Methane Skeletal Mechanism for Space Propulsion Applications

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Abstract— The skeletal reaction mechanism for methane combustion is developed to be applied in the CFD simulations of rocket combustion chamber under pressure 20 bar. The used reduction procedure analyses the model behavior under different pressures, temperature and equivalence ratios and selects the reaction and species those are redundant simultaneously for all studied processes and parameters. The rate of production analysis and sensitivity analysis were applied to simulations of experimental targets for ignition delay times (65 points) and laminar flame speed (15 targets) in intervals of p_5 = 1-50 bar, T_5= 940-210K, ϕ = 0.5–2 and p = 1-60 bar, T_0= 300K, ϕ = 0.6–1.4 correspond. The input detailed mechanism with 41 species (including Ar, He and N2) and 298 reactions has been reduced to the skeletal model with 24 species and 100 reactions. This kinetic mechanism is applicable for simulations of a wide range of combustion parameters.

I. Introduction

Within the last ten recent years, the propellant combination LOX/CH4 has received considerable attraction worldwide as a propellant combination for space propulsion applications [1-5]. The advantages are numerous: a better specific impulse than that of oxygen/kerosene, reduced cost and complexity in in handling compared to hydrogen and reduced requirements for turbomachinery. In Germany, this propellant combination is investigated both experimentally and numerically within the collaborative research center TRR40 on 'Technological foundations for the design of thermally and mechanically highly loaded components of future space transportation systems' [6-8]. Within this project, specific effort is put on developing design tools for thrust chambers which requires validated numerical tools for the prediction of combustion and heat transfer in such devices. In an effort to compare different numerical approaches, a special workshop will be organized later this year at the Technical University of Munich where teams from all over the world which apply RANS, URANS, LES and hybrid models will try to reproduce combustion efficiency and heat transfer of a test case provided by one of the TRR 40 projects [9]. Generally, different groups use not only different approaches to handle fluid mechanics as mentioned above, but also their way to treat combustion differs substantially. In order to allow more detailed comparisons of the applied numerical tools, a reduced chemical kinetic scheme has been developed and will be provided to the workshop participants. The extremely large CPU times for CFD calculations with detailed chemical mechanisms necessitate that the applied kinetic models must be as simple as possible. However, any accurate modelling of diffusion flames and in general combustion processes in liquid propellant rocket engines are of this type requires that the chemical model must be able to sufficiently describe these combustion processes for a wide range of parameters: propellant mixture, temperatures and pressures. Obviously, such a reduced mechanism can be generated only on the base of large number of different calculations, which integrate the calculation of chemical processes (ignition delays, flame speeds, concentration profiles in chemical reactors) and sensitivity analyses of different model outputs to the system parameters. The presented work results of such a reduction of a methane (CH_4) / oxygen (O_2) reaction mechanism reduction.

II. Kinetiuc Model and Reduction Procedure

The input detailed mechanism is a part of the DLR reaction data base [10], which was validated and optimized on the different experimental data for the C_1-C_{16} hydrocarbons which present n-,i-paraffines, naphthenes and aromatics. The divided CH_4 sub-model has 41 species (including Ar, He and N_2) and 298 reactions.

The reduction strategy is based on the modeling and sensitivity analyses of experimental points obtained under different conditions. To construct a skeletal mechanism, applicable for the CFD simulations of rocket combustion chamber under pressure 20 bar, the selected experimental targets for ignition delay times (65 points) cover the interval parameters of p_5 = 1-50 bar, T_5= 940-210K, ϕ = 0.5–2; for laminar flame speed (15 targets) p = 1-60 bar, T_0= 300K, ϕ = 0.6–1.4.

The global sensitivity analysis implemented in the *in-house* developed RedMaster code [11] has been applied to reduce the basic mechanism to the skeletal one. RedMaster code manages the calculation of chemical processes with CHEMKIN code [12] and the calculation of sensitivity coefficients with procedures from KINALC code [13]. The multi target reduction strategy realized in the RedMaster code, Fig.1, allows determination and elimination of unimportant species and reactions on the basis of integrated information obtained from the mechanism sensitivity analysis performed for ignition delay time and laminar flame simulations at different time points of the studied processes.

A species is considered redundant if its concentration change has no significant effect on the production rate of necessary species. The influence of a change of the

concentration of species *j* on the rate of production of a *p*-membered group of important species *i*, are calculated as the sum of squares of the *overall normalized sensitivity coefficient:*

$$B_j = \sum_i^p \left(\frac{\partial \ln R_i}{\partial \ln c_j} \right)^2 \quad , j=1,\ldots,N \qquad (1)$$

B_j yields the integrated effect of a change of the concentration of species c_j on the rate of production of species *i*, R_i, from a group of *p* important species, $i = 1, 2, \ldots, p$, *N* is a number of species. Number of *p* is changed during iterative procedure. The number of "primary" necessary species is given by the investigator based on first results of the analysis. After each step *n* ($n = N\text{-}p$) of the B_j calculation only one species with the greatest value B_j is added to the group of necessary and important species (p_n+1).

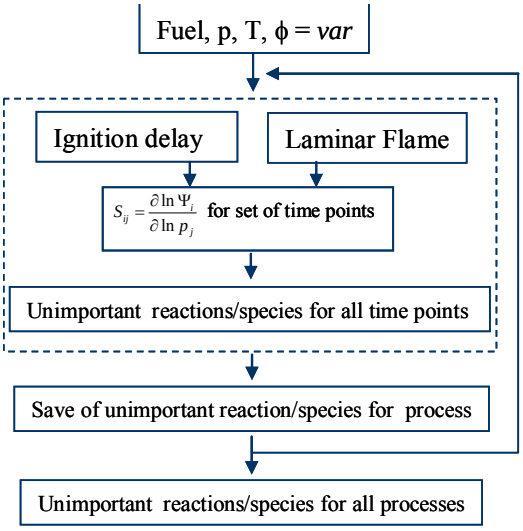


Fig. 1. Principal scheme of the RedMaster code for the multi target reaction mechanism reduction.

After calculations of B_j , those species which have the smallest value of B_j and were added to the main group at the last iterations can be considered as redundant species. In the present mechanism reduction process 11 species were nominated as "primary" necessary species H_2, CH_4, OH, O, CO, O_2, HO_2, H, CO_2, HCO, H_2O_2.

The contribution of reaction steps to the production rate is based on the sensitivity of production rates to changes in reaction rate coefficients. The effect of changing the reaction rate coefficient k_i on the rate of production of species *i*, R_i, in a mechanism with *N* species is calculated as the sum of squares of the *overall normalized sensitivity coefficient*:

$$A_i = \sum_i^N \left(\frac{\partial \ln R_j}{\partial \ln k_i} \right)^2 \qquad (2)$$

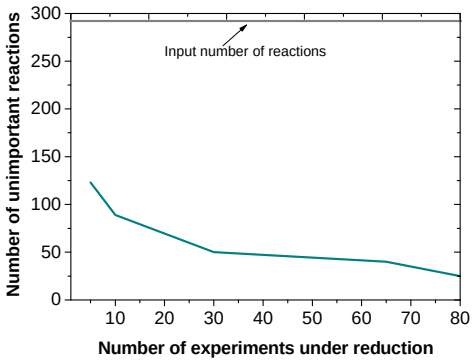
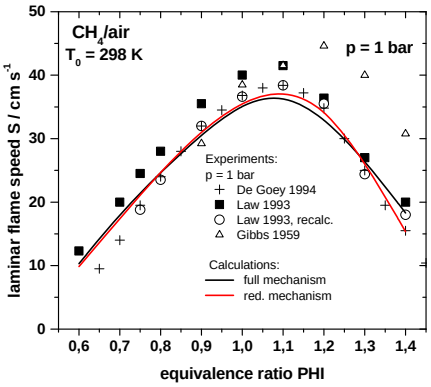


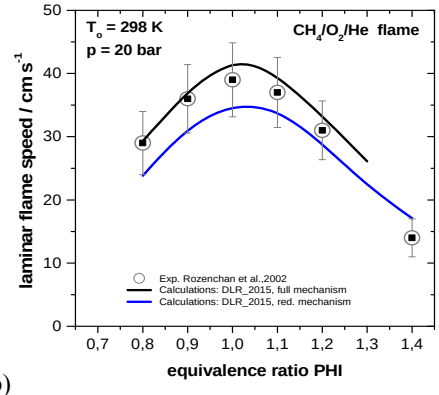
Fig. 2. Number of unimportant reactions versus number of experimental targets in consideration.

R_j - the rate of production of species *j*, k_i – rate coefficient of reaction *i*. A reaction *i* is considered important if its coefficients A_j, calculated as the sum for all species, e.g. *N*, are larger than a pre-defined threshold value Δ.

A reduction cycle has to be repeated several times until no more species and reactions are found to be unimportant and



a)



b)

Fig. 3. Modeling the laminar flame speed [14-17] with full and reduced mechanism. a) p = 1bar; b) p = 20bar.

the simulations with the resulting reduced mechanism reveal that the achieved results fulfil the pre-defined agreement requirement with experimental data.

As the mechanism reduction is in general a strongly problem oriented procedure, it is also very important to

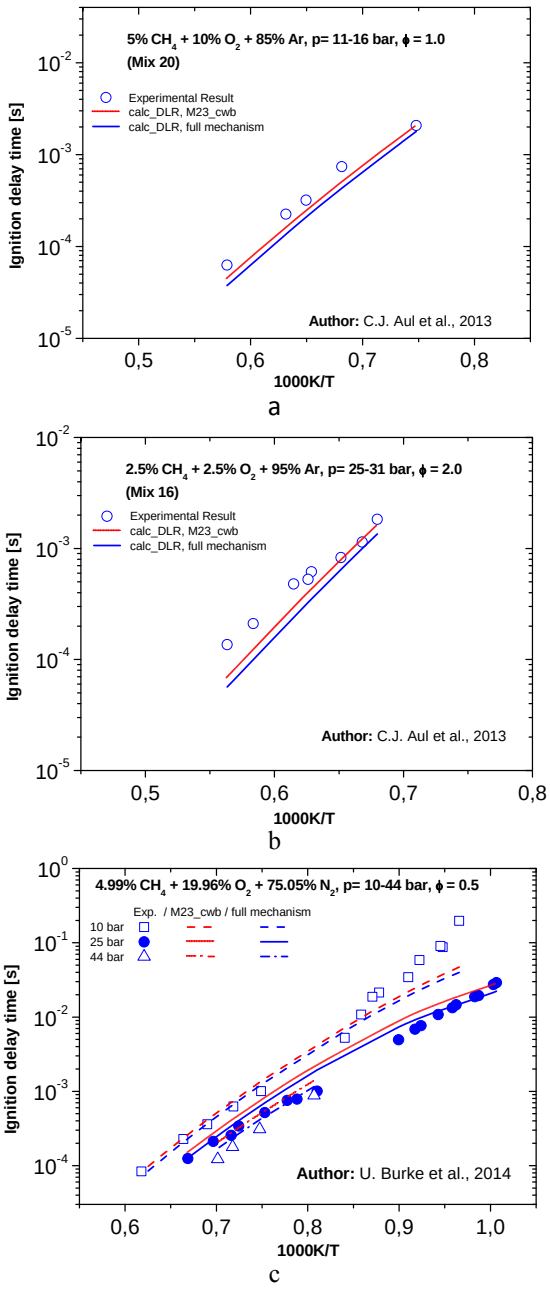


Fig. 4. Modeling the ignition delay times [18,19] with full and reduced mechanism.

perform the problem oriented selection of experimental targets for the reduced model validation. To demonstrate that, the change of number of the unimportant reactions, which are unimportant for all targets under considerations, is shown in the Fig.2 as a function of the number of targets. The quality of experimental data and their consistency, a defined threshold value for unimportant criterion Δ, and analysed time (or height) points for each target must be carefully investigated.

III. Results

The input reaction mechanism with 42 species and 298 reactions was reduced to one with 24 species and 100 reactions on the base of 65 different ignition delays simulations and 15 calculations of flame speed. This mechanism has capability to reproduce the experimental

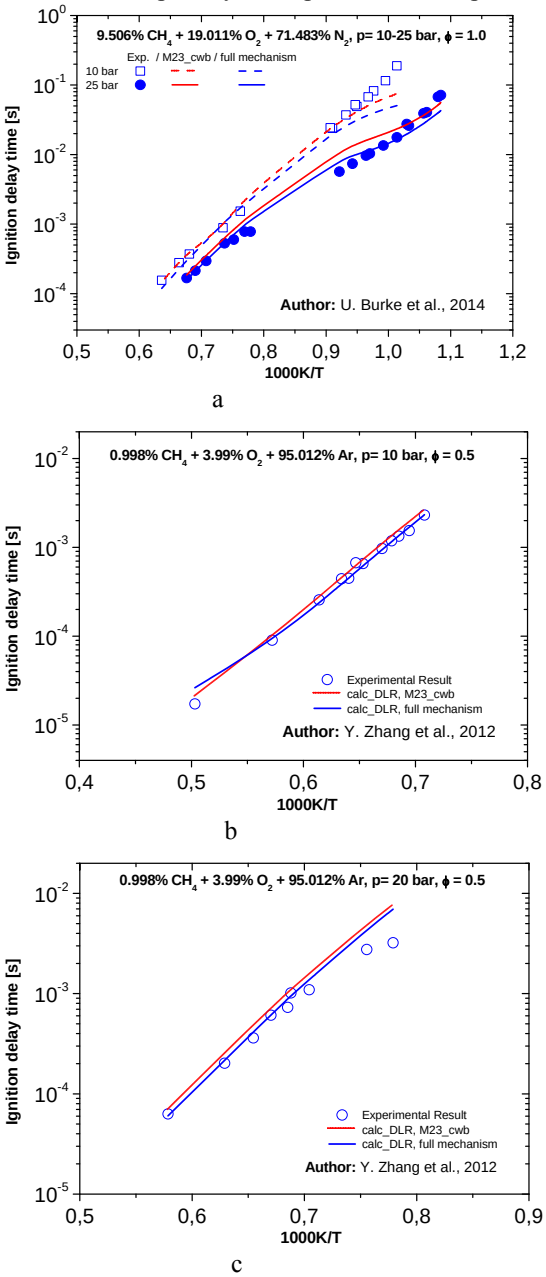


Fig. 5. Modeling the ignition delay times [19,20] with full and reduced mechanism.

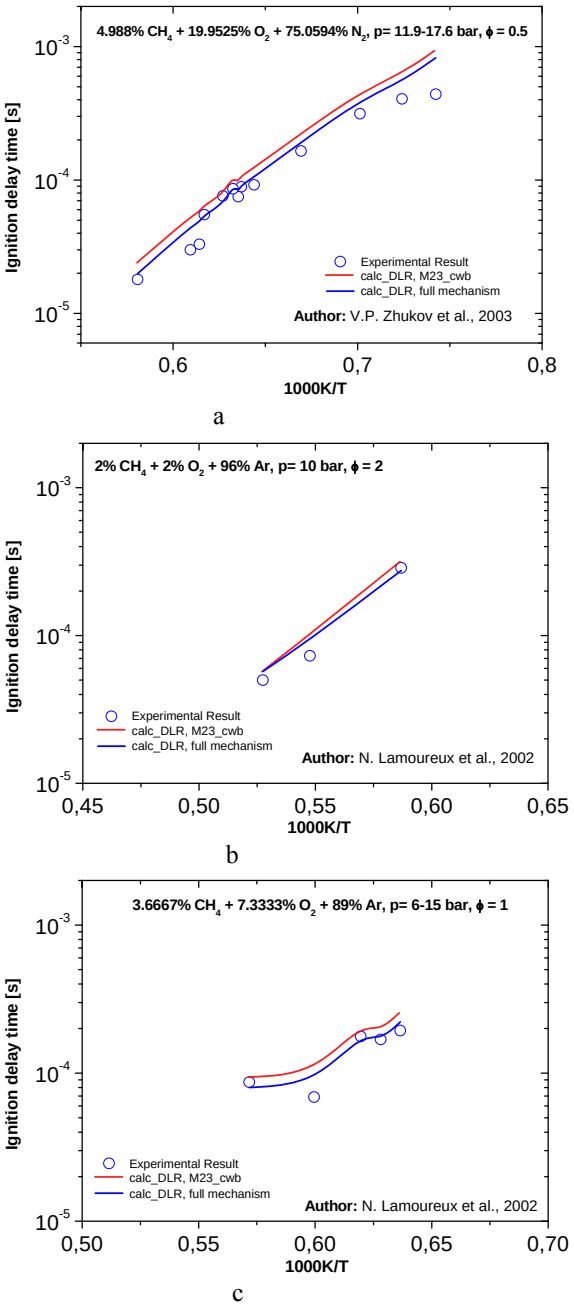


Fig. 6. Modeling the ignition delay times [21,22] with full and reduced mechanism.

data, selected for model validation, with good agreement. Each additional step for the further model reduction with applied procedure will reduce its capability sufficiently. Further reduction is possible only with chemical lumping methods and algorithms for a global model production.

On the Figs. 3 - 6 the results of calculations of ignition delay times and laminar flame speed with detailed and reduced mechanism are shown. Simulations are in good agreement with experimental data in both cases. The proposed skeletal mechanism for the methane combustion under rocket engine conditions can be successfully used in CFD modeling.

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