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

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Supplementary Material

Contents

1 Validation Results for Constant Pressure Flow Reactors

The 23 species mechanism is validated against flow reactor data from Curran *et al.* [1] which is modeled as a homogeneous adiabatic reactor at constant pressure.

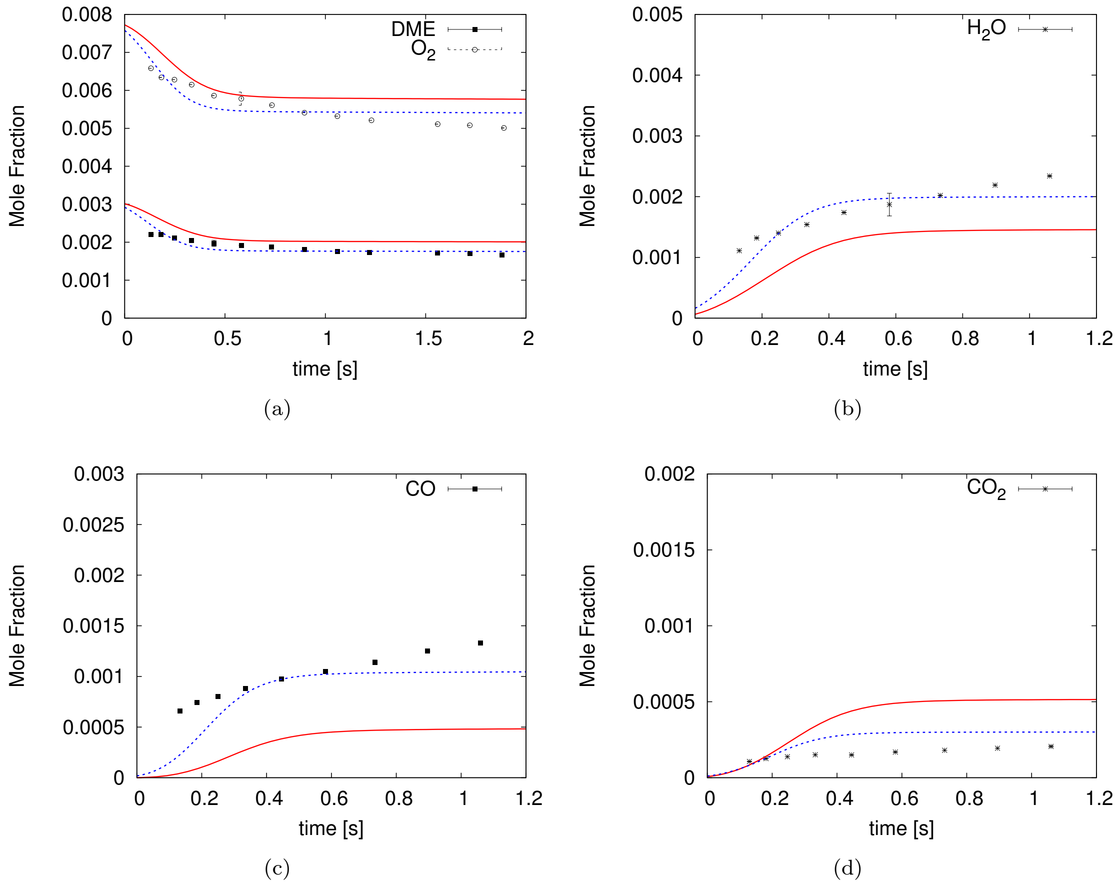


Figure S1: Major species profiles in a constant pressure flow reactor. $\phi = 1.18$, 3080 ppm DME, P = 12.5 atm, T = 593 K. Symbols – experimental data from Curran *et al.* [1]; lines – simulations: reference mechanism (solid lines), 23 species mechanism (dashed lines).

Uncertainties in Flow Reactor Residence Time

The uncertainties in the residence time should be taken into consideration for modeling an adiabatic, constant pressure flow reactor [2]. To illustrate this point, species profiles for CO at different residence times are plotted using the 23 species model in Fig. S2. For all the three residence times considered, no change is observed upto a temperature of 700 K, whereas, significant differences in the species profiles at higher temperatures (700–800 K) is noticed.

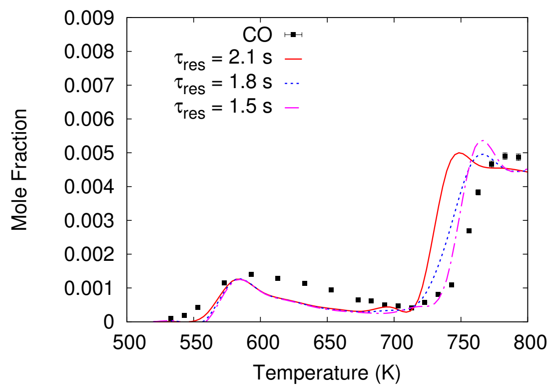
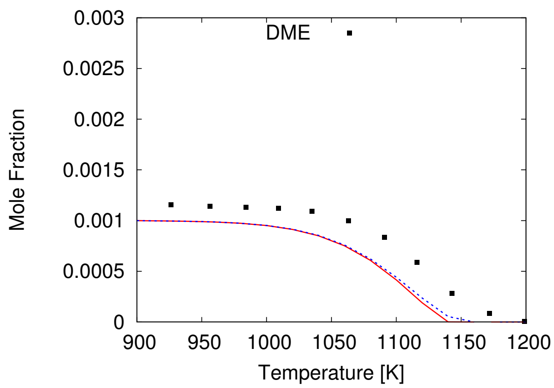


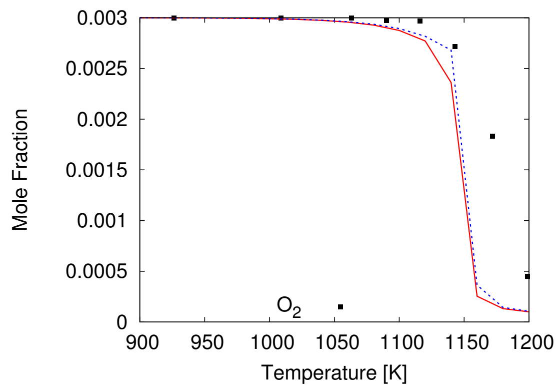
Figure S2: Predicted profiles for CO in a flow reactor using the 23 species model for different residence times. Experimental conditions: $\phi = 1.19$, 0.3% DME in N_2 at 12.5 atm. Symbols – experiments: Curran *et al.* [1]; lines – simulations: $\tau_{res} = 2.1$ (solid lines), $\tau_{res} = 1.8$ (dashed lines), $\tau_{res} = 1.5$ (dashed-dotted lines).

2 Validation Results for Jet-Stirred Reactors

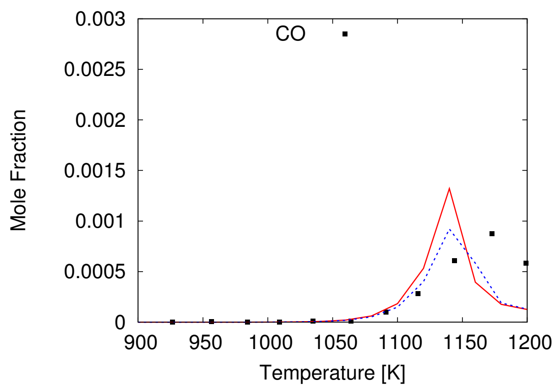
The 23 species mechanism is validated against jet-stirred reactor data from Dagaut *et al.* [3], Moshammer *et al.* [4] and Rodriguez *et al.* [5]. The JSRs are modeled as homogeneous, isothermal reactor at constant pressure.



(a)



(b)



(c)

Figure S3: Major species profiles in a jet-stirred reactor. ϕ = 1.0, 0.1% DME, P = 1.0 atm, τ = 0.1 s. Symbols – experimental data from Dagaut *et al.* [3]; lines – simulations: reference mechanism (solid lines), 23 species mechanism (dashed lines).

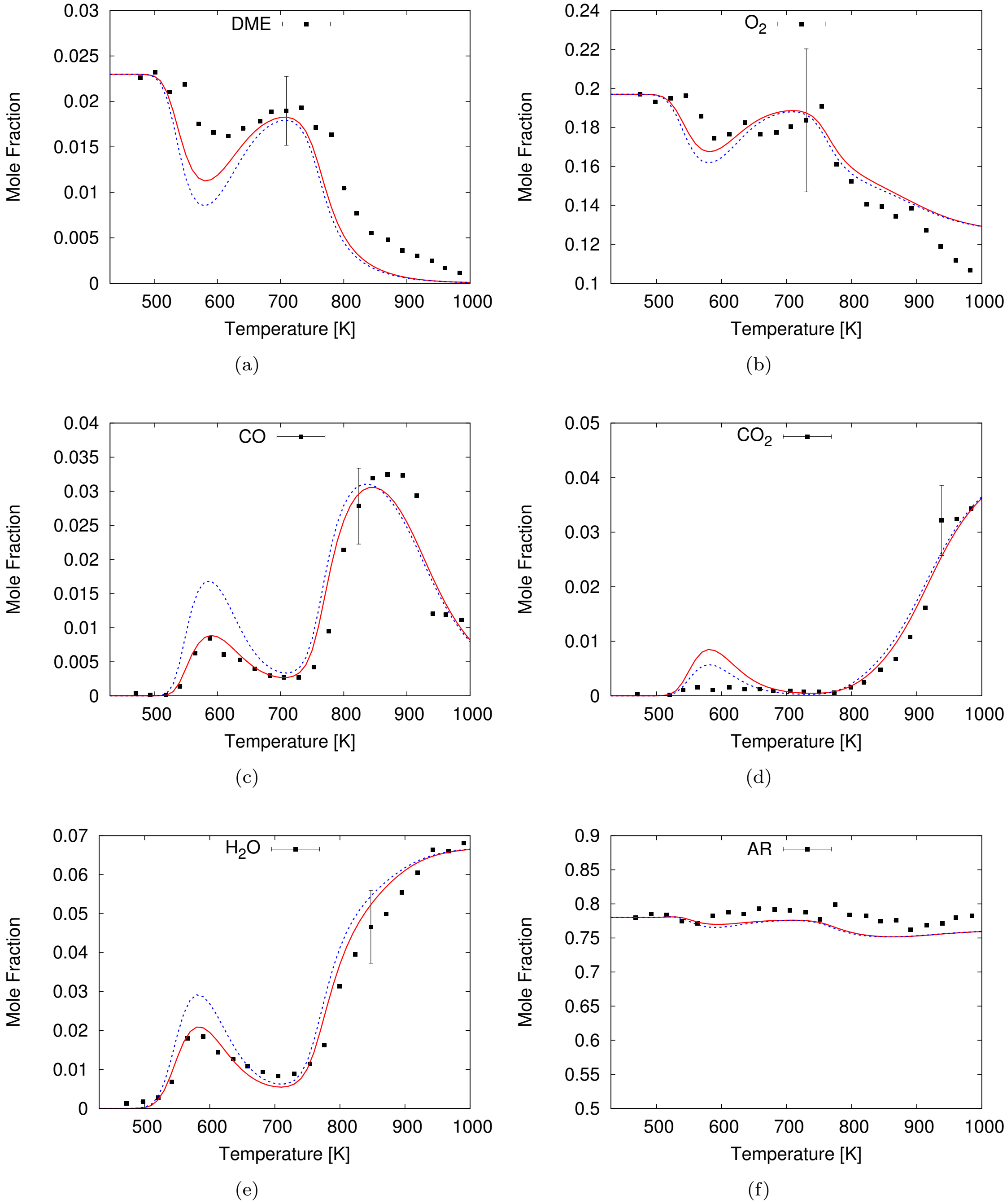


Figure S4: Major species profiles in a jet-stirred reactor. $\phi = 0.35$, 78% AR, P = 933 mbar, $\tau = 4$ s. Symbols – experimental data from Moshammer *et al.* [4] with representative error bars; lines – simulations: reference mechanism (solid lines), 23 species mechanism (dashed lines).

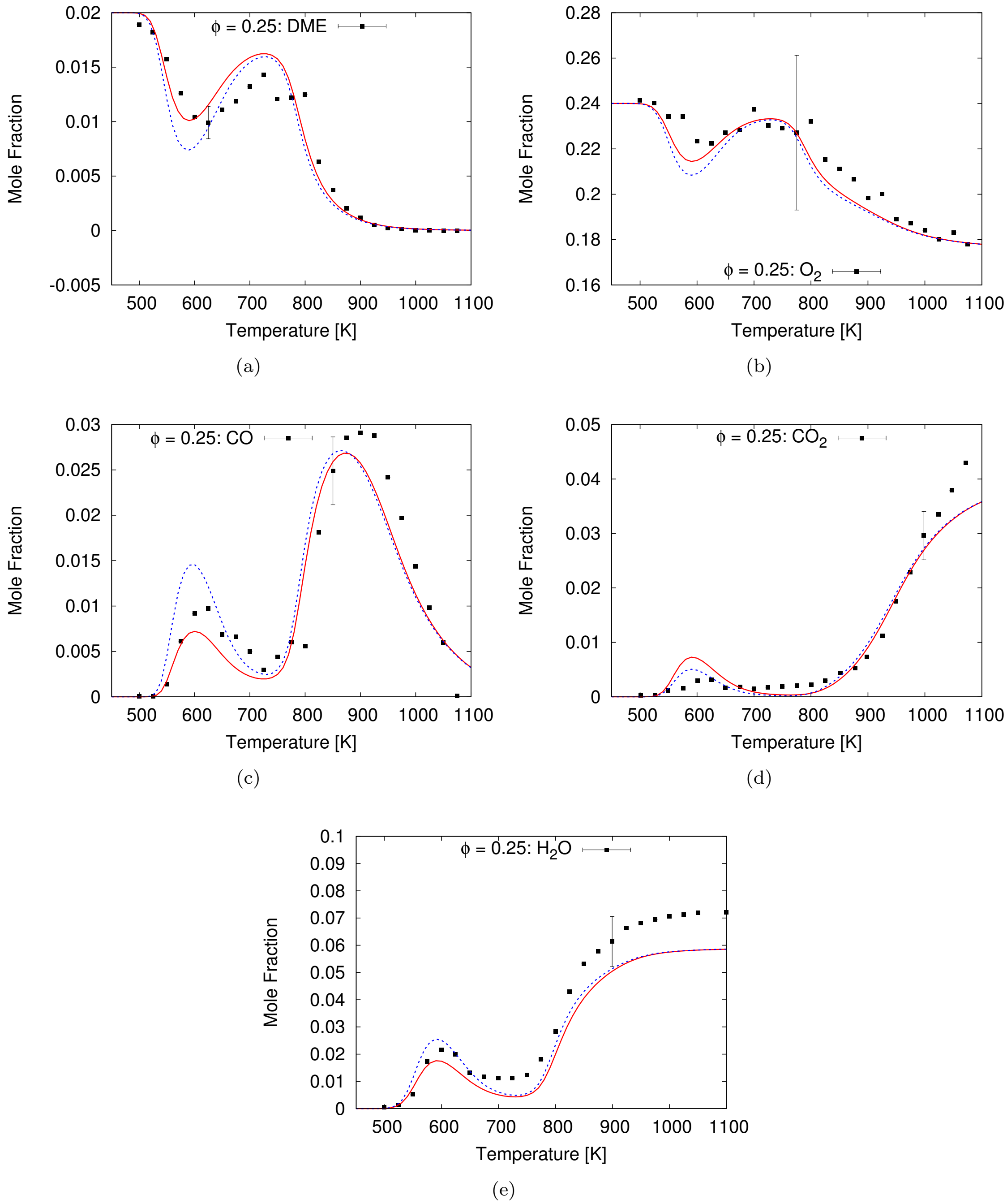


Figure S5: Major species profiles in a jet-stirred reactor. $\phi = 0.25$, $X_{dme} = 0.02$, P = 106.7 kPa, $\tau = 2$ s. Symbols – experimental data from Rodriguez *et al.* [5] with representative error bars; lines – simulations: reference mechanism (solid lines), 23 species mechanism (dashed lines).

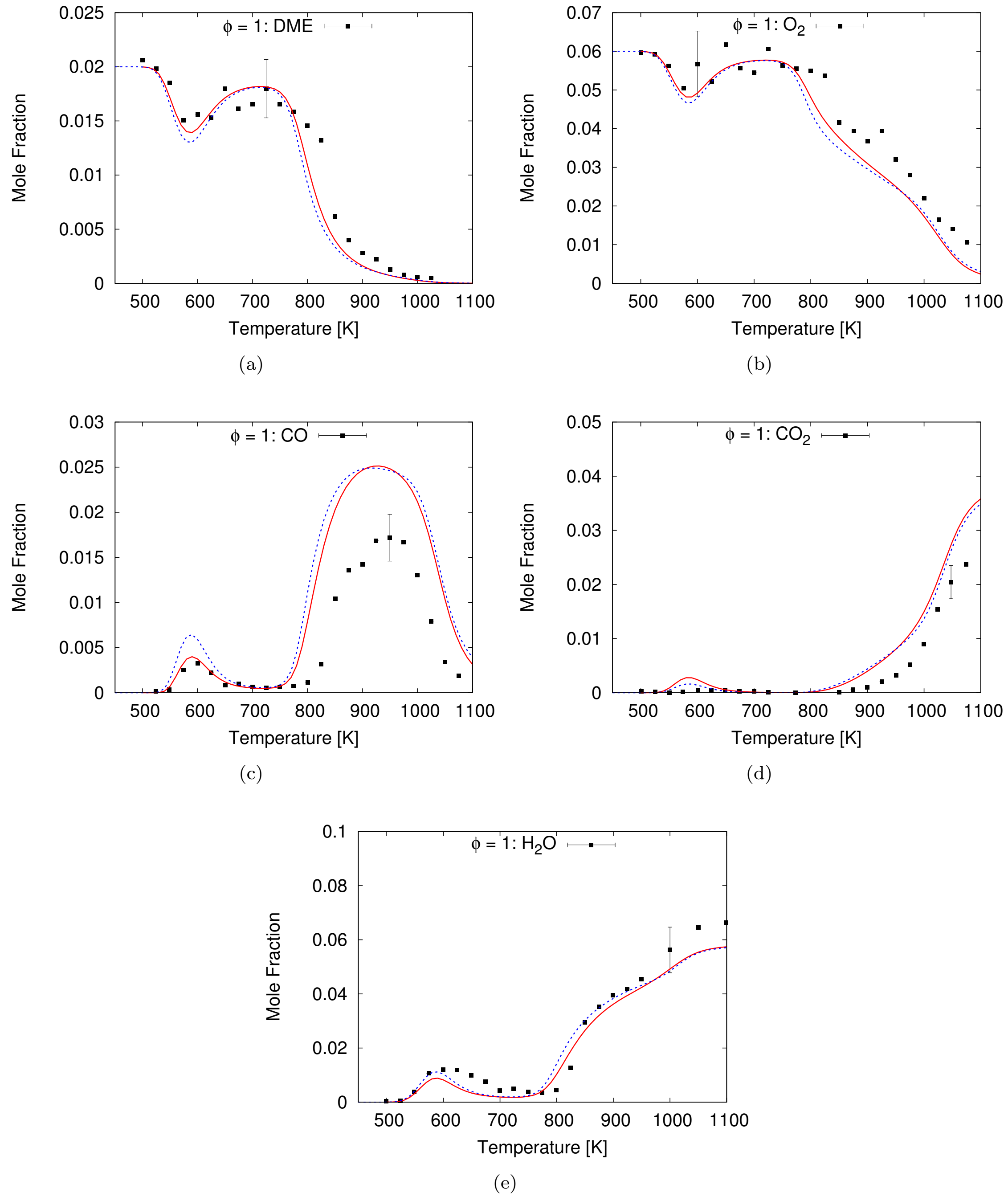


Figure S6: Major species profiles in a jet-stirred reactor. $\phi = 1.0$, $X_{dme} = 0.02$, P = 106.7 kPa, $\tau = 2$ s. Symbols – experimental data from Rodriguez *et al.* [5] with representative error bars; lines – simulations: reference mechanism (solid lines), 23 species mechanism (dashed lines).

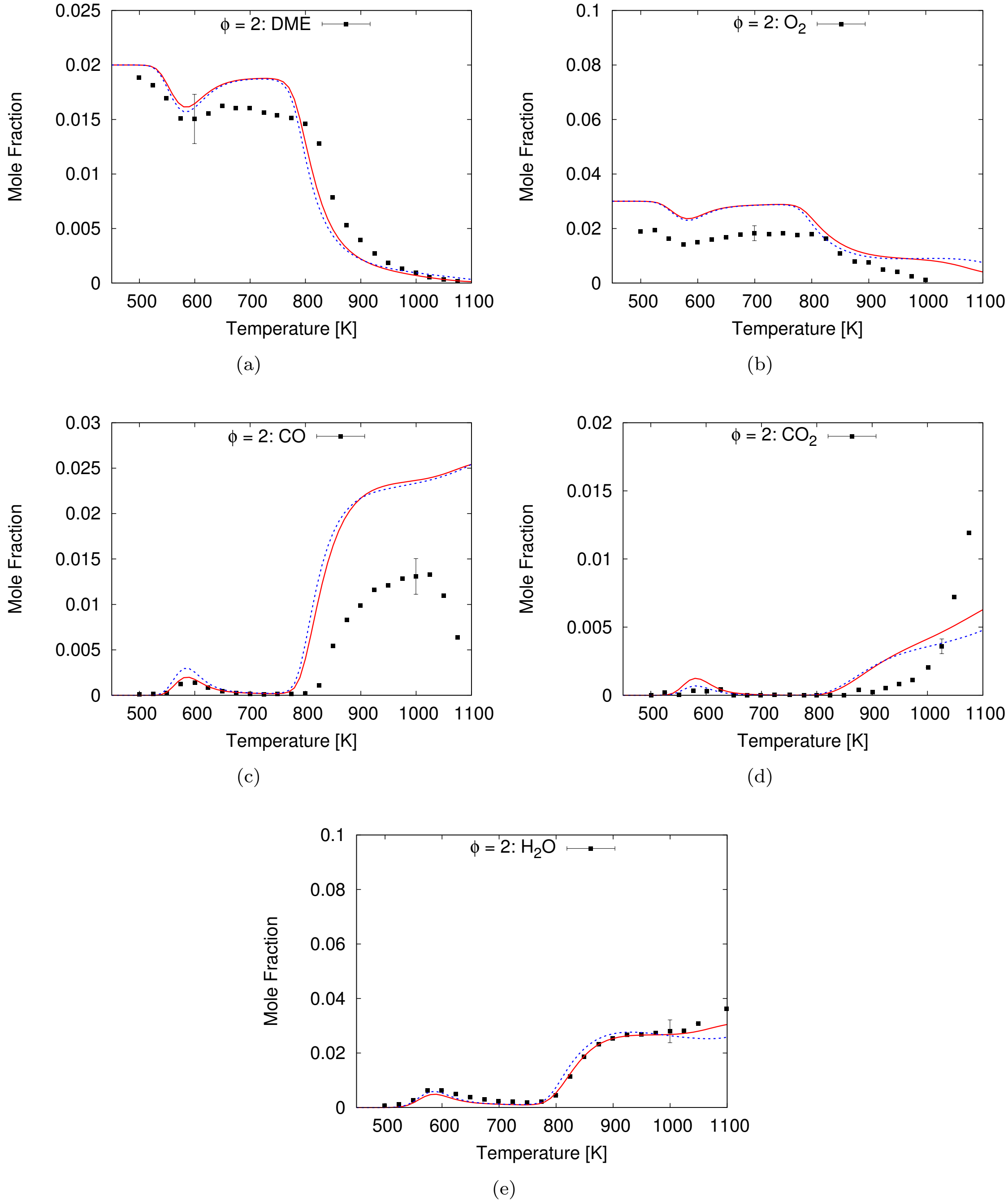
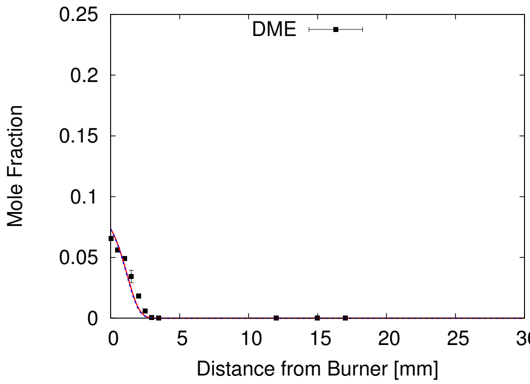


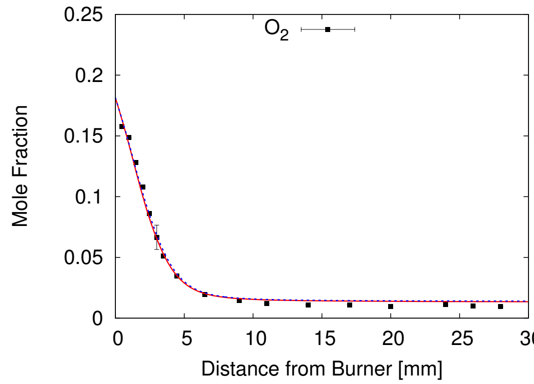
Figure S7: Major species profiles in a jet-stirred reactor. $\phi = 2.0$, $X_{dme} = 0.02$, P = 106.7 kPa, $\tau = 2$ s. Symbols – experimental data from Rodriguez *et al.* [5] with representative error bars; lines – simulations: reference mechanism (solid lines), 23 species mechanism (dashed lines).

3 Validation Results for Burner-Stabilized Premixed Flames

The 23 species mechanism is validated against burner-stabilized flame speciation data by Cool *et al.* [6]. The experimentally measured temperature profile is given as an input in performing the computations.



(a)



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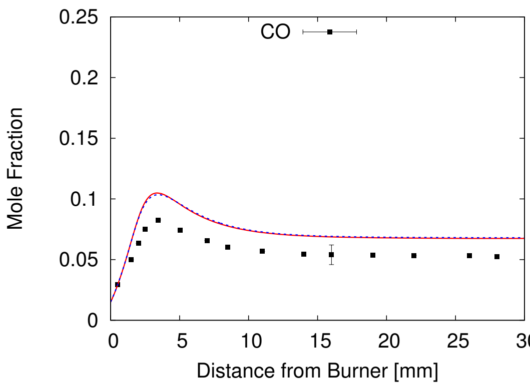

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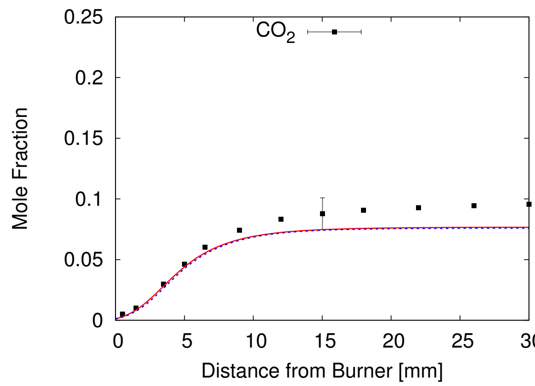
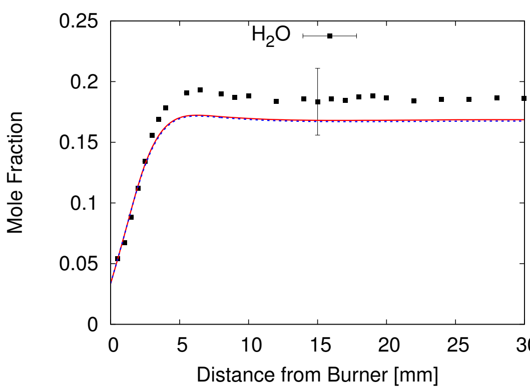
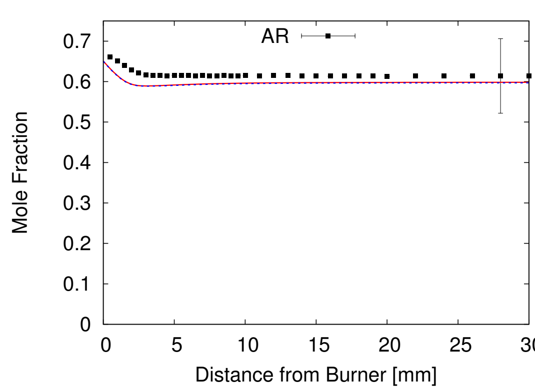


(d)



(e)



(f)

Figure S8: Mole fractions for the major species in a burner-stabilized premixed flame. $\phi = 1.2$, 70.3% AR, P = 4.0 kPa, flow velocity = 0.827 m/s. Symbols – experimental data from Cool *et al.* [6] with representative error bars; lines – simulations: reference mechanism (solid lines), 23 species mechanism (dashed lines).

4 Comparison of 23 Species Model with a Recent Detailed Model

A recent detailed model for DME oxidation by Burke *et al.* [7] is validated for some of the representative data sets shown in the main article. The results are also compared against the 23 species model computations.

- Ignition Delay:

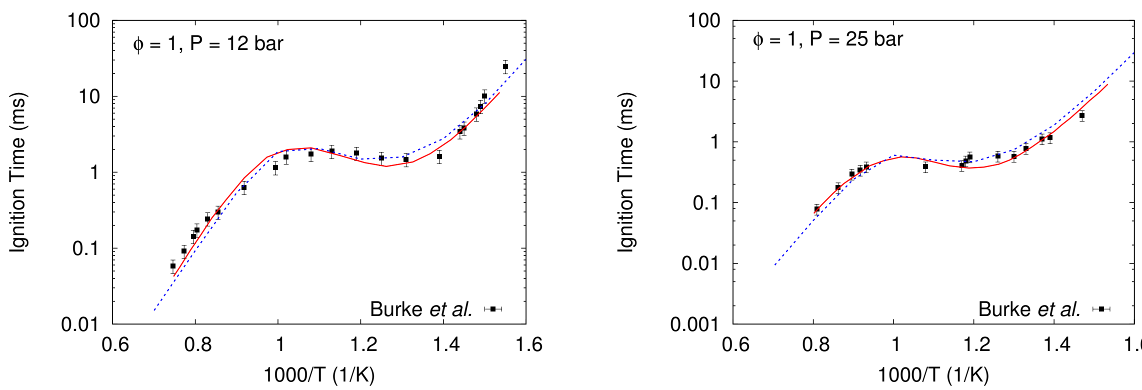
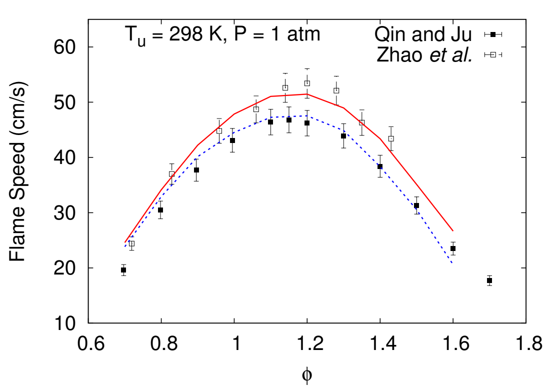
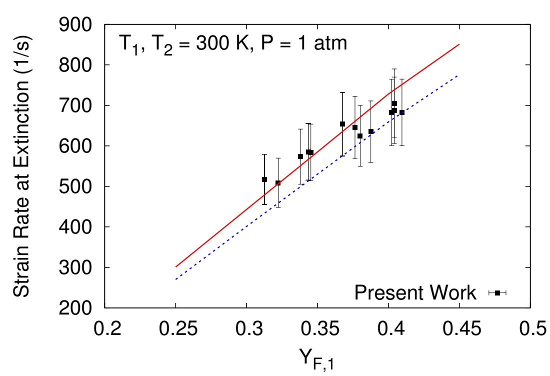


Figure S9: Ignition delay times for DME-air mixtures for $\phi = 1$ and P = 12 and 25 atm. Symbols–experimental data from Burke *et al.* [7], lines –simulations: Burke mechanism [7] (solid lines), 23-species mechanism (dashed lines).

- Flame Speed and Non-premixed Extinction:



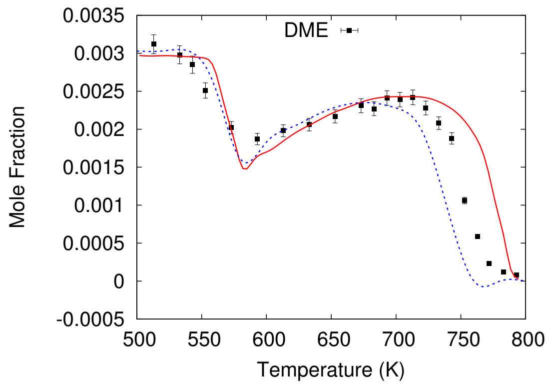
(a) Laminar burning velocities of DME-air mixtures at different equivalence ratios at 1 atm.



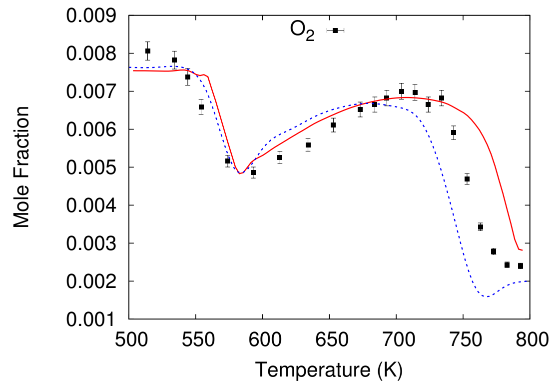
(b) Extinction strain rate, $a_{2,E}$, as a function of fuel mass fraction, $Y_{F,1}$, for DME-air mixtures.

Figure S10: (a) Symbols – experiments: Qin and Ju [8] (filled symbols), Zhao *et al.* [9] (hollow symbols); (b) Symbols – experiments: present work. Lines – simulations: Burke model [7] (solid lines), 23 species mechanism (dashed lines).

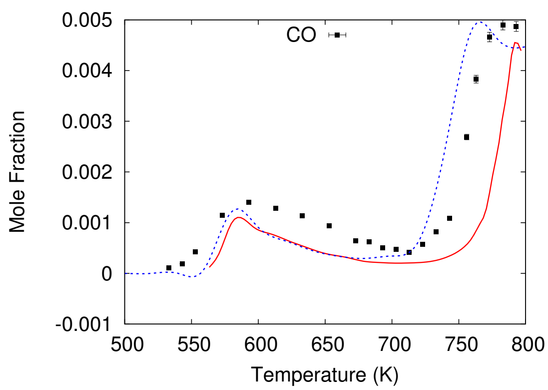
- Species Profile:



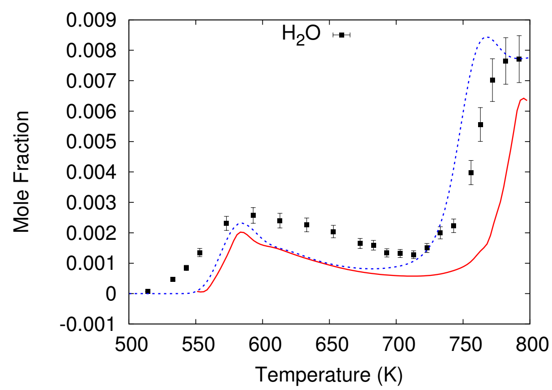
(a) Fuel



(b) Oxidizer



(c) Product: CO



(d) Product: H_2O

Figure S11: Species profiles in a constant pressure flow reactor, ϕ = 1.19, 0.3% DME in N_2 at 12.5 atm. Symbols – experimental data from Curran *et al.* [1]; lines – simulations: Burke mechanism [7] (solid lines), 23 species mechanism (dashed lines).

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