Numerical Modeling of n-Hexane Pyrolysis

Given: Plasma Gas Temperature & Flow Rate
Goal: Maximize Conversion of n-Hexane and Selectivity of C_2H_4
Find: Flow Rate of n-Hexane

Development of Chemical Kinetic Model

Goal: Development a lightweight chemical kinetic model suitable for CFD analysis
Tool: RMG

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0-D Simulation

Goal: [1] Validate the chemical kinetic model
[2] Identify suitable reaction temperature and time ranges
Tool: Chemkin-Pro

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1-D Simulation

Goal: Analyze axial profiles of temperature and species concentrations under varying feed flow rates
Tool: Chemkin-Pro

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CFD Simulation

Goal: Quantify the influence of mixing and heat transfer
Tool: Fluent