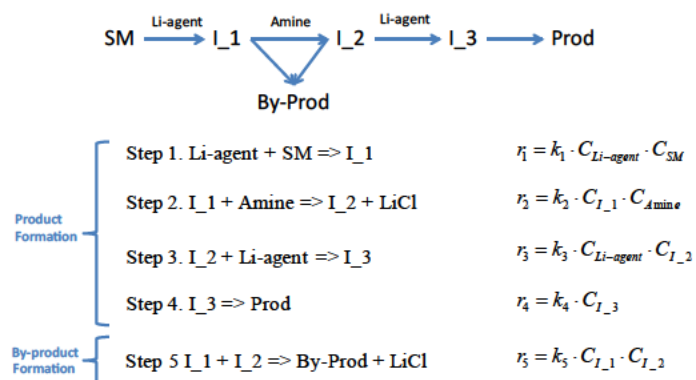


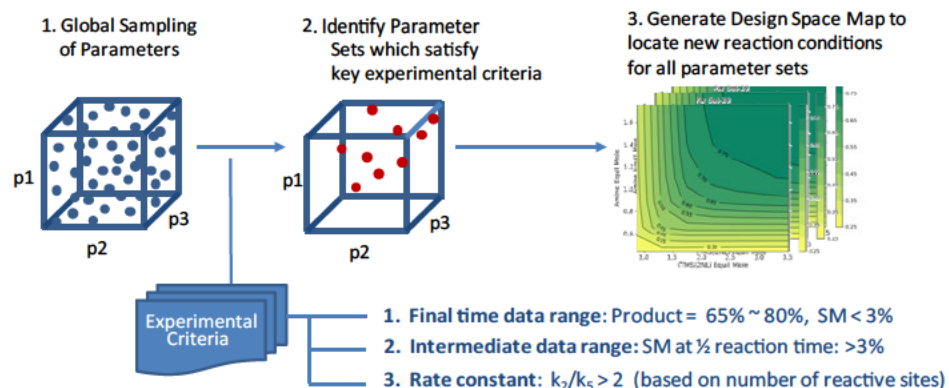
Model Generation

RES received candidate mechanism from customer and constructed a mass action model. Only one data point was provided so little information was available for model calibration.



Parameter Uncertainty & Calibration

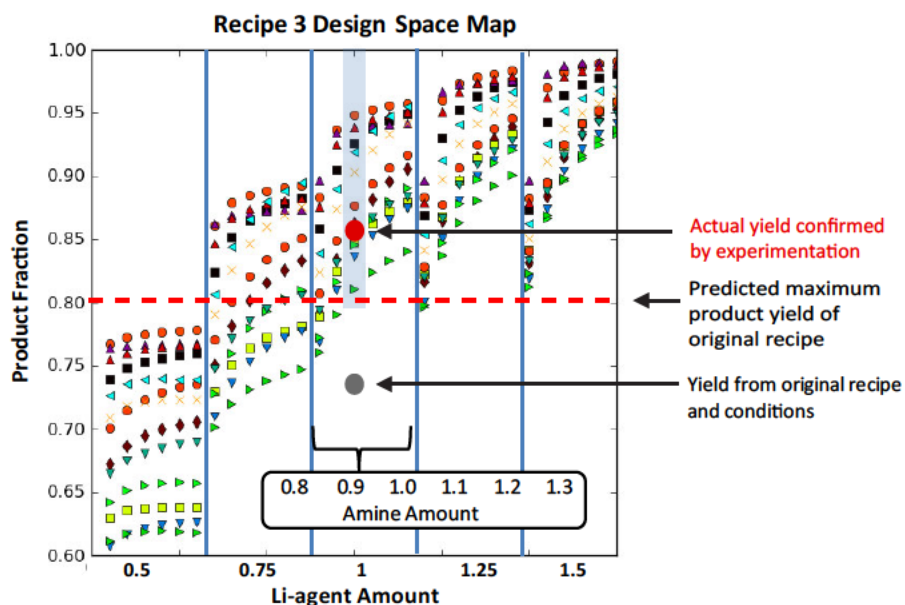
RES sampled many potential parameter sets and identified those that met experimental criteria (38/10,000). Each qualifying parameter set was simulated over all conditions to assess maximum product yield.



GO/NO-GO DECISIONS DURING CANDIDATE ROUTE SELECTION

New Reagent Order of Addition Proposed

With current order of addition, simulation showed that maximum product yield was 80% across all parameter sets. RES identified alternative recipes which predicted a significant increase in product yield (between 81% - 95%).



Value Added

- RES identified the original order of reagent addition could only achieve a maximum of 80% yield, regardless of reagent amount, avoiding further costly experimentation.
- RES proposed new recipes and operating conditions, achieving 85% yield (original recipe yielded 73%).
- Demonstrated that valuable insight can be obtained in early phase process design with only sparse data available using global sensitivity analysis and model calibration.
- RES helped the customer maximize product yield through model-guided experimental design in early phase process development, saving significant time, energy, and money.