

Numerical method for modeling the flows of reacting media

Belyaev P E^{1,2,@}, Makeeva I R^{1,2}, Pigasov E E^{1,2} and Mastyuk D A¹

¹ Federal State Unitary Enterprise “Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics”, Vasilieva 13, Snezhinsk, Chelyabinsk Region 456770, Russia

² South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

@ gbelbih@gmail.com

High-intensity flows are characterized by the appearance of features such as shock waves—regions comparable to the molecular mean free path, in which the gradients of gas-dynamic quantities tend to infinity. For a correct description of such processes, the numerical method must include the mechanism of entropy growth at the shock front. As such a mechanism, the proposed method uses a modification of the well-proven method of V.F. Kuropatenko [1] for calculating strong shock waves. This modification allows using the Kuropatenko method in Eulerian coordinates.

At the moment, there are no published works presenting the modeling of flows of chemically reacting media using the Kuropatenko method. In this work, the approach presented by Pigasov was used to simulate chemical transformations. The used sets of chemical reactions and their parameters are described in the kinetic mechanisms of Matveev [2] and Babushok [3].

This paper presents a mathematical method and a model of a multicomponent continuous medium for high-intensity flows of reacting media simulation. The results of modeling the ignition and detonation of a hydrogen-air mixture in a shock tube showed good agreement with experiment [4].

[1] Kuropatenko V F 2007 *Continuum mechanics models* (Chelyabinsk: Chelyab. gos. univers.)

[2] Matveyev V G 2001 *Combustion and explosion physics* **37**

[3] Babushok V I, Krakhtinova T V and Babkin V S 1984 *Kinetics and catalysis* **25**

[4] Wang L Q, Ma H H, Shen Z W, Lin M J and Li X J 2018 *International Journal of Hydrogen Energy* **43** 4645–4656