Methane combustion kinetic schemes in FlowVision software

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Abstract. The two-step chain reaction of methane combustion in air is integrated into the FlowVision software package. The conical flame numerical simulation under normal conditions using the built-in single-step chemical reaction was performed. A comparative analysis of the numerical results for one- and two-step schemes, as well as experimental results was made.

1. Introduction
Methane is one of the most widely used fuels due to its relatively high density in the liquefied state compared to other natural fuels, high volumetric heat value, wide range of flammability limits, environmental safety, and low cost. This leads to the high relevance of studies devoted to the methane combustion characteristics under various conditions and using the results for example for the modern burner devices optimal configuration adjustment. Along with other issues of combustion theory, a lot of research works are devoted to the optimization and the use of hydrocarbon fuels [1, 2]. Numerical simulation of combustion processes is widely used in industry for the design of various technical devices and plays a significant role in modern scientific research practice. Despite the unprecedented growth in computing power of modern cluster computing systems in the last decade, the current capabilities of three-dimensional simulation are limited to LES (large eddy simulation) modeling of burners with simple geometry or RANS (Reynolds-averaged Navier–Stokes) modeling of real burners. The main problem of the numerical simulation of methane combustion is associated with a complex kinetic combustion scheme: detailed kinetic mechanisms (DKM) contain hundreds of elementary reactions, which prevents of DKM using for combustion modeling for practical purposes. For example, the combustion of the hydrogen-oxygen mixture can be described in sufficient detail using the 19 reactions for 8 components [3], whereas methane combustion in air is best described by the GRI-Mech scheme [4,5] containing 322 reactions for 53 components [the GRI-Mech scheme was developed based on results obtained at the University of California at Berkeley, Stanford University, the University of Texas at Austin, and the SRI (Stanford Research Institute) International and sponsored by the Gas Research Institute].

For computational fluid dynamics, industrial applications optimization is an essential issue. That is obtaining adequate numerical estimations in a reasonable time under conditions of limited computing resources and minimizing computational time. Therefore, simplified kinetic schemes consisting of several reactions so-called global kinetic schemes are applied in practice. Such schemes can significantly reduce the time and computing resources providing sufficiently
accurate results. Based on the facts mentioned above, the importance to find out and apply simple and enough accurate global kinetic scheme for practical application in modern CFD (computational fluid dynamics) software is beyond doubt.

Nowadays, a number of world-renowned scientific groups are engaged in the research devoted to the reduction and improvement of methane combustion kinetic schemes. A lot of scientific works are devoted to investigations of multiple schemes implemented for various experimental conditions: laminar and turbulent flames, sub- and supersonic reacting flows, processes in internal combustion engines, and flame propagation in an enclosed volume. As usual, the new or adjusted schemes are compared to existing schemes and experimental data. Among the best well-known schemes by Lindstedt and Jones [6], Westbrook and Dryer [7], Peters [8], Andersen [9] and [10] should be mentioned. For sure, all mentioned schemes have certain limitations on applicability according to the conditions (limited range of pressure, temperature, and mixture composition), processes (for example, laminar combustion, ignition), but despite this, such schemes are actively used both for practical simulations and for scientific purposes.

To study the fundamental issues of combustion, for example, the influence of gravity forces, by experimental methods, significant resources are required. Since such experimental studies are required zero-gravity conditions, it is necessary to carry out the study either in parabolic flights, or using vacuum-dynamic stands of the Drop tower type, or in the International Space Station. All experiments under such specific conditions are “custom-made” and require careful preparation and preliminary verification, including numerical methods. Hence, there is a need to develop a methodology for high-precision numerical modeling of such processes. At the same time, minimizing the resources spent.

Bunsen (conical) flames are most commonly used in basic combustion research. Previously, the author experimentally studied the methane–air combustion under conditions gravitationally different from those on Earth [11–13]. Numerical simulation during the experiments preparations was carried out using the FlowVision software package and the built-in single-step methane combustion scheme. Such a scheme shows fairly good agreement of numerical results and experimental data according to the flame oscillation frequency [14], while the flame height, and, respectively the flame front velocity, do not. This, in turn, affects the heat release, and leads to inaccuracies and even the impossibility of modeling, for example, some types of instabilities in the flame. For example, flame instabilities that occur during the transition from normal gravity to zero gravity with a single-step combustion scheme are not simulated well enough. For the successful simulation of such processes, for the first time, the multi-step methane combustion kinetic scheme was introduced to the FlowVision software. The paper presents the results of a comparison of modelling conical methane–air flame using the kinetic schemes of Boudier (SM-2 [15,16]), a single-step scheme built into FlowVision and experimental data. It is worth noting the value of research concerning further development and improvement of software systems for numerical simulation used in industry.

2. The parameters of numerical method
Detailed simulation was carried out using the finite element method using the software package FlowVision. FlowVision is a modern Russian software package designed for numerical modeling of fluid and gas flows based on the solution of the Navier–Stokes equations by finite-volume approximation. The complex implements capabilities of modeling flows from incompressible to hypersonic, with turbulence, heat and mass transfer, multiphase, reacting flows, including on a tunable computational grid, using both conventional PCs (personal computers) and distributed cluster (including hybrid) computing systems [17].

The flame was formed in a conical-type burner with a $D_{in} = 30$ mm inlet and $D_{out} = 15$ mm output diameter. The nozzle parameters were selected in order to provide a velocity profile at the nozzle outlet section close to rectangular. The conical flame was stabilized due to the effect
of the ring at the nozzle outlet. The inner ring diameter was 10 mm. The burner geometry was identical to the experimental conditions. The numerical domain was a cylinder with height and diameter of 140 mm and 110 mm, respectively, chosen sufficiently large to avoid the influence of the walls on the reacting flow. The computational domain was filled with air (in case of two-step kinetics: oxygen and nitrogen mass fraction—0.2333 and 0.7667 respectively) under the normal conditions: temperature—298 K, pressure—101 000 Pa. A geometric model of the computational domain indicating the types of boundary conditions and a grid model is shown in figure 1. Nozzle walls, stabilizer, bottom, and sidewall were the adiabatic no-sleep wall boundary. The top wall of the numerical domain was a free stream pressure outlet boundary. The burner inlet boundary conditions were the following: mass flow rate—0.225 kg/(m$^2$s), methane mass fraction—0.055; in case of two-step kinetics: oxygen and nitrogen mass fraction—0.2205 and 0.7245 respectively. The non-uniform unstructured grid model was built from a structured grid 26×20×20 cells using grid adaptation (up to 6 orders of magnitude) in the near-wall, bluff-body, flame front and vortex regions. The final grid has more than 2.6 million of cells. Gravity had an opposite direction to the main flow. The simulation was performed before the establishment of functional discrepancies of the order of 10$^{-4}$.

3. Government equations

A complete system of Navier–Stokes equations for a viscous compressible gas was simulated:

$$
\frac{\partial \rho}{\partial t} + \nabla (\rho V) = 0,
$$

$$
\frac{\partial \rho V}{\partial t} + \nabla (\rho V \otimes V) = -\nabla P + \nabla \cdot \hat{\tau}_{\text{eff}} + F,
$$

$$
\hat{\tau}_{\text{eff}} = \mu \left( 2\hat{S} - \frac{2}{3}(\nabla \cdot V)\hat{I} \right),
$$

$$
S_{ij} = \frac{1}{2} \left( \frac{\partial V_j}{\partial x_i} + \frac{\partial V_i}{\partial x_j} \right),
$$

$$
F = (\rho - \rho_{\text{hyd}})g,
$$

where $\hat{\tau}_{\text{eff}}$ is the viscous stress tensor; $\hat{S}$ is the strain rate tensor; $\hat{I}$ is the unit tensor.
The equations of state for the components corresponded to the ideal gas model. The energy equation was following:

$$\frac{\partial (\rho H)}{\partial t} + \nabla (\rho \nabla H) = \frac{\partial P}{\partial t} + \rho \nabla F - \nabla \cdot J_q + Q,$$

$$J_q = -\lambda \nabla T + \sum_{i=\text{species}} h_i J_i = -\frac{\lambda}{C_p} (\nabla H - \nabla (\nabla \cdot V)) + \frac{\lambda}{C_p} (1 - L_e) \sum_{i=\text{species}} h_i \nabla Y_i,$$

where $J_q$ is the heat-flux density; $L_e$ is the Lewis number; $h$ is the thermodynamics enthalpy; $J_i$ is the diffusion flux for $i$-component; $Q$ is the volumetric heat release from the source of ignition. The simulation was performed without using a turbulence mode, due to a laminar premixed flame was used for test simulation—Re = 800. To solve the system of linear algebraic equations, the implicit unconstrained second-order accuracy numerical scheme was used.

4. Kinetic mechanisms

4.1. Built-in single-step kinetics

A simple single-stage combustion scheme was employed using three components: methane, air and combustion products. The stoichiometric coefficient for fuel was taken to be 1; for an oxidizer—17.167; for products—18.167.

Therefore the reaction equation was \( \text{CH}_4 + 17.167\text{Air} \rightarrow 18.167\text{”combustion products”} \). One of the “Physical processes” unit—“Combustion”—was used to solve the system of equations described below [18]. The ignition temperature of the mixture was taken equal to 923 K. For fuel component, convective diffusion equations were solved: homogeneous 8—for the restored fuel mass fraction $Y_f^*$ and inhomogeneous 9—for the real fuel mass fraction $Y_f$:

$$\frac{\partial (\rho Y_f^*)}{\partial t} + \nabla \cdot (\rho Y_f^* V) + \nabla \cdot J_f^* = 0,$$

$$\frac{\partial (\rho Y_f)}{\partial t} + \nabla \cdot (\rho Y_f V) + \nabla \cdot J_f = -Q_f,$$

where the source $Q_f$ were expressed according to the Arrhenius equation:

$$Q_f = AT_{\text{abs}}^{n_f} \exp[-E_a/(RT_{\text{abs}})] \rho^{2-n_f} Y_f^n o Y_o^{n_o},$$

where $n_f$ and $n_o$ are reaction orders. The oxidizer and products real mass fractions $Y_o$ and $Y_p$ were determined as follows:

$$Y_o = \begin{cases} Y_o^* - i_o \Delta f, & \text{if } Y_o^* > i_o \Delta f, \\ 0, & \text{else} \end{cases},$$

$$Y_p = Y_p^* + i_p \Delta f,$$

where $

$$\Delta f = Y_f^* - Y_f.$$

The temperature is found using the following equation:

$$h(T) = \sum_{i=1}^{N} h_i(T) Y_i,$$

where

$$h_i(T_{\text{abs}}) = h_0(298.15) + \int_{298.15}^{T_{\text{abs}}} C_p(T) dT.$$

The data for kinetic mechanics is represented in table 1.

The equations of state for the components corresponded to the ideal gas model. The energy equation was following:
Table 1. Built-in reaction details. The data are represented in SI: m, s, J, mol.

| Reaction                                | A   | n  | $E_a/R$ |
|-----------------------------------------|-----|----|---------|
| $\text{CH}_4 + \text{O}_2 \rightarrow \text{"reaction products"}$ | 1010 | 0  | 18400   |

Table 2. Boudier’s reaction details [16]. The data are represented in SI: m, s, J, mol.

| Reaction                                | $A$           | $n$ | $E_a/R$ | Reaction order |
|-----------------------------------------|---------------|-----|---------|----------------|
| $\text{CH}_4 + 0.5\text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$ | $2 \times 10^9$ | 0   | 17612.8 | $[\text{CH}_4]^{0.9} [\text{O}_2]^{1.1}$ |
| $\text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2$ | $2 \times 10^8$ | 0   | 6038.7  | $[\text{CO}]^1 [\text{O}_2]^{0.5}$ |
| $\text{CO}_2 \rightarrow \text{CO} + 0.5\text{O}_2$ | $8.1104 \times 10^{10}$ | 0   | 38845.8 | $[\text{CO}_2]^{1}$ |

For the “Combustion” unit the ignition was performed by using an “Ignition modifier” in a cylindrical region near the nozzle edge. This modifier temporarily replaces the Arrhenius heat release model for a model of infinite burning velocity (Zeldovich model) including cancel of the burning limits. During the ignition, the time step was taken equal to Courant–Friedrichs–Lewy condition CFL = 50. Such a modifier was used for 4 steps, after which the ignition was turned modifier action was canceled, and the step gradually decreased to CFL = 10.

4.2. Boudier’s two-step kinetics
The unit “Chemistry” was used to solve the system of equations described below for introducing a kinetic mechanism for simulation combustion of methane–air mixture.

For each substance $i$, the following equation was solved:

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho Y_i \mathbf{V}) + \nabla \cdot \mathbf{J}_i = m_i (-W_- + W_+),$$ (16)

where $W_-$ is the summ of reaction rates where $i$-substance is the reactant, $W_+$ is the summ of reaction rates where $i$-substance is the reaction product.

The global two-step reaction mechanism by Boudier [15,16,19] was used. It reproduces GRI-Mech flame speeds for various equivalence ratios very well. The details of two-step mechanism are shown in table 2. The kinetic parameters were taken in [16].

For the “Chemistry” unit, the ignition was performed with a temporarily increase of $T$ up to 1600 K. During the ignition process the time step was taken equal to CFL = 0.5. After the flame front formation similar to the experimental one, the nozzle edge ceased to be used as an ignition source and the temperature boundary condition changed to a “zero gradient”. After that, the CFL value gradually increased up to 10.

5. Results
Figure 2 illustrates the temperature fields for the case of using the integrated kinetic scheme [see figure 2(a)], and two-step Bordier’s scheme [see figure 2(b)]. A photograph of the flame chemoluminescence from [14] is also shown for illustrative purposes in figure 2(c). This image was obtained [14] using a high-speed Phantom CCD (charge-coupled device) camera with LaVision uv lens (a bandwidth > 90% in the range of 250–410 nm). The red line shows the position of the nozzle outlet cross-section. Significant temperature values differences for various schemes
Figure 2. Temperature fields for (a) the single-step and (b) two-step reaction schemes; (c) a chemiluminescence image from the experiment.

Figure 3. Flame axis profiles: A—chemiluminescence intensity; B—temperature in the case of two-step reaction scheme; C—temperature in the case of integrated single-step reaction scheme.

can be observed. In the case of using built-in single-step scheme, the maximum temperature region is located above the flame tip, the temperature is 1986 K. In the case of CM2 scheme the temperature value is 1844 K. The temperature is presented relative to the initial conditions—298 K. It corresponds to 2142 and 2282 K for built-in scheme and two-step one in absolute terms, respectively. An experimental data for an open stoichiometric methane–air flame having similar, but not identical geometric parameters, [20], show that a temperature maximum reaches 2008.1 K at the flame tip region. Thus, it worth noting that a simulation, based on CM2 kinetic scheme, giving a lower temperature is more correct.

Figure 3 shows the temperature profiles along the nozzle axis for simulation based on CM2 scheme (profile B) and on built-in one (profile C), the data are shown in Kelvins relative to the initial conditions—298 K. The position of a flame front tip for numerical results was chosen as
coordinate of the maximum temperature region. For the single-step scheme, this value equals to 17.7 mm. For the Baudier’s scheme—13.2 mm. For experimental data, a flame front position was determined as the position of maximum intensity pixels. Using a set of filters a flame front was detected as a one-pixel width curve: a cone with a rounded tip. A more detailed description of the front position procedure determination and dynamics is shown [21]. Based on the processed flame chemoluminescence image, the position of the flame symmetry axis was found. Based on the original chemoluminescence image a chemoluminescence intensity profile along the nozzle axis was plotted in figure 3 (profile A), the data are presented in arbitrary units (a.u.). Therefore an experimental flame front height is equal to 14.5 mm. Based on the results, mentioned above, it can be concluded that the flame front height is reproduced much better in the case of using Bordier’s kinetic scheme, compared to the built-in scheme. Although there are some discrepancies with the experimental results. This shows the necessity of more detailed kinetic schemes application to get more precise results.

6. Conclusions

The work is devoted to the integration of two-step kinetic scheme of methane combustion in the air under normal conditions into the FlowVision software. An important stage of this work is the development of the methodology for calculating such processes. It should be noted that a significant difference between the use of this method of describing combustion in the FlowVision software package from the built-in “Combustion” unit is a decrease in the time step by 2 orders of magnitude during the ignition process. A comparative analysis of the laminar conical flame simulation using built-in kinetic scheme and two-step scheme showed that the use of the Baudier’s scheme allows obtaining the temperature distribution and, respectively, the flame shape closer to experimental ones.

Acknowledgments

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References

[1] Zavialov I, Varov A, Salikhov R, Antsiferov E and Konyukhov A 2018 J. Porous Media 21 887–93
[2] Konyukhov A and Zavialov I 2016 J. Phys.: Conf. Ser. 774 012059
[3] Kério A et al. 2013 Combust. Flame 160 995–1011
[4] Smith G P, Tao Y and Wang H 2016 FFCM-1 URL http://nanoenergy.stanford.edu/ffcm1
[5] Smith G P et al GRI-Mech 3.0 URL http://www.me.berkeley.edu/gri_mech/
[6] Jones W P and Lindstedt R P 1988 Combust. Flame 73 233–49
[7] Westbrook C K and Dryer F L 1981 Combust. Sci. Technol. 27 31–43
[8] Peters N 1985 Numerical and asymptotic analysis of systematically reduced reaction schemes for hydrocarbon flames Numerical Simulation of Combustion Phenomena (Springer) pp 90–109
[9] Andersen J, Rasmussen C L, Giselsson T and Glarborg P 2009 Energy Fuels 23 1379–89
[10] Pryor O M, Vasu S, Lu X, Freed D and Forrest B 2018 Development of a global mechanism for oxy-methane combustion in a CO2 environment Proc. of the ASME Turbo Expo 2018: Turbomachinery Technical Conf. and Exposition vol 9
[11] Krikunova A I and Son E E 2018 Microgravity Sci. Technol. 30 377–82
[12] Krikunova A 2018 MATEC Web Conf. 209 00005
[13] Krikunova A I 2019 High Temp. 57 430–7
[14] Krikunova A I and Son E E 2018 High Temp. 56 84–91
[15] Bihrzycki J and Poinot T 2010 Arch. Combust. 30 287–96
[16] Acampora L and Marra F 2017 Chemical Engineering Transactions 57 1459–64
[17] Aksenov A A 2017 Computer Research and Modeling 9 5–20
[18] Markova T and Juklov S 2012 Razvitiye modeley goreniya v PK FlowVision Inzhenernye Sistemi—2012: Trudy Mezhdunarodnogo Foruma (Moscow: MAKS Press) pp 89–95
[19] Boudier G 2007 Methane/air flame with 2-step chemistry: 2S-CH4-CM2 Report (CERFACS)
[20] Ashrafi Z N, Ashjaee M and Askari M 2015 Opt. Commun. 341 55–63
[21] Krikunova A 2019 Phys. Fluids 31 123607