decomposition
- Chain Initiation & Thermal Initiation
- Chain Propagation
- Chain Transfer to Monomer
- Chain Transfer to Polymer
- Terminations reactions (combination & disproportionation)
- The gel effect (Trommsdorf effect) was also modeled by multiplying the termination reaction rate coefficients by a gel factor .



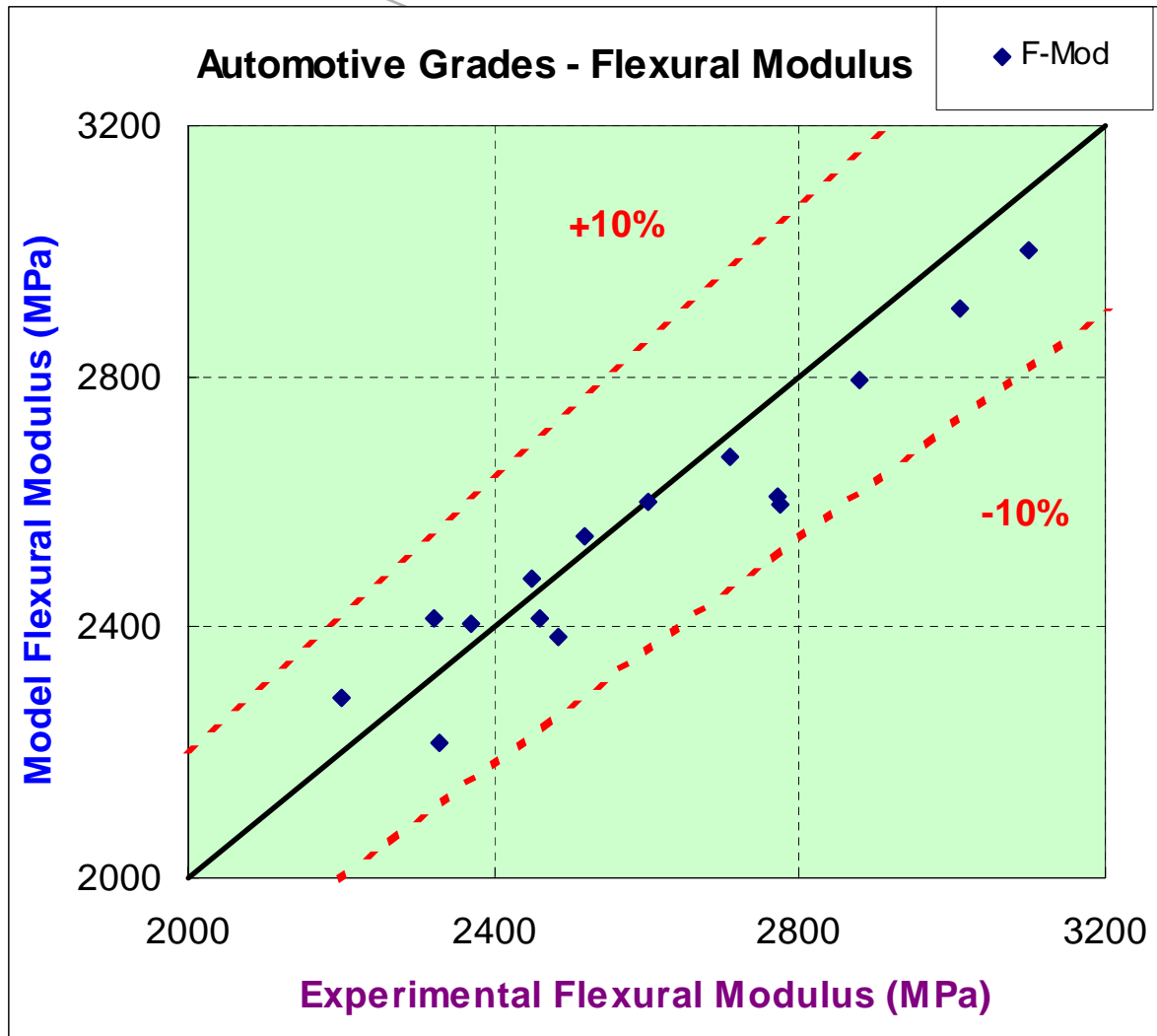
# Automotive Grades - Tensile Strength at Yield

◆ TSY

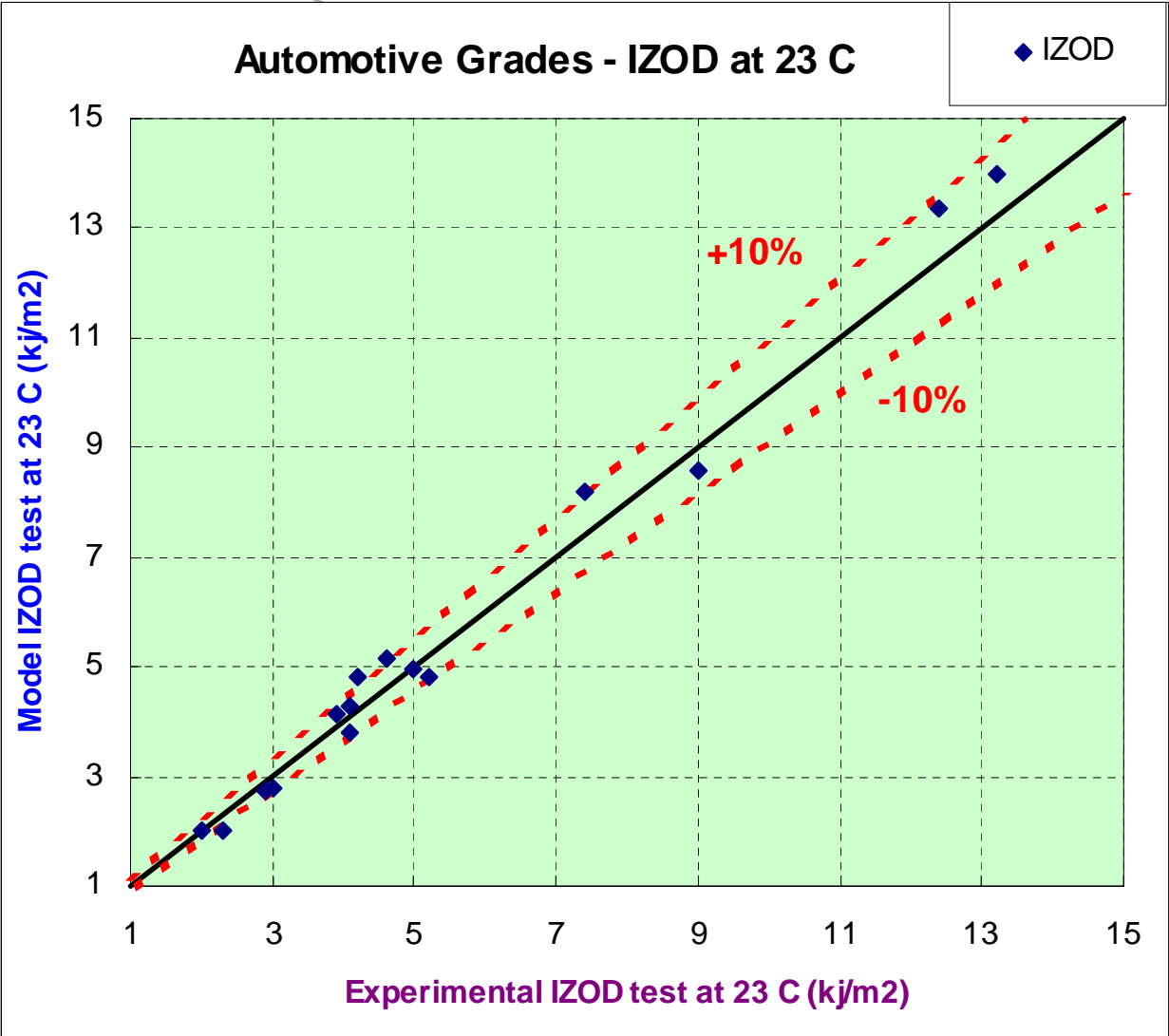




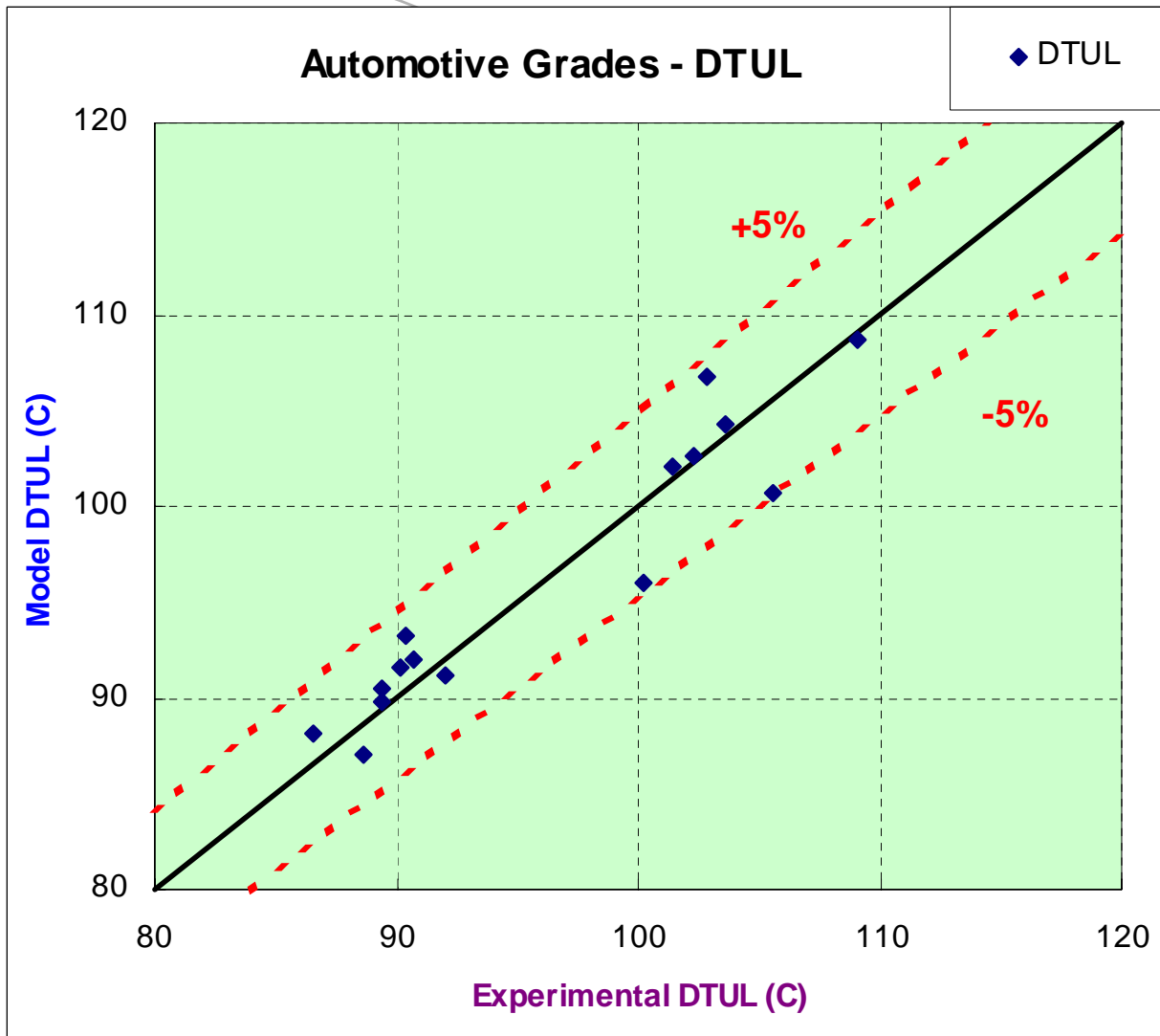
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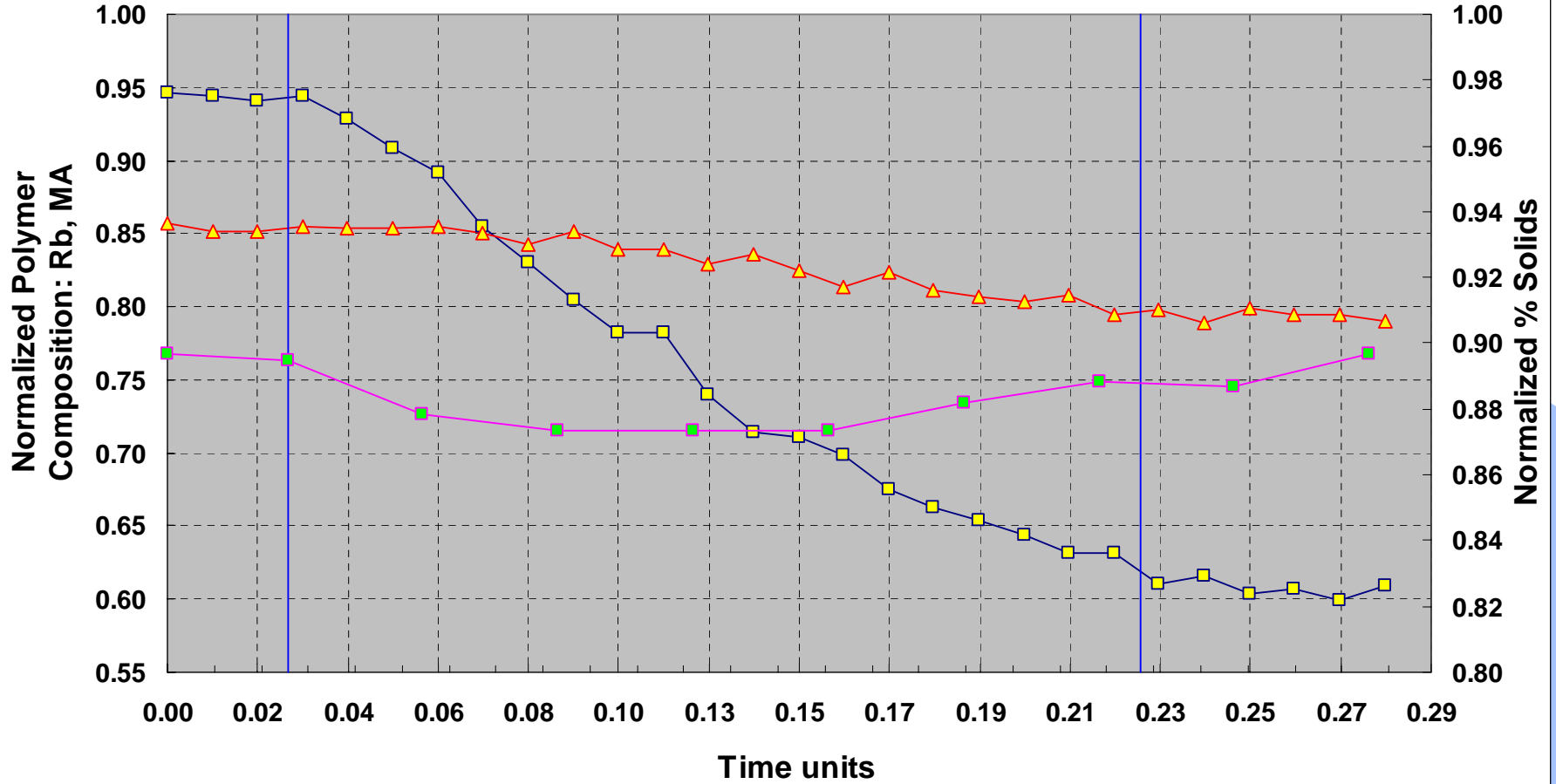


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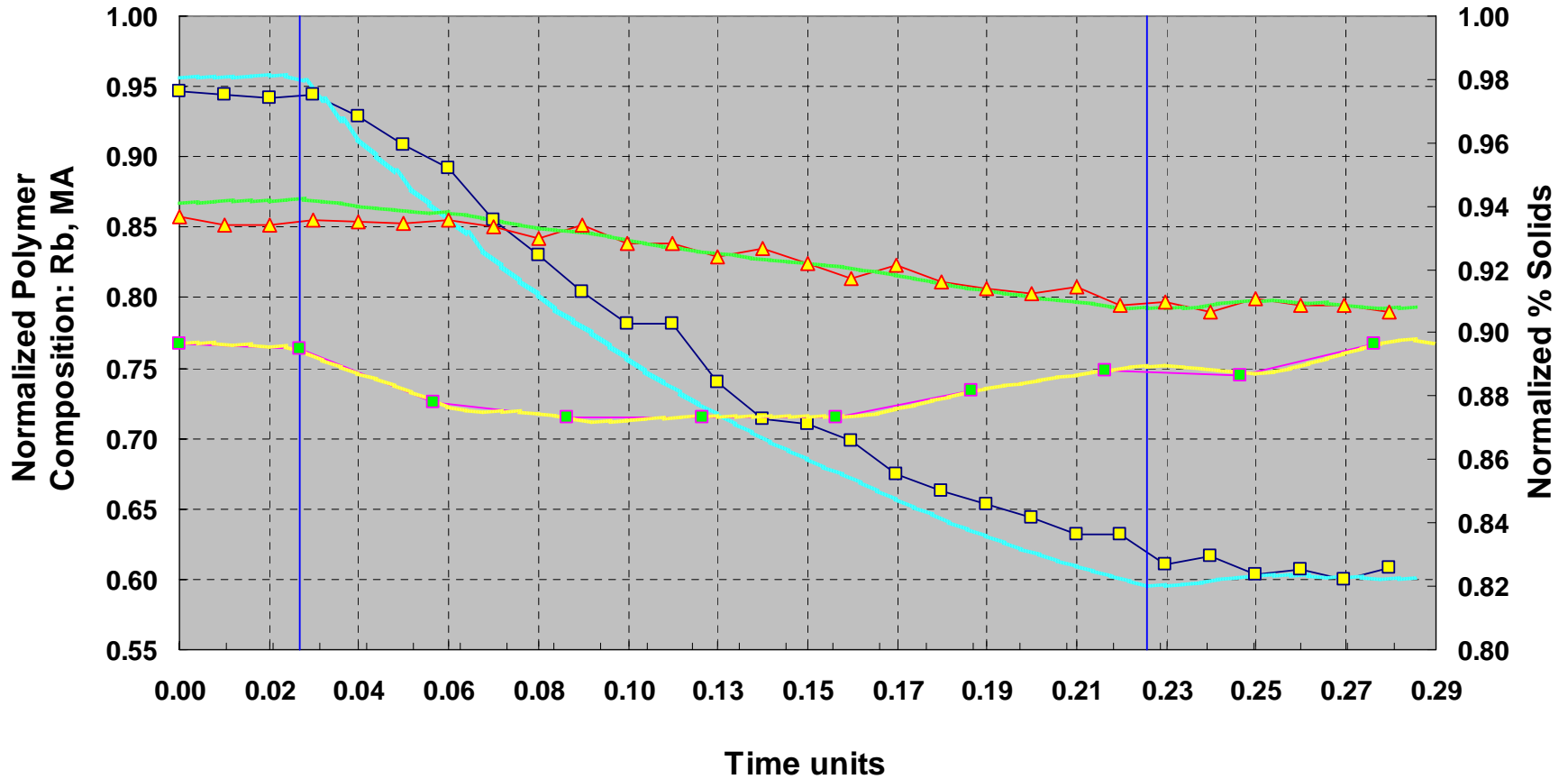
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# Plant Data



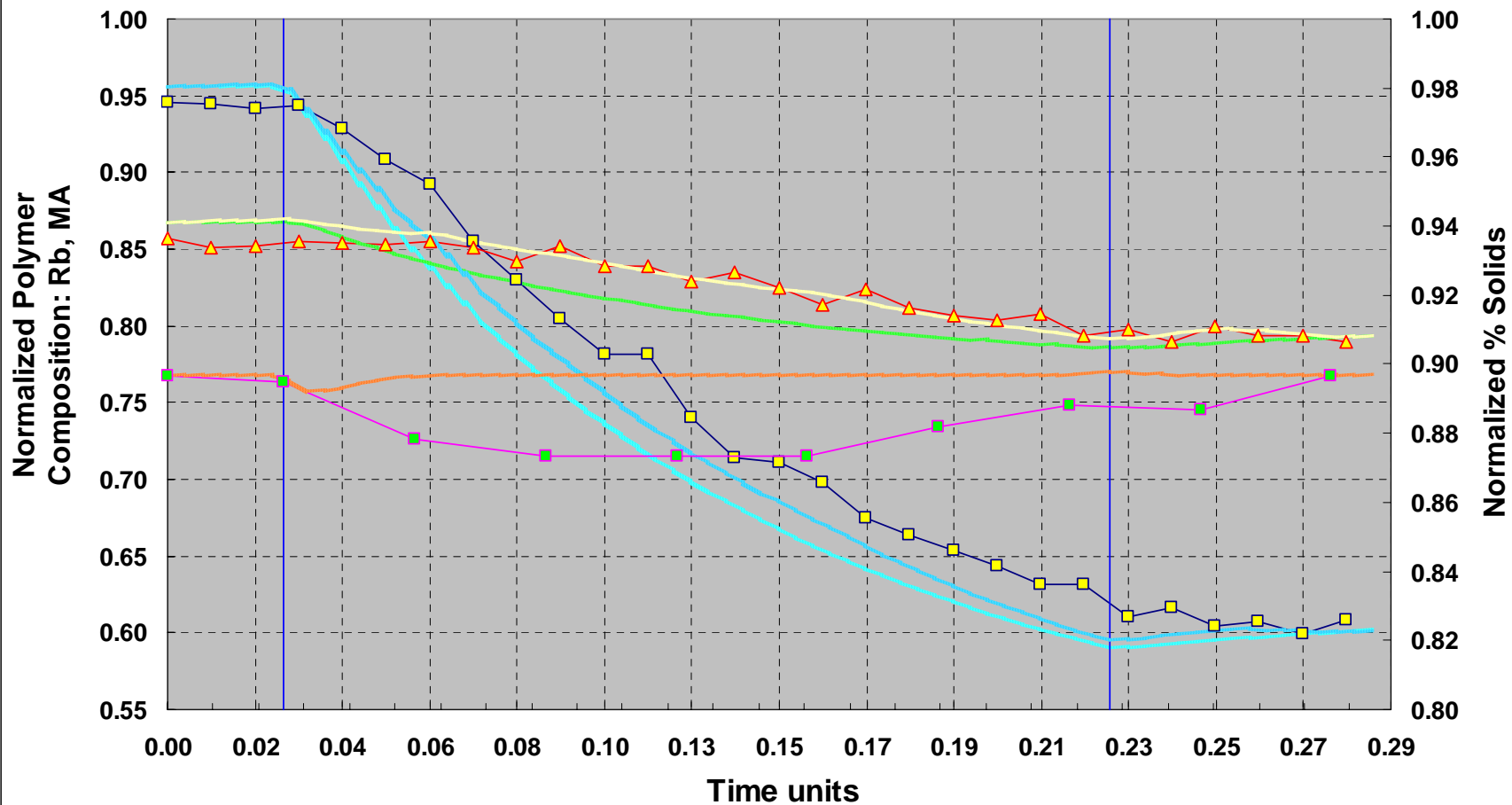
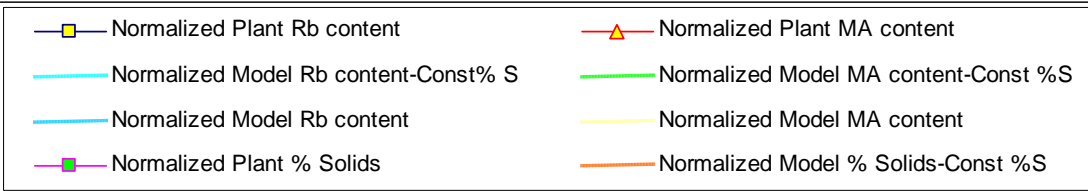
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# Plant Model Comparison



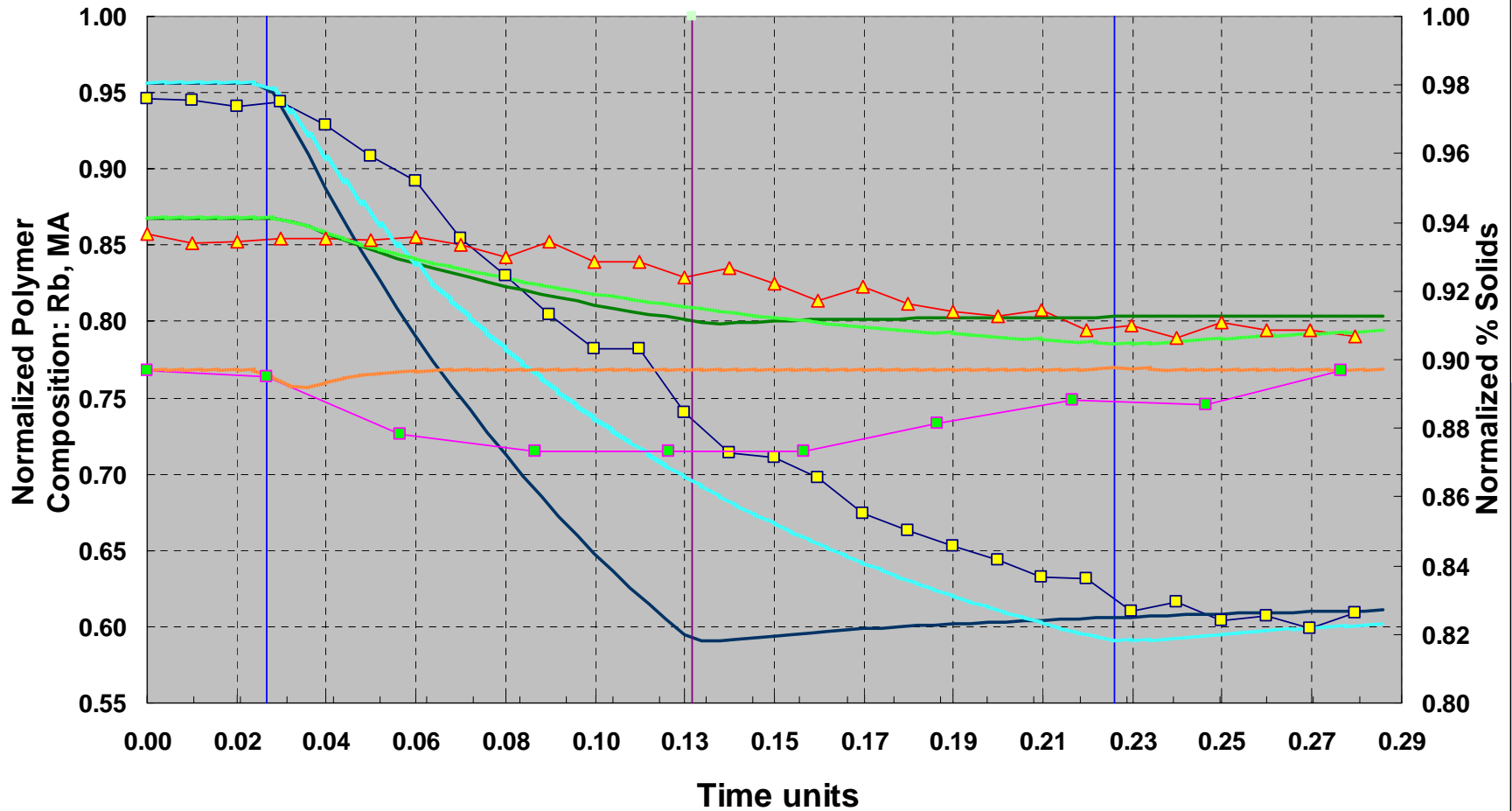
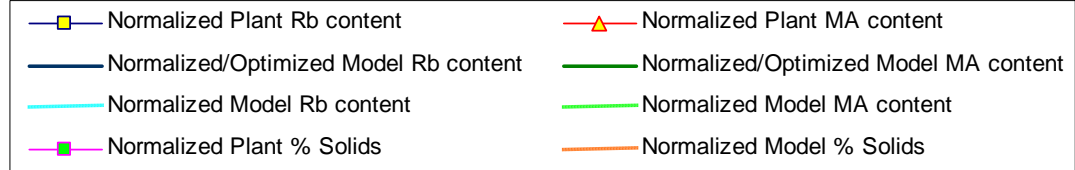
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# Plant Model Comparison (constant % solids)



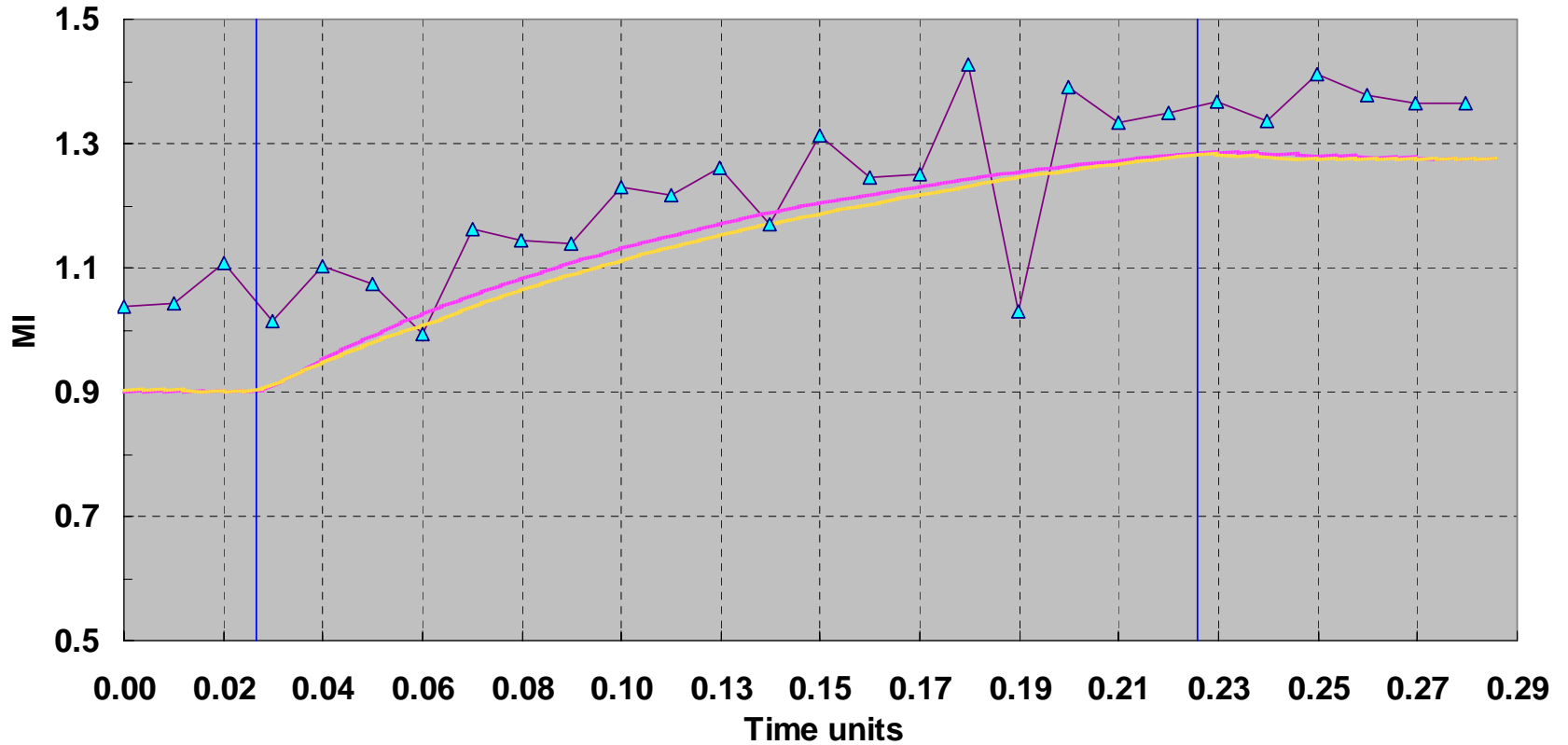
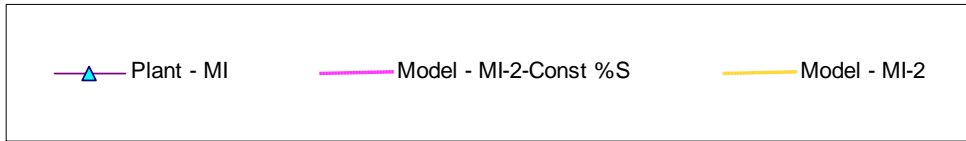
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# Plant-Model Optimization (constant % solids)



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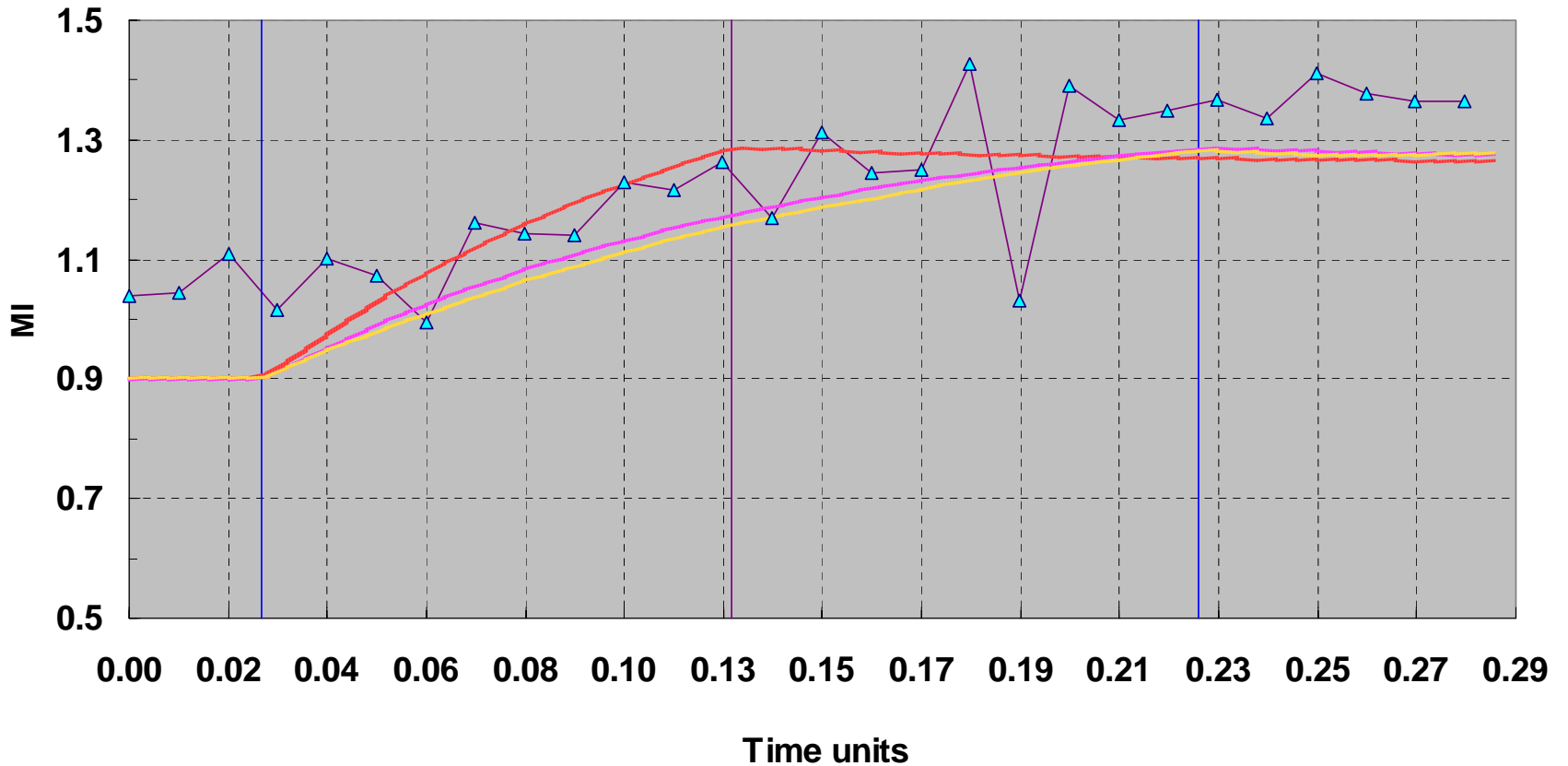
# Plant Model Comparison



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# Plant Model Optimization

—▲— Plant - MI    — Model-Mi-2-Optim    — Model - MI-2-Const %S    — Model -MI-2



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# Conclusions

- A dynamic model was successfully developed and used to estimate the kinetic constants for the free-radical polymerization scheme for the system Styrene/MA/rubber.
- Model predictions for the percentage solids in the reactor were within  $\pm 10\%$  compared to the experimental data.
- Polymer mechanical properties such as Tensile Strength, Tensile Modulus, Flexural Modulus, Heat Distortion Temperature Under Load (DTUL), and IZOD were successfully correlated and incorporated into the model.

## Conclusions (cont.)

- Polymer mechanical property correlations developed fit the experimental data within  $\pm$  5 to 10 %.
- The model was successfully validated using grade transition plant data.
- Model calculations showed that the grade transition time from polymer A to B could be cut by half, if the newly estimated reactor feed mix composition was to be used.

# Conclusions (cont.)

- Other identified model applications include:
  - Optimization of actual polymer grade recipes,
  - Development of new polymers with improved mechanical properties through the optimization of the reactor feed mix composition,
  - As a tool to investigate trends and to test the effect of various operating scenarios on the final polymer mechanical properties,
  - Use of the model as a training tool and off-line at the plant control room (with an excel interface),
  - Prediction of production line turn-down.

# Acknowledgements

- Beaver Valley analytical lab for the polymer composition analysis and the polymer molecular weights

QUESTIONS ?

COMMENTS?

