Reaction model development and optimization for 1,3,5-trimethylbenzene – an important aromatic for kerosene surrogates

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Motivation

- Chemical kinetics modeling of surrogates for Jet A-1 and sustainable aviation fuels (SAF) required for the numerical design of modern jet turbine devices
- To model soot formation in jet fuels, it is important to investigate the aromatics in the fuel surrogate [1]
- 1,3,5-trimethylbenzene (1,3,5-TMB) was identified as a suitable aromatic compound in jet fuel surrogates [2]

Objective:

- Add a compact 1,3,5-TMB sub-model to a comprehensive semi-detailed inhouse reaction mechanism
- Validate model – targets: heat release and ignition

Chemical Kinetic Modeling

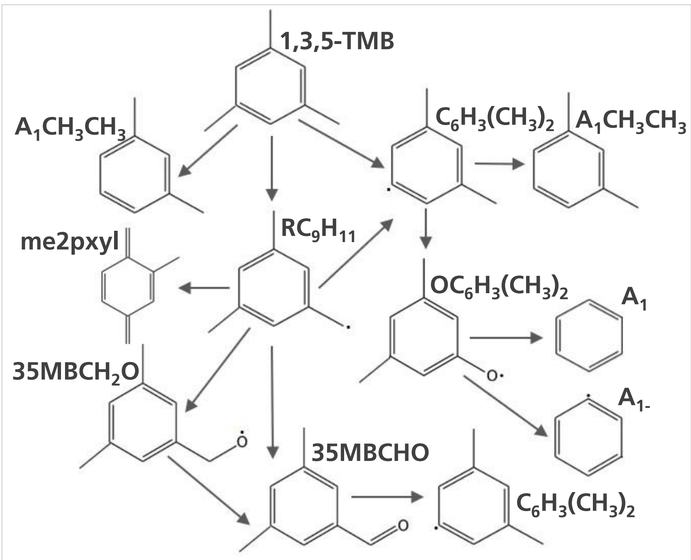
Initial model – ESTiMatE-Mech

- Build on a compact, semi-detailed in-house model [1]
- Sub model for 1,3,5-TMB proposed based on:
  - Well-known chemical kinetic mechanism of similar molecules like toluene and m-xylene (rates, paths)
  - Reactions paths adapted from literature [3, 4]

Optimized model – ESTiMatE-Mech_opt.

- Linear transformation model (linTM) [5, 6] used to generate optimized version of ESTiMatE-Mech considering:
  - Targets for optimization: laminar flame speeds and ignition delay times of 1,3,5-TMB
  - 8 sensitive reactions identified for optimization: Include 1,3,5-TMB or its decomposition product R_9H_{11}

Simplified scheme of the 1,3,5-TMB sub model

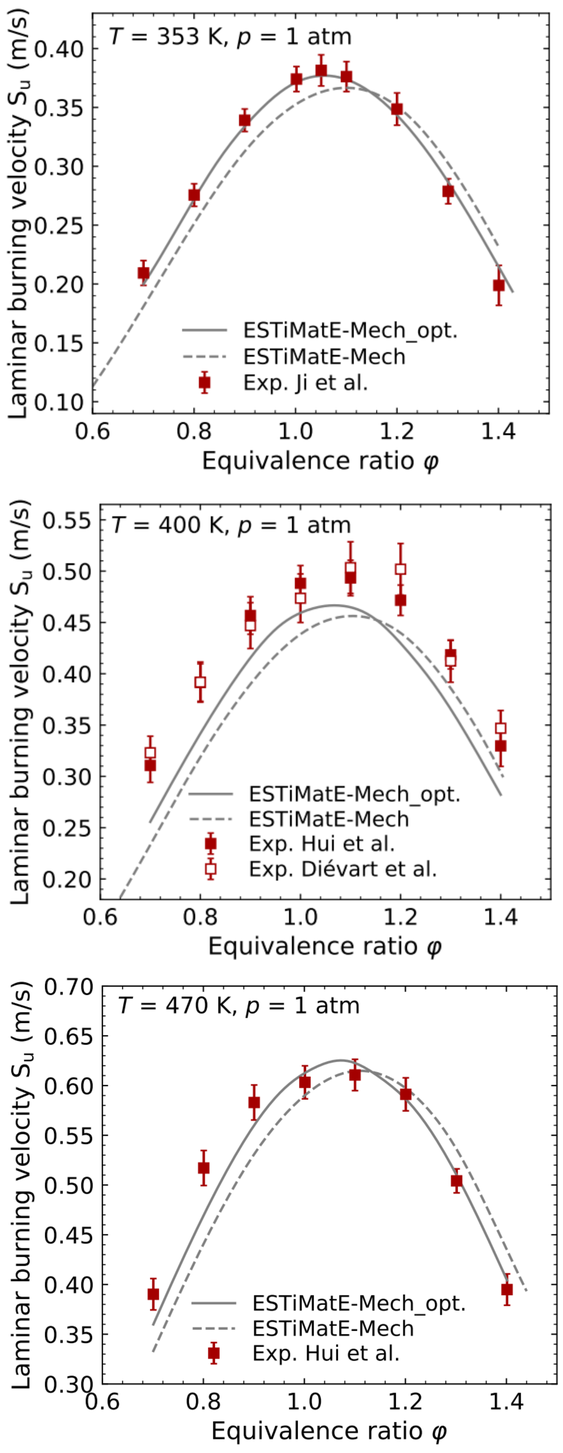


Optimized reactions

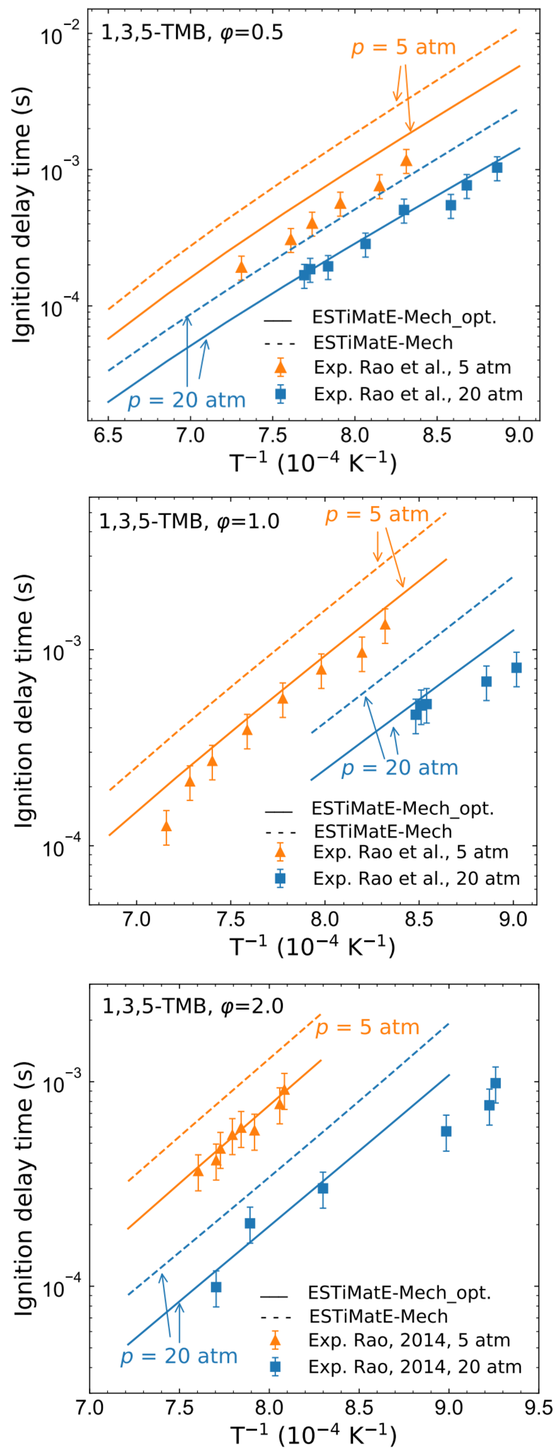
$$1,3,5\text{-TMB} \rightleftharpoons RC_9H_{11} + H$$
$$1,3,5\text{-TMB} + OH \rightleftharpoons RC_9H_{11} + H_2O$$
$$1,3,5\text{-TMB} + O_2 \rightleftharpoons RC_9H_{11} + HO_2$$
$$1,3,5\text{-TMB} + H \rightleftharpoons A_1CH_3CH_3 + CH_3$$
$$RC_9H_{11} + O \rightleftharpoons C_6H_3(CH3)_2 + CH_2O$$
$$RC_9H_{11} + HO_2 \rightleftharpoons 35MBCH_2O + OH$$
$$RC_9H_{11} \rightarrow H + me2pxyln$$
$$RC_9H_{11} + HO_2 \rightarrow OH + CH_2O + C_2H_4 + A_{1-}$$

Results – Comparison between Simulation and Measurements

- **Laminar flame speed**



- **Ignition delay times**



Conclusions and Outlook

- **Laminar burning velocities** are predicted correctly by **ESTiMatE-Mech_opt**. at ambient pressure, several preheat temperatures and φ. It Improves further the good prediction by **ESTiMatE-Mech**
- **Ignition delay times** at high pressures and temperatures are accurately calculated with **ESTiMatE_Mech_opt**. The deviations found with **ESTiMatE-Mech** are corrected
- **Future efforts** will focus on the modeling of aromatics as major soot precursors by including species concentration profiles of 1,3,5-TMB flames

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