Modeling the dynamics of hydrogen combustion using the neural network UNET

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The paper investigates the possibility of solving problems of chemical kinetics using artificial neural networks. A model of combustion of hydrogen with oxygen in air was chosen for the study. In the reaction at high temperatures (500-4000 K) hydrogen H2, oxygen O2, their derivatives (H, O, OH, H2O, HO2, H2O2), as well as neutral elements argon Ar and nitrogen N2 are interact. The whole process is described by 28 chemical reactions [1-2]. Mathematically, the problem is reduced to a system of differential equations:

$$\frac{\partial X_k}{\partial t} = \sum_{r=1}^{N_R} \nu_{rk} \omega_r \left(T, X_1, ..., X_{N_C} \right).$$

The main problem in solving such problems by numerical methods is that their complexity increases sharply with an increase in the number of parameters (more variables, more equations). Neural networks allow you to save computational costs when changing the number of input and output parameters.

n_{steps}	$\langle MSE \rangle$	σ_{MSE}	$MSE_{\max}$
1	0.00114	0.00254	0.0228
2	0.000728	0.00215	0.0268
5	0.000492	0.00113	0.0139
10	0.000217	0.000526	0.00480
20	8.97E-05	0.000189	0.00172
30	8.77E-05	0.000211	0.00170
40	0.000134	0.000541	0.00755
50	8.86E-05	0.000204	0.00221

Table 1. Error for different number of prediction steps during training

For modeling, a neural network architecture was chosen, in which there is a skip connection from input to output - such as the UNET architecture [3], only with fully connected layers. Thus, the neural network only needs to learn the change in the concentration of substances over time, which allows the parameters of the neural network to learn more quickly (usually 50-100 training epochs are enough).

In order to reduce the error incursion and improve the quality of prediction, it was proposed to include in the loss function the results of predicting the neural network several steps ahead in the recurrent mode. As a result of such training, the quality of prediction has improved significantly (Table 1), and the graphs of neural network prediction and real numerical calculation almost coincide.

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References

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