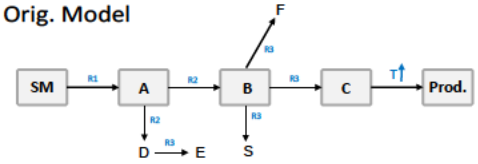
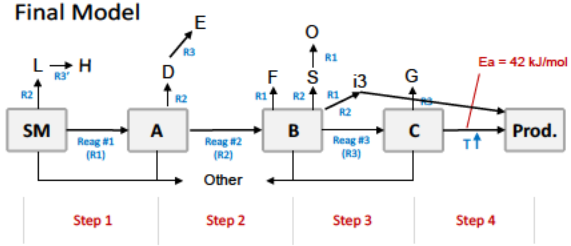
Model Generation

RES received candidate mechanism from customer and generated an improved mechanistic model.

Orig. Model

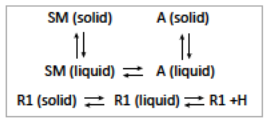


Final Model

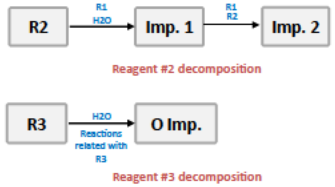


Additional Models Required:

1. Solubility Model



2. Reagent Decomposition Models

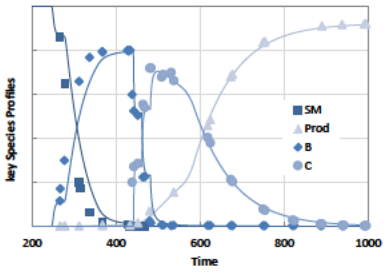


Iterative Model Evolution

Strong communication & iterative model-guided Design of Experiments, led to the generation of a well-calibrated mechanistic model.

Project Scope & Highlights	
Project Duration	~ 8 Months
Presentations Made	~ 30 (weekly)
Data Types	HPLC, NMR, IR - Raman
# Expt. Data Sets	~ 15
# Process Parameters	~ 11 (Reagents, Temp, etc.)
# Measurements	~ 12 (Prod., Impurities, etc.)

Calibration Results (Example)

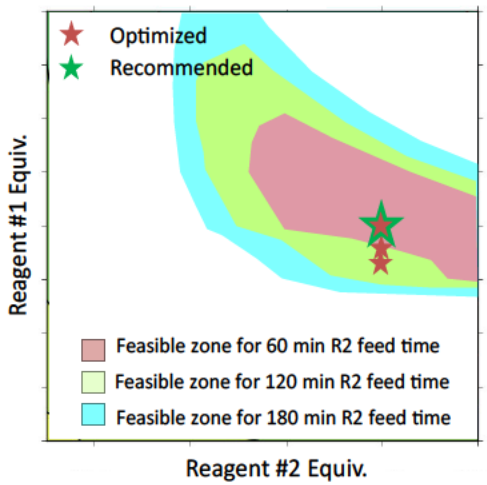


INCREASING YIELD & REDUCING COST DURING DEVELOPMENT

Process Optimization & Design Space Maps

RES simulated across many critical process parameters to both optimize the production of product while avoiding costly impurities. Uncertainty in data & model were also quantified and propagated.

Product Design Space Map



Process Parameters Studied

Reagent #1 Amount
Reagent #2 Amount
Reagent #3 Amount
Step 1 Time
Reagent #2 Feed Time
Step 2 Time
Reagent #3 Feed Time
Step 3 Time
Step 4 Temp
Step 4 Time
Solvent Volume

- Critical Process Parameter

Value Added

- RES model-guided Design of Experiments (DoE) greatly reduced the number of experiments required, saving customer resource and yielding improved mechanistic understanding of product and impurity formation.
- RES provided optimal conditions across many critical process parameters to maximize product and minimize impurities (primary project goal).
- RES generated Design Space Maps, detailing how each process parameter affects product/impurity profiles. This is not only essential for future process development and scale-up, but was also submitted to FDA fulfilling the Quality by Design (QbD) mandate.

RES Group
www.resgroupinc.com