

Rapid Construction of Validated Chemistry Models for Advanced Biofuels



Goals

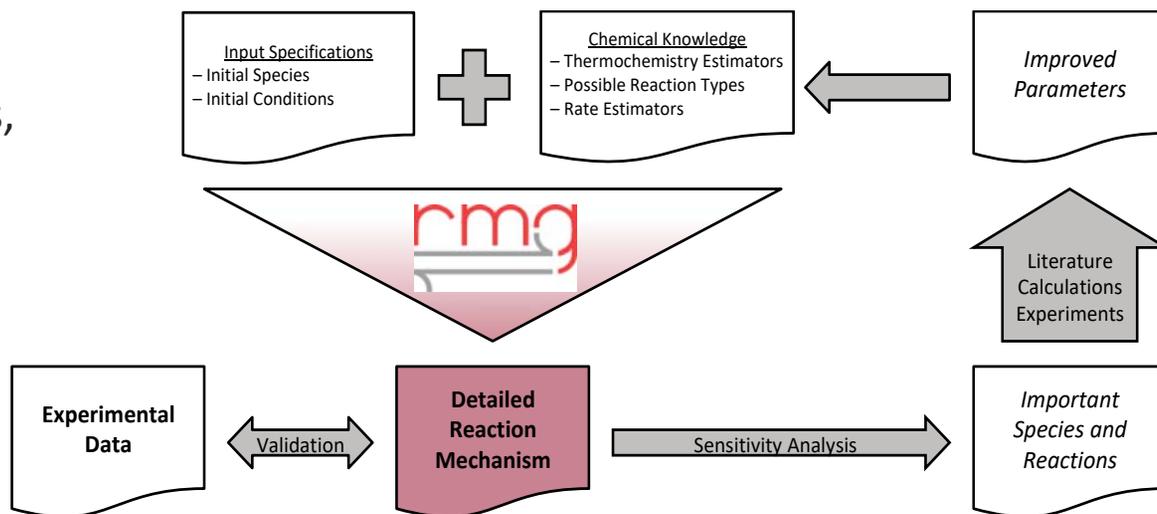
Construct models for several fuels, refine parameters with quantum chemistry, validate models with advanced laser shock tube experiments.

Approach

Dramatically accelerate the pace of fuel innovation using modern predictive chemistry computer techniques and efficient model construction-refinement-validation workflow.

Potential Impact on Co-Optima Goals

Fast evaluation of proposed fuel/engine combinations, also useful in engine simulation.



Team Members

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