NUMERICAL METHOD FOR SIMULATING REACTING MEDIA FLOWS

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Introduction

- Feasible numerical simulation of ignition and detonation of combustible compounds becomes especially important due to the growth of interest in hydrogen energetics.
- The main objective of this work is to enable simulation of reacting media flows in geometrically complex computational domains using the numerical method which previously exhibited high accuracy while simulating shock processes [1] using the modified Kuropatenko method [2].
- The approach used to simulate chemical transformations [3] and supplemented by the solver for rigid ODEs (ordinary differential equations) [4] exhibits high accuracy when describing hydrogen oxidation reactions.
- The work compares the experimental results [5] and the results of simulating deflagration-to-detonation transition of hydrogen-air mixture in a shock tube with barriers obtained with the developed modified method.

Methods

- The system of equations describing the model of multicomponent one-velocity continuous medium was solved using the finite-volume method:

$$\frac{\partial}{\partial t}\int \rho dV = -\int div\rho\vec{U}dV + \int_V S_M dV\,,$$

$$\frac{\partial}{\partial t}\int \rho U_l dV = -\oint (P\delta_{lm} - \rho U_l U_m)df_m + \int_V \rho g_l dV + \int_V S_l^J dV\,,$$

$$\frac{\partial}{\partial t}\int \rho\varepsilon dV = -\oint \rho\vec{U}\varepsilon d\vec{f} - \oint_{\partial V} \tau \bullet \vec{U} d\vec{f} + \oint_{\partial V} \chi\vec{\nabla}T d\vec{f} + \int_V \rho(\vec{g}\cdot\vec{U})dV + \int_V S_\varepsilon dV\,,$$

$$\frac{\partial}{\partial t}\int_V \rho Y_i dV + \oint_{\partial V} \rho Y_i \vec{U} d\vec{f} = \oint_{\partial V} \vec{J}_i d\vec{f} + \int_V S_{Y_i} dV\,.$$

- The system of equations is closed by the ideal gas law.
- The reaction rate is derived from the Arrhenius equation and the law of mass action:

$$W_j = z_j T^{b_j} \exp\left(-\frac{E_{\text{акт}_j}}{RT}\right)\prod_{i=1}^{n_c} C_i^{\nu_{i,j}}\,.$$

- The changes in reagent concentrations and temperatures are described as:

$$\frac{dC_k}{dt} = \sum_{j=1}^{n_r} W_j\left(\nu'_{k,j} - \nu_{k,j}\right), \quad \frac{dT}{dt} = \frac{-\sum_{k=1}^{n_c}\left[h_k(T)\frac{dC_k}{dt}\right]}{\sum_{k=1}^{n_c}[C_k c_{Pk}(T)]}, \quad k = 1\ldots n_c.$$

- The rate of mass change and energetic reaction effect computed in the following way contribute into the appropriate source terms S_M and S_ε:

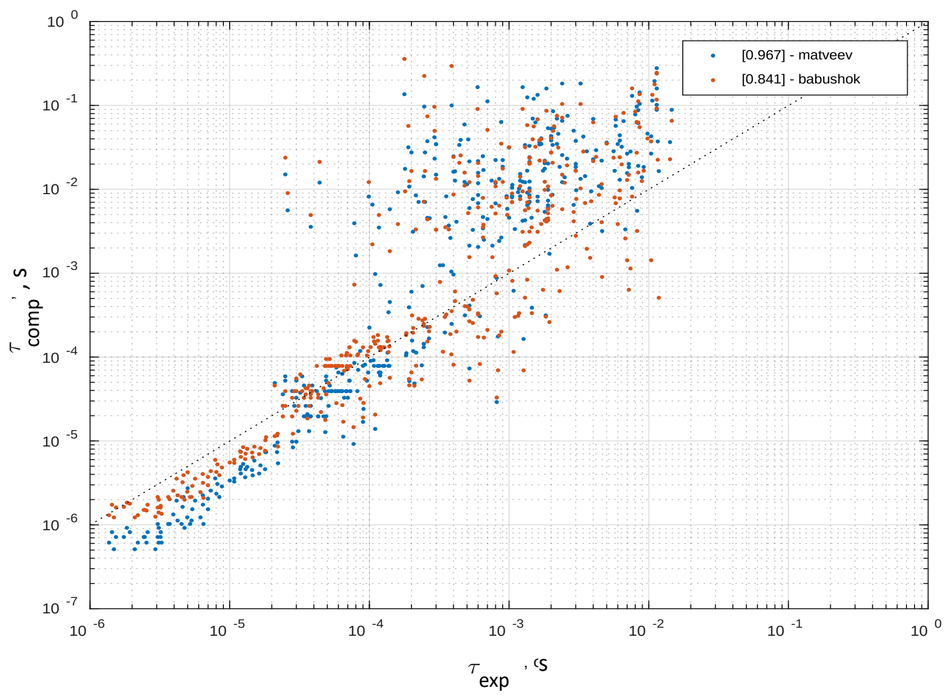
$$\omega_k = M_k\frac{dC_k}{dt}, \quad S_{\text{хим}} = \rho c_V\frac{dT}{dt}.$$

- Next to the names of the given mechanisms [6] and [7] in square brackets there is a value calculated for the mechanism using the formula:

$$\varepsilon_f = \sqrt{\frac{\sum_{i=1}^{n}\log\left(\frac{\tau_{c,i}}{\tau_{e,i}}\right)^2}{n}}.$$

Results

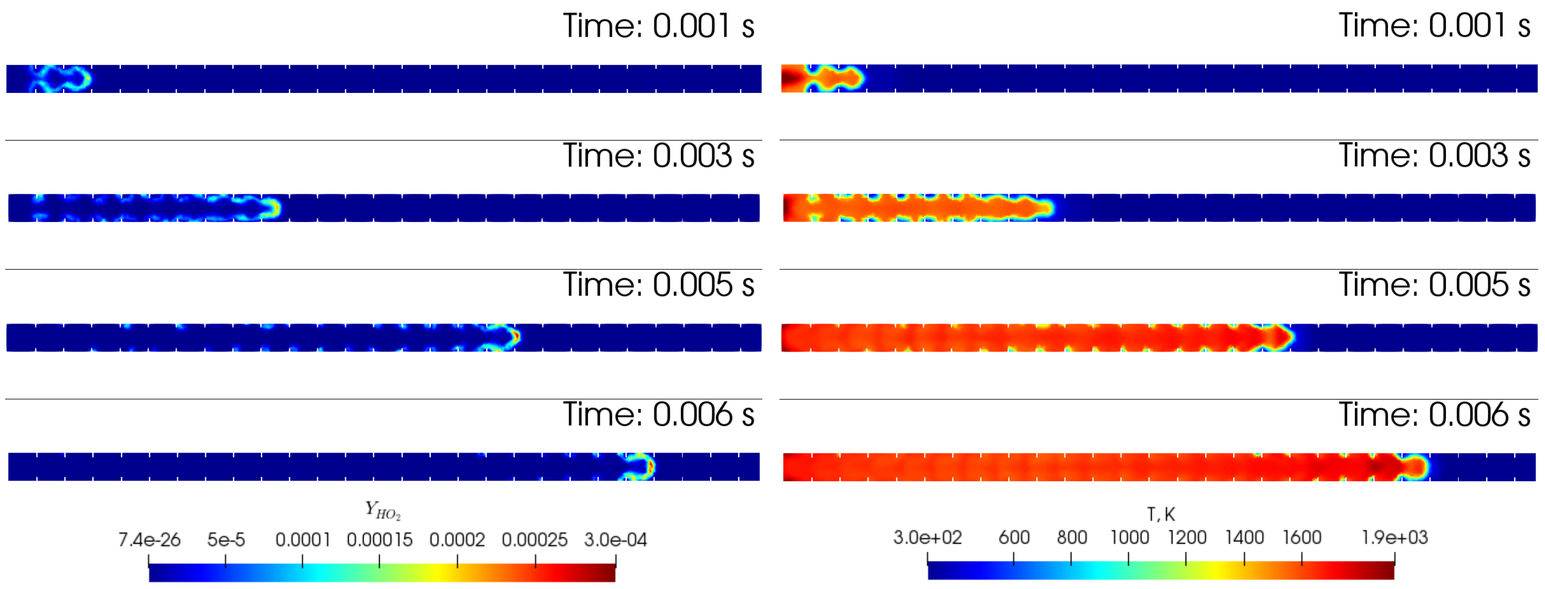
Selecting the Kinetic Mechanism

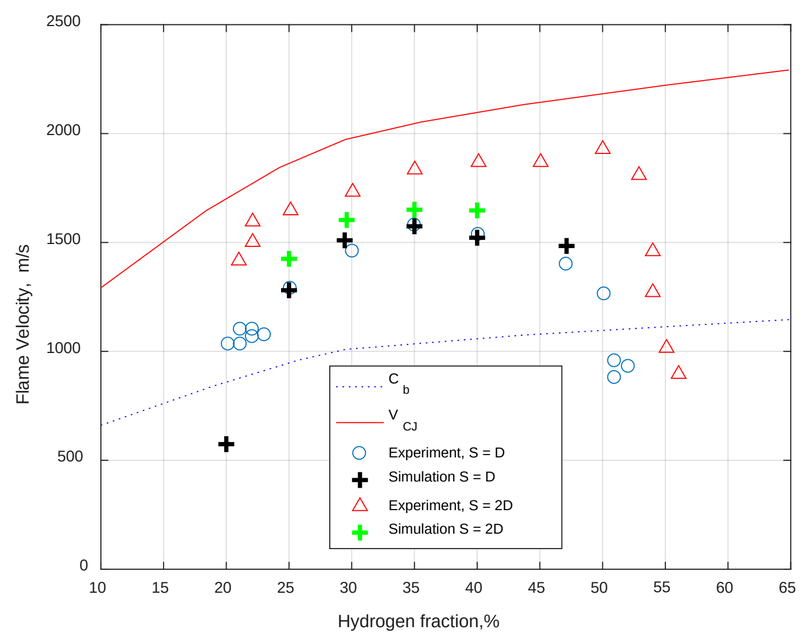


Deviation of adiabatic induction times computed using the kinetic mechanisms [6] and [7] from the experimental values [8].

Simulation of Detonation

- The calculation sets and computational domain geometry correspond to the experimental sets described in [5]. The tube has a square section with the side $D = 0.112\,m$, is 6 m long and comprises barriers spaced at a distance S. Each barrier has a round orifice whose area correlates to the tube cross-sectional area at a ratio of 0.6:1.





Comparison of detonation velocities between calculations and experiments [5].

Conclusion

- The work shows the feasibility and good accuracy of simulating detonation flows of reacting media in complex-geometry computational domain using the developed modified method.
- The absence of the models describing turbulence and radiant heat exchange results in underestimating detonation velocity in less obstructed areas and prevents deflagration-to-detonation transition in compounds which are not quite stoichiometric.
- Despite the good accuracy in determining detonation flow parameters, in further works it is intended to introduce models of turbulence and radiant heat exchange in the numerical algorithm since some applied tasks require a more detailed elaboration, and the phenomena of turbulence and radiant heat exchange are of key importance in burning and detonation processes.

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