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# Modeling and simulation of hydrogen combustion in engines



N.N. Smirnov<sup>a,b,\*</sup>, V.F. Nikitin<sup>a,b</sup>

<sup>a</sup> Moscow M.V. Lomonosov State University, Leninskie Gory, 1, Moscow 119992, Russia

<sup>b</sup> Scientific Research Institute for System Analysis of the Russian Academy of Sciences, Moscow 117218, Russia

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## ABSTRACT

Hydrogen being an ecological fuel is very attractive now for engines designers. It is already actively used in rocket engines. There exist plans to use hydrogen in pulse detonation engines. However, peculiarities of hydrogen combustion kinetics, the presence of zones of inverse dependence of reaction rate on pressure, etc. prevent from wide use of hydrogen engines. Computer aided design of new effective and clean hydrogen engines needs mathematical tools for supercomputer modeling of hydrogen–oxygen components mixing and combustion gas dynamics.

The paper presents the results of developing verification and validation of mathematical model and numerical tool making it possible to simulate unsteady processes of ignition and combustion in engines of different types and to study its peculiarities. First, verification and validation of the chemical kinetic models for hydrogen oxidation were carried out through investigations on the ignition delay time on pressure, temperature, and equivalence ratio for hydrogen–oxygen mixtures. Then, the developed solver was used to model pre-mixed and non-premixed combustion and detonation related phenomena including deflagration to detonation transition.

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## 1. Introduction

Rocket engines using hydrogen–oxygen mixture have the following peculiarity. On injecting liquid components fuel (hydrogen) having much lower critical temperature comes pre-evaporated and pre-heated in combustion chamber, while oxygen could be liquid then evaporating inside the chamber. Thus contrary to most types of engines hydrogen engine has an inverse mixture entering combustion chamber, in which fuel is gaseous and oxidant is liquid. However, taking into account rather low critical temperatures for both components estimates based on models developed in papers [1–3] show, that phase transition will take place in an order of magnitude faster than for

hydrocarbon fuels. That provides the reason to use one phase model as a first order of approximation. Onset of detonation being very dangerous for classical RAM engines could, however, serve the basis for creating new generation of engines – pulse detonating engines (PDE) [4,5]. For this issue the problems of detonation onset, decay and deflagration to detonation transition should be simulated quite accurately, because these processes strongly depend on inlet conditions, mixture composition and geometrical characteristics of combustion chamber [6–8].

Hydrogen chemistry modeling is rather complicated because regular kinetic mechanisms have hundreds stages. Many reduced kinetic mechanisms were developed. However, peculiarities of hydrogen combustion kinetics, the presence of

\* Corresponding author. Moscow M.V. Lomonosov State University, Leninskie Gory, 1, Moscow 119992, Russia.

E-mail addresses: [mech.math.msu@inbox.ru](mailto:mech.math.msu@inbox.ru), [ebifsun1@mech.math.msu.ru](mailto:ebifsun1@mech.math.msu.ru) (N.N. Smirnov).

zones of inverse dependence of reaction rate on pressure, makes developing reduced mechanisms a very difficult task, which was studied by many researchers [9–14]. In the present paper kinetic models developed based on CHEMKIN package methodology [15] will be used. The validation of these models will be performed based on experimental investigations of ignition delay times being functions of pressure, temperature and mixture composition [16,17]. The developed code will be used for simulation of premixed and non-premixed combustion and detonation related phenomena, including detonation onset, degeneration and deflagration to detonation transition.

## 2. Mathematical model

Numerical investigations of the DDT processes were performed using the system of equations for the gaseous phase obtained by Favre averaging of the system of equations for multicomponent multiphase media. The modified *k*-epsilon model was used. To model temperature fluctuations the third equation was added to the *k*-epsilon model to determine the mean squared deviate of temperature [7,8]. The production and kinetic terms were modeled using the Gaussian techniques [18,19].

The governing equations for the averaged values of parameters look as follows:

$$\partial_t(\rho) + \nabla \cdot (\rho \vec{u}) = 0, \quad (1)$$

$$\partial_t(\rho Y_k) + \nabla \cdot (\rho \vec{u} Y_k) = -\nabla \cdot \vec{I}_k + \dot{\omega}_k \quad (2)$$

$$\partial_t(\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) = \rho \vec{g} - \nabla p + \nabla \cdot \tau \quad (3)$$

$$\partial_t(\rho E) + \nabla \cdot (\rho \vec{u} E) = \rho \vec{u} \cdot \vec{g} - \nabla \cdot p \vec{u} - \nabla \cdot \vec{I}_q + \nabla \cdot (\tau \cdot \vec{u}) \quad (4)$$

The Equations (1)–(4) include mass balance in the gas phase, mass balance of *k*-th component, momentum balance and energy balance respectively. We have the following relationships between the terms in the Equations (1) and (2):  $\sum Y_k = 1$ ,  $\sum \vec{I}_k = 0$ ,  $\sum \dot{\omega}_k = 0$ . The state equations for gaseous mixture  $k$  are the following:  $p = R_g \rho T \sum Y_k / W_k$ ,  $E = \sum Y_k (c_{vk} T + h_{0k}) + \frac{u^2}{2} + k$ . The turbulent heat flux  $\vec{I}_q$  in the Equation (4) is a sum of two terms:  $\vec{I}_q = \vec{J}_q + \sum (c_{pk} T + h_{0k}) \vec{I}_k$ , where  $\vec{J}_q$  could be interpreted as turbulent conductive heat flux. The eddy kinematic viscosity  $\nu^t$  is expressed according to *k*-epsilon model as  $\nu^t = C_\mu (k^2/\epsilon)$ . The turbulent fluxes were modeled in the following way:

$$\tau = (\mu + \rho \nu^t) (\nabla \vec{u} + \nabla \vec{u}^T - (2/3)(\nabla \cdot \vec{u})U) - (2/3)\rho k U, \quad (5)$$

$$\vec{I}_k = -\rho(D + (\nu^t/\sigma_d))\nabla \cdot Y_k, \quad \vec{J}_q = -\left(\lambda + \sum_k c_{pk} Y_k \rho (\nu^t/\sigma_t)\right)\nabla \cdot T, \quad (6)$$

The *k*-th component mass origination rate  $\dot{\omega}_k$  was calculated as a sum of mass production rates  $\omega_{kj}$  in each *n*-th chemical reaction taking place in a gaseous phase. The term responsible for chemical transformations,  $\dot{\omega}_k$  is very sensitive to temperature variations, as it is usually the Arrhenius law type function for the reactions' rates. Let us regard the temperature being a stochastic function *T* with mean  $\bar{T}$  and mean

squared deviate  $\theta = \overline{T'T'}$ . The model was closed then by the equations for *k*,  $\theta$  and  $\epsilon$ :

$$\partial_t(\rho k) + \nabla \cdot (\rho \vec{u} k) = \nabla \cdot ((\mu + \rho(\nu^t/\sigma_k))\nabla k) + \tau^t : \nabla \vec{u} - \rho \epsilon \quad (7)$$

$$\partial_t(\rho \epsilon) + \nabla \cdot (\rho \vec{u} \epsilon) = \nabla \cdot ((\mu + \rho(\nu^t/\sigma_\epsilon))\nabla \epsilon) + (\epsilon/k)(C_{1\epsilon} \tau^t : \nabla \vec{u} - C_{2\epsilon} \rho \epsilon) \quad (8)$$

$$\partial_t(\rho \tilde{c}_p \theta) + \nabla \cdot (\rho \vec{u} \tilde{c}_p \theta) = \nabla \cdot \left( \left( \lambda + \sum_k c_{pk} Y_k \rho (\nu^t/\sigma_k) \right) \nabla \theta \right) + P_\theta + W_\theta - D_\theta, \quad (9)$$

Parameters in the Equations (7) and (8) are assumed to be equal to the following standard values [19] having been developed for flows in channels:

$$C_\mu = 0.09, \quad C_{1\epsilon} = 1.45, \quad C_{2\epsilon} = 1.92, \\ \sigma_d = 1, \quad \sigma_t = 0.9, \quad \sigma_k = 1, \quad \sigma_\epsilon = 1.3.$$

The Equation (10) was developed for temperature deviate evolution, where the production terms  $P_\theta$ ,  $W_\theta$  and the dissipation term  $D_\theta$  were determined by the following formulas derived in Refs. [5,8,35]:

$$P_\theta = 2\rho \sum_k c_{pk} Y_k (\nu^t/\sigma_k) (\nabla T)^2, \quad W_\theta = -\sum_k \overline{\dot{\omega}_k^T} h_{0k}, \quad D_\theta \\ = C_g \rho \sum_k c_{pk} Y_k \frac{\epsilon}{k} \frac{\theta}{\theta_m - \theta}, \quad \tilde{c}_p = \sum_k c_{pk} Y_k. \quad (10)$$

In deriving the production  $W_\theta$  due to chemistry (10) the Arrhenius law for chemical transformations was assumed. To calculate the averaged term  $\dot{\omega}_k$  the Gaussian quadrature technique was applied:

$$\overline{T'A(T)} = \theta \frac{A(\bar{T} + \sqrt{3}\theta) - A(\bar{T} - \sqrt{3}\theta)}{2\sqrt{3}\theta}. \quad (11)$$

The dissipation function  $D_\theta$  was chosen in the form (10) to satisfy the rule that the squared temperature deviate cannot exceed its maximal possible value  $\theta_m$ , because the value of  $T = \bar{T} + T'$  cannot be negative. However, production terms do not grant the presence of such a boundary. To guarantee it we incorporate the multiplier  $1/(\theta_m - \theta)$  into the dissipation term (the other multipliers are standard [19]). In order to estimate the value of  $\theta_m$ , we should take into account that the probability for the deviate value to exceed 2 times the mean deviate value is less than 1% for the normal distribution. Also, we should take into account that the mean temperature deviate in experiments published by Philip [18] did not exceed half of the maximal mean temperature. With this, we estimate  $\theta_m$  as follows:  $\theta_m = \bar{T}^2/4$ . The dissipation constant  $C_g$  in (10) was determined based on the experiments [18], which had been carried out for similar geometrical confinement:  $C_g = 2.8$ .

The boundary conditions for turbulent parameters  $k$ ,  $\epsilon$ ,  $\theta$  are constructed according to the wall laws [5]:

$$k = 0, \quad \frac{\partial \epsilon}{\partial \vec{n}} = 0, \quad \frac{\partial \theta}{\partial \vec{n}} = 0, \quad (12)$$

where  $\vec{n}$  is the normal vector to the wall. To take into account the wall damping effect the coefficients of the original turbulence model are modified in accordance with the Lam-Bremhorst low Reynolds models [21]:

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