A comprehensively validated compact mechanism for dimethyl ether oxidation: an experimental and computational study

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Motivation

- DME – promising alternative fuel.
- Reduced soot, improved flame stability.

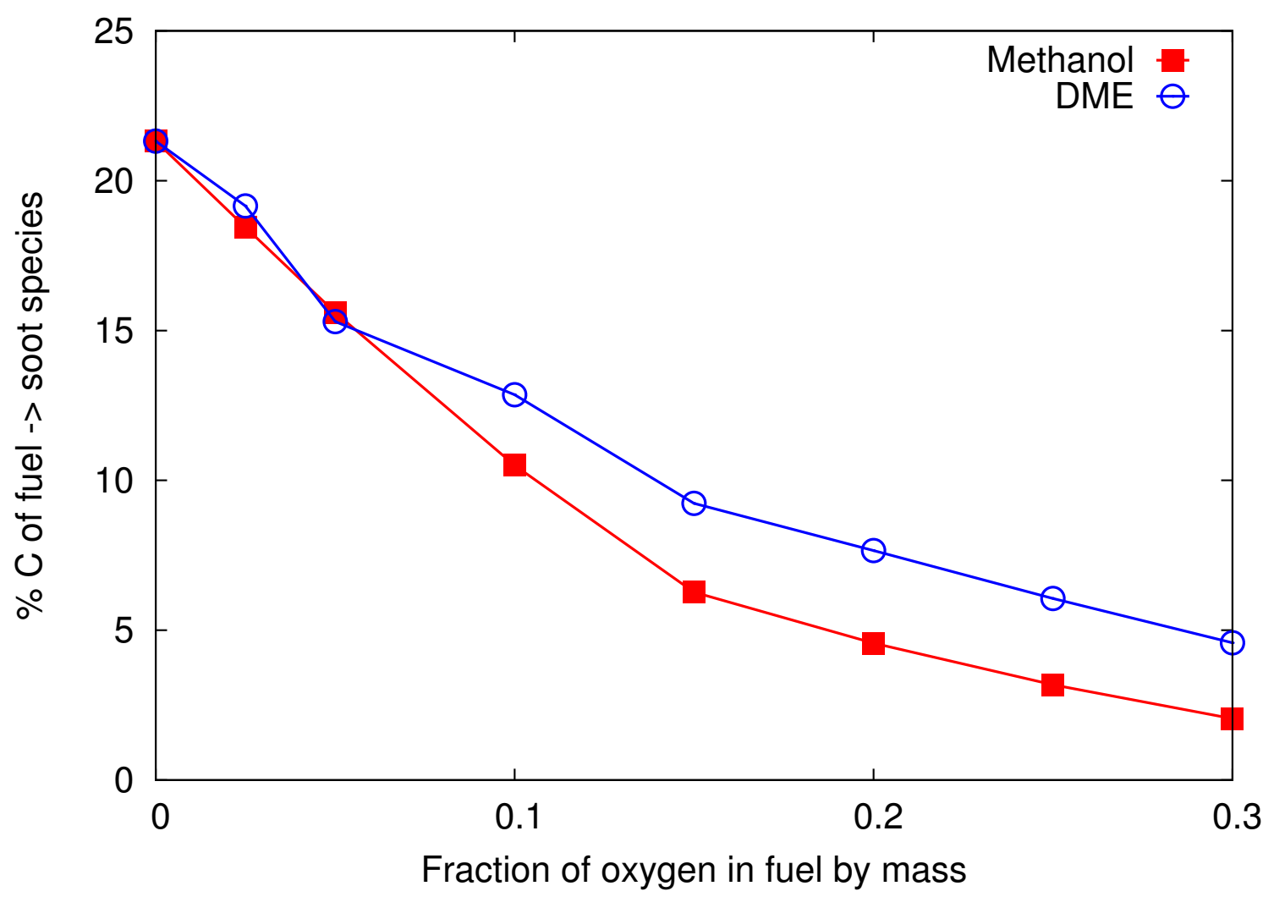


Figure 1: Soot reduction with diesel/DME blend [1].

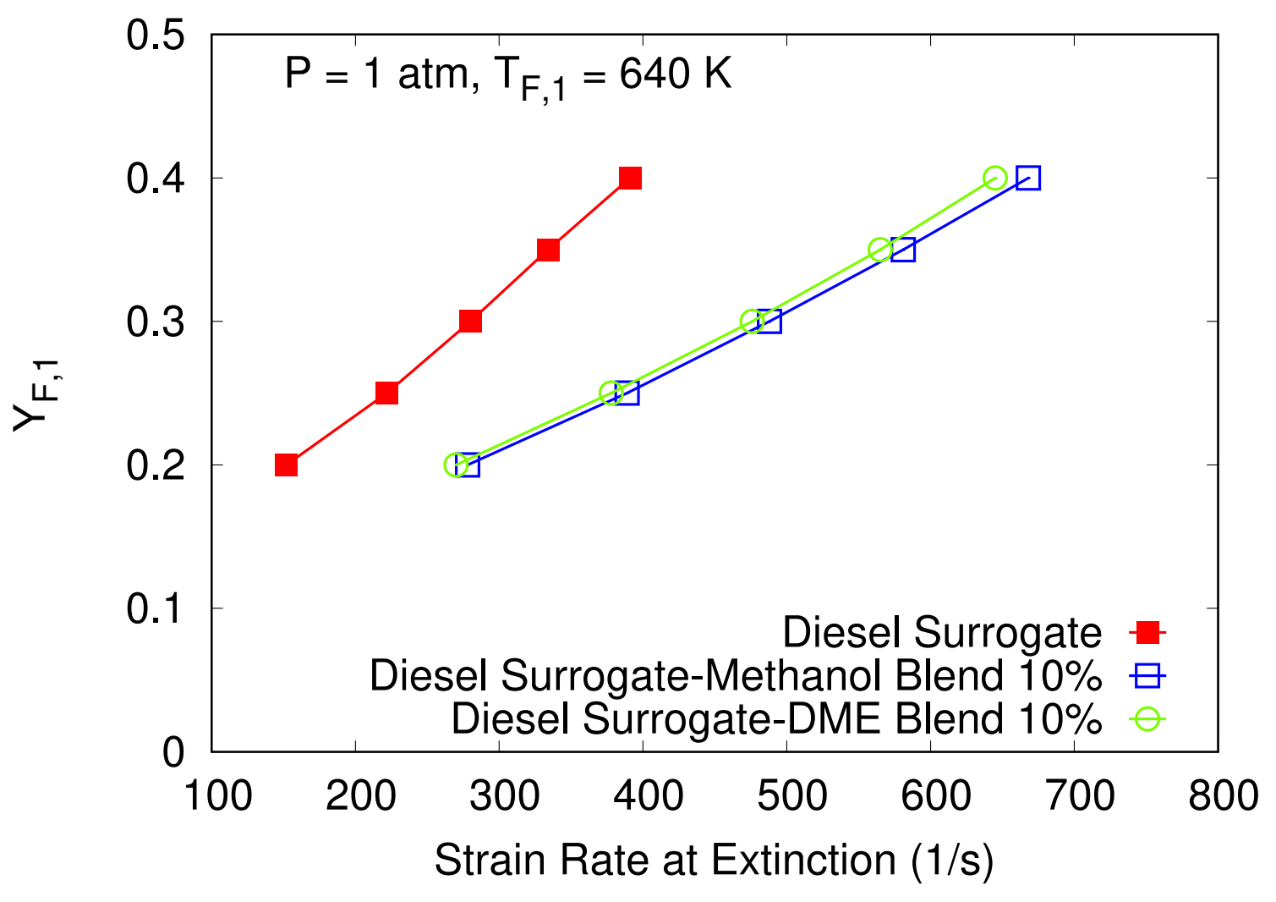


Figure 2: Increased resistance to extinction using diesel/DME blends [2].

Objectives

- Develop a short mechanism for DME oxidation that is as compact as possible, still containing the essential kinetics.
- Validated the proposed mechanism comprehensively and thus establish its ability to accurately predict a wide range of configurations of practical relevance to combustion.
- Obtain extinction strain rates of DME-air mixtures in a laminar 1D counter-flow non-premixed flame to provide an additional data set for model validation.

Counter-flow Burner Experiments

- Experiments are conducted at atmospheric pressure and temperature.
- Flame is established by controlling the flowrate of DME through fuel duct and stabilized by switching on the exhaust system.
- Flat flame is established by allowing air through the oxidizer duct.
- Curtain nitrogen flow is switched on to minimize the ambient interference.
- Fuel is gradually diluted with nitrogen (in a mixing chamber) until flame extinguishes.

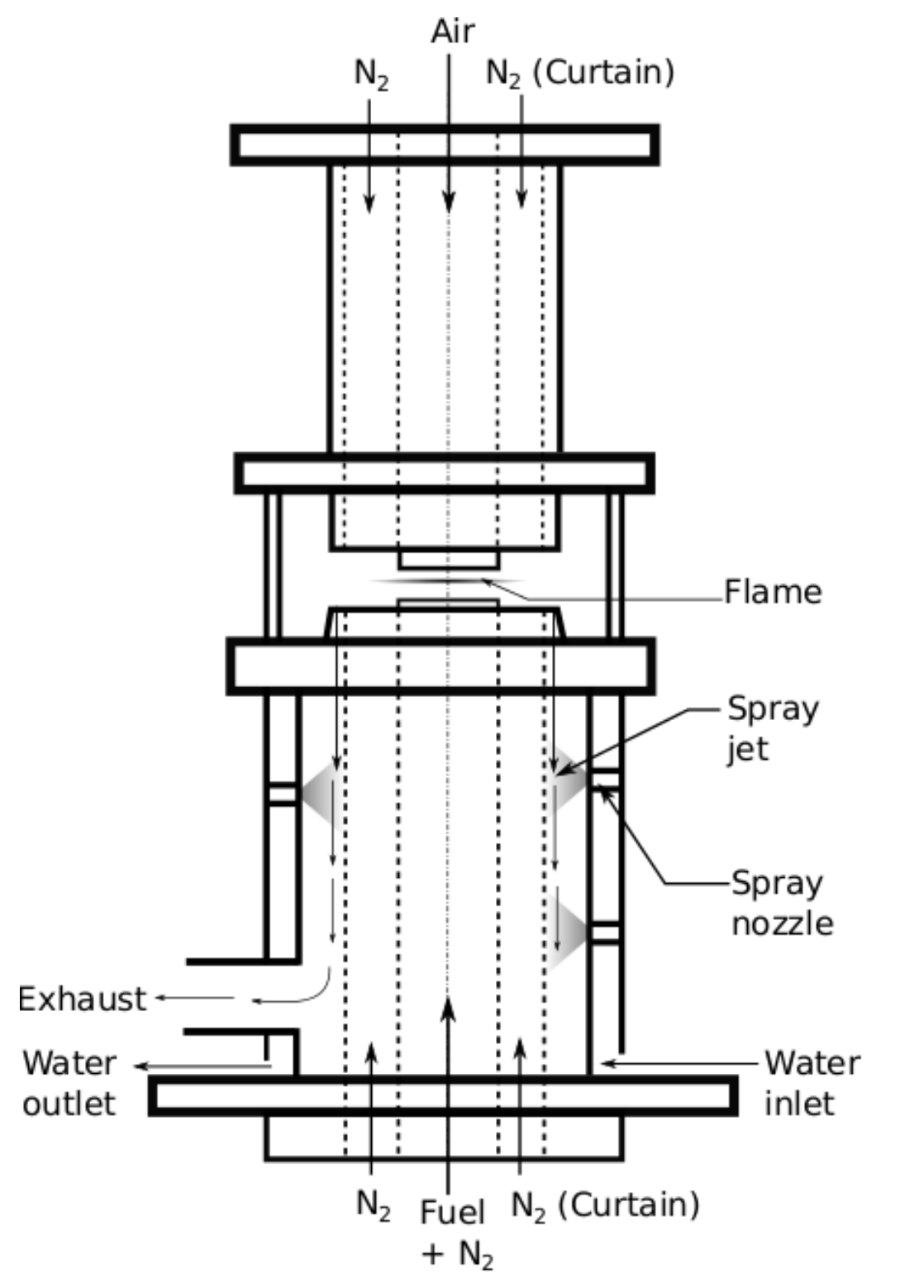
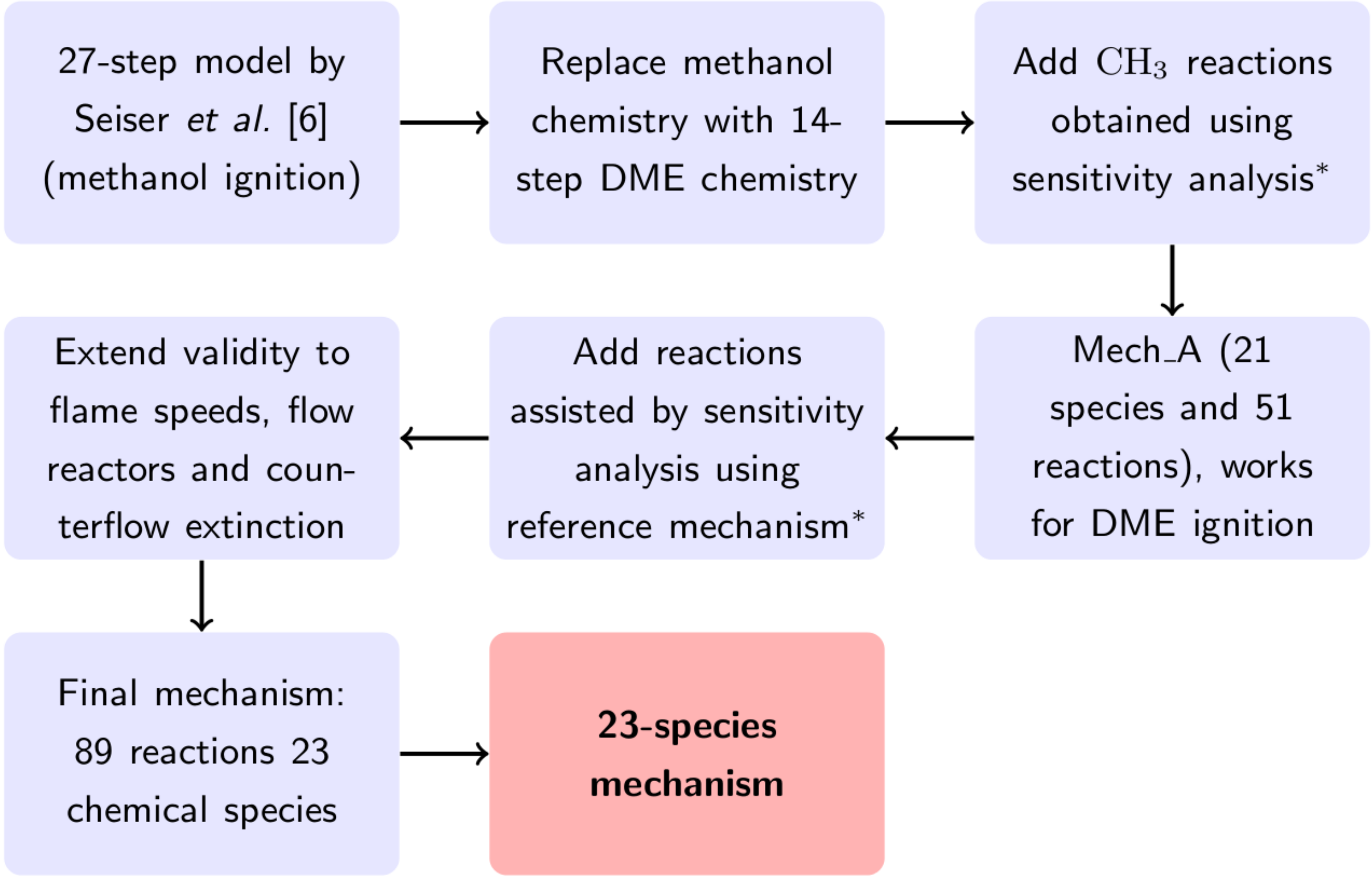


Figure 3: Schematic of the counter-flow burner setup.

- Extinction phenomenon is observed through visual inspection.
- Flowrates of DME, dilutant nitrogen, and air at extinction are recorded.
- Strain rate at extinction is plotted as a function of the mass fraction of fuel.

Development of Compact Mechanism

- A bottom-up approach is adopted to develop the short compact mechanism based on the work of Tarrazo *et al.* [3]; San Diego mechanism [4,5] used as reference mechanism.



27-step model by Seiser *et al.* [6] (methanol ignition)

Replace methanol chemistry with 14-step DME chemistry

Add CH_3 reactions obtained using sensitivity analysis*

Mech_A (21 species and 51 reactions), works for DME ignition

Add reactions assisted by sensitivity analysis using reference mechanism*

Extend validity to flame speeds, flow reactors and counterflow extinction

Final mechanism: 89 reactions 23 chemical species

23-species mechanism

- Smallest among the reduced mechanisms proposed for DME oxidation consisting predominantly of elementary reactions without tuning any of the rate parameters.

* **List of important reactions and species are listed on the right top box.**

Kinetics Important for Different Configurations

1. *Ignition Delay* : $CH_3 + CH_3 \rightleftharpoons C_2H_6 + M$ is the most important reaction to predict the high temperature ignition delays.
2. *Flame Speeds* : Sensitivity analysis results reveal the importance of reactions involving CH_3 and **HCO** to predict flame speeds accurately.
3. *Species Profiles* : Ensuring complete consumption pathways for intermediate species, such as HO_2 and CH_4, was found important to match CO profiles at high temperatures in flow reactors. Addition of reaction $HO_2CH_2OCHO \rightarrow CH_2O + CO + 2\ OH$ significantly improved the low temperature species profiles.
4. *Counterflow Non-premixed Extinction* : Sensitivity analysis towards peak temperatures reveal the importance of C_2H_4, C_2H_5, and C_2H_6 species. Significant improvement in the extinction results is obtained with addition of elementary steps involving these species.

Validation of the 23 Species Mechanism

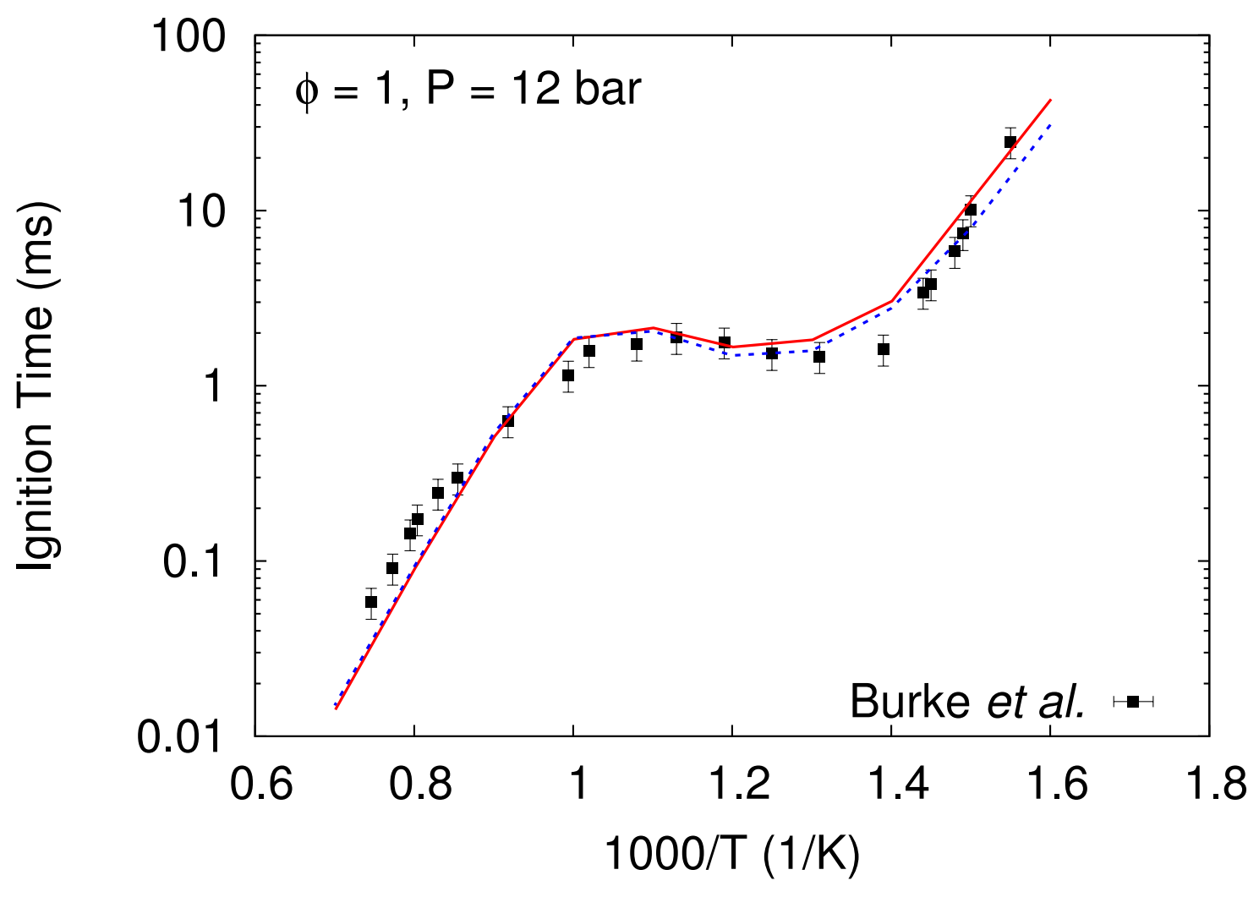


Figure 4: Ignition Delay

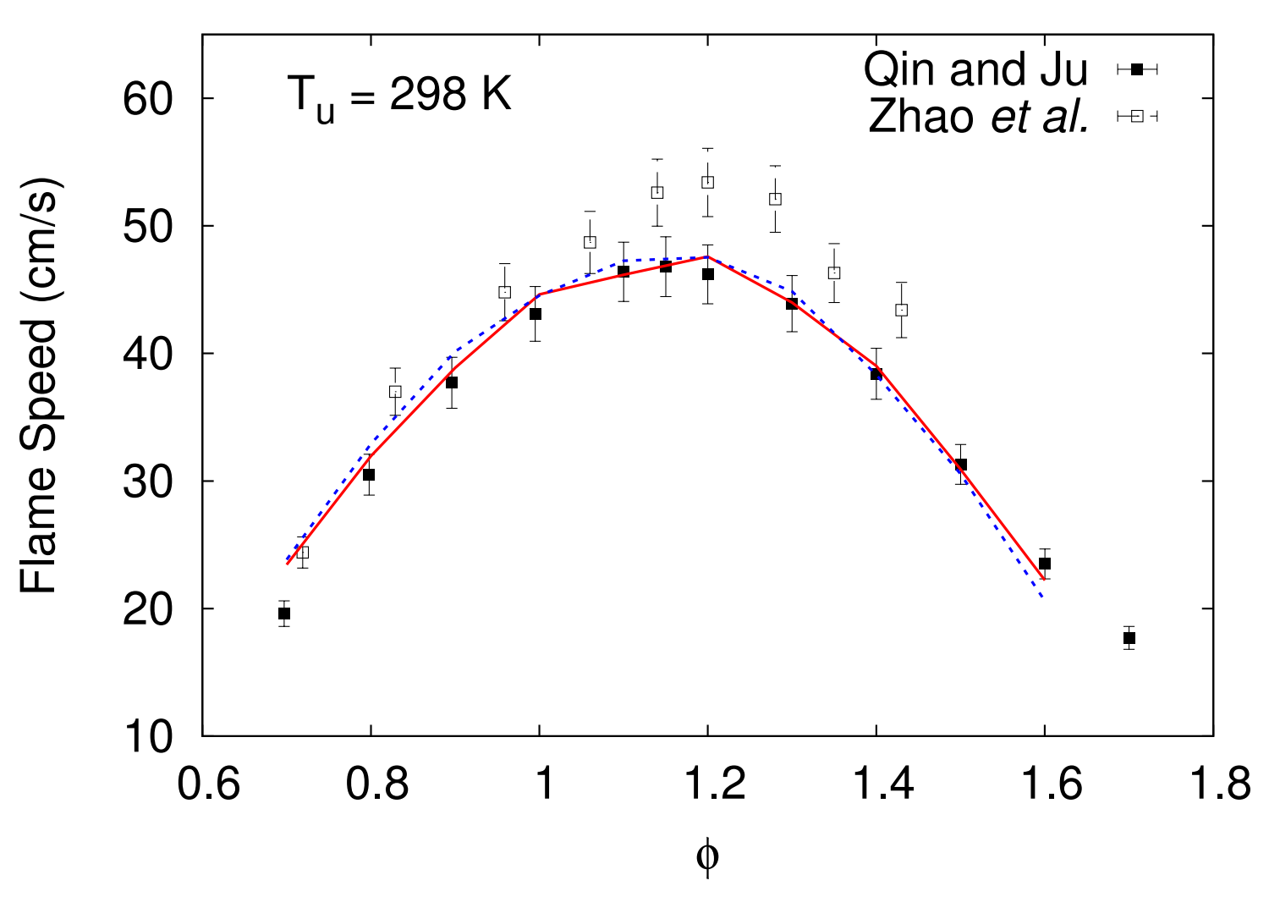


Figure 5: Laminar Burning Velocity

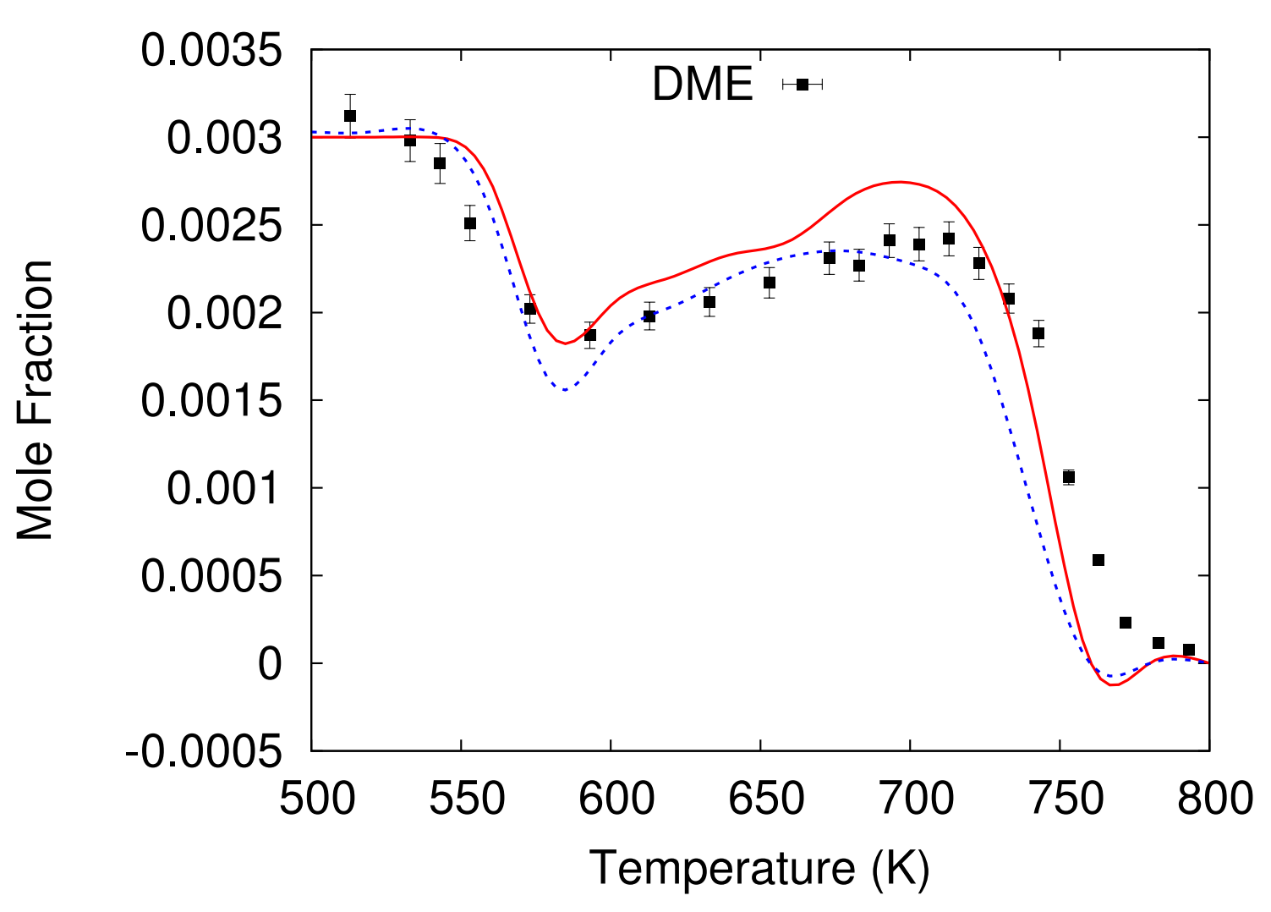


Figure 6: Flow Reactor Species Profile

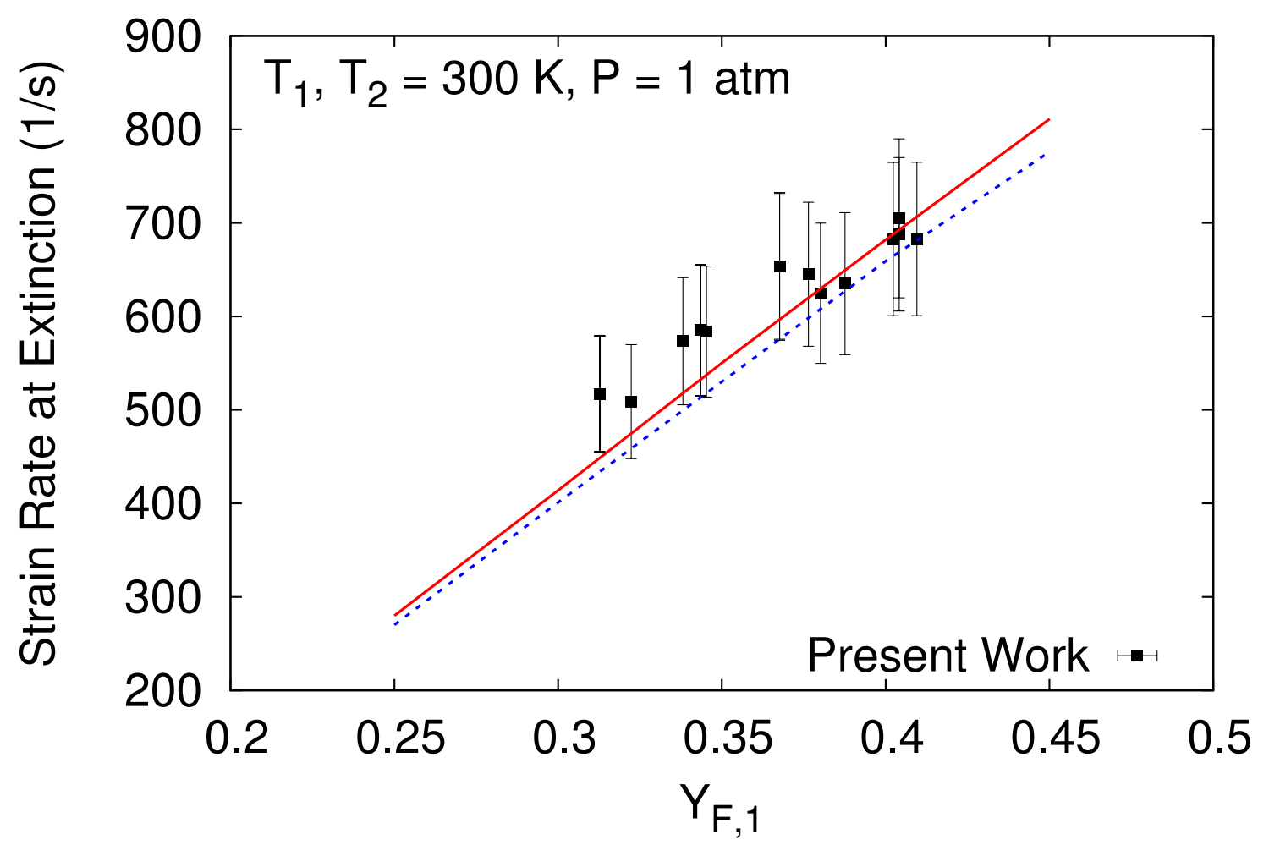


Figure 7: Counter-flow Non-premixed Extinction

Symbols: experimental data; Lines: reference mechanism (solid red lines), 23 species mechanism (dotted blue lines).

Quasi-Steady State Assumption

- A 14-step reduced mechanism is obtained by introducing quasi-steady state assumption for six intermediate species.
- A reduction code has been developed which gives the 14 global steps along with its rate expressions in terms of individual rates.
- The code is made available online at `https://bitbucket.org/ccube_iitm/qss_reduction`.
- The 14-step mechanism has also been comprehensively validated against available experimental data and shows similar level of agreement as the 23-species mechanism.

Conclusions

- Experimental data for extinction strain rates of DME-air mixtures have been obtained for the first time in an opposed flame set up, which serves as a fundamental data set for reaction mechanism validation in non-premixed environments.
- A compact 23-species mechanism for DME oxidation as well as 14-step reduced mechanism have been developed and validated comprehensively against experimental data in homogeneous and heterogeneous systems.
- The comprehensive validation and compact size of the kinetic model makes it suitable to be used in CFD calculations.

References

(1) Khare *et al.* SEEC (2017).
(2) Khare *et al.* 10th U.S. Combustion Meeting (2017).
(3) Tarrazo *et al.* Combust. Theor. Model. 20 (2016).
(4) `web.eng.ucsd.edu/mae/groups/combustion/mechanism.html`.
(5) J.C. Prince, F.A. Williams, Combust. Flame 162 (2015).
(6) R. Seiser *et al.* Combust. Flame 158 (2011).

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