## UDC 662.612.31: 519.876.5 **doi: 10.32620/reks.2024.4.21**

# **Oleh TRYFONOV, Olga SHYPUL, Vadym GARIN, Vitalii MYNTIUK, Denys TKACHENKO**

*National Aerospace University "Kharkiv Aviation Institute", Kharkiv, Ukraine*

# **A NUMERICAL SIMULATION STUDY OF HYDROGEN-AIR MIXTURE COMBUSTION IN A CLOSED CHAMBER AT LOW INITIAL PRESSURE**

*This study investigates the combustion of a hydrogen-air mixture at low initial pressure in a closed chamber, focusing on thermal energy methods (TEM) used for processing thermoplastics. This study aims to develop and validate a numerical model capable of predicting critical combustion parameters, specifically, the pressure and temperature distribution profiles over time, to ensure safe and efficient TEM processing. The tasks included constructing and validating the hydrogen-air combustion model using experimental data for high accuracy and applicability in TEM systems. The methods involved numerical simulation of the hydrogen-air mixture combustion in ANSYS Fluent using the GRI-Mech 3.0 mechanism, employing fourth-degree polynomial functions to define the thermodynamic properties of the species. Validation against previous experimental data yielded highly accurate results with peak pressure deviations of less than 3%. The following validation, the model was applied to simulate combustion in an industrial TEM chamber, which is representative of real operational conditions. Results showed consistent flame front development, including the formation of turbulent cellular structures, which are essential for achieving optimal temperature distribution and stability within the chamber. These insights allow for strategic part placement to maximize processing quality, which is especially important when using low-pressure hydrogen-air mixtures. In conclusion, the validated model emphasizes the potential of green hydrogen-based fuels as eco-friendly alternatives for energy-intensive industrial processes, thereby advancing climate-neutral manufacturing. Future work will expand on combustion studies using plastic parts in TEM chambers to improve processing precision and safety for broader adoption in sustainable thermoplastics manufacturing.*

*Keywords: hydrogen-air mixture; CFD simulation; combustion; TEM processing; model validation.*

#### **1. Introduction**

#### **1.1. Motivation**

With the establishment of the New Industrial Strategy, Climate and Energy Policy Framework, and SRRI Roadmap (2021), all energy sources must comply with a policy of friendliness to the surrounding environment. In this regard, many studies are devoted to the issues of production, storage, and use during the replacement of fossil fuel-based energy sources with naturally produced hy-drogen: thermal processes; biological processes; water splitting; hydrogen purification. For a clear understanding of the technological, economic, and environmental consequences of using hydrogen as an energy source and analyzing its strengths and weaknesses, opportunities, and threats, a SWOT analysis is performed in the work [1], which emphasizes the high energy density of hydrogen and zero emissions but notes the high costs of production and storage problems. In [2], the authors describe and compare different technologies for hydrogen production, storage, and usage (especially in fuel cell applications). The feasibility of transitioning to free-carbon processing technology not only reduces emissions and is in line with the concept of a climate neutral industry, but also brings industrial technologies to a level of high production safety. The analysis in [3] shows that green hydrogen ultimately wins in terms of climate impact under the four scenarios developed (with green hydrogen, with blue hydrogen, without green hydrogen, and the baseline scenario), largely offset by its net using and supplying electricity from renewable sources, and the total monetized life cycle impact cost of green hydrogen production is relatively lower than the cost of blue hydrogen production.

The use of the combustion energy of fuel mixtures is relevant for industrial processes involving material processing technologies, for example, thermal energy methods (TEM) [4], and they are also subject to a policy of friendliness to the surrounding environment [5]. Herewith, it is known the experience of using TEM with hydrogen-oxygen mixtures at low pressure for removing burrs, fogging, and partial surface polishing of parts made of thermoplastic materials such as acrylic, polyurethane, polyethylene, etc. [6, 7].



At the same time, for the implementation of TEM with mixtures based on green hydrogen for processing plastics with the predicted processing quality, it is necessary to study the effective modes of combustion of the mixture in the machine chamber, depending on the initial conditions. The initial conditions in this case include the component composition of the fuel mixture, degree of homogeneity, initial low pressure, and ignition energy. The dependence of the laminar combustion speed of explosive gas mixtures as a function of pressure, temperature, and the air-to-fuel ratio is of great importance for evaluating the influence of fuels on the efficiency of work processes in the combustion chambers of thermal machines. From this point of view, such studies have not been conducted for existing equipment for the thermal energy processing of plastics.

#### **1.2. State of the art**

Computer simulation is a proven effective tool for studying the complex rapid processes of chemically reactive substances. Modern mathematical models and simulation studies of fuel mixture combustion, including hydrogen-based ones, are related to the next. Coupled with the 30-step methane combustion mechanism simplified by GRI3.0, a three-dimensional computational fluid dynamics (CFD) simulation of the combustion chamber of a partially premixed gas water heater was carried out to investigate the impact of blending natural gas with hydrogen on the combustion performance [8]. The development of efficient and ecologically clean emission combustion systems is a particularly important research area, where modeling the combustion of fuel mixtures and the creation of reliable prognostic models have become important research tools [9]. Using the CHEMKIN simulation software, the qualitative and quantitative evaluation of the dynamic behavior characteristics of hydrogen explosion in a confined space under different initial conditions was conducted, and the variation law of the physical process of hydrogen explosion under different influencing factors in a confined space was revealed from macro-micro perspectives [10]. In [11], the flame propagation and overpressure characteristics of hydrogen-air mixtures ignited under atmospheric pressure were simulated, and the effects of the hydrogen volume fraction (20 %...45 %) and the pipe blockage ratio (0/0.4) on the hydrogen combustion and explosion processes were analyzed. In the paper [12], the multi-phenomena deflagration model was developed to simulate the deflagrative combustion of several fuel–air mixtures in various scale closed vessels, and the experimental verification of the model's capability for a variety of fuels and vessel sizes was performed.

We can conclude that previous studies have mainly focused on experimental and theoretical investigations

for too complex fuel blends [9] or for a very wide range of initial parameters [10, 11] in standardized combustion chambers and channels to determine general parameters of the combustion process and its dependence on initial conditions.

In this study, we focused on the development of mathematical models for accurate prediction of the combustion parameters at low initial pressure hydrogenair mixtures in both the laboratory and industrial combustion chambers of TEM equipment. For the TEM processing of plastic parts, it is important to predict not only the general parameters of the combustion process but also the volumetric distribution of the combustion product temperature in a closed chamber, considering the peculiarities of the convective heat exchange during cooling. It is very important to choose the location of parts inside a chamber and to select regimes for plasticpart TEM processing.

Therefore, the required mathematical model sufficiently differs from already known models and should be developed from the beginning considering the particularities of the combustion process during the TEM processing of plastic parts.

#### **1.3. Objective and the approach**

In our previous study, a numerical investigation of the hydrogen-air mixture generation in a TEM chamber was carried out to determine the ability to achieve the required component composition and the degree of homogeneity [13]. This study`s objective is the state critical combustion parameters of hydrogen-air mixture in a TEM chamber at low initial pressure. This study aims to simulate the combustion process of a hydrogen-air mixture with a given component composition and degree of homogeneity and to estimate the pressure and temperature distribution profiles at arbitrary moments in time.

The current study's approach is to develop a mathematical model of a hydrogen-air mixture combustion and to verify the developed model by comparing the simulation results with experimental data to assess its applicability for further investigations. The closest similarity of the investigated processes is described in the work [14], where the burning velocities of hydrogen-air mixtures are investigated in a spherical constant-volume combustion bomb varying the initial conditions of pressure, temperature, and fuel/air equivalence ratios. Thus, experimental data [14] were used to verify the developed model.

To achieve the stated goals of the work, it is necessary to solve and complete the following tasks:

1) to develop a mathematical model and set solver parameters of a hydrogen-air mixture combustion numerical model (Section 2);

2) to evaluate the accuracy of the proposed model by comparing simulation results with known experimental results (Section 3 point 1);

3) estimate the pressure and temperature distribution profiles in the combustion chamber of the TEM machine at arbitrary moments in time (Section 3 point 2);

4) analyze the obtained results, identify limitations , and determine the direction of further research (Section 4);

5) summarizing the main contributions and practical significance of the obtained results (Section 5).

#### **2. Materials and Methods**

#### **2.1. Governing Equations**

The combustion of gases is governed by a set of equations describing the conservation of mass, momentum, energy, and species. Excluding the mass forces, baro – and thermal diffusion the equations are given by [4]:

$$
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \cdot \mathbf{u}) = 0, \tag{1}
$$

$$
\frac{\partial(\rho \cdot \mathbf{u})}{\partial t} + \nabla \cdot (\rho \cdot \mathbf{u} \cdot \mathbf{u}) = -\nabla \mathbf{P} + \nabla \cdot \mathbf{\tau}_{\text{eff}}, \qquad (2)
$$

$$
\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\mathbf{u} \rho h) = \frac{\partial \mathbf{P}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{P} + \nabla (\lambda_{eff} \nabla T - \nabla \Sigma_i h_i \mathbf{J}_i + \tau_{eff} \cdot \mathbf{u}) + \sum_{i=1}^{N} Q^i - Q_{rad}, \quad (3)
$$

$$
\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) = \nabla \cdot \left( (\rho D_i + \frac{\mu_t}{c_{\text{ct}}}) \nabla Y_i \right) + R_i , (4)
$$

$$
\mathcal{L}_{\mathcal{A}}(x)
$$

where  $\rho$  is the density, [kg/m<sup>3</sup>];

**u** is the velocity vector;

t is the time, [s];

**P** is the pressure, [Pa];

 $\tau_{\text{eff}} = (\mu + \mu_t)(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - 2/3 \mathbf{I} \cdot (\nabla \cdot \mathbf{u}))$  is the effective stress tensor (i.e., the sum of the viscous and turbulent stresses);

 $\mu$  is the viscosity, [Pa·s];

 $\mu_t$  is the turbulent viscosity;

**I** is the unit tensor;

h is the enthalpy of the mixture, [J];

 $\lambda_{\text{eff}} = \lambda + \lambda_t$  is the effective thermal conductivity;

 $\lambda$  is the laminar heat conductivity [J/(m·s·K];

$$
\lambda_t = C_p \mu_t Pr_t^{-1}
$$
 is the turbulent heat conductivity;

$$
C_p
$$
 is the specific heat, [J/K];

Pr<sub>t</sub> is turbulent Prandtl number;

T is the temperature, [K];

 $h_i = \int_{T_{ref}}^{T} C_{p,i} dT$ , where  $T_{ref}$  is 297 K, is the enthalpy of species i, [J];

 $J_i$  is the diffusion rate vector of species i;

 $Q^i = h_i^0 R_i / M_i$  is the heat of chemical reactions that the species i participate in, [J];

 $Q_{rad}$  is the radiation heat, [J];

Y<sup>i</sup> is the mass fraction of species i;

 $D_i$  is the diffusion coefficient of species i in the mixture,  $[m^2/s]$ ;

 $Sc<sub>t</sub>$  is the turbulent Schmidt number;

 $R_i$  is the rate of production of species i by chemical reaction.

For the current study, an SST turbulence model was used, which showed good results for simulating wall surface flows [15].

For the combustion simulation, we used Premixed FGM model in the Reaction Progress Variable Space which solves a transport equation for the mean reaction progress variable, с, as well as the mean mixture fraction, and the mixture fraction variance  $\overline{f'^2}$ . Ahead of the flame  $(\bar{c} = 0)$ , the fuel and oxidizer are mixed but are not burnt. Behind the flame  $(\bar{c} = 1)$ , the mixture is burnt.

The reaction progress variable is defined as the normalized sum of the mass fractions of the product species [16]:

$$
c = \frac{\sum_{k} \alpha_{k} (Y_{k} - Y_{k}^{u})}{\sum_{k} \alpha_{k} (Y_{k}^{eq} - Y_{k}^{u})} = \frac{Y_{c}}{Y_{c}^{eq}},
$$
(5)

where superscript u denotes the unburnt reactant;

 $Y_k$  denotes the k<sup>th</sup> species mass fraction;

superscript eq denotes chemical equilibrium at the flame;

 $\alpha_k$  are constants that are typically zero for reactants and unity for a few products species.

For cases, such as  $H_2$  combustion, Ansys Fluent uses  $\alpha_k = 0$  for all species other than  $\alpha_{H O_2} = 10$  and  $\alpha_{\text{H}_2\text{O}} = 1$ , by default.

Premixed flame equations can be transformed from the physical space to the reaction progress space, neglecting differential-diffusion, are [17, 18]:

$$
\rho \frac{\partial Y_k}{\partial t} + \frac{\partial Y_k}{\partial c} \dot{\omega}_c = \rho \chi_c \frac{\partial^2 Y_k}{\partial c^2} + \dot{\omega}_k, \tag{6}
$$

$$
\rho \frac{\partial T}{\partial t} + \frac{\partial T}{\partial c} \dot{\omega}_c = \rho \chi_c \frac{\partial^2 T}{\partial c^2} - \frac{1}{Cp} \sum_k h_k \dot{\omega}_k + + \frac{\rho \chi_c}{Cp} \left( \frac{\partial Cp}{\partial c} + \sum_k C_{p,k} \frac{\partial Y_k}{\partial c} \right) \frac{\partial T}{\partial c},
$$
(7)

where  $Y_k$  is the  $k^{\text{th}}$  species mass fraction;

T is the temperature;

ρ is the fluid density;

t is time;

 $\dot{\omega}_k$  is the k<sup>th</sup> species mass reaction rate;

 $h_k$  is the total enthalpy;

 $C_{p,k}$  is the  $k^{th}$  species specific heat at constant pressure.

The scalar-dissipation rate,  $\chi_C$  in Equation 6 and Equation 7 is defined as follows

$$
\chi_{\rm C} = \frac{\lambda}{\rho C_{\rm p}} |\nabla c|^2, \tag{8}
$$

where  $\lambda$  is the thermal conductivity.

#### **2.2. Solver Settings**

In this study, the simulation of combustion was carried out for the fuel gas – hydrogen, and oxidant – air using a commercial code ANSYS Fluent for numerical simulations [16]. The GRI-Mech 3.0 mechanism [19] was used. For all species, thermodynamic properties were established as fourth-degree polynomial functions [19].

The calculation grid near the wall was built according to the recommendations for  $y^+$  grid spacing in the SST model. The simulation was performed using transient analysis. To cope with high pressure and velocity gradients, a time step of 1e-5s was used for the pressure-based solver.

A summary of the parameters used as solvers is presented in Table 1.

> Table 1 Summaries of the solver parameters



To reduce computational resources during model development, we considered a ¼ section of a constantvolume combustion bomb (CVCB) with symmetrical boundaries on its sides (Figure 1, a). A hybrid polyhexacore mesh with 308197 total number of cells was used (Figure 1, b).

## **3. Results**

## **3.1. Model verification**

To evaluate the accuracy of the proposed model, a comparison of simulation results and experimental results was performed. An experimental investigation of the hydrogen air mixture in the closed chamber was carried out by Reyes et al. [14]. The experimental setup is shown in Figure 2, and it was designed for the combustion of various fuels. However, to verify the developed model, only experimental data for the hydrogen-air mixture.

The experimental setup was a constant-volume combustion bomb (CVCB), made of stainless steel and a spherical cavity of 200 mm in diameter, with pressure and temperature transducers [14]. There are two electrodes located inside the bomb, which start the combustion at the geometric center of the sphere.

To verify the developed model, as described above, we considered the combustion of stoichiometric mixtures of hydrogen and air for different initial pressures at a fixed initial temperature. A summary of the considered cases is presented in Table 2. The mixture was assumed to be homogeneous and immovable.



Fig. 1. Computational model:  $a -$ domain;  $b -$ mesh



Fig. 2. Schematics of the combustion bomb with the gas filling lines and data acquisition system [14]

Table 2



During the simulation, the pressure inside the bomb was monitored at the point that corresponded to the location of the pressure sensor in the experimental setup.

The flame propagation was similar in both cases at different initial pressures. The spherical propagation of the flame can be observed. The temperature profiles inside the chamber during mixture combustion for 0.15 MPa initial pressure are shown on Figure 3.

Over time, the flame front becomes turbulent, forming a cellular structure (Figure 4).

The numerical and experimental pressure profiles are compared in Figure 5. The experimental and simulation results demonstrate good match of the pressure values in both cases (difference between pressure and time peak values does not exceed 3%). This confirms the applicability of the proposed model to further investigations.



Fig. 3. The instances of static temperature profiles during mixture combustion (0.15 MPa initial pressure)



Fig. 4. Changes in the flame front structure over time

# **3.2. Simulation of the stoichiometric hydrogen-air mixture combustion in a chamber of TEM machine**

The next task of this study was to estimate the pressure and temperature distribution profiles in the combustion chamber of the TEM machine at arbitrary moments in time. The experimental setup of a TEM combustion chamber with a volume of 3.9 litres (Figure 6, a) and its CAD model (Figure 6, b) has two specified separate inlets for filling fuel and oxidizer. The Hybrid Poly-Hexacore computation mesh comprises 269508 cells.

Previous investigations [13] have shown that when the holding time is provided, the mixture inside the chamber becomes homogeneous and immovable. This assumption was used in the current hydrogen-air simulation.

TEM treatment of plastics is usually carried out at low initial mixture pressure [7]. Thus, for the current study, it was the case listed in Table 3.

The obtained temperature pattern is shown in Figure 7. In the validation cases, the flame front became turbulent and acquired a cellular structure (Figure 8). The pressure inside the chamber rose over time and reached its maximum value after 0.016 s of ignition. The pressure

vs time diagram at hydrogen-air mixture combustion in the chamber is shown in Figure 9.



Fig. 5. Comparison of the numerical and experimental (unfiltered) pressure profiles:  $a$  – initial mixture pressure of 0.1 MPa; b – initial mixture pressure of 0.15 MPa

Table 3







Fig. 6. The industrial combustion chamber for TEM deburring:  $a - TEM$  chamber;  $b - 3D$  model of the chamber;  $c -$ Computational mesh of the chamber inner space



Fig. 7. The instances of static temperature profiles at hydrogen-air mixture combustion in industrial chamber



Fig. 8. The instances of the flame front structure at hydrogen-air mixture combustion in the industrial chamber



at hydrogen-air mixture combustion in industrial chamber

## **4. Discussions**

A combustion in a closed chamber corresponds to the uneven temperature distribution of the reaction products after combustion (Figure 10, a). When combustion is initiated by an ignition source, the burning rate of the fuel mixture is determined by the flame propagation speed. Since the combustion speed is much lower than the speed of sound, the pressure equalizes across the chamber volume at any given moment. In simple terms, combustion occurs at each moment in a thin layer called the flame front. One layer reacts after another, and this type of combustion is known as layered combustion.



Fig. 10. Flow field of the reaction products:  $a$  – uneven temperature distribution of the reaction products after combustion; b – vectors of flow velocity of the reaction products after combustion

A consequence of layered combustion in closed chambers is the emergence of heterogeneous states in the reaction products. An elementary gas layer that initially burned immediately after ignition reached a reaction product temperature corresponding to the pressure under which this layer burned. A further increase in the temperature of this elementary volume occurs due to adiabatic compression by adjacent layers, which compress continuously as the pressure rises due to the burning of neighbouring layers until reaching the final pressure after the entire fuel mixture has burned. It is noteworthy that the layers that burned last, after the reaction completion, did not experience additional compression; thus, their temperature remained unchanged, which was determined only by the initial conditions before combustion began. Thus, after the entire fuel mixture burns in a closed chamber, the combustion products exhibit different temperatures depending on the distance from the ignition point: a higher temperature near the ignition point, i.e., the layers that burned first and then adiabatically compressed to the final state; and a lower temperature in the most distant layers that burned last. The specified phenomenon of the characteristics of the flow rate of combustion products (Fig. 10, b) is important for the effective assignment of the operating modes of TEM processing, including the placement of technological equipment considering the prohibited areas for the arrangement of parts and rational positioning of ignition systems.

Adequate models of mixture formation, combustion, and heat exchange with plastics considering physical and geometric nonlinearity and the dependence of thermoplastic properties on temperature can be used to create ROM models of digital twins of technologies according to the requirements of Industry 4.0.

Promising areas for further research are experimental and numerical studies on the combustion of a hydrogen-air mixture in the presence of plastic parts inside the chamber for determination of the effective heat fluxes and the time of action necessary to achieve the desired quality of processing of thermoplastic parts.

# **4. Conclusions**

The main contribution of the current study is the developed and verified mathematical model of the combustion of a hydrogen-air mixture in a closed chamber at a low initial pressure, which, unlike the known ones, takes into account the peculiarities of the convective heat exchange in the combustion chamber during the cooling of the combustion products and allows to predict with a certain accuracy critical combustion`s parameters.

The model was verified by comparing the simulation results with the known experimental data. The obtained results demonstrate a good coincidence of the pressure values in both cases (the difference between the pressure values and the time peak does not exceed 3%). This confirms the suitability of the proposed model for further research.

The combustion of a hydrogen-air mixture was simulated for the case of an industrial combustion chamber used in TEM processing equipment at low initial pressure. The practical study`s significance lies in the fact that the computational model makes it possible to assess the pressure in the combustion chamber and obtain a temperature distribution profile in the combustion chamber at arbitrary moments in time. This allows the effective assignment of the operating modes

of TEM processing, including the placement of technological equipment considering the prohibited areas for the arrangement of parts, rational positioning of ignition systems, etc., in a wide range of initial conditions.

Note that in this work, the deflagration combustion of a stoichiometric hydrogen-air mixture was investigated in the specified volumes. For other initial conditions, for example, temperatures and pressures, as well as when changing the geometric shape of the chamber or its volume, conditions for the transition from combustion to the detonation regime may arise. In this case, other numerical models should be used, in particular, solver settings, time steps, and the resolution of the computational grid. This limits the possibilities for using the model described by the authors. At the same time, the detonation regime of combustion of a stoichiometric hydrogen-air mixture was not considered in this study because it is not suitable for TEM processing of plastics, as stated in the introduction.

**Contributions of authors:** conceptualization, **Olga Shypul**; methodology, **Oleh Tryfonov** and **Olga Shypul**; software, **Vadym Garin**; validation, **Oleh Tryfonov**; formal analysis, **Olga Shypul**; investigation, **Oleh Tryfonov**; resources, **Vadym Garin**, **Denys Tkachenko** and **Vitalii Myntiuk**; data curation, **Oleh Tryfonov** and **Olga Shypul**; writing—original draft preparation, **Olga Shypul** and **Oleh Tryfonov**; writing– review and editing, **Denys Tkachenko** and **Vitalii Myntiuk**; visualization, **Oleh Tryfonov**; project administration, **Olga Shypul**; funding acquisition, **Olga Shypul.**

All authors have read and agreed to the published version of the manuscript.

#### **Conflict of Interest**

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research, and its results presented in this paper.

#### **Financing**

This project has received funding from the EURIZON project, which is funded by the European Union under grant agreement No.871072.

#### **Data Availability**

The data associated with this work are stored in the data repository.

#### **Use of Artificial Intelligence**

The authors confirm that they did not use artificial intelligence methods in their work.

#### **Acknowledgments**

The authors express their gratitude to CADFEM UA LLC, the Channel Partner of Ansys Inc. in Ukraine, for their help with software licensing. This study was partially supported by the European Union Assistance Instrument for the Fulfilment of Ukraine's Commitments in the Horizon 2020 Framework Program for Research and Innovation of the European Union as part of the scientific research project No. 0124U004371.

#### **References**

1. Kamran, M., & Turzynski, M. Exploring hydrogen energy systems: A comprehensive review of technologies, applications, prevailing trends, and associated challenges. *Journal of Energy Storage*, 2024, vol. 96, article no. 112601. DOI: 10.1016/j.est.2024.112601.

2. Di Nardo, A., Calabrese, M., Venezia, V., Portarapillo, M., Turco, M., Di Benedetto, A., & Luciani, G. Addressing Environmental Challenges: The Role of Hydrogen Technologies in a Sustainable Future. *Energies*, 2023, vol. 16, no. 23, article no. 7908. DOI: 10.3390/en16237908.

3. Shen, H., Crespo del Granado, P., Jorge R. S., & Loffler, K. Environmental and climate impacts of a largescale deployment of green hydrogen in Europe. *Energy and Climate Change*, 2024, vol. 5, article no. 100133. DOI: 10.1016/j.egycc.2024.100133.

4. Plankovskyy, S., Popov, V., Shypul, O., Tsegelnyk, Y., Tryfonov, O., & Brega, D. *Advanced thermal energy method for finishing precision parts*. In Advanced Machining and Finishing; Gupta, K., Pramanik, A., Eds.; Elsevier: Amsterdam, the Netherlands, 2021, pp. 527-575. [DOI: 10.1016/B978-0-](https://doi.org/10.1016/B978-0-12-817452-4.00014-2) [12-817452-4.00014-2](https://doi.org/10.1016/B978-0-12-817452-4.00014-2).

5. Plankovskyy, S., Shypul, O., Tsegelnyk, Y., Brega, D., Tryfonov, O., & Malashenko, V. *Basic Principles for Thermoplastic Parts Finishing with Impulse Thermal Energy Method*. In Handbook of Research on Advancements in the Processing, Characterization, and Application of Lightweight Materials; Kumar, K., Babu, B., Davim, J., Eds. IGI Global: Hershey PA, USA, 2022, pp. 49-87. DOI: 10.4018/978-1-7998-7864-3.ch003.

6. Galliková, J., Grenčík, J., Barta, D., Barlok, M. FMECA analysis of thermal deburring machine EXTRUDE HONE TEM P-350. *Scientific Journals of the Maritime University of Szczecin*, 2020, vol. 63, pp. 9- 16. DOI: 10.17402/434.

7. Kulik, P. *Thermal deburring machine and method of thermal deburring*. WO patent 2019/054886 Al, European Patent Office, 2017.

8. Li, S., Li, X., Jin, H., Liu, Y., & Wu, Y. A Numerical Simulation Study on the Combustion of Natural Gas Mixed with Hydrogen in a Partially Premixed Gas Water Heater. *Energies*, 2024, vol. 17, no. 16, article no. 4069. DOI: 10.3390/en17164069.

9. Amzin, S., & Mohd Yasin, M. F. Modelling of a Bluff-Body Stabilised Premixed Flames Close to Blow-Off. *Computation*, 2021, vol. 9, article no. 43. DOI: 10.3390/computation9040043.

10. Ma, X., Nie, B., Wang, W., Zhao, D., Zhang, Y., Yang, Y., Ma, C., Hu, B., Chang, L., & Yang, L. Effect of hydrogen concentration, initial pressure and temperature on mechanisms of hydrogen explosion in confined spaces. *Combustion and Flame*, 2024, vol. 269, article no. 113696. DOI: 10.1016/j.combustflame. 2024.113696.

11. Han, H., Ma, Q., Qin, Z., Li, Y., & Kong, Y. Experimental study on combustion and explosion characteristics of hydrogen-air premixed gas in rectangular channels with large aspect ratio. *International Journal of Hydrogen Energy*, 2024, vol. 57, pp. 1041-1050. DOI: 10.1016/j.ijhydene.2024.01.125.

12. Rudy, W., Pekalski, A., Makarov, D., Teodorczyk, A., & Molkov, V. Prediction of Deflagrative Explosions in Variety of Closed Vessels. *Energies*, 2021, vol. 14, no. 8, article no. 2138. DOI: 10.3390/en14082138.

13. Shypul, O., Garyn, V., Tryfonov, O., Myntiuk, V., Egedy, A. Study of the green hydrogen-air mixture formation in closed chamber with given composition. *Hungarian Journal of Industry and Chemistry*, 2024, vol. 52, no. 2. (In press).

14. Reyes, M., Tinaut, F. V., Horrillo A., & Lafuente, A. Experimental characterization of burning velocities of premixed methane-air and hydrogen-air mixtures in a constant volume combustion bomb at moderate pressure and temperature. *Applied Thermal Engineering*, 2018, vol. 130, pp. 684-697. DOI: 10.1016/j.applthermaleng.2017.10.165.

15. Menter, F. Two-equation eddy-viscosity transport turbulence model for engineering applications. *AIAA Journal,* 1994, vol. 32, pp. 1598-1605. DOI: 10.2514/3.12149.

16. *Fluent Theory Guide*. Available at: https://ansyshelp.ansys.com/account/secured?returnurl=/ Views/Secured/corp/v242/en/flu\_th/flu\_th.html (accessed 29.10.2024).

17. Nguyen, P., Vervisch, L., Subramanian, V., & Domingo, P. Multi-Dimensional Flamelet-Generated Manifolds for Partially Premixed Combustion. *Combustion and Flame*, 2010, vol. 157, no. 1, pp. 43-61. DOI: 10.1016/j.combustflame.2009.07.008.

18. Lodier, G., Vervisch, L., Moureau, V., & Domingo, P. Composition-Space Premixed Flamelet Solution with Differential Diffusion for In Situ Flamelet-Generated Manifolds. *Combustion and Flame*, 2011, vol. 158, no. 10, pp. 2009-2016. DOI: 10.1016/j.combustflame.2011.03.011.

19. *GRI-Mech 3.0*. Available at: http://combustion.berkeley.edu/gri-mech/version30/ text30.html (аccessed 23.09.2024).

*Received 17.07.2024, Accepted 18.11.2024*

# **ЧИСЛОВЕ МОДЕЛЮВАННЯ ГОРІННЯ ВОДНЕВО-ПОВІТРЯНОЇ СУМІШІ В ЗАКРИТІЙ КАМЕРІ ПРИ НИЗЬКОМУ ПОЧАТКОВОМУ ТИСКУ** *О. В. Трифонов, О. В. Шипуль, В. О. Гарін, В. Б. Минтюк, Д. А. Ткаченко*

У цій роботі досліджується процес горіння воднево-повітряної суміші при низькому початковому тиску в закритій камері, з фокусом на можливості обробки пластиків за термоенергетичним методом (ТЕМ). **Мета** дослідження полягає в тому, щоб розробити й верифікувати числову модель, здатну передбачити критичні параметри горіння, зокрема профілі розподілу тиску та температури в часі, щоб забезпечити безпечну та ефективну обробку ТЕМ. **Завдання** включали побудову та перевірку моделі горіння водень-повітря з використанням експериментальних даних для високої точності та застосовності в системах ТЕМ. Дослідження виконано CFD **методом** у системі ANSYS Fluent з використанням кінетичного механізму горіння GRI-mech 3.0 та поліноміальні функції четвертого ступеня для визначення термодинамічних властивостей реагентів та продуктів горіння. Порівняння розробленої моделі з відомими експериментальними даними дала точні результати з піковими відхиленнями тиску менше 3%. Після верифікації модель було застосовано для імітації горіння в промисловій ТЕМ-камері, яка відповідає реальним умовам експлуатації. **Результати** показали послідовний розвиток фронту полум'я, включаючи утворення турбулентних коміркових структур, які є важливими для досягнення оптимального розподілу температури та стабільності всередині камери. Ці знання дозволяють стратегічно розмістити деталі, щоб максимізувати якість обробки, що особливо важливо при використанні воднево-повітряних сумішей низького тиску. **Висновки**. Розроблена й верифікована числова модель доводить потенціал використання палива на основі зеленого водню як

екологічної альтернативи для енергоємних промислових процесів, що сприяє розвитку кліматично нейтрального виробництва. Майбутня робота буде розширена на дослідження оплавлення пластиків у ТЕМ камерах, покращуючи точність обробки та безпеку для ширшого застосування у стійкому виробництві деталей з термопластів.

**Ключові слова:** воднево-повітряна суміш; низький початковий тиск; термопластичні матеріали; обробка ТЕМ.

**Трифонов Олег Валерійович** – канд. техн. наук, доц., доц. каф. технології виробництва літальних апаратів, Національний аерокосмічний університет ім. М. Є. Жуковського «Харківський авіаційний інститут», Харків, Україна.

**Шипуль Ольга Володимирівна** – д-р техн. наук, доц., доц. каф. технології виробництва літальних апаратів, Національний аерокосмічний університет ім. М. Є. Жуковського «Харківський авіаційний інститут», Харків, Україна.

**Гарін Вадим Олегович** – канд. техн. наук, старш. досл., старш. наук. співроб. каф. технології виробництва літальних апаратів, Національний аерокосмічний університет ім. М. Є. Жуковського «Харківський авіаційний інститут», Харків, Україна.

**Минтюк Віталій Борисович** – канд. техн. наук, доц. каф. проєктування літальних апаратів, Національний аерокосмічний університет ім. М. Є. Жуковського «Харківський авіаційний інститут», Харків, Україна.

**Ткаченко Денис Анатолійович** – старш. викл. каф. міцності літальних апаратів, Національний аерокосмічний університет ім. М. Є. Жуковського «Харківський авіаційний інститут», Харків, Україна.

**Oleh Tryfonov** – Candidate of Technical Sciences, Associate Professor, Associate Professor at the Department of the Technologies of Aircraft Manufacturing, National Aerospace University "Kharkiv Aviation Institute", Kharkiv, Ukraine,

e-mail: o.v.trifonov@gmail.com, ORCID: 0000-0001-8058-8649, Scopus Author ID: 57192959255.

**Olga Shypul** – Doctor of Technical Sciences, Associate Professor, Associate Professor at the Department of the Technologies of Aircraft Manufacturing, National Aerospace University "Kharkiv Aviation Institute", Kharkiv, Ukraine,

e-mail: o.shipul@khai.edu, ORCID: 0000-0002-1356-5831, Scopus Author ID: 57192959380.

**Vadym Garin** – Candidate of Technical Sciences, Senior Researcher, Senior Researcher at the Department of the Technologies of Aircraft Manufacturing, National Aerospace University "Kharkiv Aviation Institute", Kharkiv, Ukraine,

e-mail: v.garin@khai.edu, ORCID: 0000-0001-7788-0593, Scopus Author ID: 57219015898.

**Vitalii Myntiuk** – Candidate of Technical Sciences, Associate Professor at the Department of Aircraft Design, National Aerospace University "Kharkiv Aviation Institute", Kharkiv, Ukraine,

e-mail: vitalii.myntiuk@khai.edu, ORCID: 0000-0002-4047-0192, Scopus Author ID: 57201067344.

**Denys Tkachenko** – Lecturer of the Department of Aircraft Strength, National Aerospace University "Kharkiv Aviation Institute", Kharkiv, Ukraine,

e-mail: d.tkachenko@khai.edu, ORCID: 0000-0002-5006-6775, Scopus Author ID: 57463439000.