

Multiscale aviation kerosene modeling: from *ab initio* quantum chemistry to the combustion chamber simulations.

V. L. Kovalev[†], S. O. Adamson[§], A. S. Vetchinkin^{*†}, A.V.Vagner[†]

[†]Department of Mechanics and Mathematics, Lomonosov Moscow State University, Leninskie Gory 1, Moscow 119991, Russia

[§]Laboratory of Molecular Structure and Quantum Mechanics, Department of Chemistry, Moscow State University, Leninskie Gory, Moscow 119991, Russia

^{*}NN Semenov Institute of Chemical Physics, Kosygina str., 4, Moscow 119991, Russia

The development of propulsion systems operating on commercial fuels demands multi-dimensional modeling of reactive flows inside the device. Most aviation fuels are mixtures of a large number of hydrocarbons and the chemical kinetic processes occurring in combustion of such fuels at high temperatures have not been sufficiently validated. The modeling of gas chamber systems demands the development of reduced kinetic mechanism of a gas fuel combustion. In addition to the investigation of Frolov et al [1],[2] and, lately, Strelkova et al [3], we developed the reduced mechanism of n-butane and, then, aviation kerosene combustion, based partly on the detail Curran et al [4] kinetic mechanism. Then we provide the industrial combustion chamber simulation. The work contains three stages.

At first stage, we calculate the n-butane and the aviation kerosene ignition time according to Dean experiment [5]. We modeled a shock tube 76 mm in diameter and 5.5 m length. A high-pressure valve with a forced start was employed as high-pressure chamber for creating incident shock wave. The ignition delay time was defined as the time difference between shock arrival at the end wall and the start of rapid growth of OH concentration. The simulation has been provided by the ANSYS FLUENT packet [6]. The good agreement between the stimulated and experimental data [4],[7] has been achieved.

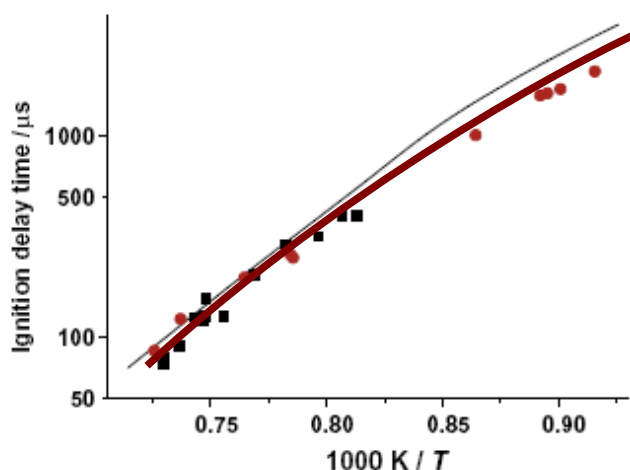


FIGURE 1. The n-butane ignition time delay on dependence of temperature. Thin line is H.J. Curran et al detail mechanism simulation [4], fat line is our simulation, the circle points are Curran et al [4] experimental data, the square points are from Burcat et al experiments [7]. 2.5% n-butane, 25% O₂, 81.25% Ar, P = 10 atm.

The second stage of the investigation is the correct simulation of the final stage of the kerosene flame, i.e. the acetylene combustion. The new kinetic mechanism of the C₂H₂+OH, CH₃+CO and C₂H₂O+H has been developed, based on the quantum chemistry investigations of potential energy surfaces and geometry of the molecules and intermediate complexes. The potential energy surface for the reactions of acetylene with OH – radical which are leading to C₂H₂O+H and CH₃+CO products was calculated using the density functional theory. The calculations of the unsaturated alcohol HOCH=CH formation [8-10] (the first stage of the studied reaction) and of the van-der-waals complex HC=CH..OH (C_{2v} symmetry) [11,12] were carried out to choose the optimal computational technique. It is found that the combination of the aug-cc-pVTZ basis set with the density functional M06-2X [13] provide the relative energies which are close to the results of CC-SD(T) и RQ-CISD(T)/CBS calculations (Fig. 1) [8,9]. The GAMESS US package is used in all calculations [14].

The rate constants are calculated for the all reactions paths and the mechanism is constructed for the C₂H₂+OH reaction using the calculated PES.

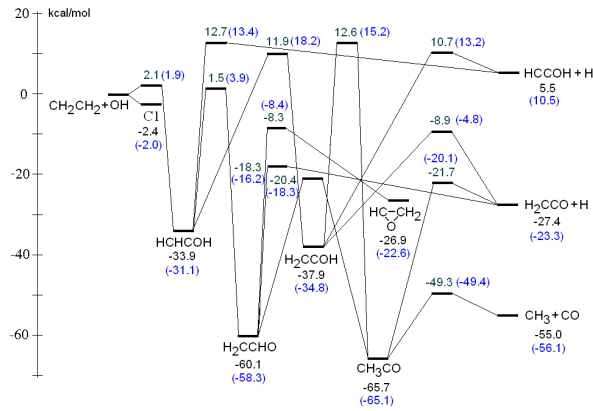


FIGURE 2. The Potential energy surface of the $C_2H_2 + OH$ reaction. The RQ-CISD(T)/CBS results are in the round parentheses [9]. All energies are presented in kcal/mol.

The third stage of the work is the fluent simulation of the industrial combustion chamber. We used the aviation kerosene kinetic mechanism, improved during the previous two stages. The simulation has been provided by the ANSYS FLUENT 13.1 packet [6]. The grid contains about 32 millions points.

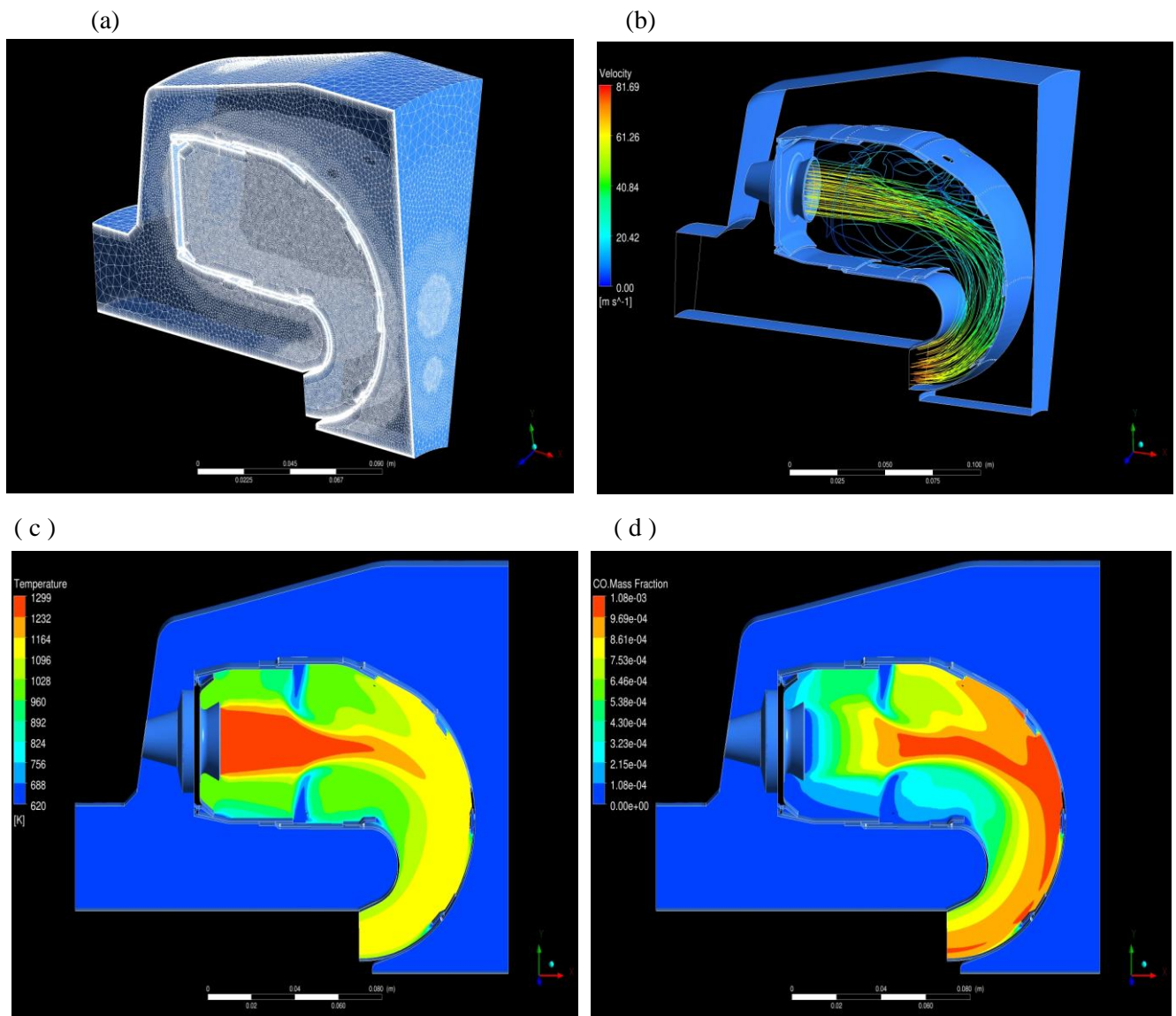


FIGURE 3. The segment of the combustion chamber. The picture (a) is the grid, (b) is the flow velocity distribution in m/s, (c) is the temperature, K and (d) is the output CO flow (normalized mass fraction).

The kerosene is injected by the sprayer. The fuel consists on $C_{10}H_{22}$ $1.64e-2$, C_6H_{14} $1.24e-3$, C_6H_6 $2.2e-3$, O_2 $2.2e-1$ mole fraction. Total pressure is about 9 atm. Output mass flow is about 0.1 kg/s. The results are shown on the FIGURE 3. The calculated species output is in a good agreement with the experimental data.

The authors acknowledge the support Russian Foundation for Basic Research under Project № 11-01-12041-ofi-m.

LITERATURE

1. V. Ya. Basevich, A.A. Belyaev, S.M. Frolov et al, *Rus. J. of Physical Chemistry B*, 2007, **2**, pp. 477-484
2. S. M. Frolov et al, *Journal of Loss Prevention in the Process Industries*, 2007, **20**, pp. 562–569
3. M.I. Strelkova et al, *Combustion and Flame*, 2010, **157**, pp. 641–652
4. H. J. Curran et al, *Combustion and Flame*, 2010, **157**, pp. 1526–1539
5. A.J. Dean, O.G. Penyazkov, K.L. Sevruck, B. Varatharajan, *Proceedings of the Combustion Institute*, 2007, **31**, pp. 2481–2488.
6. ANSYS FLUENT, ANSYS Ltd., <http://www.ansys.com>
7. Burcat et al, *Combustion and Flame*, 1971, **16**, pp. 29
8. Yi-hong Ding, Xiang Zhang, Ze-sheng Li, Xu-ri Huang, and Chia-chung Sun, *J. Phys. Chem. A*, 2001, **105**, pp. 8206–8215
9. J. P. Senosiain, S. J. Klippenstein, J. A. Miller, *J. Phys. Chem. A* 2005, **109**, pp. 6045-6055.
10. A. Galano, L. G. Ruiz-Suárez, A. Vivier-Bunge, *Theor. Chem. Account*, 2008, **121**, pp.219–225.
11. C. Sosa, H. Schlegel, *J. Am. Chem. Soc.*, 1987, **109**, pp. 4193-4198.
12. J. Davey, M. Greenslade, M. Marshall, M. Lester, M. Wheeler, *J. Chem. Phys.*, 2004, **121**, pp. 3009-3018.
13. Yan Zhao, D. Truhlar, *Acc. Chem. Res.*, 2008, **41**, pp. 157-167.
14. M. W. Schmidt et al., *J. Comput. Chem.*, 1993, **14**, pp. 1347-1363.