Уважаемый рецензент,

Благодарим вас за предоставленный отзыв и сделанные комментарии. Ниже представлены наши ответы и внесенные изменения на полученные замечания:

1. Представить современное состояние решаемой проблемы (state of arts) и четко сформулировать новизну и преимущество предлагаемого подхода по сравнению с имеющимися; в текущем варианте есть только ссылки [3, 5–7] без анализа/оценки их результатов; возможно следует указать работы и других авторов; - На страницах 1-2 добавлен обзор современного состояния проблемы:

In computational fluid mechanics the implementation of machine learning algorithms for subset of the complete system of gas dynamics equations approximation has been recently started [8–10]. For instance, in [10] a simplified neural network model as an algebraic turbulence model is developed within CFD simulation, addressing challenges in rapidly converging solutions for the Reynolds Averaged Navier-Stokes (RANS) equations, demonstrating its improved convergence compared to traditional methods. In [9] a data-driven approach to turbulence modeling in RANS simulations is explored, leveraging supervised learning algorithm sto improve the accuracy of turbulence closure terms in CFD simulations, with the aim of enhancing predictive capabilities and potentially offering an alternative to traditional turbulence models. The study [8] is dedicated to large-eddy simulations (LES), where LES is employed for a methane-hydrogen flame, and comparison of structured tabulation and neural networks for chemistry representation is given. The novel optimal neural network approach to LES is applied. The accurate representation with controlled errors is ensured. Comparable accuracy with structured tables and highlight the neural networks potential for enhancing predictions in reactive flows is shown. In the same manner, the calculation of transport coefficients can be executed autonomously at each computational time step, taking into account the governing hydrodynamic equations. The main advantage of such an approach is that computational costs of computation of transport coefficients justifies the application of regression [3]. In the previous research [3], neural networks are implemented to assess transport coefficients in atomic and molecular gases, taking into account internal degrees of freedom. Comparison of results to exact calculations demonstrates promising accuracy and speed enhancements, particularly in multi-component mixtures. In the paper [5] the implementation of machine learning algorithms is investigate for mitigation of the computational cost of state-to-state numerical simulations in high-speed reacting flows. The achievement of accurate predictions for relaxation source terms is shown. State-to-state Euler equations through data-driven machine learning regression models are solved. The results are coupled with the strategies to accelerate an in-house solver, and deep neural networks for direct solution inference. Finally, in [7], machine learning algorithms are utilized to compute state-to-state transport coefficients in nonequilibrium reacting gas flows.

Under conditions of strong coupling between vibrational-chemical kinetics and gas dynamics, the transport coefficients of thermal conductivity, shear viscosity, and bulk viscosity are considered. Dedicated software application is developed for solving the regression problem, enabling model configuration, training, and evaluation, resulting in a multi-layer perceptron regression model applied to a binary molecular and atomic nitrogen mixture  $(N_2, N)$  taking into account 48 vibrational states of  $N_2$ . Comparing with rigorous kinetic theory calculations substantial acceleration up to two orders of magnitude for neural network regression is shown. The potential for significantly reducing of computational efforts in nonequilibrium flow simulations is emphasized.

- 2. Более детально обосновать выбор гиперпараметров для методов на основе машинного обучения; в частности, вызывает удивление выбор столь простой и небольшой нейронной сети перцептрона с одним скрытым слоем, в то время как общей тенденцией является использование глубоких нейросетей; краткое упоминание того, что использовался grid search approach представляется недостаточным; Добавлены соответствующие комментарии на страницах 5 и 7:
  - For the sake of simplicity, in the present study a multilayer perceptron with one hidden layer is used. Since a universal approximation theorem is established [25], in case of solution convergence, the problem of memory limitation in our research becomes the crucial one. Therefore, no additional calculation complications associated with the deep neural network have to be required.
  - The choice of the optimal neural network architecture remains a relevant challenge for a future research: increasing the depth while maintaining overall compactness and evaluation speed can improve regression performance, and, therefore, overall modeling accuracy.
- 3. В разделе 4 (CONCLUSION) четче сформулировать наличие или отсутствие преимуществ методов машинного обучения/нейросетей для решения задач в рассматриваемой прикладной области. Дополнено заключение на странице 6: The utilization of these techniques enables the application of computationally intensive accurate transport algorithms to practical scenarios, as well as facilitating comparison and implementation even under constraints of limited computational resources.

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