Numerical Modeling of Hydrogen Combustion: Approaches and Benchmarks

Ivan Yakovenko * and Alexey Kiverin

Abstract: The paper is devoted to the analysis of two different approaches for the numerical simulation of gaseous combustion. The first one is based on a full system of Navier-Stokes equations describing the dynamics of the compressible reactive medium, while the second one utilizes low-Mach number approximation. The compressible model is realized by the traditional low-order numerical scheme and the contemporary CABARET method. The low-Mach approach is implemented on the base of a widely known FDS numerical scheme. The benefits and disadvantages of compressible and low-Mach approaches are discussed and demonstrated on a specially developed set of problem setups, applicable for validation and verification of the numerical methods for combustion analysis. In particular, the laminar flame velocity test, spherical bomb test, and multidimensional modeling of combustion development inside the rectangular closed vessel are performed via both techniques that allowed to determine the applicability limits of the low-Mach number approximation.

Keywords: numerical modeling; gaseous combustion; compressibility effects; low-Mach approximation; validation and verification

1. Introduction

Today numerical modeling became a powerful tool for complex combustion process analysis. Together with the experimental observations, computational techniques allow comprehensive investigation of various combustion modes, which can develop in volumes filled with reactive gaseous mixtures. Numerical modeling is particularly important for studying high-speed processes, such as flame acceleration and deflagration-to-detonation transition in gaseous mixtures [1,2], in complex fuels [3], and the propagation of detonation waves [4]. Determination of the mechanisms responsible for various combustion modes formation and transitions between them and prediction of the damages related to the dynamic and thermal loads associated with the combustion development is crucial for reliable combustion and explosion safety systems design and risk mitigation measures.

Despite the sufficient progress in techniques and resources available for computations, reliable combustion modeling is still a challenging problem. Tight coupling between gas-dynamic flows, chemical kinetics, and molecular transfer makes it very demanding to perform detailed numerical modeling on spatial and temporal scales characteristic for real-world applications, especially for analyzing large-scale fires or combustion within propulsion and energy devices. Model simplifications commonly used to cut computational costs include reduced or lumped chemical kinetic schemes, sub-grid turbulence models, and various approximations of the flow features. Among the latter, the low-Mach approximation is one of the most used. It allows softening restrictions on the time step related to the necessity to reproduce individual acoustic perturbations propagating with the speed of sound. Instead, the average acoustic field is calculated as a continuous distribution of the pressure perturbation. As a result, the calculation time step can be sufficiently increased, and calculations may be performed on greater spatial and temporal scales than with techniques developed for a Navier-Stokes equations system describing dynamics of
compressible medium. For today low-Mach model is extensively used for the computations of flame instability development [5,6], turbulent mixing inside a cylinder of the internal combustion engine [7], jet flames [8] and other problems. However, such an approximation has only a limited range of possible applications. High-speed reactive flow development, associated with the formation of intense shock waves and complex acoustic fields, cannot be reliably reproduced with a low-Mach approach. For these problems, it is required to fully resolve compressibility effects, such as the generation and propagation of compression and shock waves and interactions between waves, flame, and acoustic fields.

Among various computational techniques realizing low-Mach number approximation, the approach implemented in Fire Dynamics Simulator (FDS) computational package [9] proves itself very useful for modeling large-scale compartment fires [10,11]. Originally it utilized lumped species chemical kinetic scheme, LES subgrid model of turbulent combustion, and constant heat capacity of the mixture. The FDS approach was not widely utilized for comprehensive numerical simulations of combustion using detailed chemical kinetic schemes, and precise molecular transport models and real equations of state. For the first time, such calculations via FDS approach were recently performed for the analysis of the buoyancy-driven combustion in premixed ultra-lean hydrogen-air mixtures [12] and allowed determining mechanisms of the flame extinguishing due to convective flows. Here the implementation of the FDS approach for solving conservation laws on the basis of the in-house computational software NRG [13] is employed to evaluate further the capabilities of low-Mach number approximation and the FDS numerical algorithm for detailed combustion modeling. NRG package contains models for heat transfer, viscosity, multicomponent diffusion, and capability for using detailed chemical kinetic schemes. Together with the FDS approach for solving gas dynamic governing equations in low-Mach approximation, the NRG package contains the traditional low-order finite-difference method “coarse” particles method (CPM) [14] and the contemporary computational technique CABARET for solving the Navier-Stokes equation system for the compressible gaseous mixture [15,16]. CPM is a robust computational approach that allows for solving a wide range of combustion problems. However, the main drawback of this technique is a relatively high numerical dissipation. On the one side, high dissipation makes it very versatile and applicable to studying general features of different modes of gas-dynamic flows, but on the other side small-scale flow features, such as acoustic and vortical perturbations, cannot be reliably reproduced. In turn, CABARET has several distinct features making this numerical scheme highly suitable for modeling complex flows in reactive gaseous mixtures. Among the most important advantages are the compact computational stencil, convenient for high-performance computations, low dissipation and dispersion errors, and the absence of artificial flux limiting procedures.

An acute problem in the field of computational analysis of combustion is related to the reproducibility of the obtained results and methods for the evaluation of numerical schemes in terms of applicability for the reliable modeling of complex transient reactive flows. Although there is a vast amount of test problems in conventional computational fluid dynamics, there is still a lack of generally accepted approaches for validation and verification of the numerical techniques used for combustion modeling [17]. Combustion is accompanied by a large number of processes, such as molecular transport, chemical kinetics, and gas dynamics. The correctness of the reproduction of those processes can be estimated separately, but it does not guarantee the overall accuracy of the reactive flow modeling. There are attempts to establish validation and verification routines for particular combustion problems, such as gas turbine combustors modeling [18], simulation of jet flames [19], and premixed turbulent flames [20]. An overview of experimental data that can be used for validation purposes can be found in [21,22]. However, most of the experimental data and proposed validation and verification approaches are developed for complex combustion processes and particular applications. Such problems require implementing approximate subgrid turbulence models and simplified chemical kinetic schemes. Thereby correct identification of the source of discrepancies is a complicated
problem, not to mention determining their reasons. For engineering purposes, such an approach is justified, but in academic research more rigorous and controlled routines for validation and verification are required. This paper is devoted to the evaluation of the ability for combustion modeling by three numerical approaches, FDS, CPM, and CABARET, based on the proposed set of test problems with a step-by-step increase in complexity of the flow, starting from steady one-dimensional combustion and ending at non-steady multidimensional flame development. The testing methodology follows that proposed in [17] and is intended to assess possible limitations of the computational techniques and underlying physical models of hydrogen combustion.

2. Mathematical Model

A full set of Navier-Stokes equations of the multicomponent reactive hydrogen-air mixture taking into account compressibility, viscosity, heat transfer, multiphase and detailed scheme of chemical kinetics scheme [23] is solved via a contemporary CABARET numerical scheme and traditional approach CPM. Governing equations are given below:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0
\]  

(1)

\[
\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial (\rho u_i Y_k)}{\partial x_i} = \frac{\partial \left( \rho Y_k V_{kj} \right)}{\partial x_i} + \rho \dot{\omega}_k
\]  

(2)

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_i} = \left[ \frac{\partial}{\partial x_i} (\sigma_{ji} - \delta_{ij} p) \right]
\]  

(3)

\[
\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho u_i E)}{\partial x_i} = \left[ \frac{\partial}{\partial x_i} (u_i \sigma_{ji} - u_i p) \right] + \left[ \frac{\partial}{\partial x_i} (\kappa(T) \frac{\partial T}{\partial x_i}) \right] + \rho \sum_k \frac{h_k}{m_k} \left( \frac{\partial Y_k}{\partial t} \right)
\]  

(4)

\[
\sigma_{ij} = \mu(T) \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \rho}{\partial x_m} \right)
\]  

(5)

where \(x_i\)—spatial coordinates, \(t\)—time, \(\rho\)—density, \(Y_k = \rho_k / \rho\)—k-th species mass fraction, \(p\)—pressure, \(T\)—temperature, \(u_i\)—mass velocity vector, \(V_{kj}\)—k-th species diffusion velocity vector, \(E = \varepsilon + \frac{1}{2} \left( \sum_i u_i^2 \right)\)—specific total energy, \(\varepsilon\)—specific inner energy, \(\dot{\omega}_k\)—chemical source term, \(\kappa(T)\)—thermal conductivity, \(D_k(T)\)—diffusion coefficient of k-th species, \(\mu(T)\)—viscosity coefficient, \(h_k\)—enthalpy of formation of k-th species, \(m_k\)—k-th species molar mass, \(\sigma_{ij}\)—shear stress tensor components, \(\delta_{ij}\)—Kronecker delta.

Mixture averaged transport coefficients such as viscosity \(\mu(T)\), thermal conductivity \(\kappa(T)\) and diffusion \(D_k(T)\) are calculated from the first principles of the molecular kinetic theory. Mixture averaged viscosity coefficient \(\mu(T)\) is obtained as:

\[
\mu(T) = \frac{1}{2} \left[ \sum_k X_k \mu_k + \left( \sum_k \frac{X_k}{\mu_k} \right)^{-1} \right]
\]  

(6)

where \(X_k\)—molar fraction of k-th species and viscosity coefficient of k-th species \(\mu_k\) is calculated as follows [24]:

\[
\mu_k(T) = \frac{5}{16} \frac{\sqrt{\pi M_k k_B T}}{\pi \sigma_k^2 \Omega(2.2)}
\]  

(7)
where \( \Omega^{(2,2)} \)—reduced collision integral depending on reduced temperature \( T^* = k_B T/\epsilon_k \) [25], \( \sigma_k \)—collision diameter, \( M_k \)—\( k \)-th atomic (molecular) mass, \( \epsilon_k \)—Lennard-Jones potential well depth, \( k_B \)—Boltzmann constant. Values of \( \sigma_k, \epsilon_k \) were taken from transport table accompanying chemical mechanism from [26].

Mixture averaged thermal conductivity:

\[
\kappa(T) = \frac{1}{2} \left[ \sum_k X_k \kappa_k + \left( \sum_k \frac{X_k}{\kappa_k} \right)^{-1} \right]
\]

while thermal conductivity \( \kappa_k \) for each species [24]:

\[
\kappa_k(T) = \frac{25}{32} \frac{\sqrt{\pi} M_k k_B T}{\pi \sigma_k^2 \Omega^{(2,2)}} c_{V_k}
\]

Diffusion velocities were calculated via zeroth-order approximation [27]:

\[
V_{k,i}^* = \left( \frac{D_k(T)}{Y_k} \frac{\partial Y_k}{\partial x_i} \right)
\]

where mass-averaged diffusion coefficient of \( k \)-th species \( D_k \) is obtained as [28]:

\[
\frac{1}{D_k} = \sum_{j \neq k}^N \frac{X_j}{D_{kj}} + \frac{X_k}{1 - \sum_{j \neq k}^N \frac{Y_j}{D_{kj}}}
\]

where \( X_k \)—molar fraction of \( k \)-th component, \( D_{kj} \)—binary diffusion coefficient of a compound \( k \) into a compound \( j \). Binary diffusion coefficients are calculated as follows [27,28]:

\[
D_{kj} = \frac{3 \sqrt{2\pi k_B^3 T^3 / m_{kj}}}{p \pi \sigma_{kj}^2 \Omega^{(1,1)}}
\]

Diffusion velocity is corrected to satisfy \( \sum_N Y_k V_{k,i} = 0 \) [23,29] and is given by:

\[
Y_k V_{k,i} = Y_k \left( V_{k,i}^* - V_{c,i} \right) = \left( D_k(T) \frac{\partial Y_k}{\partial x_i} \right) - Y_k \sum_{N} \left( D_k(T) \frac{\partial Y_k}{\partial x_i} \right)
\]

Equations of state are based on temperature dependencies of specific enthalpies of \( k \)-th species \( h_k \) and specific constant volume heat capacities of \( k \)-th species \( c_{V_k} \), expressed in NASA polynomial form with coefficients taken from [26].

\[
p = \rho R T / \overline{M}
\]

\[
d\epsilon = c_V(T) dT
\]

where \( R \)—universal gas constant, \( \overline{M}^{-1} = \sum_k Y_k / m_k \)—the average molar mass, \( c_V = \sum_k c_{V_k} Y_k \)—specific constant volume heat capacity of the mixture, \( c_{V_k} \)—specific constant volume heat capacity of \( k \)-th species.

Balance-characteristic form of the CABARET algorithm [30] with second-order accuracy in space and time is utilized to solve the governing equations system (1)–(4). Traditional CPM approach [31] with first-order accuracy in space and second-order accuracy in time is implemented for comparison purposes and investigation of numerical viscosity effects. In both approaches, the time step is dynamically adjusted according to the Courant–Friedrichs–Lewy condition \( CFL = \Delta t \left( \frac{||u|| + c}{\Delta x} \right) < 1 \), where \( c = \sqrt{\frac{p}{\rho}} \)—velocity of sound.
The FDS approach utilizes low-Mach number approximation of the Navier-Stokes equations. According to this approximation, the total pressure $p$ is decomposed into background pressure and perturbation [32]: $p(\vec{r}, t) = \bar{p}(t) + \tilde{p}(\vec{r}, t)$. The background pressure $\bar{p}(t)$ is calculated from the equation of state (14). Perturbation pressure $\tilde{p}(\vec{r}, t)$ is obtained from the Poisson equation, derived from the momentum transport Equation (3):

$$\nabla^2 H = -\left[ \frac{\partial}{\partial t} (\nabla \cdot \vec{u}) + \nabla \cdot \vec{F} \right]$$

(16)

where $H \equiv |\vec{u}|^2/2 + \bar{p}/\rho$, $\vec{F} = -\vec{u} \times \vec{\omega} - \frac{1}{\rho} \left[\nabla \sigma_{ij} \right] - \bar{p} \nabla \left( \frac{1}{\rho} \right)$, $\vec{\omega} = \nabla \times \vec{u}$—vorticity vector.

The Equation (16) is solved via V-cycle geometric multigrid approach [33]. The overall solution procedure follows the explicit second-order predictor/corrector scheme described in [9]. The time step is adjusted dynamically based on the Courant-Friedrichs-Lewy constraint $CFL = \Delta t \left( \frac{|\vec{u}|}{Ax} + |\nabla \cdot \vec{u}| \right) < 1$. TVD transport scheme with CHARM flux limiter [34] is used for scalar transport equations.

All three numerical techniques are realized on the base of the same in-house computational software NRG. Thereby all the molecular transport models and implementation of the chemical kinetics are preserved for considered numerical methods. A detailed chemical scheme consisting of 19 reactions between 8 chemically active components is used for the hydrogen oxidation process description [26].

3. Problem Setup

Three problem setups are considered. The first one is the laminar burning velocity test, namely the determination of the laminar burning velocity via one-dimensional calculations of the planar flame. Two different approaches are used. According to the first one, flame develops in a one-dimensional semi-closed channel and propagates toward the opened end after the ignition near the closed end of the channel. The solid wall boundary condition is implemented on the left end of the computational domain and the free outflow condition is set up on the right end of the computational domain. Here laminar burning velocity $S_b$ can be obtained by tracking the flame velocity in the laboratory frame of reference $U_{f,L}$ and can be estimated as $S_b = U_{f,L} / \theta$, where expansion ratio $\theta = \rho_f / \rho_b$ is the ratio of densities of the fresh mixture $\rho_f$ and burnt products $\rho_b$. The second approach for determining laminar burning velocity is also based on calculations in an opened channel. The inflow of the fresh mixture boundary condition is set on the left end of the computational domain, while the free outflow of combustion products is implemented on the right end of the computational domain. Here flame front is subjected to the counterflow of the fresh mixture, and via dynamic change of the fresh mixture flow velocity, one can obtain a flow velocity value corresponding to the flame stabilization, so the flame front becomes stationary. By definition, this flow velocity value coincides with the laminar burning velocity. This approach is used only with the FDS technique, as it occurs to be very sensitive towards acoustic perturbations, which impede flame stabilization.

The second problem is the flame development inside the spherical vessel of 20 cm diameter (1.3 L volume). Here calculations are performed in spherical symmetry. The left end of the computational domain is a symmetry point, and the solid wall condition is stated on the right end of the domain. This problem is intended to investigate combustion features under the influence of compression wave propagation at the background of the continuous pressure rise. In particular, it is of interest to define the limits of the low-Mach number approximation in the context of developed acoustic fields accompanying combustion.

The third problem is devoted to the analysis of the flame dynamics within the two-dimensional closed vessel and the influence of the compression waves on the flame front structure. Here the rectangular volume with dimensions $25 \times 25$ mm filled with hydrogen-air mixtures of various compositions is considered. All the boundaries represent solid walls. Flame is initiated in the middle of the volume and propagates outwardly.
4. Discussion

4.1. Laminar Burning Velocity Test

The results of the routine for determining the laminar burning velocity are presented in Figure 1a. Here meshes with different cell sizes are used to perform the convergence analysis. All considered techniques and methods for obtaining laminar burning velocity provide close results with mesh refining. Moreover, calculated values of the laminar burning velocity are within the scatter of the experimental data. It can be concluded that implemented techniques are capable of reproducing features of laminar combustion if the compression waves are not playing a crucial role in the flame dynamics. From the Figure 1a, it can be seen that the convergence rate is highest in the case of burning velocity estimation on the basis of flame dynamics in the opened channel. In semi-closed channels, convergence rates on the example of obtaining laminar burning velocity in stoichiometric mixture via CPM, FDS, and CABARET approaches are 1.2, 1.7, and 4.7, respectively. It can be concluded that a cell size of 100 µm provides a reliable estimation of the laminar burning velocity for the CABARET and FDS methods. In turn, the results obtained via the CPM method are generally overestimated and become close to experimental values only with the cell size of 50 µm. The small convergence rate and the necessity to utilize smaller cell sizes is a manifestation of the high numerical dissipation of the CPM technique compared to other considered methods. Based on that result, a cell size of 100 µm is employed in further calculations via CABARET and FDS, while for CPM computational cell with a cell size of 50 µm is used. Figure 1b provides the values of the expansion ratio obtained with different numerical schemes. The expansion ratio does not depend on the chosen approach for gas dynamics computations. That parameter depends solely on the thermodynamics and kinetics of combustion.

4.2. Spherical Vessel

Experimental facilities with a reaction chamber of spherical shape are commonly used for the analysis of the spherical freely propagating flame. Based on the obtained data, one can measure important characteristics of the flame evolution, such as combustion intensity, laminar burning velocity [37], cellular patterns due to instability development on the flame front [38], and many others. In Figure 2, time histories of the pressure inside the chamber calculated with FDS, CPM, and CABARET techniques for different mixture compositions are presented. It can be seen that low-Mach approximation causes an underestimation of the pressure rise increment in the considered mixtures. The results obtained via the FDS method are close to the compressible model only in the initial stages of combustion of lean compositions with moderate chemical reactivity. In the cases of higher chemical activity,
the compression waves play an important role in the flame dynamics already in the earlier stage of flame development and cause sufficient intensification of the combustion process. In turn, the overestimation of laminar burning velocity by the CPM technique leads to the overall increase in combustion process intensity compared to another compressible method CABARET. Figure 3 provides a clear visualization of how compression waves modify temperature and velocity profiles in the fresh mixture and combustion products. Here one can see that due to lower dissipation error, the compression waves pattern is more developed when using CABARET in comparison with the CPM result.

Figure 2. Pressure measurements on a wall of the spherical vessel. (a) 15.0% H₂-Air mixture, (b) 29.5% H₂-Air mixture, (c) 40.0% H₂-Air mixture. Solid black lines—FDS method, solid red lines—CABARET method (moving average), solid green lines—CPM method (moving average).

Figure 3. Temperature and velocity profiles in a spherical vessel filled with stoichiometric hydrogen-air mixture in a coordinate system related to the flame front location. Solid lines—velocity, dashed lines—temperature. Black lines—FDS method, red lines—CABARET method, green lines—CPM method. Time instant 4 ms.

4.3. Multidimensional Flame Development

Here we analyze flame evolution in a closed rectangular vessel obtained via CABARET, CPM, and FDS approaches. Compression waves emitted by the flame front during its evolution define the flow structure ahead of the flame. Peculiarities of the flow can have a crucial impact on the overall flame dynamics. Thus, in the case of combustion in the semi-opened channel, the development of the flow determines the flame acceleration in the initial stages of the combustion process [39]. In closed volume, the reflection of the compression waves from the reactor walls and its further interaction with the flame can sufficiently alter the topology of the flame, causing additional flame front corrugation [40]. In turn, the rise of the flame front surface due to the perturbation development increases combustion intensity. Thus, the correct reproduction of the acoustic patterns ahead of the flame is crucial for precise flame dynamics modeling. From the pressure curves depicted in Figure 4, one can
conclude that the correct reproduction of acoustic effects together with laminar burning velocity value has a substantial influence on the overall combustion dynamics. In Figure 5, flame front structures and vorticity distributions for the lean 15% hydrogen-air mixture (left column) in the cases of using FDS, CPM, and CABARET approaches are presented. It can be seen that the flame front obtained via the CABARET technique is more developed compared to the FDS and CPM results. Interaction between the compression waves ahead of the flame defines the formation of complex flow patterns containing small-scale vortical structures. These vortices interact with the flame, causing its local perturbation that leads to flame corrugation, intensification of the flame instability development, and increased intensity of the combustion process, which can be correctly modeled via the CABARET technique.

In the case of the CPM method, the propagation of compression waves is also resolved within the model. However, the numerical dissipation leads to significant smearing of all flow perturbations. Thereby the effect of acoustic fields on the combustion dynamics is reduced. The FDS approach, on the contrary, cannot reproduce the acoustic pattern in the fresh mixture. Thus the flame front evolution here is governed solely by the intrinsic instability development. In the initial stage of the process, when the flame develops nearly as in an unconfined space, the leading role belongs to the laminar burning velocity value. Overestimation of this parameter leads to more intense combustion development at that stage in the case of the CPM approach compared to other methods (see Figure 4). Further, as the flame comes closer to the walls of the vessel, acoustic perturbations and instability development start to play a much more important role. Here only the CABARET approach can correctly predict the acoustic pattern and flame front corrugation, which make flame evolution more rapid. Despite higher combustion intensity, in the case of a stoichiometric H\textsubscript{2}-Air mixture, this effect is less noticeable as the combustion is less prone to instability development. Here the leading role belongs to the correct reproduction of the laminar burning velocity parameter. A comparison of flame front structures and vorticity fields for a stoichiometric hydrogen-air mixture is presented in Figure 5 (right column).

![Figure 4. Pressure rise in a rectangular vessel filled with 15% hydrogen-air mixture (dashed lines) and 29.5% hydrogen-air mixture (solid lines) obtained via CABARET (moving average, red lines), FDS (black lines) and CPM (moving average, green lines) techniques.](image-url)
5. Conclusions

The paper presents the analysis of the capabilities of low-Mach number approximation implemented in the FDS approach in comparison with the compressible model realized by the CABARET and CPM numerical schemes.

- In opened systems, where the interaction between the compression waves and the flame front is not intense, the low-Mach approximation provides reliable solutions close to those obtained with the compressible model. Thus the difference in the estimation of laminar burning velocity via CABARET and FDS techniques is less than 6% for $\Delta x = 50 \mu m$.

- It is shown that the flame development within closed vessels, strongly affected by compression waves propagation, is not precisely reproduced within the framework of the low-Mach number approximation. The calculations in a spherical vessel show that the low-Mach model tends to underestimate the dynamics of pressure rise. The interaction between individual compression waves and the flame front causes its local acceleration or deceleration that leads to the overall greater intensity in the combustion process and faster pressure build-up.
- From the results of multidimensional calculations, it is shown that the combustion intensity is not the key factor defining the compression waves’ impact. In mixtures susceptible to instability development, such as lean hydrogen-air mixtures, even low intense compression waves can trigger instability development and multidimensional evolution of the flame front, leading to a substantial change in the dynamics of the combustion process.

- On the example of the traditional CPM numerical method, it is shown that numerical dissipation errors act in a similar way to acoustic filtering in low Mach approximation, smearing acoustic perturbations and reducing their influence on the flame front structure evolution.

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Abbreviations

The following abbreviations are used in this manuscript:

- FDS Fire Dynamics Simulator
- CABARET Compact Accurately Boundary Adjusting-REsolution Technique
- JANAF Joint Army-Navy-Air Force
- LES Large Eddy Simulation
- CPM “Coarse” Particles Method
- TVD Total Variation Diminishing
- CHARM Cubic-parabolic High Accuracy Resolution Method

Nomenclature

- $R$ universal gas constant
- $k_B$ Boltzmann constant
- $x_i$ spatial coordinates
- $t$ time
- $\rho$ density
- $Y_k$ mass fraction of $k$-th species
- $X_k$ molar fraction of $k$-th species
- $p$ total pressure
- $T$ temperature
- $E$ specific total energy
- $c$ velocity of sound
- $\varepsilon$ specific inner energy
- $u_i$ mass velocity vector
- $\omega_i$ vorticity vector
- $\sigma_{ij}$ shear stress tensor components
- $\kappa(T)$ thermal conductivity
- $D_k(T)$ mass-averaged diffusion coefficient of $k$-th species
- $\mu(T)$ viscosity coefficient
\( \kappa_k \) \( \mu_k \) \( D_{kj} \) \( V_{k,i} \) \( m_k \) \( M_k \) \( \bar{M} \) \( h_k \) \( \Omega^{(2,2)} \) \( T^* \) \( \sigma_k \) \( \epsilon_k \) \( c_V \) \( c_{Vj} \) \( \bar{\rho} \) \( H \) \( \delta_{ij} \)

- thermal conductivity coefficient of \( k \)-th species
- viscosity coefficient of \( k \)-th species
- binary diffusion coefficient of a compound \( k \) into a compound \( j \)
- \( k \)-th species diffusion velocity vector
- \( k \)-th specie molar mass
- atomic (molecular) mass of \( k \)-th species
- mixture average molar mass
- \( k \)-th species diffusion velocity vector
- \( k \)-th specie molar mass
- \( k \)-th species atomic (molecular) mass
- reduced temperature
- collision diameter of \( k \)-th species
- Lennard-Jones potential well depth
- specific constant volume heat capacity of the mixture
- specific constant volume heat capacity of \( k \)-th species
- background pressure
- total pressure divided by the density (Bernoulli integral)
- Kronecker delta

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