Verification, Validation and Testing of Kinetic Models of Hydrogen Combustion in Fluid Dynamic Computations

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Abstract

A one-step, a two-step, an abridged, a skeletal and three detailed kinetic schemes of hydrogen oxidation have been tested in CFD simulations. A new skeletal kinetic scheme of hydrogen oxidation has been developed. The CFD calculations were carried out using ANSYS CFX software. Ignition delay times and speeds of flames were derived from the computational results. The computational data obtained using ANSYS CFX and CHEMKIN, and experimental data were compared. The precision, reliability, and range of validity of the kinetic schemes in CFD simulations were estimated. The impact of kinetic scheme on the results of computations was discussed. The relationship between grid spacing, timestep, accuracy, and computational cost were analyzed.

1. Introduction

The processes of verification and validation are very important in CFD [1]. They are ground steps in obtaining a numerical solution. By verification we check that we solve the equations right while through valiadation we prove that we solve the right equations. Normally, the whole numerical model, which includes equations of fluid dynamics, equation of state and the model of turbulence, is already verified by the developer of the CFD code and the user should verify only its own user defined models. Our ultimate aim is the modelling of the flow in a rocket combustion chamber. In such case we cannot rely on the predefined numerical model, but should use the models which takes into account the specifics of this complicated case. Here we are focusing on the usage of the chemical kinetic models of hydrogen combustion. In the most cases the assumption of thin flame (infinitely fast chemical reactions) gives reliable results, so there is no actual need of the use of kinetic mechanisms in CFD simulations. However, the assumption of thin flame is not completely satisfied in rocket combustion chamber where the turbulence is very high. By this reason the model of the chemical kinetics should be used for the modelling of the combustion in rocket engine, but before the model should be verified and validated.

In our case the verification can be done by the comparison with CHEMKIN [2] which solves a system of kinetic equations. This gives us a chance to find (eliminate) misprints and to prove that the numerical parameters like time-step and grid do not determine the solution. The next step should be the validation. After entering into a CFD code a chemical kinetic model became a part of large physical–chemical numerical model. Generally, kinetic mechanisms are already validated extensively by their authors, but in CFD codes a chemical kinetic mechanism should be validated in the conjunction with the other submodels of the numerical model. Of course chemical reactions drive combustion, but indeed combustion processes depend on heat and mass transfer too. Although turbulence model, equations of state, transport coefficients, chemical kinetic mechanism can be validated separately, the resulting physical–chemical model needs the final validation as a whole.

Probably the first example of the verification and the validation of hydrogen reaction mechanism in CFD simulations is the work by Mani *et al.* [3]. Supersonic flow in a constant-area channel was simulated. The employed kinetic scheme consisted of 8 reactions without kinetics of peroxides. Supersonic combustion of hydrogen–air mixture at high temperature was modelled. The simple kinetic scheme reproduced experimental data properly, what is expected when the initial temperature is about 1400 K.

While there examples of successful verification, validation and application of hydrogen reaction mechanisms in CFD simulation of supersonic combustion ramjet [4–6], the problem of CFD simulation of hydrogen combustion in rocket engine is not closed. Scramjet is a specific case and the results obtained for supersonic combustion cannot be extended over the case of rocket engine. Combustion in rocket engine has its own characteristic features: high pressures (50–250 atm), the wide span of temperatures from 100 K to 3500 K, the absence of dilutant (nitrogen). In the case of scramjet verification and validation can be done by simulating supersonic combustion directly what is not possible in case of combustion in rocket engine yet. In recent work [7] the group of researchers from five research centres made the CFD simulations of a flow in the combustion chamber. The each participant of the project modelled the same object using own methodology. It was the sub-scale rocket engine with 1.5 inch inner diameter, with one co-axial injector. The combustion chamber had an axial symmetry, which allowed to carry out the comparison of 2D and 3D modelling. The authors compared steady Reynolds–Average Navier–Stockes (RANS), unsteady Reynolds–Average Navier–Stockes (URANS) and three different Large Eddy Simulation (LES) models with the experiment. The comparison showed that all approaches give the noticeably different results and only in one case (LES — stochastic reconstruction model) the obtained results were comparable with experimental data. Indeed the most precise modelling results were obtained with the finest mesh of $255 \cdot 10^6$ cells and using the highest computational power of 2 million cumulative CPU hours. However at the current moment it is not totally clear how the initial model assumptions affected the accuracy of the final results, and what assumption or parameter impaired the other models. Such comparison is very important from the practical point of view because the computational cost and precision vary strongly from one numerical model to another.

The performance of chemical kinetic models of hydrogen oxidation in CFD simulation has been estimated in the current work. The aims of the work are the ranking of the selected hydrogen kinetic models, the development of the verification, validation and ranking procedures. In the current work the performance of the kinetic models are assessed using the experimental data on hydrogen ignition [8] and hydrogen flame [9]. CFD simulations are carried out using complex physical models. The simulations have a secondary aim to estimate the validity region within the space of the computational parameters: mesh, computational scheme, time step. The precision (difference between calculations and experiments) and the computational cost (required CPU time) were estimated on the each test. Global reaction model [10], two-step scheme [11], abridged Jachimowski's model [6], a new skeletal mechanism, three detailed hydrogen mechanisms [12–14] have been tested. Thus the results of the work should show what chemical kinetic model should be used, at which parameters the model should be used, how much computing power it is necessary to have for the fulfilment of a task. The further development of the current work should be the CFD modelling of the experiments carried out at our test facility [15, 16].

2. Skeletal kinetic model

In this work the skeletal kinetic scheme was developed, which has the same set of species as detailed hydrogen mechanisms, but the reduced set of reaction. This light scheme speeded up the formulation of the computational problem. The problem definition required to perform a certain set of the calculations. Different meshes and models of diffusion and thermal conductivity were tried before getting the final results. The light skeletal scheme reduced the amount of the expended CPU hours at the preliminary stage. The new scheme fills the gap between abridged Jachimowski's model [6], which has 7 reactions and 6 species, and detailed hydrogen mechanisms [12–14] (19–21 reactions, 8 species and bath gases) as well as it allows to separate the influence of the amount of reactions and species.

The new scheme was developed from the skeletal model by Kreutz and Law [17]. Their skeletal kinetic model has 9 unidirectional reactions and 8 species. Considering H_2/O_2 system it may assume that the set of 9 species: H_2, O_2, H_2O, H, O, OH, HO_2, H_2O_2 and bath gas is complete and other species (O_3, OH^-, $OH^*(A)$, etc.) can play role only in marginal cases. It is necessary to note that at high pressures, what is the case of rocket combustion chambers, chain branching proceeds via the formation of HO_2, H_2O_2 radicals due to the high rates of recombination processes [20]. For example, reaction R1, which is the most important in atmospheric hydrogen flames, is suppressed by reaction R9 at pressures above 50 bar. The model by Kreutz and Law [17] has a 5 times smaller set of reactions as detailed hydrogen mechanisms and can adequately predict ignition delay time and ignition limits. On the other hand the scheme consists of the irreversible reactions, which means that the concentrations of species never reach the equilibrium state. The afterburning processes are omitted, which is not important during ignition, but leads the mispredictions of species profiles. By these reason the reaction set was extended by 6 reactions from detailed hydrogen model [14]. The reaction of the quadratic recombination of HO_2 radicals

$$HO_2 + HO_2 \longrightarrow H_2O_2 + O_2$$

was substituted by reactions R11 and R13, see Tables 1, 2. Such extension increases the computational weight of the model, but it increases the adequacy of the model as well. The new added reactions involve the processes of radical recombinations, which are important in post flame zone.

Table 1: New skeletal mechanism.

Ref. No	Reaction	A^*	n	E_a	Ref.
R1	$H + O_2 \longrightarrow OH + O$	1.91e+14	0.0	16.44	[17]
R2	$H_2 + O \longrightarrow H + OH_2$	5.08e+4	2.67	6.292	[17]
R3	$H_2 + OH \longrightarrow H + H_2O$	2.16e+8	1.51	3.43	[17]
R5	$H_2 + M \longleftrightarrow H + H + M$	4.57e+19	-1.4	105.1	[14]
R6	$O + O + M \longleftrightarrow O_2 + M$	6.17e+15	-0.5	0.0	[14]
R7	$H + O + M \longrightarrow OH + M$	4.72e+18	-1.0	0.0	[14]
R8	$H + OH + M \longrightarrow H_2O + M$	4.5e+22	-2.0	0.0	[14]
R9	$H + O_2 + M \longrightarrow HO_2 + M$	6.17e+9	-1.42	0.0	[17]
R10	$H + HO_2 \longrightarrow H_2 + O_2$	1.66e+13	0.0	0.82	[14]
R-10	$H_2 + O_2 \longrightarrow H + HO_2$	3.68e+13	0.203	54.46	[17]
R11	$H + HO_2 \longrightarrow OH + OH$	1.69e+14	0.0	0.87	[17]
R13	$OH + HO_2 \longrightarrow H_2O + O_2$	2.89e+13	0.0	-0.5	[14]
R15	$H_2O_2 + M \longrightarrow OH + OH + M$	1.2e+17	0.0	45.5	[17]
R-17	$H_2 + HO_2 \longrightarrow H + H_2O_2$	3.42e+12	0.202	27.12	[17]

* $k = A \cdot T^n \cdot \exp(-E_a/RT)$; units: mol, cm^3, K, kcal; thermodynamic data [2]; the reverse rate constants (R5, R6) are calculated from the forward rate constants through the equilibrium constants.

Table 2: Efficiency factors for third body term.

Ref. No	H	H_2	H_2O	H_2O_2	HO_2	O	O_2	OH
R5	1.0	2.5	12	1.0	1.0	1.0	1.0	1.0
R6	0.83	2.5	12	1.0	1.0	0.83	1.0	1.0
R7	0.75	2.5	12	1.0	1.0	0.75	1.0	1.0
R8	1.0	0.73	12	1.0	1.0	1.0	1.0	1.0
R9	1.0	2.5	12	1.0	1.0	1.0	1.0	1.0
R15	1.0	2.5	12	1.0	1.0	1.0	1.0	1.0

3. Calculations

The CFD calculations have been done with the use of the ANSYS CFX 11 solver [18], which utilizes the Finite Volume Element Method (FVEM).Two types of tests (simulations) were done in the work. The first test case is a quasi 0-dimensional simulation of hydrogen ignition to verify and validate the models against the experimental data on ignition delay times [8]. The second test case is an 1-dimensional simulation of hydrogen flame propagation to test the models against the data on the speeds of laminar flame [9].

Ignition in perfect adiabatic constant volume reactor has been modelled The computational domain represents eighth part of the 1 mm sphere with rigid adiabatic walls. The mesh consists of 21 nodes and 38 tetrahedron elements. At the initial moment the whole domain is filled with a stoichiometric hydrogen–air ($0.79N_2$+$0.21O_2$) mixture at pressure of 1 atm and temperature in the range of 900–1400 K. The problem has been solved as a transient task, i.e. time evolution of gas conditions has been sought. The object of these calculations is the estimation of the ignition delay times and the comparison of the calculated delay times with the experimental data from shock tube [8], see Fig. 1. In the calculations the ignition delay times were defined as the time of temperature increase up to 500 K relative to the initial temperature.

During the 1D tests freely propagating hydrogen flame has been modelled. The computational domain consists of 1604 nodes and 400 rectangular prism elements. All elements are placed along one axis so that the thickness of the domain equals to one element in the two other coordinate axes. The mesh spacing equals to 5 μm in the direction of flame propagation. The separate study of the influence of grid spacing was carried out where the spacing was varied from 0.2 μm to 200 μm. The domain represents the rectangular with symmetry boundary conditions on the side walls.

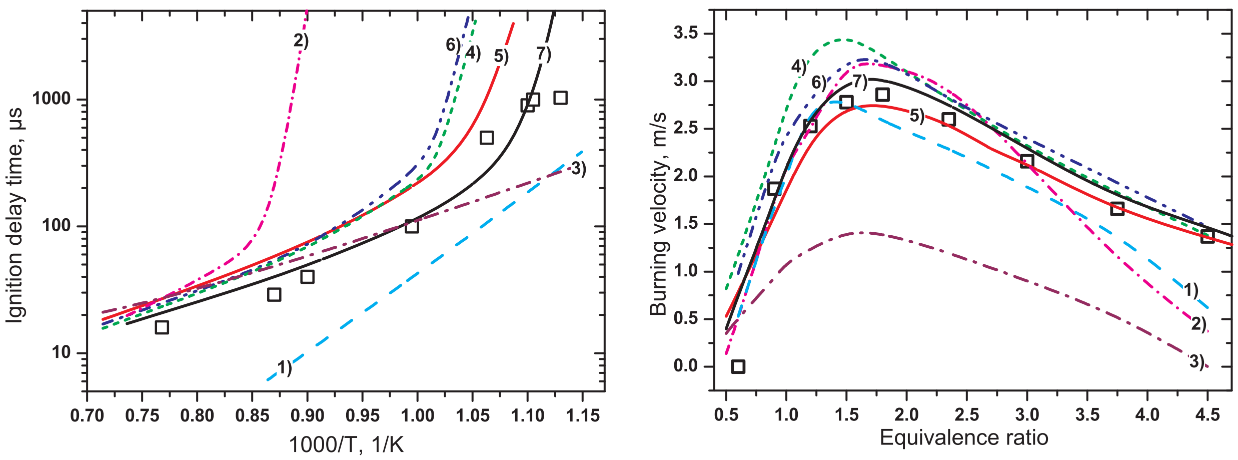

Figure 1: Ignition delay times (stoichiometric) and burning velocities of hydrogen–air mixture at 1 atm. Black squares — [8, 9]; 1) cyan dash line — Marinov et al. [10]; 2) magenta short dash dot line — Lee and Kim [11]; 3) purple dash dot line — the abridged Jachimowski's model [6]; 4) green short dash line — Zhukov (this work); 5) red solid line — O'Conaire et al. [14]; 6) blue dash dot dot line — Gutheil et al. [12]; 7) solid black line (closest to exp. data) — Konnov [13].

The domain has one inlet and one outlet (on the side opposite to inlet). At the outlet static pressure is specified and equals to 1 atm. At the inlet a hydrogen–air ($0.79N_2$+$0.21O_2$) mixture at 298 K and 1 atm flows inside the domain. The velocity of the mixture is specified at the inlet in the range of 0.5–3.5 m/s so that the velocity of the flame front reaches a small value in the laboratory system of coordinates. The mixture composition was varied from equivalence ratio of ER = 0.5 to ER = 4.5. The simulations were run as a transient task. Stationary burning velocity was sought. Speed of flame depends essentially on the transport properties of gas, so the temperature dependent thermal conductivity and diffusion coefficients were used. Thermal diffusion was not taken into account.

4. Results and discussion

4.1 Verification. Comparison with CHEMKIN.

Both tasks were also solved in CHEMKIN II [2]. The results of the simulations with the help of CHEMKIN were used as a reference data and helped to eliminate the errors in the definitions. During the calculations with ANSYS CFX the same equations were employed for the rate constants, the thermodynamic functions and the equations of states. The results of the simulations is depicted in Fig. 2, where ANSYS CFX shows the good agreement with CHEMKIN after eliminating of the errors. Indeed it is necessary to note that CFX solves the 3-dimensional Navier–Stokes equations while CHEMKIN uses the 0-dimensional equation of energy conservation or 1-dimensional equations in the case of the modelling of flame propagation.

In the case of freely propagating laminar flame Zeldovich–Frank-Kamenetskii equation, which connects flame velocity and reactivity, gives us a clear view on the problem:

$$u_{lam} = \sqrt{\frac{\alpha}{\tau}}, \tag{1}$$

where τ is the chemical time scale in reaction zone, and α is the coefficient of temperature conductivity, which summarizes the effect of diffusion and heat conductivity through Lewis number $Le = 1$. In contrast to the previous case kinetic and transport properties have an equal importance in flame propagation.

The flame speeds were estimated using ANSYS CFX and PREMIX [19] (subroutine of the CHEMKIN), Fig. 2. The same temperature depended coefficients of thermal conductivity, viscosity and binary diffusion were used in PREMIX and ANSYS CFX, but diffusion fluxes in multicomponent mixture were approximated by different ways.

By default ANSYS CFX estimates the coefficient of thermal conductivity and viscosity of gas mixture using mass averaging, and the coefficients of diffusion are calculated from the mixture bulk viscosity. The problem becomes

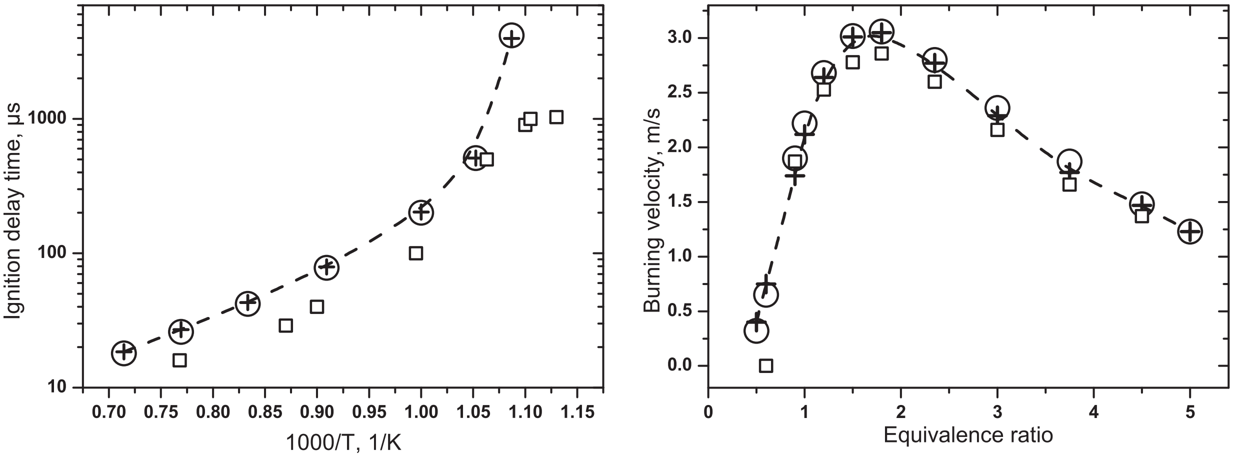

Figure 2: Comparison of the simulating data obtained using ANSYS CFX and CHEMKIN. Squares — the experimental ignition delay times of a stoichiometric hydrogen–air mixture at 1 atm [8] and burning velocities of a hydrogen–air mixture at 1 atm and 298 K [9]; the kinetic model by O'Conaire et al. [14]: dash line (B-spline) and crosses — ANSYS CFX, big circles — CHEMKIN.

significant in the case of combustion in rocket engine where the mixture is not diluted by nitrogen. This problem can be resolved in ANSYS CFX using CFX Expression Language (CEL) by defining the transport properties through the user expressions.

In the current work the diffusion coefficients are calculated by the empirical formula

$$D_i = \frac{1 - w_j}{\sum X_j / D_{ij}}, \tag{2}$$

where w_i is the mass fraction of i-species; X_j is the mole fraction of j-species; D_{ij} is the binary diffusion coefficient. After that the diffusion coefficients of individual species are put into the equation which is responsible for transport in CFX:

$$\rho_i(U_{mix} - U_i) = -\frac{D_i}{\rho_{mix}} \frac{\partial \rho}{\partial x}, \tag{3}$$

where $\rho_i(U_{mix} - U_i)$ is the relative mass flux of i-species. The equation is not solved for one constraint component (in our case nitrogen), whose mass fraction is calculated from the constraint that the sum of mass fractions of all species equals to 1. PREMIX (CHEMKIN) uses a more accurate definitions of the diffusion and thermal conductivity in gas mixture, and takes into account the thermal diffusion of H and H_2. "Mixture-averaged" option, which was used here in PREMIX, employs eq. (2), but does not have a constraint species. In this case PREMIX employs an additional term — correction velocity, which makes the net species diffusion flux equal to zero.

The flame velocities obtained with the use of CFX and CHEMKIN coincide practically with each other. The difference in the results, which is small (Fig. 2), should be associated with the distinction in the formulation of the diffusion fluxes. Coffee and Heimerl [21] compared various methods of approximating transport properties of premixed laminar flames, in particular the methods which have been used in CFX and CHEMKIN. They found that the difference in flame speed is small for these methods, but the method, which is employed in CHEMKIN, is more accurate than the method with constrained species (CFX), which is inaccurate in computing the diffusion velocity for constrained species. As for the comparison with experimental data it was shown in recent work [22] that such small overshooting around the stoichiometry, which is observed on Fig. 2, results from the neglecting Soret effect (thermodiffusion).

4.2 Validation and testing

Let us consider the results of the first "0D" test case, which is depicted in Fig. 1. The detailed models [12–14] agree with experimental data well, while non-detailed kinetic models [10, 11], abridged Jachimowski's model [6] and the new skeletal model have the agreement with experimental data only in the limited range. On the graph it is possible to see the transition from high–temperature ignition to low–temperature ignition around 950 K. The only kinetic model by

Konnov [13] agrees with experimental data below 1000 K, but its validity below 900 K is also questionable. Generally the models show the common trend: more details — higher accuracy. This conclusion is supported by the results of the 1D test case too. It is possible to conclude from the results that one or two reactions are not enough to describe the ignition of hydrogen. Probably the sophistication of abridged Jachimowski's model (7 reactions and H, O, OH as intermediates) is a reasonable minimum for the modelling of hydrogen combustion in the high temperature region ($T > 1000\,\mathrm{K}$). For the modelling in a wide temperature range the formation of H_2O_2 and HO_2 should be taken into account.

In the 1D test case the agreement of simulating data with experimental data is better in sum than in the "ignition" case, see Fig. 1. Practically all models agree with experimental data. The other distinctive feature of the obtained results is the bad agreement of abridged Jachimowski's model [6] and the good agreement of one-step model [10]. The results of 1D simulations can be interpret in terms of eq. (1). Abridged Jachimowski's model [6] is significantly slower at high temperatures ($T_{flame} \approx 2000$ K) which means the lower burning velocity. As for one-step model [10], which is the fastest at high temperatures, it does not include atomic hydrogen. In this case the fast kinetics is compensated by the "slower" transport (the flame propagates only by thermal conductivity).

Numerical parameters such as time step, grid spacing, type of difference scheme, etc. should not determine the results of modelling. The proper values of time step and grid spacing should correspond via the coefficients of physical model to the physical time and space scales. On practical ground the upper limits of time step and grid spacing are more important, because computational cost is generally inversely proportional to timestep and amount of nodes (for the employed grid the amount of nodes is reciprocally proportional to the grid spacing), see Fig. 3. The employed values of time step and grid spacing are normally close to the upper limit. The upper limit is quite specific to the details of a task. It is necessary to estimate the maximum time and mesh steps in each case separately. At too high time step the solution diverges. Numerical noise and residuals can be used as the measure of the proximity to the upper limit of time step. In this work the adaptive time step has been used and it has been defined by the residual. The time step was decreased or increased until the value of the residuals reached the desired level. To estimate the upper limit of mesh step several simulations were carried out with different spacing, see Fig. 3. On the plot we can see a plateau for cell size below 5 μm. The upper limit, which is located near 10 μm, is related to the flame thickness. In flame front the concentration of hydrogen increases in 2–4 times each 10 μm. The maximum grid spacing is universal for all hydrogen–air flames at 1 atm and is defined by the transport properties and reactivity of the system while the maximum time step is individual for each kinetic model.

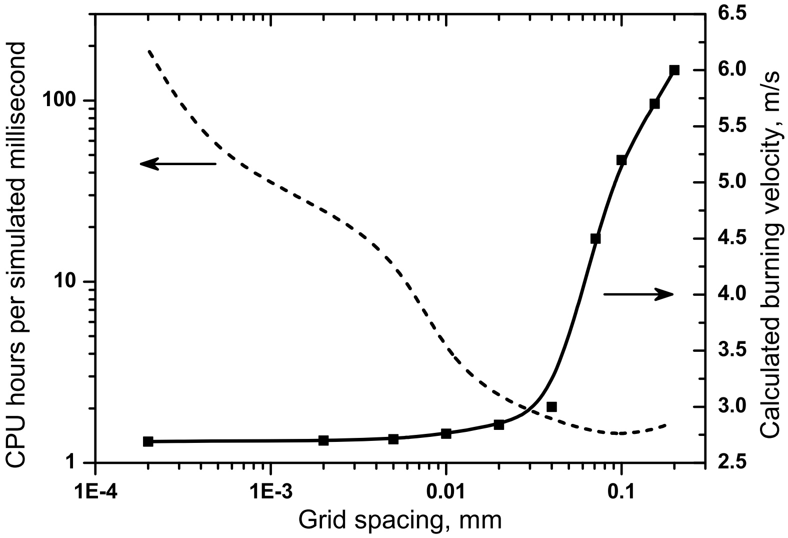

Figure 3: Simulating results and computational cost as the function of grid spacing. A hydrogen–air mixture at 1 atm, kinetic model by Zhukov (this work).

Grid spacing, the physical dimensions of computational domain and computational cost are connected with each other. At these conditions grid spacing can limit the applicability of kinetic model. In Table 3 the computational costs, which are required for the simulation of the evolution of the system during 1 ms on 1 CPU (Pentium 4) at 2 GHz, are presented for the all tested models. In the identical conditions computational cost varies by orders from one model to another. It is impossible from the data of Table 3 to see any direct connection of the computational cost with the number of reactions and species. However there is a trend: detailed kinetic models require much more computational power than reduced models. Thus the high computational cost limits the application of detailed kinetic mechanisms in CFD calculations seriously. The grid spacing has the limit near 40 μm after which simulations give absolutely unrealistic results. Detailed models can be employed only in special tasks with the computational domains of small sizes due to the high computational cost and the small grid spacing.

Table 3: Parameters of kinetic models and the computational costs (used CPU hours per 1 ms of simulation time). Case 1 — the test case "ignition", 38 cells; Case 2 — the test case "flame propagation", 400 cells.

Model	**Number of equations***	**Number of species**	**Case 1, CPU hours**	**Case 2, CPU hours**
Marinov et al. [10]	1	3 (H_2, O_2, H_2O) + N_2	0.18	0.14
Lee and Kim [11]	2	4 (3 + H) + bath gas	0.43	0.20
abridged Jachimowski's [6]	7	6 (3 + H, O, OH) + bath gas	1.7	5.2
Zhukov (this work)	13	8 + bath gas	1.6	19
Gutheil et al.[12]	21	8 + bath gas	2.5	67
O'Connaire et al. [14]	23	8 + bath gas	1.8	71
Konnov [13]	29	8 + bath gases	2.3	36

* The number of equations could exceed the number of reactions because of the possible presence of double reactions and of third-body reactions where the activation energy depends on collisional partner.

Computational cost increases strongly from global reaction models to detailed kinetic mechanisms, but the number of chemical equations and species does not completely determine the computational cost. The cost depends strongly on stiffness which is the embedded parameter of each kinetic model.

5. Conclusions

The seven different kinetic models of hydrogen oxidation were verified, validated and tested in the CFD simulations what was done using ANSYS CFX 11 software. Two cases: ignition in adiabatic constant volume reactor and propagation of free laminar flame were considered. The verification of the kinetic models was done through the comparison with the results obtained with the help of the CHEMKIN software. The verification allowed to eliminate misentries and to define correctly the thermodynamical, kinetic and transport properties.

The subsequent validation showed that the detailed kinetic schemes are more precise than the reduced. While it was not found any direct dependence between the ”speed“ of kinetic model and the number of reaction and species, the reduced kinetic scheme are faster than detailed. The simulations showed the common trend for kinetic models: more details — higher computational cost — higher precision where the detailed mechanisms requires considerable amount of the computational power. The simulation of the ignition of hydrogen–air mixture showed that the results are sensitive to the choice of kinetic model. However in the case of flame propagation the results are more sensitive to the model of the transport properties while the reasonable results can be achieved even with the use of global reaction mechanism.

The comparison of the simulating data with the experimental data [8, 9] showed that detailed kinetic schemes [13, 14] agree with experiments well, while the non-detailed schemes agree with the experiments only within a limited range. The kinetic model by Konnov [13] has the best agreement with the experimental data among the tested models. The application of reduced kinetic schemes of hydrogen combustion, which do not take into account chemical reactions with HO_2 and H_2O_2, is possible only with the strong limitations.

For the debugging purposes the new skeletal kinetic scheme was developed which represents the good compromise between the computational cost and the accuracy.

Acknowledgments

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References

[1] Roache, P.J., "Verification of Codes and Calculations," AIAA Journal, Vol. 36, No. 5, May 1998, pp. 696-702.

[2] Kee, R. J., Rupley, F. M., and Miller, J. A., "CHEMKIN-II: A Fortran Chemical Kinetics Package for the Analysis of Gas-Phase Chemical Kinetics", Sandia National Laboratories Report, SAND89–8009, 1989.

[3] Mani, M., Bush, R.H., Vogel, P.G., AIAA Paper 91-3299-CP, Jan. 1991.

[4] C.J. Jachimowski, An analytical study of hydrogen–air reaction mechanism with application to scramjet, NASA Technical Paper 2791 (1988) Feb.

[5] Gerlinger, P., Nold, K., and Aigner, M., Int. J. Numer. Meth. Fluids 2010; 62:1357–1380.

[6] Eklund D.R. ,Stouffer S.D., AIAA Paper 94–2819, 1994.

[7] P.K. Tucker, S. Menon, C.L. Merkle, J.C. Oefelein, V. Yang, 44-th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, 21–23 July 2008, Hartford, CT USA, AIAA 2008–5226.

[8] Slack, M., Grillo, A., Investigation of Hydrogen-Air Ignition Sensitized by Nitric Oxide and by Nitrogen Oxide, NASA Report CR-2896, 1977.

[9] Kwon, O.C., Faeth, G.M., Combust. Flame, 124 (2001) 590–610.

[10] Marinov, N.M., Westbrook, C.K. and Pitz, W.J., Detailed and Global Chemical Kinetic Model for Hydrogen, Transport Phenomena in Combustion Volume 1, Taylor and Francis, Washington DC, 1996.

[11] Lee, S.R., Kim, J.S., Korean J. Chem. Eng. 16(2) (1999) 253–259.

[12] Gutheil, E., Balakrishnan, M.D., Williams, F.A., "Structure and Extinction of Hydrogen-Air Diffusion Flames", Reduced Mechanisms for Application in Combustion Systems, Springer-Verlag, Berlin, Heidelberg, 1993.

[13] Konnov, A.A., Development and validation of a detailed reaction mechanism for the combustion of small hydrocarbons. 28-th Symposium (Int.) on Combustion, Edinburgh, 2000. Abstr. Symp. Pap. p. 317.

[14] M. O'Conaire, H.J. Curran, J.M. Simmie, W.J. Pitz and C.K. Westbrook, Int. J. Chem. Kinet. 36 (2004), pp. 603–622.

[15] Gurliat, O., Schmidt, V., Haidn, O.J., Oschwald, M., Aerospace Science and Technology 7 (2003) 517–531.

[16] Suslov, D., Lux, J., Haidn, O., Investigation of porous injector elements for LOX/CH4 and LOX/H2 combustion at sub- and super-critical conditions, 2nd European Conference for Aerospace Sciences 1–6 July, 2007, Brussels, Belgium.

[17] Kreutz T.G. and Law C.K., Combust. Flame, 114:436–456, 1998.

[18] ANSYS CFX, http://www.ansys.com/products/cfx.asp

[19] Kee, R.J., Grcar, J.F., Smooke, M.D., and Miller, J.A., "A Fortran Program For Modeling Steady Laminar One-Dimensional Premixed Flames", SAND89–8240, 1985.

[20] Zhukov, V. P., Combustion Theory and Modelling, 13:3, 427–442, 2009. DOI: 10.1080/13647830902767302

[21] Coffee, T.P., and Heimerl, J.M., Combust.Flame 43 (1981) 273–289.

[22] F. Yang, C.K. Law, C.J. Sung, H.Q. Zhang, Combust.Flame 157 (2010) 192–200.