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NEURAL NETWORK ACCELERATION OF NUMERICAL SIMULATION OF METHANE COMBUSTION IN A GAS TURBINE ENGINE

Chepurnyi A.V.*, Jakovics A.

Institute of Numerical Modelling, University of Latvia, Riga, Latvia
*Corresponding author: vasfed12345@gmail.com/

Abstract. *Gas turbines are essential for high-power energy generation, but growing demands to reduce NO_x and CO_2 emissions make traditional combustion chamber design increasingly complex and costly. This work proposes a new modeling paradigm that combines high-fidelity Computational Fluid Dynamics using neural network learning to accelerate emission prediction. A Computational Fluid Dynamics model was developed using the Reynolds-averaged Navier-Stokes equations with the k–ε turbulence model and a non-premixed Probability Density Function approach to simulate turbulent methane combustion. NO_x emissions were calculated post-simulation using the Zeldovich mechanism. Model validation included varying fuel flow, excess air ratio, and wall heat loss. To speed up evaluations, a multilayer perceptron neural network was trained on Computational Fluid Dynamics results to predict NO_x and CO_2 emissions based on key inputs (fuel rate, air excess, temperature, pressure, cooling). The model achieved high accuracy with a coefficient of determination (R^2) of 0.998 for NO_x and 0.956 for CO_2 on an independent test set. Results showed good agreement with both experimental data and a Network of ideal reactors model using detailed kinetic scheme of methane combustion - Mech 3.0. This neural network serves as a fast surrogate model for emissions assessment, enabling rapid optimization of low-emission combustor designs. The approach is suitable for digital twins and combustion control systems and is adaptable to alternative fuels like hydrogen and ammonia.*

Keywords: neural network, combustion, gas turbine engine, numerical simulation.

Abbreviations:
PDF - Probability Density Function (in context - the estimated PDF of the mixture)
RANS - Reynolds-averaged Navier-Stokes equations
RNG k–ε - Turbulent k–ε model with group renormalization
CRN - Network of ideal reactors (method of calculating chemical kinetics)
GRI-Mech 3.0 - Detailed kinetic scheme of methane combustion
MLP - Multilayer Perceptron
ANN - Artificial neural network
PCA - Principal Component Analysis
POD - Method of eigen orthogonal functions
RBF - Radial basis function / radial basis neural network
LES - Large Eddy Simulation
RSM - Reynolds stress model
P1 - Radiation model P1 (first approximation)
SIMPLE - Semi-explicit method for pressure-velocity relationship
MPC - Model-based control (predictive)
CPU - Central Processing Unit
GTE - Gas Turbine Engine
PINN - Physically-informed neural network
CNN - Convolutional Neural Network

1. Introduction

Gas turbine engines (Fig. 1) are widely used in power engineering and aviation, but increasingly stringent NOx and CO_2 regulations require combustion chambers that operate reliably at high pressures and temperatures while producing minimal emissions. The full development cycle of such chambers traditionally relies on expensive experimental stands and resource-intensive Computational Fluid Dynamics (CFD) calculations: modeling turbulent combustion with detailed chemistry takes hours to days, which significantly slows down development. Machine learning, in particular neural networks, offers a way out: a neural network trained on a set of CFD and experimental data instantly predicts flame temperature, product composition, and emission levels. This opens the way to rapid mode selection, optimization, and reduction of design costs.

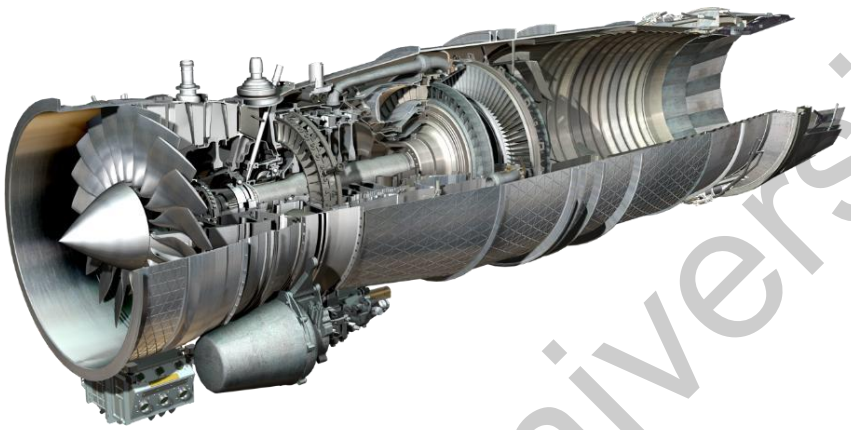


Fig.1. The gas turbine engine - Eurojet EJ200 is a low-bypass turbofan used as the powerplant of the Eurofighter Typhoon (image taken from the official manufacturer's website [https://www.eurojet.de/innovation/])

The aim of the work is to show that a multilayer perceptron trained on a sample of CFD models of methane flame provides engineering-acceptable accuracy of NOx/CO_2 prediction at a computational cost an order of magnitude lower than classical CFD, thereby radically accelerating the process of developing combustion chambers for gas turbine engines.

In recent years, interest in combustion and emissions has increasingly led to the use of neural networks [1]. Wang and Yang showed that such models predict NOx formation significantly more accurately [2, 3]. Earlier work already demonstrated the usefulness of artificial neural networks (ANN) for describing combustion processes [4]. Thus, in [5], a single-layer network predicted NOx emissions, vibrations, and pressure fluctuations based on the operating parameters of a gas turbine engine. Lamont et al. confirmed that ANNs provide accurate estimates of NOx, CO, and chamber outlet temperature with metered fuel supply [6].

"Fast" simplified models are also being developed. Wang et al. created a compact neural network that replaces complex calculations of turbulent combustion and preserves the flow shape with good accuracy [7]. Aversano and colleagues combined principal component analysis and kriging interpolation, constructing a "digital twin" of a burner for a fast parametric study. Similarly, the eigenfunction method in conjunction with the radial basis network made it possible to speed up calculations of a large furnace several times with an acceptable error [8]. For a direct emission forecast, Sun et al. used an RBF network: the maximum errors were ≈ 12% for NOx and ≈ 3% for CO, the average errors were < 5% and 1%, respectively [9]. The hybrid approach "CFD + network of simple reactors" turned out to be promising. It takes the flow field from CFD and calculates the chemistry in a network of elementary reactors, reducing the NOx discrepancy to ≈ 5% (versus 10–20% for pure CFD) [10]. Such a mechanism is implemented, for example, in the ENERGICO energy package, where the CHEMKIN module provides an accuracy of < 5% and reduces the calculation time from weeks to days [11]. Experience shows that neural networks and their combination with classical calculations effectively approximate complex interrelations in combustion and help reduce emissions [12].

In this paper, this approach is developed: detailed CFD modeling is used to train an MLP network that forms an "express model" of methane combustion chamber emissions.

The object of the study is the turbulent non-premix flame of a methane-air mixture in the combustion chamber (Fig. 2) of a gas turbine engine. A steady-state combustion mode is considered: methane (CH_4) is fed

through a burnr, mixed with an oxidizer (air) and burns in the chamber. The main reaction during complete combustion is:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

with the release of heat.

However, in real conditions the flame is turbulent and some of the fuel may not burn completely (CO is formed), and at high temperatures nitrogen oxides are generated from atmospheric nitrogen (thermal NOx by the Zeldovich mechanism). To adequately describe the process, it is necessary to solve a system of coupled equations of gas flow and heat/mass transfer taking into account chemical kinetics.

The gas flow was described by the system of Reynolds-averaged Navier-Stokes (RANS) equations for conservation of mass, momentum, energy, and species transport. The flow was assumed to be steady, turbulent, and chemically reacting.

These equations track how the composition of the gas mixture changes as a result of convection, diffusion, and reactions. For turbulent combustion, a direct solution of a detailed kinetic scheme (including dozens of reactions and intermediate radicals) in conjunction with the Navier–Stokes equations are practically unrealizable due to the enormous computational complexity. Therefore, turbulent combustion models are used that simplify the description of chemistry while preserving the main effects. In this paper, a non-premix combustion approach is used using a variable mixture fraction and the assumption of fast combustion. A scalar value Z is introduced – the fractional content of fuel (mixture) in the gas. The value Z = 0 corresponds to a pure oxidizer, Z = 1 – to pure fuel. It is assumed that turbulent mixing occurs much slower than the chemical reaction (fast chemical reaction mode), therefore, at each point, chemical equilibrium is established instantly based on the local Z and the mixture formation parameter (for example, enthalpy). Thus, the concentration fields of products (CO_2, H_2O), residual O_2 and main pollutants are calculated assuming local chemical equilibrium at given Z. Turbulent fluctuations of Z are taken into account by means of the assumed PDF (probability density function, Fig. 3) model [13].

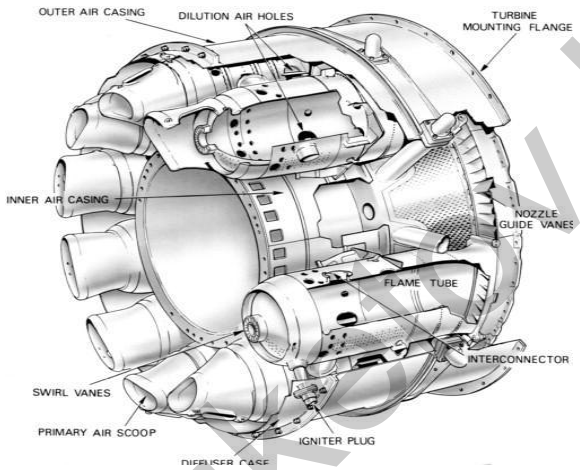


Fig.2. Tubo-annular combustion chamber (Rolls-Royce) [12].

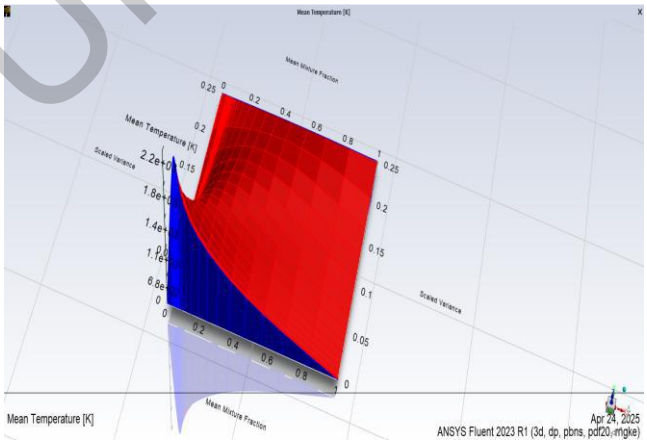


Fig.3. Three-dimensional surface from the flamelet-PDF library generated in the Flamelet-PDF module of ANSYS Fluent for a stationary laminar diffusion flame [14].

The red part of the surface shows hot combustion products (up to ~2250 K) near the optimal fuel-air ratio; blue - cold areas where reactions have not yet begun. The stronger the mixing (the greater the dispersion), the lower the peak temperature: turbulence "stretches" the flame and cools it. The 3-D surface provides a visual representation of how the mixture, turbulence and chemistry work together to form a flame.

A P(Z) distribution within the cell is assumed (usually a beta distribution), allowing the turbulence-averaged product fractions and heat release to be calculated. This approach is known as the unmixed combustion PDF model and is implemented in ANSYS Fluent, among others. It greatly simplifies the calculations by reducing the integration of the rigid kinetics to a preliminary calculation (of a chemical equilibrium table or "flamlet"), and then only the algebraic operations to determine the Z compositions are performed during the CFD solution.

The approach is based on the hypothesis of instantaneous (infinitely fast) combustion, which is true for the main reactants, but NOx formation does not fit into this concept, since NOx formation is a relatively slow process compared to fuel combustion. Therefore, a separate calculation (postprocessing) is used for NOx, taking into account the final reaction rate, as discussed below.

Boundary and initial conditions.

At the chamber inlet, a fuel and air inflow with a certain flow rate and temperature is specified. At the chamber outlet, a boundary condition of the outlet (outlet pressure or ambient condition) is specified. The chamber walls are considered either adiabatic or considering heat exchange. Model validation (see "Verification and validation of models") includes a comparison of variants with heat loss (convective heat removal and radiation) and without it. To summarize, the formulated problem is a stationary turbulent combustion of a methane-air mixture in a direct-flow combustion chamber. The solution method is numerical integration of the averaged Navier-Stokes equations with a turbulent combustion model (mixture model with PDF), supplemented by calculating NOx formation in the postprocessor. The selected turbulence and combustion models and the rationale for their use are described below.

The RNG k–ε turbulence model [15] is used to close the averaged system of flow equations. This is a modification of the standard k–ε model with an additional term in the equation for ε, which increases the accuracy in describing rapidly decaying flows and takes into account the swirl. This is especially important for gas turbine engine combustion chambers, where the flow swirls to stabilize the flame. The model also provides more reasonable values for some constants (e.g., Prandtl numbers) and is able to take into account effects at low Re. Compared to the standard k–ε, RNG k–ε better describes curvilinear and vortex flows with a moderate computational load [15]. The non-premixed PDF approach (see Section 3) is used to describe combustion, where combustion is assumed to be limited by the mixing rate and chemistry is instantaneous. Turbulence affects the flame through fluctuations in the mixture parameter Z, which is described by the beta distribution. The method is suitable for methane diffusion flames, where combustion is determined by the reactant feed.

Since the model assumes instantaneous chemistry, NOx formation is calculated separately after the main calculation, taking into account the final reaction rate according to the Zeldovich mechanism and prompt-NO (the NOx model in Fluent) [16]. When using detailed kinetics directly in the calculation (e.g. via the PDF transport equation), the accuracy can increase to the level of 6% RMS for NOx [17], but this requires significantly more resources. Thus, the combination of RNG k–ε and PDF model is chosen as a balanced solution between accuracy and efficiency, widely used for modeling methane combustion with satisfactory results in terms of temperature and product composition.

Numerical simulation was performed in ANSYS Fluent. The geometry of the flame tube of a typical straight-through tubular-annular combustion chamber with a swirler was built in the SolidWorks' program, the mesh was built in ANSYS Meshing (~5×10^5 cells). A model of almost incompressible gas with the ideal gas equation of state was used. The finite volume method and the Second Order Upwind scheme were applied to approximate the equations (momentum, energy, k, ε, composition). The difference between the 1st and 2nd order schemes on a fine mesh was <2%. The relationship between pressure and velocity was implemented using the SIMPLE algorithm. Convergence criteria: residuals $<10^{-6}$, integral parameters are stabilized with an accuracy of 0.1%. Grid convergence analysis was performed: when doubling the number of cells (to 10^6), the temperature changed by <1%, NOx by ~2%, which confirmed the adequacy of the base grid. A step-by-step strategy was used: first, the main combustion (without NOx) was calculated, then NOx emissions in the postprocessor based on the Zeldovich mechanism (Fluent NO-postprocessor), with recalculation to 15% O_2

Taking into account heat transfer through the walls turned out to be critical: in the base case - adiabatic conditions, then - a scenario with heat loss through convection ($h = 100$ W/m² K, T_ext = 500 K) and radiation (model P1, emission = 0.7).

To ensure the generalization capability of the neural network and meet statistical requirements, the training dataset was expanded to 200 operating points. The dataset covers a wide range of operating conditions characteristic of gas turbine combustion chambers:

- Fuel mass flow rate**:** 0.004 – 0.006 kg/s;
- Air inlet temperature**:** 300 – 600 K;
- Air excess ratio (α): 1.2 – 2.0.

The neural network was trained in MATLAB using the Levenberg-Marquardt algorithm. The dataset was randomly divided into three subsets: Training (70%) for weight adjustment, Validation (15%) to prevent overfitting, and Testing (15%) for independent performance evaluation.

Training dataset structure

Each row in the table corresponds to one unique CFD simulation with its own set of input and output parameters. These parameters are divided into two groups:

Inputs: These are the 4 variables that determined the operating conditions of the combustor in the simulation. The neural network learns from them to make predictions.

mf_fuel_kg_s: mass flow rate of fuel (methane) in kg/s.

mf_air_primary_kg_s: mass flow rate of primary air (for combustion) in kg/s.

mf_air_secondary_kg_s: mass flow rate of secondary air (for cooling) in kg/s.

T_air_in_K: inlet air temperature in Kelvin.

Outputs: these are the 2 target variables that the neural network learns to predict:

Mass fraction NOx - mass fraction of nitrogen oxides (NOx) in the combustion products.

CO2_pct - percentage of carbon dioxide (CO_2) in the combustion products.

The purpose of using this table is to train the neural network (multilayer perceptron) to recognize the complex relationships between the operating parameters of the combustion chamber and the resulting NOx and CO_2 emissions, so that it can make instant predictions without the need for lengthy CFD calculations.

At this stage, 200 CFD calculations may be sufficient for preliminary analysis and creation of the neural network model, this allows to assess the main trends and check what is happening, but it is planned to increase the number of calculations to 500 - 2000 options. The neural network was trained in MATLAB (Neural Network Toolbox): 4 inputs, one hidden layer of 10 neurons, 2 outputs (NOx, CO_2), the backpropagation method (Levenberg–Marquardt algorithm). MSE reached a minimum in ~100 epochs. Calculation of 1 point <0.01 s — comparable to a thousand-fold acceleration compared to CFD. For additional validation, CHEMKIN (via ANSYS Chemkin-Pro) was used — equilibrium composition, verification of the NO formation mechanism. Calculations were also performed in ANSYS Energico — the chamber model as a network of PSR reactors (Fig. 4), the GRI-Mech 3.0 mechanism. NOx values were obtained with an accuracy of 5–10% of the experimental ones, confirming the reliability of the models. Thus, the integrated approach combined the tools of CFD (Fluent), detailed chemistry (Chemkin/Energico) and neural network modeling (MATLAB), which allowed a comprehensive study and validation of the proposed methodology.

2. Materials and Methods

Numerical verification.

To check the numerical stability, a grid convergence analysis was performed on three grids: 0.3, 0.5, and 1.0 million elements. With increasing resolution, the maximum temperature increased (~1940 K → ~2010 K), and NOx increased from 45 ppm to 55 ppm. The changes in the transition from 0.5 to 1 million were ~6%, which is considered acceptable. The base grid (0.5 million) was used further, and the spread was taken into account as an estimate of the discretization error. Approximation schemes were also investigated: the 1st order scheme underestimated the temperature and NOx (1960 K and 48 ppm), so the 2nd order scheme was used in the calculations. Taking into account heat losses (convection and radiation model P1) reduced the temperature by 100–150 K and decreased NOx by ~15%. For example, with an equivalent coefficient of 0.6, the NOx concentration decreased from 50 to ~42 ppm. The main features of the flow were preserved.

Experimental validation.

The numerical data are compared with the results from [18], where NOx ~25 ppm at T_output ~1673 K were obtained in a laboratory chamber on methane. The CFD results (22–30 ppm at ~1650–1700 K) fall within this range. The expected exponential dependence of NOx on temperature, characteristic of the thermal mechanism of its formation, is also confirmed [19]. For example, increasing the temperature from 1500 to 1700 K increased NOx from 10 to 50 ppm.

The temperature distributions in CFD correspond to the laser diagnostics data: the maximum of ~2000 K is localized in the flame above the burner, with a subsequent decrease towards the outlet (~1600 K). The observed recirculation zone behind the swirl is consistent with the literature data for swirling turbulent methane flames [20]. Additionally, a comparison was made with the CRN reactor model using GRI-Mech 3.0. The obtained NOx level (~50 ppm) practically coincides with the CFD results (~52 ppm), confirming the reliability of the model. The CO_2 yield was in the range of 8–10%, which is close to the theoretical value. The CO concentration did not exceed 10 ppm (at the nominal mode), indicating almost complete combustion.

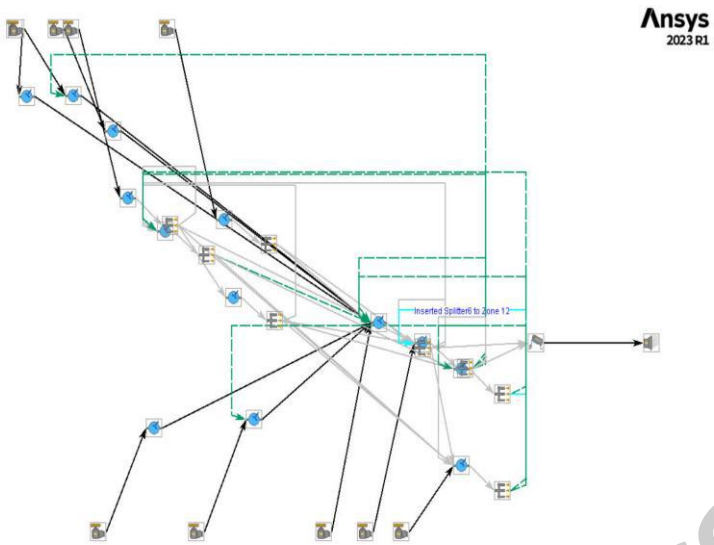


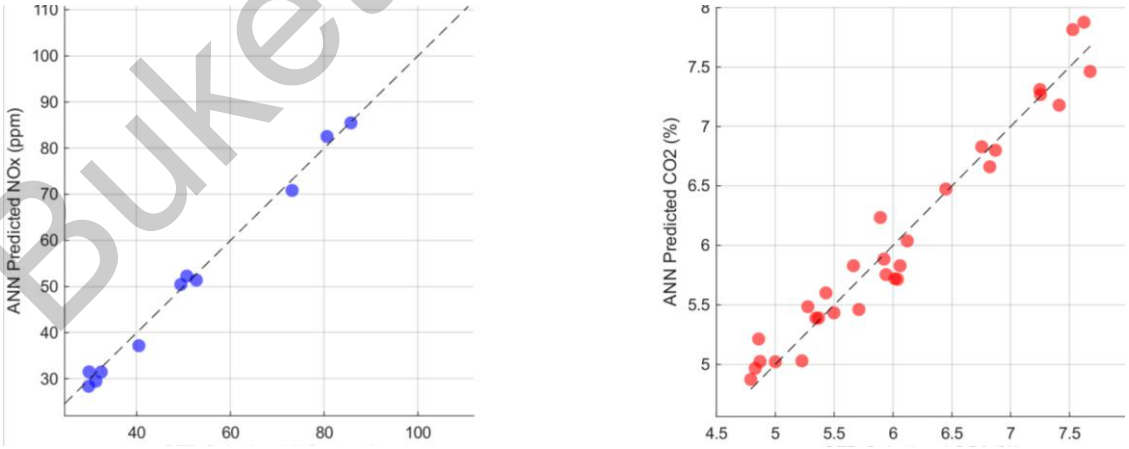
Fig.4. Network of serial/parallel PSR (Perfectly Stirred Reactor) reactors with visual flow grouping tools.

Testing the neural network model.

An extended dataset (200 cases) was used. The prediction performance was evaluated on an independent test set of 30 scenarios (15% of the database). The results are presented in Fig. 5. The model demonstrated high accuracy: the coefficient of determination (R^2) reached 0.998 for NOx and 0.956 for CO_2. The Mean Absolute Error (MAE) and Root Mean Squared Error (RMSE) values confirm that the neural network successfully reproduces the complex non-linear dependencies of pollutant formation without significant overfitting. The maximum deviation for NOx (~10%) was observed in extreme lean modes.

Table 1. Neural network performance metrics on the independent test dataset.

Variable	R^2 (Determination Coefficient)	MAE (Mean Absolute Error)	RMSE (Root Mean Squared Error)
NOx (ppm)	0.998	1.774	2.450
CO_2 (%)	0.956	0.202	0.263



a) b)

Fig.5. Neural Network Validation Results: a) NO_x prediction (R^2=0.998); b) CO_2 prediction (R^2=0.956).

In general, the neural network correctly reproduced the main dependencies (increase in NOx with temperature, decrease in CO_2 with lean mixtures), which corresponds to literature data [9]. This confirms the adequacy of both the CFD model and the neural network trained on its basis.

3. Results and discussion

In Fig. 6 the temperature profile in the combustion chamber is shown under typical conditions (air excess coefficient α ≈ 2.0, close to the nominal load). The maximum temperature reaches ~2100 K in the main flame zone immediately behind the swirl.

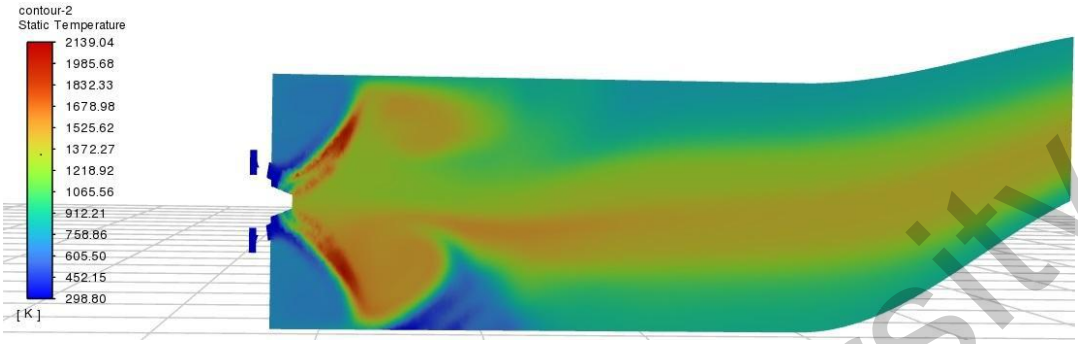
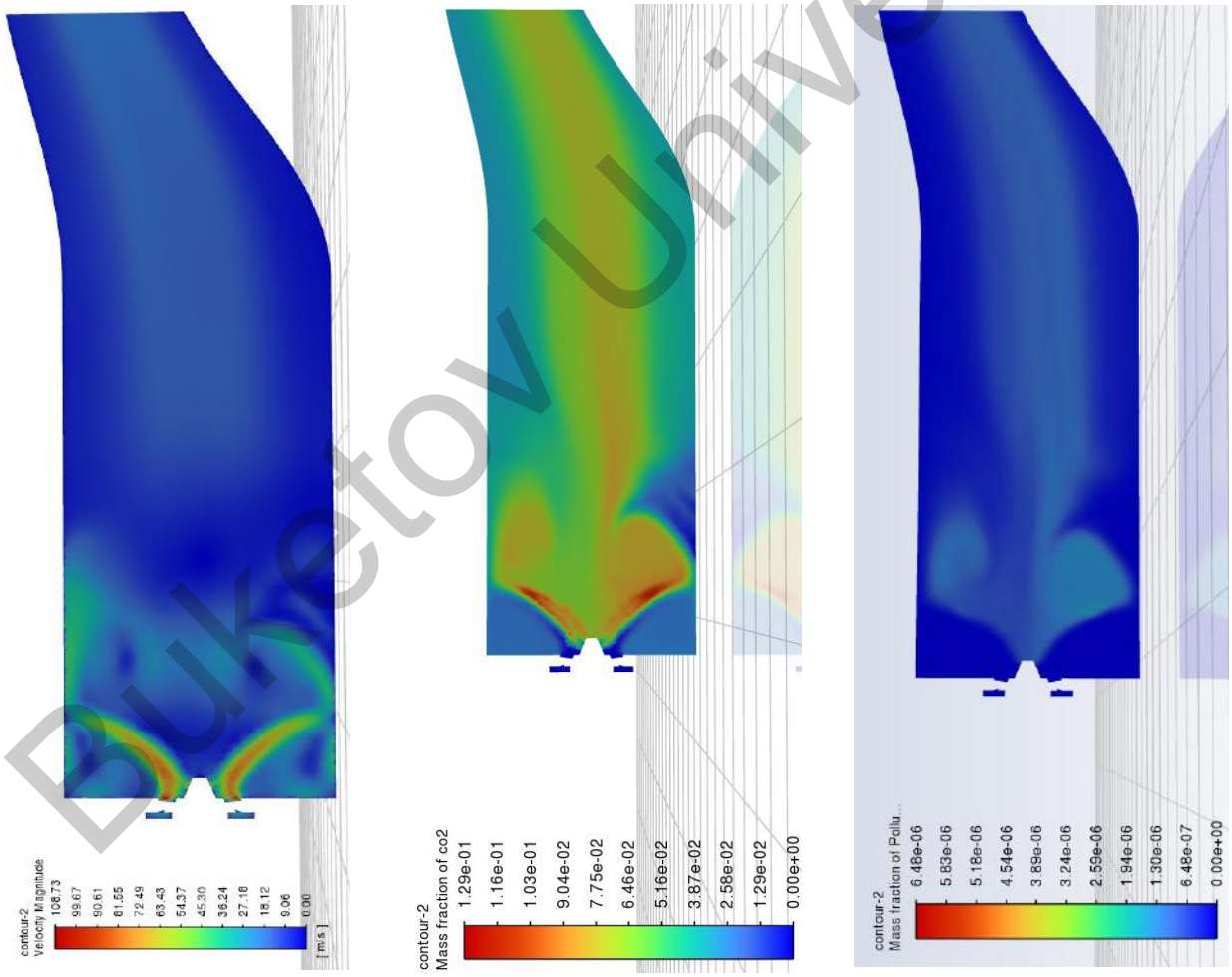


Fig.6. Temperature profile in the flame tube under typical conditions (described in the text)



a) b) c)

Fig.7. Distribution along the flame tube of the:
a) velocity magnitude; b) mass fraction of CO2; c) mass fraction of NOx (mode with a "lean" fuel-air mixture).

In the central part of the chamber, a combustion product recirculation zone is formed, which is expressed in an area with an elevated temperature (about 1500 K) – this helps maintain combustion and re-burn unreacted

methane, Fig 7. Closer to the walls, the temperature is lower (about 1000 K or less, due to the supply of secondary air), which is important to prevent overheating of the chamber material. Velocity field (Fig 7a) is characterized by a strong swirl of the flow: immediately behind the inlet nozzle, a swirling air flow is visible, creating a toroidal recirculation zone behind the flame plume. This zone captures part of the combustion products and returns them to the base of the flame, promoting stable combustion. Such a structure (the so-called internal recirculation torus) is typical for chambers with vortex stabilization.

The distribution of concentrations of the main products (CO_2, H_2O) exactly repeats the temperature field - the highest concentration of CO_2 is observed in the same place where the temperature is high, confirming that the fuel mainly burns in the torch behind the swirl. Oxygen is almost completely consumed in the flame zone, and ~15% O_2 remains at the outlet (in terms of dry gas, (during fuel combustion, water vapor (H_2O) is formed. But when analyzing the composition of combustion products, it is removed (moisture condenses), and only the dry part of the gas is analyzed - CO_2, CO, O_2, NOx, etc.)) with an excess of air of 2.0, which is consistent with the mass balance), Fig. 7b., Fig. 7c.

The CFD model showed that NOx is formed in the high-temperature flame zone (Fig. 7c, reaching 20–30 ppm behind the combustion zone. The concentration decreases towards the outlet due to dilution. The final emission is ~50 ppm without cooling, ~40–45 ppm with cooling, which corresponds to the standards (temperature <2000 K). An increase in temperature (for example, when α decreases from 2.0 to 1.8) causes a sharp increase in NOx (~15 → 70 ppm), which is due to the exponential dependence according to Arrhenius. The opposite trend is observed for lean mixtures: at α=2.5 – only ~10 ppm. The air temperature at the inlet also has an effect. The neural network successfully reproduces these dependencies, accelerating the analysis of modes. CO_2 prediction and combustion efficiency: at nominal modes, CO_2 is ~3–4%, which indicates complete combustion. At α=3.0, CO_2 drops to ~2%, and CO grows (~5e–6), which reflects deterioration of combustion in a diluted and cooled flame.

4. Conclusions

This paper presents a study aimed at improving the efficiency of numerical modeling of methane combustion in a gas turbine engine combustion chamber by using neural networks. A technique has been developed that combines high-precision CFD modeling of turbulent combustion with subsequent training of a multilayer perceptron for rapid prediction of harmful emissions.

The main conclusions and results are as follows:

1 A CFD model of a methane combustion chamber (flame tube) has been developed based on the RNG k–ε turbulent model and a combustion model assuming fast chemical reaction with PDF.

2 The model has been successfully verified (grid sensitivity analysis, comparison of orders of approximation) and validated against literature data: temperature and concentration distributions, as well as predicted NOx levels (~tens of ppm) are close to those observed experimentally. This confirms the suitability of the selected models for assessing processes in a real chamber.

3 A numerical study of the factors influencing NOx and CO_2 emissions was conducted. It was shown that the key role is played by the combustion temperature regime, determined by the mixture composition (excess air coefficient) and cooling conditions. Thermal NOx increases sharply with an increase in the maximum flame temperature, which corresponds to the exponential nature of its kinetics. Moderate wall cooling can reduce NOx by 10–20% by reducing thermal peaks. Methane combustion efficiency (in terms of CO_2 and CO concentrations) is reduced at too lean mixtures, which limits the ability to minimize NOx by leaning alone. These results are consistent with physical concepts and previously published data on emissions in chamber flare flames [21].

4 A neural network model (MLP) has been developed that approximates the dependence of NOx and CO_2 emissions on the chamber operating mode parameters. The model has been trained on an expanded dataset (200 cases) obtained from CFD and provides a coefficient of determination (R^2) of 0.998 for NOx and 0.956 for CO_2 relative to CFD.

5 In practice, this means that the neural network can replace CFD calculations for emission assessment purposes, producing results in a fraction of a second. Thus, a significant increase in efficiency has been achieved: a quick forecast is possible in real time or during multiple runs during optimization calculations.

6 The neural network reproduces physical patterns: analysis of weights and responses showed that the model captures the exponential nature of NOx growth with temperature, the effect of residence time and oxygen concentration, although these dependencies were not explicitly specified. This demonstrates the ability

of AI tools to identify hidden dependencies in complex multidimensional combustion process data. In essence, the neural network has become a digital twin of the camera, to which various scenarios can be applied and a reliable response estimate can be obtained.

Application prospects. The proposed approach can be directly used in the design of low-emission combustion chambers. A neural network surrogate trained on CFD data can be integrated into optimization algorithms for finding the best configuration (e.g. swirl geometry, flame tube diameter ratio, etc.) based on the criteria of minimizing NOx/CO while maintaining combustion stability. In addition, such a surrogate can serve as the basis for a combustion monitoring and control system: receiving operational sensor data (temperature, flow rate, pressure), the trained network could predict the emission level and signal the need to adjust the mode, which essentially implements the concept of control based on the MPC (Model Predictive Control) model for emissions.

The plan is to move on to modeling ammonia combustion by training a neural network surrogate that simultaneously predicts NO_x, CO, and soot. For this, full-size CFD dumps, and more complex architectures (CNN, PINN) will be used, which will allow reproducing the spatial-temporal structure of the flame and assessing thermoacoustic stability. Additionally, the introduction of AI models directly into the CFD code is being considered to correct for turbulence and reaction rates, providing faster and more accurate calculations.

Conflict of interest statement

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.

CRediT author statement

Chepurnyi A.: Conceptualization, Software, Validation, Investigation, Data curation, Writing – original draft, Visualization; **Jakovics A.:** Methodology, Analysis of calculations results and scientific editing of draft. The final manuscript was read and approved by all authors.

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The author, Andrii Chepurnyi, dedicates this article to his entire large and educated family, who instilled in him a love of science, especially his mother Lyudmila Chepurna, and grandfather Ivan Chepurnyi.

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AUTHORS' INFORMATION

Chepurnyi, **Andrii** – PhD student, University of Latvia, Riga, Latvia; https://orcid.org/0009-0005-4410-5458; vasfed12345@gmail.com

Jakovics, Andris – Doctor of Physical and Mathematical Sciences, Head of Laboratory of Multiphysical Processes, University of Latvia, Riga, Latvia; https://orcid.org/0000-0003-3410-5081; Andris.Jakovics@lu.lv