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A MULTIPURPOSE MECHANISM FOR ETHANOL COMBUSTION

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Abstract

A new and shorter multipurpose kinetic mechanism for ethanol combustion comprising 80 reactions and 32 species is presented. The selected benchmark problems are the premixed planar flame propagation (under different equivalence ratio, temperature and pressure), the isobaric autoignition time, and both premixed and non-premixed flame extinction in a counterflow configuration. The selected mechanisms are: The San Diego mechanism (SD), AramcoMech2.0 (ARAMCO), C1-C3 mechanism from Politecnico di Milano University (CRECK), Lawrence Livermore National Laboratory (LLNL) and the mechanism developed by Eötvös Lorant University (ELTE). The accuracy and computational cost evaluation of above mentioned mechanisms identifies the San Diego Mechanism not only as the most precise mechanism but also as the most convenient option from the point of view of computational cost. Chemistry reduction is achieved by analyzing the sensitivity of intermediate species to eliminate the reactions involving the less reactive species. The resulting skeletal mechanism compares favorably with the 235-step, 47 species detailed Mechanism in all cases studied, reducing the computational cost in more than a 50%.

Introduction

Literature survey identifies the state-of-the-art mechanisms to be tested in the wide range of canonical problems representative of combustion applications. The selected mechanisms are: the San Diego mechanism [1] (SD), AramcoMech2.0 [2] (ARAMCO), C1-C3 mechanism from Politecnico di Milano University [3] (CRECK), Lawrence Livermore National Laboratory [4] (LLNL) and the mechanism developed by Eötvös Lorant University [5] (ELTE). These mechanisms emerge as the most popular ethanol combustion mechanisms based in the amount of research papers published that made use of them.

Main models evaluation

The accuracy of the mechanisms is evaluated by comparing the predictions with the experimental results ignition delay time, τ_{ig}, of homogeneous mixture at constant pressure ([6]), propagation velocity, V_L, of laminar premixed flames ([7], [8], [9], [10], [11], [12] and [13]) and strain-induced extinction, a_{2E}, of premixed and diffusion flames ([14] and [15]). A figure of merit is characterized the relative performance of all mechanisms as

$$\Delta_\psi = \frac{100}{N}\sum_{i=1}^{N_c}\sum_{j=1}^{N_{s,i}}\frac{|\psi_{sim,i,j}-\psi_{exp,i,j}|}{\psi_{exp,i,j}} \quad N=\sum_{i=1}^{N_c} N_{s,i}, \tag{1}$$

where $\psi_{sim,i,j}$ is a macroscopic value simulated, $\psi_{exp,i,j}$ is the experimental measurement, obtained from the literature, for the experimental point j measured in a set of conditions i in all the configurations under scrutiny. $N_{s,i}$ is the number of experimental measurements located for the case i and N_c is the total number of cases available.

The following table summarizes the results for the different mechanisms and shows the characteristic CPU time needed to compute each configuration, starting from the same initial conditions and using the same solver settings in Cosilab [16].

Mechanism	Error (%) defined by (1)				Average CPU time		
	$\Delta_{\tau_{ig}}$	Δ_{V_L}	$\Delta_{a_{2E,premix}}$	$\Delta_{a_{2E,diff}}$	$t_{\tau_{ig}}$(s)	t_{V_L}(min)	$t_{a_{2E}}$(min)
SD	82.06	7.00	17.54	16.63	<1	5	138
LLNL	137.51	9.00	16.56	18.15	1	8	218
ARAMCO	76.02	6.61	*	*	101	4601	*
CRECK	72.58	7.50	16.96	24.97	18	56	1331
ELTE	89.13	13.85	36.82	34.04	<1	5	155

* Simulations did not converge after running ten times more longer than the next slower mechanism.

Development of skeletal mechanism

Based on the previous table, the SD mechanism is selected as the starting point to develop the skeletal mechanism. To reduced the number of reactions, we used a reaction-pathway analysis and the sensitivity analysis implemented in Cosilab. In order to achieve an even shorter mechanism, we eliminate progressively those elementary reactions likely to play a minor role in the chemistry. As a result, after eliminating all unimportant species and reactions, we get the 80-step, 32 species skeletal mechanism whose performance is shown in the figures below. The following table shows the errors and the computational time associated to our calculations using the skeletal mechanism.

Mechanism	Error (%) defined by (1)				Average CPU time		
	$\Delta_{\tau_{ig}}$	Δ_{V_L}	$\Delta_{a_{2E,premix}}$	$\Delta_{a_{2E,diff}}$	$t_{\tau_{ig}}$(s)	t_{V_L}(min)	$t_{a_{2E}}$(min)
$Skeletal_{80}$	107.28	6.60	17.28	11.36	<1	2	58

References

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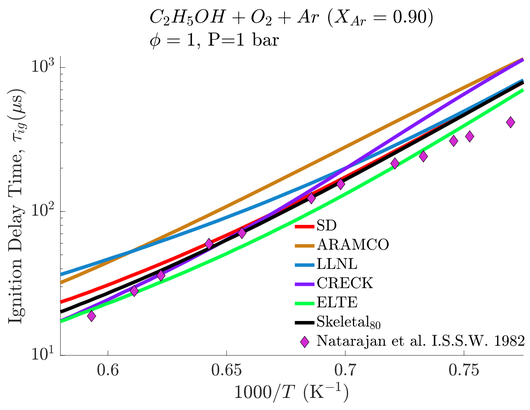
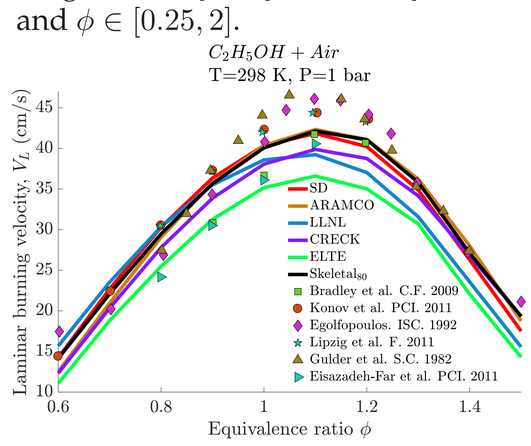
Results

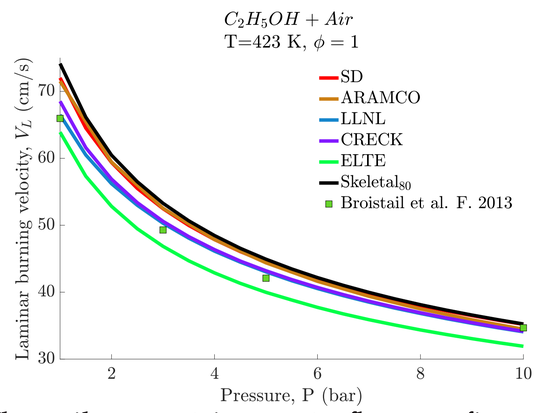
A summary of the results is presented below.



Ignition delay time as a function of temperature for a stoichiometric mixture ($\phi = 1$) at constant pressure ($P = 1$ bar). The symbols represent experimental measurements [6] while the curves are the predictions obtained with the different mechanisms, including the skeletal. Simulations were carried out for pressure, P, temperature, T and equivalence ratio, ϕ, in their ranges. $P \in [1, 50]$ bar, $T \in [800, 1700]$ K and $\phi \in [0.25, 2]$.

Laminar burning velocity as a function of the equivalence ratio ϕ for atmospheric conditions ($P = 1$ bar and $T = 298$ K).





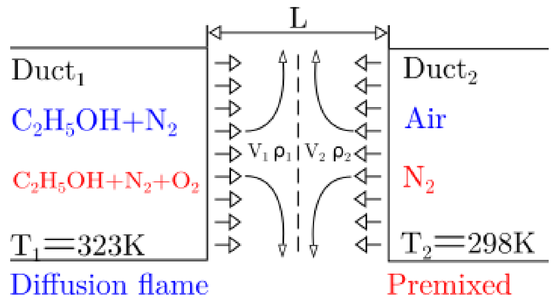
Laminar flame propagation velocity as a function of pressure for a stoichiometric mixture ($\phi = 1$) at temperature $T = 423$ K.

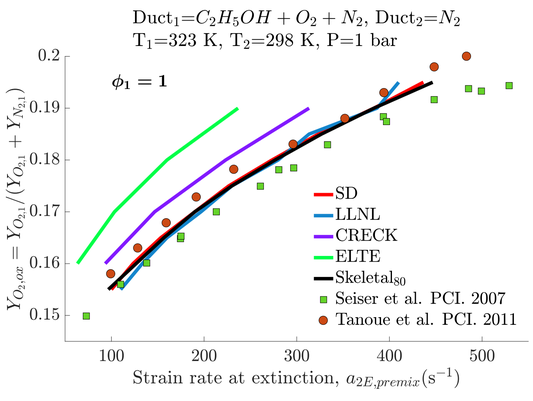
Laminar burning velocities were evaluated for $P \in [1, 10]$ bar, $T \in [298, 423]$ K and $\phi \in [0.6, 1.5]$.

The axilsymmetric counterflow configuration under analysis is sketched in the figure. The global strain rate is defined as

$$a_{2E} = \frac{2|V_2|}{L}\left(1 + \frac{|V_1|\sqrt{\rho_1}}{|V_2|\sqrt{\rho_2}}\right).$$

Where v_i, ρ_i, and T_i are, respectively, the exit velocity, the density and the temperature of the stream at the exit of duct i, and L is the distance between the ducts.





Strain rate of extinction for a premixed flame as a function of the mass fraction of the oxidizer, $Y_{O_2,ox} = Y_{O_2,1}/(Y_{O_2,1} + Y_{N_2,1})$.

Conclusions and Future Work

A minimum mechanism for ethanol combustion has been obtained. Starting from the full San Diego mechanism, a significant reduction in computational cost has been obtained while maintaining the accuracy of the original mechanism. Further reduction will be pursued before proceeding to analyze species in steady-state and reactions in partial equlibrium, with the final goal of reducing the computational cost by one order of magnitude with comparable accuracy to that of the San Diego mechanism.

Acknowledgements

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