

NUMERICAL SOLUTION OF THE OPTIMAL
CONTROL PROBLEM OF VISCOUS
HEAT-CONDUCTING GAS FLOW USING THE PINN
METHODK.S. KUZNETSOV  AND E.V. AMOSOVA *Dedicated to 85th birthday of academician Vladimir G. Romanov*

Abstract: The numerical solution of the problem of optimal control of the non-stationary flow of a viscous, heat-conducting compressible medium in the one-dimensional case is considered. The initial state velocity and velocity at the right boundary are used as control. To solve the problem, the PINN method, is used. To do this, the problem of minimizing a quadratic functional is solved. The functional includes terms for the residuals of the equations, boundary and initial conditions, and also, for the inverse problem, additional information. Numerical experiments were performed in cases where the velocity, density and temperature separately are minimized to the given functions. The parameters of the medium correspond to the physical parameters of real gases at high Reynolds numbers, $Re = 1.5 \cdot 10^7 - 2.4 \cdot 10^8$, and Peclet numbers, $Pe = 3 \cdot 10^7 - 1.6 \cdot 10^8$. The method allows to solve numerically complex nonlinear problems of optimal control without discretization, linearization and solving optimality systems.

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1 Introduction

Numerical solution of the system of equations including the equation of motion, the continuity equation, and the heat equation is an actual problem of modern mathematics, in particular, due to its significant importance in the context of solving scientific and technical problems. It is worth noting that the solution of these equations is especially difficult when they describe the motion of a compressible medium. In this case, the system of equations differs from the equations of hydrodynamics by the type of differential equations and the presence of large heterogeneity in the medium, caused by the presence of small coefficients before the second derivatives. It is worth noting that the behavior of this system of equations for a compressible medium was fully studied in [1, 2], but only in the one-dimensional case.

The solution of inverse problems of gas dynamics is of particular interest due to its practical significance, for example, in problems of aerodynamics [3, 4], power engineering [5, 6]. Problems of optimal control of gas flow are also relevant when working with gas turbines and compressors [7]. The ability to control gas flow can increase their operating efficiency, as well as improve their reliability and durability, achieving optimal performance of the mechanism.

The authors propose to use a method called Physics Informed Neural Networks (PINN) to solve the optimal control problem. It involves approximating unknown functions using neural networks by minimizing a quadratic quality functional, which includes terms for the residual equations, boundary and initial conditions, as well as the term with an additional information in the case of solving an inverse or ill-posed problem. The method was first presented in the pioneering study [8] as a new way to solve partial differential equations, and has since been widely used.

In [9] the method is considered to solve the direct problem of metal melting, in which the motion of the liquid phase is described the Navier-Stokes and heat equations. The authors solve the problem in a non-stationary one-dimensional case without using additional information, making a comparison with calculations performed using the finite element method. In addition, the authors calculate the system of equations for a quasi-stationary three-dimensional case, using data obtained by the finite element method as additional information for the neural network, after which they verify the obtained results by comparing them with data from physical experiments.

In the paper [10] the application of PINN to solve the Reynolds equations in two dimensional case at Reynolds numbers in the range $Re = 10^2 - 2 \cdot 10^5$ is considered, also verifying the result by comparison with experimental data.

In the paper [11] the authors use the method to calculate laminar flows of the Navier-Stokes equations in two dimensional case, comparing the results with the exact solution.

In addition, the method is also used to solve various inverse and ill-posed problems. For example, in [12], the application of the PINN method to reconstruct the parameters of the medium in solid mechanics problems was studied, comparing the results with the exact solution. In [13], the solution of the inverse problem of determining the optimal parameters of a multiphase flow is considered. In [14–16], variations of the PINN method suitable for solving inverse problems are proposed.

Solving optimal control problems for gas dynamics equations is difficult due to the high nonlinearity of the system of equations, which requires linearization, as well as solving nonlinear conjugate optimality systems. The presence of zones of rapid function growth requires the use of a small step of the spatial grid, which also apply high computational costs. Using PINN allows one to avoid both the need for linearization and solving optimality systems. In addition, the method allows one to solve systems with high heterogeneity of the medium, caused by large Reynolds numbers [10] on a uniform sample of training data, which does not require thickening in the area of rapid function growth.

The papers [17] and [18] consider solving gas dynamics problems using the DeepONet method, first presented in [19]. The principle of the method is to use the theorem on the approximation of any nonlinear operator by a fully connected neural network with one hidden layer [20]. However, the DeepONet method differs from the PINN method proposed in the current paper. [17] also mentions that the PINN method is more effective in solving inverse problems.

In this paper, the approach proposed in [8] is used to solve the problem of optimal control of the state of the system of motion, continuity, and heat equations for a compressible medium, where the gas velocity initial and right boundary conditions are used as control functions. The possibility of controlling the unknown gas velocity, density, and temperature is studied. The optimal control problem was first considered in [21], where the existence of optimal control was proven, the necessary optimality conditions were derived, and the compactness of the solution set was established. A numerical experiment is calculated and presented for cases of control of each of the unknowns. The advantages of the method used and the potential for its application to solving inverse and ill-posed problems of gas dynamics are shown.

2 Mathematical model

The mathematical model describing the non-stationary flow of a viscous heat-conducting gas in one-dimensional space together with boundary and initial conditions has the following form in dimensionless variables:

$$Sh\rho\frac{\partial u}{\partial t} + \rho u\frac{\partial u}{\partial x} - \frac{1}{Re}\frac{\partial^2 u}{\partial x^2} + k\frac{\partial}{\partial x}(\rho\theta) = 0, \quad (1)$$

$$Sh\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(u\rho) = 0, \quad (2)$$

$$Sh\rho\frac{\partial \theta}{\partial t} + \rho u\frac{\partial \theta}{\partial x} - \frac{1}{Pe}\frac{\partial^2 \theta}{\partial x^2} - \frac{1}{Re}\frac{\pi}{k}\left(\frac{\partial u}{\partial x}\right)^2 + \pi\rho\theta\frac{\partial u}{\partial x} = 0, \quad (3)$$

$$u|_{t=0} = u_0, \quad \rho|_{t=0} = \rho_0, \quad \theta|_{t=0} = \theta_0, \quad (4)$$

$$u|_{x=0} = u_1, \quad \rho|_{x=0} = \rho_1, \quad \theta|_{x=0} = \theta_1, \quad (5)$$

$$u|_{x=1} = u_2, \quad \theta|_{x=1} = \theta_2, \quad x \in [0, 1], \quad t \in [0, 1]. \quad (6)$$

Here u , ρ , θ – are unknown velocity, density and temperature of the gas consequently, Sh – is the Strouhal number, Re – is the Reynolds number, Pe – is the Peclet number, k , π – are dimensionless coefficients. The listed above coefficients can be calculated as follows:

$$Sh = \frac{X}{Tu_s}, \quad Re = \frac{u_s X}{\nu}, \quad \nu = \frac{\mu}{\rho_s},$$

$$Pe = \frac{u_s \rho_s c_v X}{\kappa}, \quad k = \frac{R\theta_s}{u_s^2}, \quad \pi = \frac{R}{c_v},$$

where u_s , ρ_s , θ_s – are reference values of velocity, density and temperature of the gas consequently, X – is the reference size value of the domain, T – is the total time of the process, μ – is the dynamic viscosity of the gas, c_v – is the specific heat capacity of the gas, R – is the universal gas constant.

In [21], the optimal control of the state of the system $\mathbf{s}(\mathbf{v}) = \{u(\mathbf{v}); \rho(\mathbf{v}); \theta(\mathbf{v})\}$ is considered, which is a generalized solution of the system (1)–(6), where the gas velocity initial state, u_0 , and velocity at the right boundary, u_2 , are chosen as the control $\mathbf{v} = \{u_0; u_2\}$. Then the optimal control problem to minimize the following functional:

$$J_\alpha = J(\mathbf{s}) + \alpha_1 \int_0^1 \frac{\partial u_0(x)}{\partial x} dx + \alpha_2 \int_0^1 \frac{\partial u_2(t)}{\partial t} dt, \quad (7)$$

$$J_\alpha \rightarrow \min, \quad (8)$$

where α_1 , α_2 – are non-negative constants, and the following functionals can be used as $J(\mathbf{s})$:

$$J_u(\mathbf{s}) = \int_0^1 \int_0^1 (u - u_d)^2 dx dt, \quad (9)$$

$$J_\rho(\mathbf{s}) = \int_0^1 \int_0^1 (\rho - \rho_d)^2 dx dt, \quad (10)$$

$$J_\theta(\mathbf{s}) = \int_0^1 \int_0^1 (\theta - \theta_d)^2 dx dt, \quad (11)$$

where $u_d = u_d(x, t)$, $\rho_d = \rho_d(x, t)$, $\theta_d = \theta_d(x, t)$ – are given functions.

We use the usual notation $L^p(W_p^l)$ for spaces of functions integrable to degree $p \geq 1$ (together with generalized derivatives up to order $l \geq 0$).

By $L^2(0, T; X)$ we denote the space of measurable functions mapping the interval $(0, T)$ into the space X , such that

$$\|f\|_{L^2(0, T; X)}^2 = \int_0^T \|f\|_X^2 dt < \infty.$$

By H^s we denote the space W_2^l , $l > 0$,

$$H^{2,1} = \{q \in L^2(0, T; H^2(\Omega)) : q \in H^1(0, T; L^2(\Omega))\}.$$

Let us denote

$$Y = \{q_1; q_2; q_3 : q_1, q_3 \in H^{2,1}(Q) \cap L^\infty(0, T; H^1(0, 1)),$$

$$q_2 \in L^\infty(0, T; H^1(0, 1)), q_{2t} \in L^\infty(0, T; L^2(0, 1)) \cap L^\infty(0, T; H^1(0, 1))\}.$$

Definition. A generalized solution of problem (1)–(6) is a vector-function $\mathbf{s} = \{u; \rho; \theta\}$ belonging to the space Y , satisfying equations (1)–(6) almost everywhere in $(0, 1) \times (0, T)$ and accepting boundary and initial conditions in the sense of traces of functions from the specified classes.

As shown in [22], when the conditions on the initial data are satisfied,

$$u_0, \rho_0, \theta_0 \in H^1(0, 1), \quad u_1, u_2, \rho_1, \theta_1 \in H^1(0, T)$$

there exists a unique generalized solution u, ρ, θ of problem (1)–(6) that has the following properties:

$$0 < m \leq \rho, \theta \leq M < \infty, \quad \|\mathbf{s}\|_Y \leq C,$$

where the constant C does not depend on T .

We define the set of admissible controls as follows:

$$U = \{\mathbf{h} = \{h_1, h_2\} : h_1 \in H^1(0, 1), h_2 \in H^1(0, T), h_1(1) = h_2(0)\},$$

which is a closed convex set in $H^1(0, 1) \times H^1(0, T)$.

The optimal control problem is formulated as follows. Let the state of the system $\mathbf{s} = \{u; \rho; \theta\}$ be defined as a generalized solution of the problem (1)–(6). It is required to find $\mathbf{v}_0 \in U$ such that

$$J_\alpha(\mathbf{v}_0) = \inf_{\mathbf{v} \in U} \{J_\alpha(\mathbf{v})\}.$$

Here $J_\alpha(\mathbf{v})$ is defined in (7).

In [21] the following theorem is proved.

Theorem. Let $\alpha_1 > 0, \alpha_2 > 0$. Then there exists at least one solution to the optimal control problem.

3 PINN method

The PINN method involves the approximation of unknown functions using neural networks by minimizing the quadratic functional R . To solve the direct problem (1)–(6), the functional R must include terms for the residuals of

equations (1)–(3), R_r , as well as terms $R_0^u, R_1^u, R_2^u, R_0^\rho, R_1^\rho, R_0^\theta, R_1^\theta, R_2^\theta$, corresponding to the initial and boundary conditions (4)–(6):

$$R = R_r + R_0^u + R_1^u + R_2^u + R_0^\rho + R_1^\rho + R_0^\theta + R_1^\theta + R_2^\theta, \quad (12)$$

$$R_r = \frac{W_r}{N_r} \sum_{j=1}^{N_r} \left[r_1^2 \left(\hat{u}(x_j^r, t_j^r), \hat{\rho}(x_j^r, t_j^r), \hat{\theta}(x_j^r, t_j^r) \right) + r_2^2 \left(\hat{u}(x_j^r, t_j^r), \hat{\rho}(x_j^r, t_j^r) \right) + \right. \\ \left. + r_3^2 \left(\hat{u}(x_j^r, t_j^r), \hat{\rho}(x_j^r, t_j^r), \hat{\theta}(x_j^r, t_j^r) \right) \right],$$

where $\hat{u}, \hat{\rho}, \hat{\theta}$ – are approximations of unknowns u, ρ, θ by neural networks, $r_1(x, t), r_2(x, t), r_3(x, t)$ are residuals of equations (1)–(3), $x_j^r \in (0, 1), t_j^r \in (0, 1]$.

All other terms of the functional have the form:

$$R_i^u = \frac{W_i}{N_i} \sum_{j=1}^{N_i} [\hat{u}(x_j^i, t_j^i) - u_i(x_j^i, t_j^i)]^2, \quad i = 0, 1, 2,$$

$$R_i^\rho = \frac{W_i}{N_i} \sum_{j=1}^{N_i} [\hat{\rho}(x_j^i, t_j^i) - \rho_i(x_j^i, t_j^i)]^2, \quad i = 0, 1,$$

$$R_i^\theta = \frac{W_i}{N_i} \sum_{j=1}^{N_i} [\hat{\theta}(x_j^i, t_j^i) - \theta_i(x_j^i, t_j^i)]^2, \quad i = 0, 1, 2,$$

where $x_j^0 \in [0, 1], t_j^0 = 0, x_j^1 = 0, t_j^1 \in [0, 1], x_j^2 = 1, t_j^2 \in [0, 1]$.

In the current work, a separate neural network is used to approximate each unknown function. This approach is used due to the fact that each unknown function has its own dependence on spatio-temporal characteristics. Each approximation of the unknown function can be represented as a superposition of activation functions and weight matrices of the neural network:

$$\hat{u}(X) = H_{swish}(H_{tanh}(H_{tanh}(XW_1^u)W_2^u)W_3^u)W_4^u, \quad (13)$$

$$\hat{\rho}(X) = H_{swish}(H_{tanh}(H_{tanh}(XW_1^\rho)W_2^\rho)W_3^\rho)W_4^\rho, \quad (14)$$

$$\hat{\theta}(X) = H_{swish}(H_{tanh}(H_{tanh}(XW_1^\theta)W_2^\theta)W_3^\theta)W_4^\theta, \quad (15)$$

where $X = (x, t)$, $H_{swish} = x/(1 + e^{-x})$, $H_{tanh} = (e^x - e^{-x})/(e^x + e^{-x})$, W_i^j – is the weight matrix between hidden i and the previous layer for a neural network approximating function j , where $i = 1, 2, 3, 4, j = u, \rho, \theta$.

The activation functions used are the hyperbolic tangent functions, R_{tanh} , which have shown the best results in solving partial differential equations [8], [10], and the modified logistic function, R_{swish} , which, according to [23], allows to solve the vanishing gradient problem [9], arising in neural network related problems.

The neural networks used in the work are feedforward. Every neural network have the same architecture, which simplifies the task of finding hyperparameters. The architecture of the neural networks is shown at the figure 1 using the example of a neural network for approximating an unknown

function u . In three hidden layers, 64, 32 and 16 neurons were used sequentially, starting from the first hidden layer.

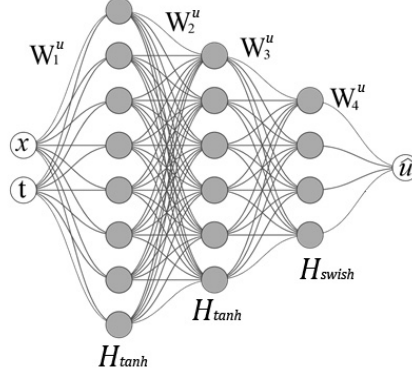


FIG. 1. Architecture of a neural network approximating an unknown function u .

The training dataset for the neural network is a set of points, where denotation $j = 1$ corresponds to the left boundary, $j = 2$ corresponds to the right boundary, $j = r$ corresponds to the domain $\Omega = \{x, t : 0 < x < 1, 0 < t \leq 1\}$. The points are generated using a random sampling from a uniform distribution. In the current work, an approach is used when the pre-generated data inside the region Ω at the initial setup of training of the neural network is selected not over the entire intervals, but with a small indentation from the boundaries. This is done so that the neural network can approximate the transition layer at the boundaries in the solution, caused by the presence of small coefficients before the second derivatives in the equations of motion (1) and thermal conductivity (3). As the neural network is training, the indentation from the boundaries decreases until it becomes equal to the step of the spatio-temporal grid. The training sample at the beginning and end of the training process is schematically shown at figures 2.a and 2.b, respectively.

To solve the optimal control problem, the terms R_0^u and R_2^u in the quadratic functional (12), are not taken into account, but the functional J_α , responsible for control, are added. Then the quadratic functional of the neural network for solving the optimal control problem R_i will take the following form:

$$R_i(s) = R_r + R_1^u + R_0^\rho + R_1^\rho + R_0^\theta + R_1^\theta + R_2^\theta + J_i(s) + \alpha_1 \int_0^1 \frac{\partial u_0(x)}{\partial x} dx + \alpha_2 \int_0^1 \frac{\partial u_2(t)}{\partial t} dt, \quad (16)$$

where, depending on the selected index $i = u, \rho, \theta$, by minimizing this functional, the problem of controlling the gas velocity, (9), gas density, (10),

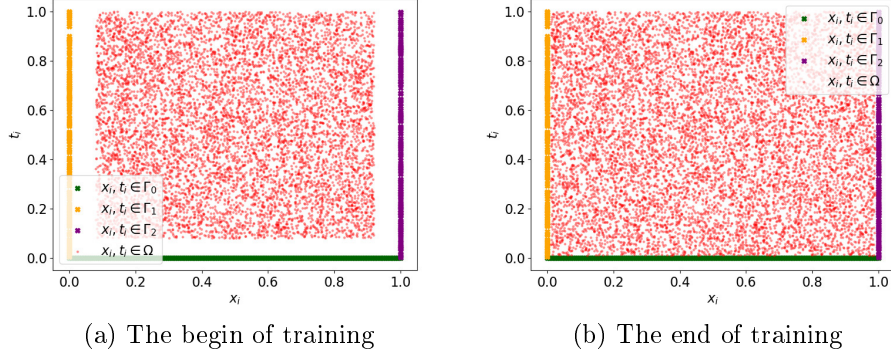


FIG. 2. Training dataset a) at the begin of neural network training, b) at the end of neural network training.

or gas temperature, (11) to the given functions will be solved:

$$R_i(s) \rightarrow \min. \quad (17)$$

4 Numerical experiments

In the current work, three numerical experiments were calculated to solve the optimal control problem (17) for the cases of gas velocity, density, and temperature control.

As described earlier, the gas temperature at the beginning of the process, $u_0(x)$, and at the right boundary, $u_2(t)$, are used as control. The following coefficients were used in all numerical experiments:

$$\alpha_1 = \alpha_2 = 10^{-3}, \quad W_r = 1, \quad W_0 = W_1 = W_2 = 15,$$

As a training sample, 10,000 points were generated in the XT space and 200 points for each of boundary and initial state. The PINN method implementation is performed using the Tensorflow [24] library of the Python programming language. The Adam [25] algorithm is used as a training method, and the constant $lr = 10^{-4}$ is used as a learning rate.

For the first numerical experiment, the functional (9) is chosen for $i = u$, which corresponds to the problem of optimal control of the gas velocity to match the given function $u_d(x, t)$. The physical characteristics of the medium correspond to carbon dioxide. The reference values of the unknown functions, dimensionless coefficients, and other parameters are as follows:

$$\begin{aligned} u_s &= 15 \left[\frac{\text{m}}{\text{s}} \right], & \rho_s &= 2 \left[\frac{\text{kg}}{\text{m}^3} \right], & \theta_s &= 444 [\text{K}], \\ X &= 50 [\text{m}], & T &= 3600 [\text{s}], \\ Sh &= 9.26 \cdot 10^{-2}, & Re &= 3.0 \cdot 10^7, & Pe &= 4.7 \cdot 10^7, \end{aligned}$$

$$\begin{aligned} u_1(0, t) &= 0.5 - 0.1t, & \rho_0(x, 0) &= 0.7 + 0.1x^2, & \rho_1(0, t) &= 0.7 + 0.1t, \\ \theta_0(x, 0) &= 0.8 + 0.1x^2, & \theta_1(0, t) &= 0.8 + 0.1t, & \theta_2(1, t) &= 0.9 + 0.1t. \end{aligned}$$

The function u_d is as follows:

$$u_d(x, t) = 0.5 - 0.1t - 0.01x^2. \quad (18)$$

The obtained solution is shown at figures 3.a, 3.b, 3.c, 3.d at different moments of time.

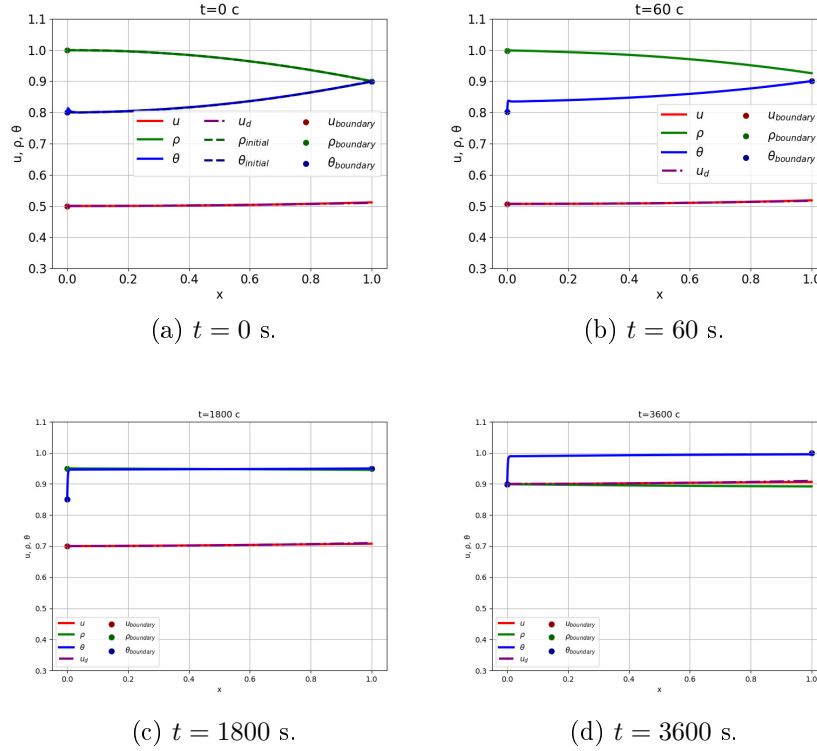
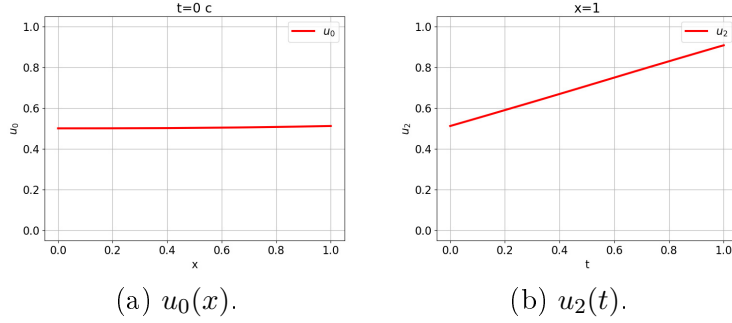


FIG. 3. Solution of the optimal control problem (17) with condition (18) at different moments of time.

The control profile of functions u_0 and u_2 is presented at figures 4.a and 4.b.

For the second experiment, the functional (10) is chosen for $i = \rho$, which corresponds to the problem of optimal control of gas density to match the given function $\rho_d(x, t)$. The physical characteristics of the medium correspond to air. All other process parameters were chosen as follows:

$$\begin{aligned} u_s &= 10 \left[\frac{\text{m}}{\text{s}} \right], & \rho_s &= 1.35 \left[\frac{\text{kg}}{\text{m}^3} \right], & \theta_s &= 403 [\text{K}], \\ X &= 100 [\text{m}], & T &= 600 [\text{s}], \end{aligned}$$

FIG. 4. Control profile, a) u_0 , b) u_2 .

$$\begin{aligned}
Sh &= 2.77 \cdot 10^{-3}, & Re &= 2.4 \cdot 10^8, & Pe &= 1.6 \cdot 10^8, \\
u_1(0, t) &= 0.85 - 0.35t, & \rho_0(x, 0) &= 1.0, & \rho_1(0, t) &= 1.0 - 0.1t, \\
\theta_0(x, 0) &= 1.0 - 0.1x^2, & \theta_1(0, t) &= 1.0 - 0.1t, & \theta_2(1, t) &= 0.9 - 0.1t.
\end{aligned}$$

Function ρ_d has the following form:

$$\rho_d(x, t) = 1.0 - 0.1t. \quad (19)$$

The obtained solution is shown in figures 5.a, 5.b, 5.c, 5.d at different moments of time.

The control profile of functions u_0 and u_2 is presented in figures 6.a and 6.b.

For the third numerical experiment, the functional (17) is chosen for $i = \theta$, which corresponds to the problem of optimal control of the gas temperature to match the given function $\theta_d(x, t)$. The physical characteristics of the medium also correspond to carbon dioxide. The reference values of the unknown functions, dimensionless coefficients, and other process parameters are as follows:

$$\begin{aligned}
u_s &= 15 \left[\frac{\text{M}}{\text{c}} \right], & \rho_s &= 2 \left[\frac{\text{kg}}{\text{m}^3} \right], & \theta_s &= 343 [\text{K}], \\
X &= 25 [\text{m}], & T &= 60 [\text{s}], \\
Sh &= 2.78 \cdot 10^{-2}, & Re &= 1.5 \cdot 10^7, & Pe &= 3.0 \cdot 10^7, \\
u_1(0, t) &= 0.5 - 0.025t, & \rho_0(x, 0) &= 0.8 + 0.025x^2, & \rho_1(0, t) &= 0.8, \\
\theta_0(x, 0) &= 1.0 - 0.025x^2, & \theta_1(0, t) &= 1.0 - 0.025t, & \theta_2(1, t) &= 0.975 - 0.025t.
\end{aligned}$$

The function θ_d has the following form:

$$\theta_d(x, t) = 1.0 - 0.025t - 0.025x^2. \quad (20)$$

The obtained solution is shown in figures 7.a, 7.b, 7.c, 7.d at different moments of time.

The control profile of functions u_0 and u_2 is presented in figures 8.a and 8.b.

The calculation of all experiments was stopped upon reaching the value of $R_i = 10^{-4}$, which the authors consider an optimal value for such problems [8].

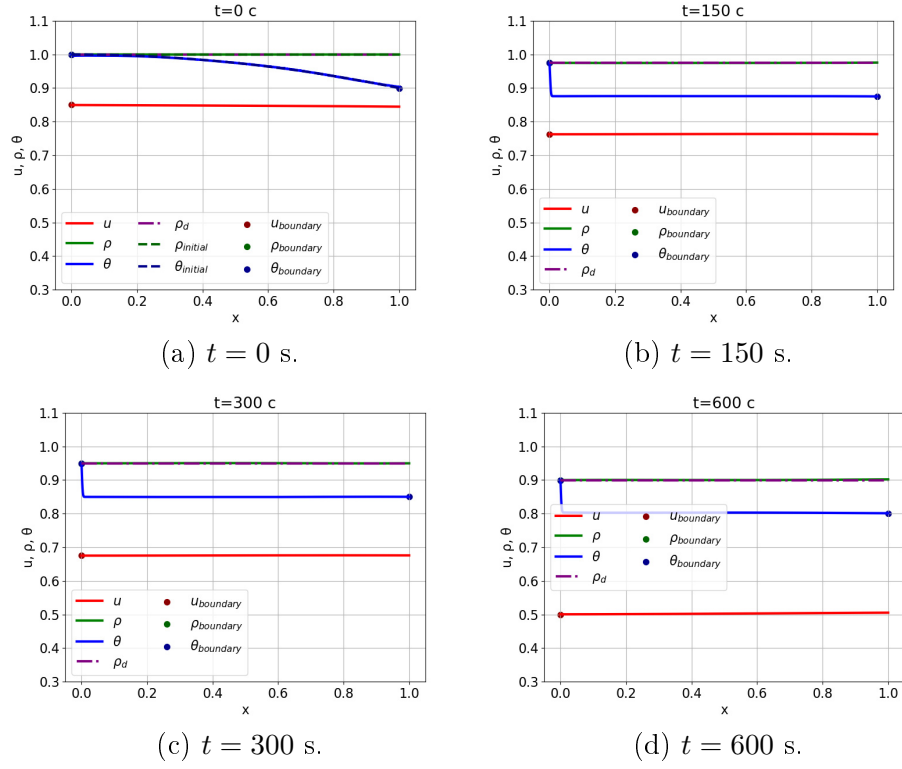


FIG. 5. Solution of the optimal control problem (17) with condition (19) at different moments of time.

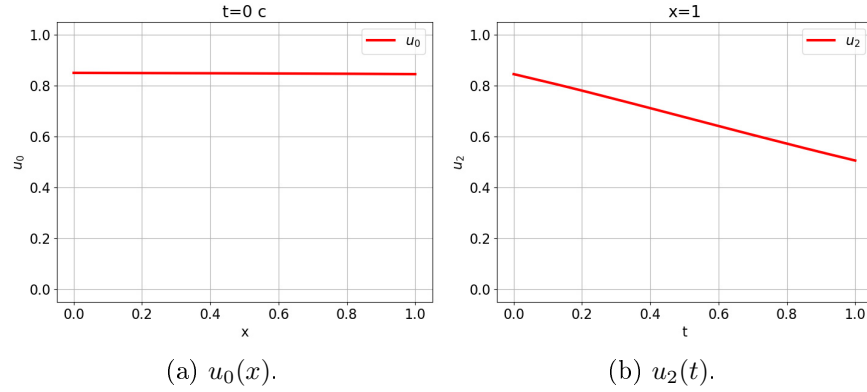


FIG. 6. Control profile, a) u_0 , b) u_2 .

The training of PINN for each numerical experiment took approximately 2 hours. From the presented graphs it is evident that the approximated functions u, ρ and θ almost completely match the specified functions u_d, ρ_d ,

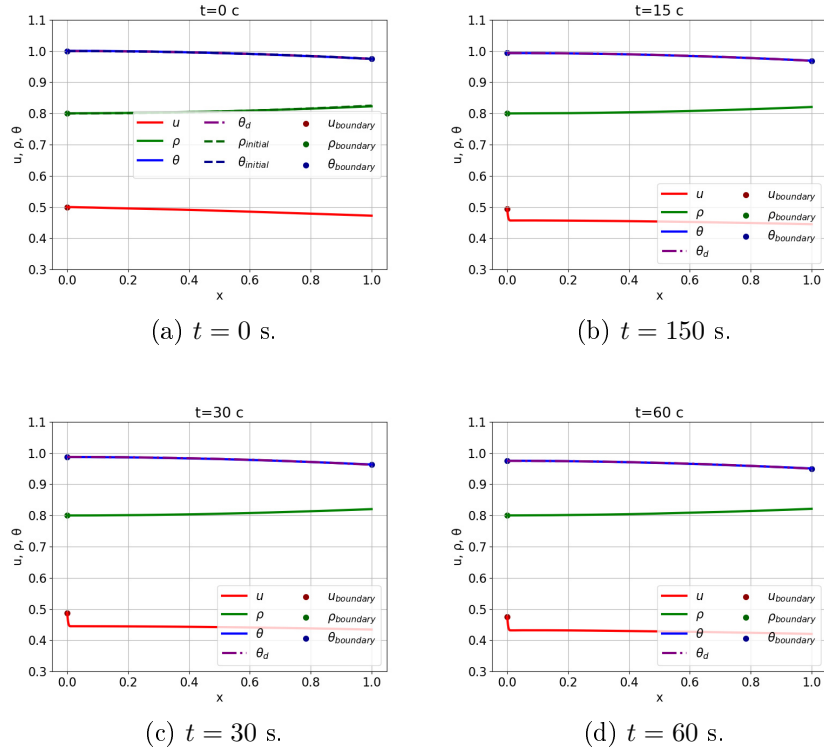


FIG. 7. Solution of the optimal control problem (17) with condition (20) at different moments of time.

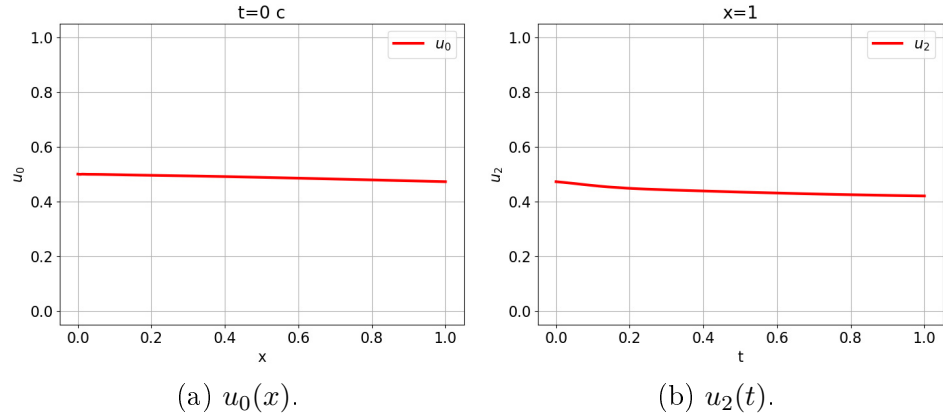


FIG. 8. Control profile, a) u_0 , b) u_2 .

θ_d . In this case, the control profile is actually linear. It is also worth noting that the solution of the optimal control problems was performed on a uniform

grid even in the presence of transition layers in the solution due to very high Reynolds and Strouhal numbers.

All numerical experiments were performed using the following computational resources: Inter core i7-12700H CPU, NVIDIA GeForce RTX 3070 TI laptop GPU, 8 GB VRAM.

5 Conclusion

The current work presents a numerical experiments of the viscous heat conducting gas flow control problem. The parameters of the medium in performed experiments are close to the real parameters of the gases, including very high Reynolds and Peclet numbers. Due to the complexity of the system of equations for a compressible medium, the calculation was performed with the case of one-dimensional gas flow. In the future, it is planned to study the possibility of applying the developed technique to the multidimensional case.

It is worth noting that this is the first case of a numerical solution of the inverse problem for the Navier-Stokes equations in the case of a compressible medium, taking into account viscosity and thermal conductivity. Previously, such problems were considered only theoretically, since the numerical solution of even a direct problem by other numerical methods seems difficult. The possibility of numerically solving inverse problems of gas dynamics, shown in the work, can lay the foundation for solving many practical problems that arise in engineering and oil production.

The advantage of using the PINN method to solve the inverse problem of a highly nonlinear, singularly perturbed system of equations is shown. Those are the absence of the need to linearize the system and solve the optimality system, as well as the possibility of solving the problem on a relatively small amount of training dataset (about 10^4 points), while classical methods require a extremely small step of the computational grid for such cases. It is shown that the use of the method does not require excessive computing resources for operation.

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KIRILL SERGEYEVICH KUZNETSOV
FAR EASTERN FEDERAL UNIVERSITY,
AJAX BAY 10, RUSSKY ISLAND,
690922, VLADIVOSTOK, RUSSIA,
INSTITUTE OF APPLIED MATHEMATICS FEB RAS,
RADIO STR., 7,
690041, VLADIVOSTOK, RUSSIA
Email address: kuznetsovks17@gmail.com

ELENA VLADIMIROVNA AMOSOVA
FAR EASTERN FEDERAL UNIVERSITY,
AJAX BAY 10, RUSSKY ISLAND,
690922, VLADIVOSTOK, RUSSIA,
INSTITUTE OF APPLIED MATHEMATICS FEB RAS,
RADIO STR., 7,
690041, VLADIVOSTOK, RUSSIA
Email address: el_amosova@mail.ru