Predictive modeling of the Chemical Kinetics in Jet-A/Air for High-Temperature Combustion and Gas Phase Detonations: Multi-scale Approach

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1 Introduction

As the complexity of the power and energy system increases, it becomes more and more difficult to improve their efficiency and cleanness with the design approaches, which were standard previously – development of the prototypes and their modification until the desired result will be attained. The situation is complicated by a huge amount of the controlling parameters and complex physical processes, which should be varied and accounted for simultaneously to attain the optimum conditions.

Today there are two ways to go forward. The first one is to make much more experiments, than before, to gain a notable improvements in the efficiency of the energy conversion and use. The second one is to move to multi-scale predictive modeling of the energy and power system, which is based on the fundamental, first principle based approaches.

The last approach seems to be valuable for several reasons. Firstly, the main parametric studies could be conducted theoretically (computationally), while the experiment will be used for verification of the approaches or models used and for the decisive tests of the final solutions. Second, inventive search for the best solutions could be carefully scheduled by turning into consideration one kind of the physical processes and turning off the another, which are not important according to the engineer's intuition. Consequently, implementation of this approach allows to reduce the expenses in terms of money and time and to reduce the risks related with the development of the innovative products and technologies. Therefore, the development of the scientific grounds for this approach is important and necessary for the power and energy systems of the future.

The intensive direction of the research is the development of predictive reduced kinetic mechanisms of the real fuel combustion, based on detailed physical-chemical mechanism and acceptable from the viewpoint of the multidimensional modeling. The realization of this task requires solution of the several problems: construction of the predictive detailed kinetic mechanisms, its

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verification and reduction, verification of the obtained reduced mechanisms against the detailed one and a set of experimental data, relevant for the particular target application.

In the present paper the hybrid multi-scale first-principle based approach to the construction of the detailed and reduced kinetic mechanisms, developed by the collaborative group of the researchers, is described and illustrated on the example of the detonative combustion of the commercial aviation kerosene-air mixtures.

2 The hybrid multi-scale first-principle based approach

The following approach to the construction of the detailed physical-chemical mechanism, its reduction and validation of the mechanisms according to target application is developed. It includes the following stages:

1. Compilation and model based acquisition of the detailed kinetic mechanism
   - Refining of the thermo-chemical data and elementary reaction rate constants using data, available in the literature;
   - Refining of the thermo-chemical data and elementary reaction rate constants using quantum-chemical and micro-kinetic calculations;
   - Validation of the detailed mechanism against experimental data;
2. Reduction of the detailed mechanism
   - Systematical derivation of the reduced and overall kinetic mechanisms for target application;
   - Validation of the reduced and overall kinetic mechanisms against experimental data;
3. Application targeted validation of the reduced and overall kinetic mechanism
   - Selection of the experiments, which include all principal physical phenomena from the target application. For example, if the detonation problems are considered, the test case should include the gas dynamics phenomena and shock wave ignition.

The developed approach covers several physical scales: from atomic scale to macro-scale of the real flow inside the device. It contains several steps including the verification at the every step.

3 Case-study: Jet A / air mechanisms of detonative combustion.

Detailed kinetic mechanism.

Based on this hybrid multi-scale first-principle based approach we elaborated detailed mechanism of the Jet A surrogate combustion. Three-species (72.7 wt % decane + 9.1 wt % hexane + 18.2 wt % benzene) surrogate mixture representing Jet A fuel was chosen. The mechanism was built in a logical, hierarchical manner taking into account hydrocarbon chemistry as determined by reactivity of the few functional groups. The rate constants of the elementary reactions entering the detailed mechanism were verified based upon most recent compilation of experimental rate constants of reactions important in combustion, qualitative physical and chemical arguments (spin conservation, orders of magnitude of pre-exponential factors) and thermo-chemical data. For cases when the accuracy of thermo chemical and kinetic data for important reactions and species were considered as insufficient the first principle study based on modern quantum chemistry and microscopic theory of chemical reactions was initiated using the KHIMERA code [1].

This detailed mechanism, consisted of 417 reversible reactions and 71 components, was validated against available experimental data for Jet A combustion at pressure of 1 atm, 10 atm for lean, stoichiometric and rich Jet A /air mixtures (φ = 0.5, 1, 2) within the temperature range of 1000 -1700 K.

Reduced kinetic mechanism

Sensitivity and rate of production analysis and also quasistationary approximation were used for successive reduction of the detailed mechanism to the reduced mechanism. For reduction the detailed mechanism were used the procedures – sensitivity analysis, rate of production analysis tool, special

tool for "mechanism visualization" based on the atomic fluxes analysis (Reaction Pathway diagram builder) [2]. The reduced mechanism, consisted of 38 reactions and 24 species, was validated upon experimental data [4] and on the results of detailed mechanism and showed good agreement It can be utilized in wide range of temperatures, pressures and equivalent ratios. Detailed and reduced mechanisms in detailed are described in [3].

Overall kinetic mechanism

The reduced mechanism can be useful tool to study combustion and detonation processes by using 1D CFD code. But it becomes generally impractical for multidimensional modeling from point of view of large CPU times and computer memory. Nevertheless, the reduced mechanism could serve as a basis for the development of the overall mechanisms of the desired degree of the detail. So the overall mechanism, which was derived from reduced mechanism by quasy-stationary approach, is more suitable. This mechanism consisted of 11 forward reactions and 10 species was validated against the detailed reaction mechanism and experimental results for the following conditions: initial temperatures 1000-1800 K, pressures 1, 10, and 100 atm, and equivalence ratios 0.5, 1, and 2.

Validation

In Fig.1 comparison induction times, calculated by using Jet A surrogate detailed, reduced and overall mechanisms at Po=10 atm with experimental data for equivalence ratio phi=1 is shown. It is clear that the induction times, simulated by these elaborated mechanisms are in a good agreement between others and are agreed with experimental data rather good.

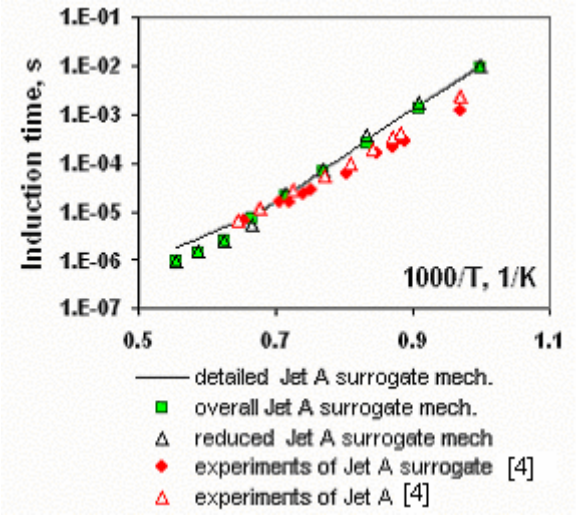

Fig.1. Induction times, simulated by detailed, reduced, overall mechanisms for Jet A surrogate combustion in comparison with experimental data for To=10 atm, φ=1.

Validation overall mechanism of Jet A surrogate combustion in the CFD simulations. The overall 11-step mechanism for the Jet-A surrogate was used to simulate the experiments on detonation initiation in stoichiometric gaseous Jet A/air mixture behind reflected shock waves [3]. This set of the experiments is considered as and *application target validation case* due to its strictly defined methodology and well reproducibility. Except the ignition delay times, which can be compared with the experimental data just in the pure kinetic simulations, another targeted parameter – the speed of the reflected wave is introduced, as it reflects not only the ignition, but the detonation formation process as well. In the Fig. 2 the reflected wave speed at the distance 0.073 m from the wall is presented as function of the incident shock wave Mach number. Conditions of the experiments: initial temperature 340 K, pressure behind reflected shock wave is fixed and equal to 9 – 10 atm. It is seen that the results of the one-dimensional CFD simulations agree with the experimental data, difference between the data does not exceed 10%.

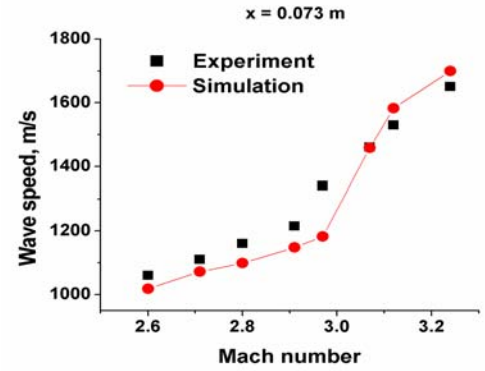

Fig.2. Results of the comparison of the reflected wave speed at the 0.073 m from the reflecting wall after detonation initiation behind plane reflected shock wave, measured in experiments [3] and predicted with the reduced kinetic mechanism. Gaseous stoichiometric Jet-A/air mixture, initial temperature 340 K, pressure behind reflected shock wave 9 – 10 atm.

4 Conclusions.

In the present paper the hybrid multi-scale first-principle based approach for the development of predictive kinetic mechanisms for the combustion and detonation is presented. Utilizing this approach the kinetic mechanisms for Jet A / air detonative combustion were developed: detailed mechanism (417 reversible reactions, 71 components), reduced mechanism (38 reactions, 24 species), overall mechanism (11 forward reactions, 10 species). These mechanisms were validated upon the available experimental data.

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