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RESEARCH ARTICLE

Neural operators for hydrodynamic modeling of underground gas storage facilities

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Abstract
Objectives. Much of the research in deep learning has focused on studying mappings between finite-dimensional spaces. While hydrodynamic processes of gas filtration in underground storage facilities can be described by partial differential equations (PDE), the requirement to study the mappings between functional spaces of infinite dimension distinguishes this problem from those solved using traditional mapping approaches. One of the most promising approaches involves the construction of neural operators, i.e., a generalization of neural networks to approximate mappings between functional spaces. The purpose of the work is to develop a neural operator to speed up calculations involved in hydrodynamic modeling of underground gas storages (UGS) to an acceptable degree of accuracy.
Methods. In this work, a modified Fourier neural operator was built and trained for hydrodynamic modeling of gas filtration processes in underground gas storages.
Results. The described method is shown to be capable of successful application to problems of three-dimensional gas filtration in a Cartesian coordinate system at objects with many wells. Despite the use of the fast Fourier transform algorithm in the architecture, the developed model is also effective for modeling objects having a nonuniform grid and complex geometry. As demonstrated not only on the test set, but also on artificially generated scenarios with significant changes made to the structure of the modeled object, the neural operator does not require a large training dataset size to achieve high accuracy of approximation of PDE solutions. A trained neural operator can simulate a given scenario in a fraction of a second, which is at least 10^6 times faster than a traditional numerical simulator.
Conclusions. The constructed and trained neural operator demonstrated efficient hydrodynamic modeling of underground gas storages. The resulting algorithm reproduces adequate solutions even in the case of significant changes in the modeled object that had not occurred during the training process. The model can be recommended for use in planning and decision-making purposes regarding various aspects of UGS operation, such as optimal control of gas wells, pressure control, and management of gas reserves.

Keywords: mathematical modeling, deep learning, artificial intelligence, neural networks, neural operators, Fourier neural operators, hydrodynamic modeling, underground gas storage facilities

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НАУЧНАЯ СТАТЬЯ

Нейронные операторы для гидродинамического моделирования подземных хранилищ газа

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Резюме
Цели. Значительная часть исследований в области глубокого обучения сосредоточена на изучении отображений между конечномерными пространствами. Гидродинамические процессы фильтрации газа в подземных хранилищах, описываемые дифференциальными уравнениями в частных производных (ДУЧП), требуют изучения отображений между функциональными пространствами бесконечной размерности, что отличает данную задачу от традиционных. Одним из перспективных подходов является построение нейронных операторов – обобщение нейронных сетей для аппроксимации отображений между функциональными пространствами. Цель работы – создание нейронного оператора для ускорения расчетов гидродинамического моделирования подземных хранилищ газа (ПХГ) при допустимых потерях точности.
Методы. В работе построен и обучен модифицированный нейронный оператор Фурье для гидродинамического моделирования процессов фильтрации газа в ПХГ.
Результаты. Показано, что данный метод может быть успешно применен для задач трехмерной фильтрации газа в декартовой системе координат на объектах с множеством скважин. Разработанная модель обеспечивает высокое качество при моделировании объектов с неравномерной сеткой дискретизации и сложной геометрией, несмотря на использование в архитектуре алгоритма быстрого преобразования Фурье. При этом нейронному оператору не требуется большой размер обучающей выборки для достижения высокой точности аппроксимации решений ДУЧП, что демонстрируется не только на тестовой выборке, но и на искусственно сгенерированных сценариях с внесением существенных изменений в структуру моделируемого объекта. Обученный нейронный оператор осуществляет моделирование заданного сценария за доли секунды, что, по меньшей мере, в 10^6 раз быстрее, чем традиционный численный симулятор.
Выводы. Построенный и обученный нейронный оператор показал хорошую эффективность в задаче гидродинамического моделирования ПХГ. Полученный алгоритм воспроизводит адекватные решения даже в случае существенных изменений в моделируемом объекте, которых не было в процессе обучения. Все это делает возможным применение данной модели в задачах планирования и принятия решений в отношении различных аспектов эксплуатации ПХГ, таких как оптимальное использование скважин, контроль давления и управление запасами газа.

Ключевые слова: математическое моделирование, глубокое обучение, искусственный интеллект, нейронные сети, нейронные операторы, нейронные операторы Фурье, гидродинамическое моделирование, подземные хранилища газа

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INTRODUCTION

Underground gas storage facilities (UGS) are technological complexes designed for gas injection, storage and withdrawal. They typically comprise the following functional components: aboveground engineering and technical facilities; a subsurface area limited by a mining allotment; a gas storage facility; control reservoirs; a gas buffer volume; a stock of wells for various purposes. Hydrodynamic modeling of UGS reservoirs, which is required to improve the accuracy and reliability of predicting UGS behavior, represents an integral part of the planning and decision-making processes for various aspects of UGS operation, such as optimal well utilization, pressure control, and gas reserve management.

Simplified balance models and more accurate numerical hydrodynamic models (HDMs) can be used in modeling of filtration processes of underground gas storage. Balance models are typically used where there is a lack of sufficient initial data to build three-dimensional numerical models or limited computing power. Such models solve the reservoir-filtration equation using simplified dependencies without considering complex geological and hydrodynamic processes that can have a significant impact on the behavior of UGS. Modern hydrodynamic simulators for numerical modeling of gas filtration processes are used to obtain more detailed information on the distribution of parameters in UGS reservoir beds and assess the impact of various factors on the processes of underground gas storage. However, the use of the finite volume method to approximate the system of differential equations in space, as well as an implicit scheme for time approximation for modeling, can be a computationally expensive procedure.

At present, numerical HDMs are mainly used to solve the problems of hydrodynamic modeling of UGS facilities. Due to the possibility of adapting such models to the accumulated history of field development (in the case of UGS in depleted fields) and the actual history of UGS operation, the modeling and model adaptation horizon can exceed 60 years. Moreover, taking into account the considerable amount of geological and field data supplied to the HDM as input data (geophysical survey results, pressure measurements, gas flow rates, etc.), the time of a single calculation can reach several hours.

Thus, the speed of calculations is one of the determining factors affecting managerial decisions related to the distribution of gas injection/withdrawal by wells and by area. One of the most promising approaches for accelerating hydrodynamic calculations involves the use of contemporary deep learning methods.

A substantial part of works in the field of deep learning is devoted to the construction of mappings between finite-dimensional (e.g., Euclidean) spaces [1, 2]. However, the use of partial differential equations (PDE) to describe physical processes of gas filtration in UGS distinguishes this problem due to the requirement to learn mappings between function spaces of infinite dimensionality [3].

According to the universal approximation theorem [4, 5], a fully connected network with a *sufficient* number of parameters can approximate any continuous function defined on a compact set to a predetermined accuracy. In [6–8], theoretical possibilities for approximating nonlinear mappings between function spaces are demonstrated. In addition, [9] provides estimates of the complexity bounds of the approximation error of neural networks, relating the number of model parameters and the dimensionality of the problem to the value of the approximation error.

However, the theoretical possibility to approximate mappings between infinite-dimensional spaces does not imply information on how to do it efficiently in practice. It is known that existing neural network architectures vary in terms of their performance when solving specific problems. For example, the same fully connected networks show significantly lower quality in image processing compared to the widely used convolutional architectures [2]. In order to further investigate the issue of effective training of neural networks, [10] decomposes the overall model error into three components: approximation error, optimization error, and generalization error. The approximation error depends on the number of network parameters and the dimensionality of the problem, while the optimization error is related to the loss function, and the generalization error depends on the training sample size [11].

One of the important points in generalizing the dependencies described by the PDE using neural networks is the problem of dimensionality ("curse of dimensionality") [12, 13], especially when modeling objects having complex UGS geometry or equations with multidimensional parameter spaces (the basic gas filtration equation) [3]. In order to generalize the basic dependencies and relations, deep learning models require a sufficiently large training sample size. According to [11], the upper bound on the generalization error is: $E_{\text{gen}} \sim \frac{1}{\sqrt{N}}$, where N is the number of training samples. Consequently, to obtain a relative generalization error of 1%, a sample size of $O(10^4)$ is required.

In the case of modeling hydrodynamic processes in reservoir systems, obtaining a data set of similar size can be a difficult task, since the data set is formed from calculations on a numerical simulator, representing a computationally expensive procedure. Consequently, when taking into account the above features, the development of neural network architecture for the effective solution of problems of this type becomes a nontrivial and relevant issue.

Over the last few years, deep learning has actively penetrated the field of scientific computing to become a new paradigm.[1, 2] Many novel methods have emerged to offer faster alternatives to numerical simulation.

Of course, there are works based on traditional deep learning approaches in the form of constructing finite-dimensional operators, which use the results of numerical simulations as a training set. For example, convolutional-, recurrent- and generative-adversarial architectures for solving fluid dynamics problems are investigated in [14–16]. However, due to their failure to use knowledge about the structure of the simulated dependencies, the presented methods are demanding on the object geometry and discretization grid, thus requiring a large amount of data.

A group of methods [17–19] belongs to a specialized class of algorithms known as *physically informed neural networks*. While this approach is also based on finite-dimensional mappings, it incorporates the PDE directly into the algorithm's error function using the automatic differentiation mechanism [20]. In this way, physics is taken into account in the learning process as the model seeks to minimize the discrepancies between the left and right parts of the equation, representing initial and boundary conditions. However, the main disadvantage of this approach is its limitation to approximate a particular realization of the PDE. Consequently, physically informed neural networks do not provide a significant speed advantage relative to traditional numerical methods for many applied problems.

An alternative and relatively new approach is to train *neural operators*, which represent mappings between function spaces [21–23]. Since trained neural operators can approximate any nonlinear continuous operators, do not depend on the sampling grid, and require only a single training, they can be trained and evaluated on different sampling grids and PDE implementations. These methods demonstrate better efficiency when approximating PDEs in comparison with other existing approaches based on deep learning, including for hydrodynamic modeling problems.

Operator learning in spaces of infinite dimensionality is currently an active area of research. Work is ongoing to improve the efficiency and applicability of this approach in various applications.

1. TASK STATEMENT

Mathematical model of gas filtration process

The present work considers the process of hydrodynamic modeling of porous-type UGS facilities. For such objects, various parameters describing gas motion in porous medium (filtration) have a strong time dependence [3]. Such processes are called unsteady (nonstationary).

The basic equation of three-dimensional unsteady single-phase filtration of a compressible fluid (gas) in a porous medium is obtained by substituting the law of conservation of momentum (Darcy's law of filtration) into the law of conservation of mass [24]:

$$\frac{\partial}{\partial x}\left(\frac{A_x k_x}{\mu_g B_g}\frac{\partial p}{\partial x}\right)\Delta x + \frac{\partial}{\partial y}\left(\frac{A_y k_y}{\mu_g B_g}\frac{\partial p}{\partial y}\right)\Delta y + \frac{\partial}{\partial z}\left(\frac{A_z k_z}{\mu_g B_g}\frac{\partial p}{\partial z}\right)\Delta z = \frac{V_{\text{bulk}}\phi T_{\text{sc}}}{p_{\text{sc}}}\frac{\partial}{\partial t}\left(\frac{p}{Z}\right) - q_{\text{gsc}}, \quad (1)$$

where p is pressure; q_{gsc} is the gas flow rate under standard conditions; $B_g = \frac{p_{\text{sc}} TZ}{T_{\text{sc}} p}$ is the gas phase

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[1] Lavin A., Krakauer D., Zenil H., et al. *Simulation Intelligence: Towards a New Generation of Scientific Methods*. 2022. http://arxiv.org/abs/2112.03235. Accessed April 25, 2023.

[2] Cuomo S., di Cola V.S., Giampaolo F., et al. *Scientific Machine Learning through Physics-Informed Neural Networks: Where we are and What's next*. 2022. http://arxiv.org/abs/2201.05624. Accessed April 25, 2023.

volume coefficient; Z is the gas supercompressibility coefficient; μ_g is the gas viscosity; T_{sc} is the temperature under standard conditions; p_{sc} is the pressure under standard conditions; V_{bulk} is the rock volume; ϕ is porosity; k is permeability; A is the cross-sectional area of rock perpendicular to the filtration direction; Δx, Δy, Δz are length, width, and height of rock volume (final volume), respectively.

The PDE (1) is nonlinear due to the dependence of μ_g, B_g, and Z on pressure and is similar to the diffusion equation, however, by its dynamic characteristics the flow described by this relation is not diffusion but filtration flow.

Neural operator training

The purpose of the present work is to approximate the gas filtration equation in UGS (1) by constructing a neural operator that maps between two infinite-dimensional spaces from a finite set of pairs of pairs of initial, boundary conditions, and PDE solutions.

Let us fix the spatiotemporal dimension $d \in \mathbb{N}$ and denote by $D \subset \mathbb{R}^d$ the area in $\mathbb{R}^d$. Then we can consider a mapping that is inherently an operator of the solution of PDE:

$$G : A(D;\mathbb{R}^{d_a}) \to U(D;\mathbb{R}^{d_u}),\quad a \to u := G(a), \tag{2}$$

$a \in A(D;\mathbb{R}^{d_a})$ is the function of the input data of the type $a : D \to \mathbb{R}^{d_a}$; $u \in U(D;\mathbb{R}^{d_u})$ is the function of the output data of the type $u : D \to \mathbb{R}^{d_u}$. $A(D;\mathbb{R}^{d_a})$ and $U(D;\mathbb{R}^{d_u})$ are Banach spaces.

In order to train the operator, it is necessary to assume a finite set of pairs of initial, boundary conditions and solutions of PDE $\{a_j, u_j\}_{j=1}^N$, where $a_j \sim \mu$ (μ is a probability measure) is a sequence of probability measures defined on A and $u_j = G(a_j)$. These pairs are obtained from the HDM of the current UGS, which uses a finite volume method to approximate the system of differential equations in space and an implicit scheme to approximate in time. Thus, the training of the neural operator can be formulated as follows. The input data generated by the numerical simulator is essentially the result of a nonlinear mapping satisfying the gas filtration equation: $G(a_j) = u_j$. Consequently, it is possible to construct a neural operator N_{θ^*} by selecting the parameters $\theta \in \Theta$ in such a way as to approximate the initial mapping $N_{\theta^* \approx G}$. Then the learning process, which can be reduced to the problem of minimizing the loss function C: U × U → $\mathbb{R}$, has the following form:

$$\min_{\theta} E_{a\sim\mu}[C(N_\theta(a), G(a))], \tag{3}$$

where $E_{a\sim\mu}$ is the mathematical expectation.

2. CONSTRUCTION OF A NEURAL OPERATOR MODEL

In accordance with the problem statement, a neural operator should be trained to approximate the solution of the gas filtration PDE in UGS. When developing such methods, it is convenient to adhere to the following sequence of steps in the model architecture [23]:

1. P is the operator of transformation of input data into the hidden space of higher dimensionality;
2. Iterative application of the kernel of the integral operator L;
3. Q is the projection operator from the hidden space to the initial output space.

Thus, the structure of the neural operator has the form (4):

$$N(a) = Q \circ L_L \circ L_{L-1} \circ \ldots \circ L_1 \circ P(a), \tag{4}$$

where the given depth of layers is $L \in \mathbb{N}$, $P : A(D;\mathbb{R}^{d_a}) \to U(D;\mathbb{R}^{d_v})$, $d_v \geq d_a$, $Q : U(D;\mathbb{R}^{d_v}) \to U(D;\mathbb{R}^{d_u})$.

By analogy with classical finite-dimensional neural networks, $L_1, \ldots, L_L$ are nonlinear layers of the operator, $L_l : U(D;\mathbb{R}^{d_v}) \to U(D;\mathbb{R}^{d_u})$, $v \to L_l(v)$, which can be written as:

$$L_l(v)(x) = \sigma(W_l v(x) + (K(a;\theta_l)v)(x)),\ \forall x \in D, \tag{5}$$

where σ is the activation function, W_l is the linear transformation, $K : A \times \Theta \to L(U(D;\mathbb{R}^{d_v}), U(D;\mathbb{R}^{d_v}))$.

Operator $K(a, \theta_l)$ [22] is an integral operator of the form:

$$(K(a,\theta_l)v)(x) = \int_D \kappa_\theta(x, y, a(x), a(y))v(y)dy,\ \forall x \in D. \tag{6}$$

The kernel κ_θ, which is a neural network with parameters $\theta \in \Theta$, can have various structures. Different kinds of neural operator are derived from this, for example, graph neural operators (GNO) and multipole graph neural operators (MGNO) [22], as well as low-rank neural operators (LNO) and Fourier neural operators (FNO).

At present, one of the promising methods for approximating solutions of filtration equations is FNO, which is used to parameterize the kernel of the integral operator in Fourier space [25]. This method demonstrates better efficiency in fluid filtration problems in porous media as compared to traditional neural network algorithms and other operator architectures (GNO, MGNO, LNO, DeepONet) [23]. At the same time, [26] shows, using the example of the approximation of the transport equation, that the complexity of FNO grows *logarithmically*

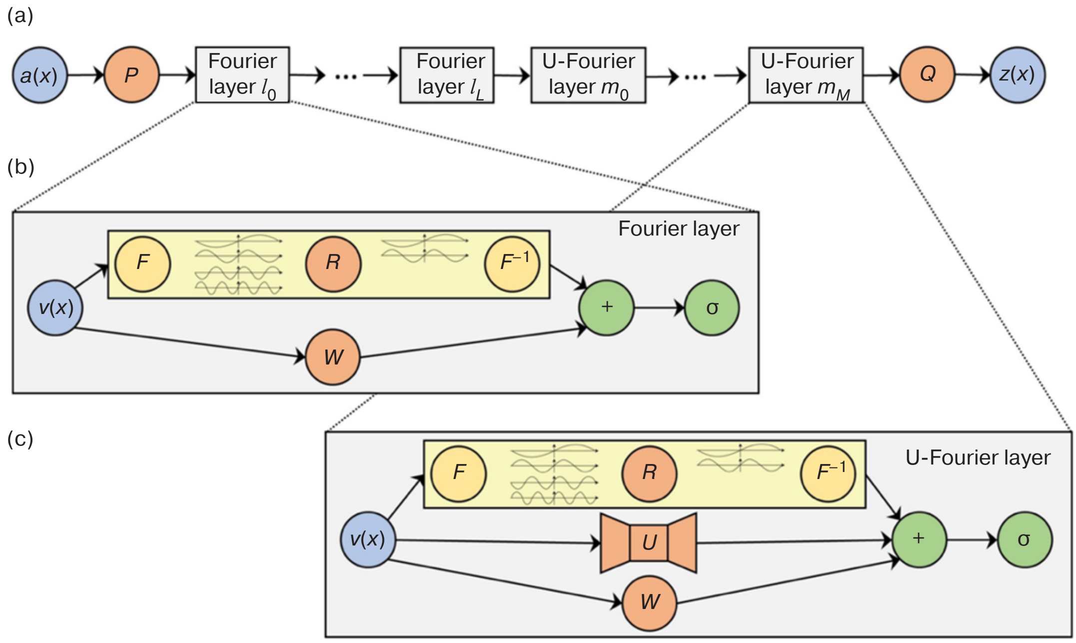

Fig. 1. (a) Model architecture: *P* and *Q* are fully connected layers, *z*(*x*) is the model output; (b) Fourier layer: *R* represents the parameterization in Fourier space, *W* is the linear displacement; (c) modified Fourier layer: *U* is the U-Net operator, other notations have the same meaning as in the Fourier layer

to achieve a given error; this contrasts with the alternative DeepONet architecture [21], which grows *quadratically*.

The Fourier neural operator [25] belongs to the class of neural operators in which the kernel can be written as a convolution:

$$(\mathrm{K}(a,\theta_l)v)(x)=\int_{\mathrm{D}}\kappa_\theta(x-y)v(y)dy,\ \forall x\in \mathrm{D}. \quad (7)$$

In order to parameterize the kernel efficiently according to the convolution theorem, this method considers the image v in Fourier space using the fast Fourier transform F and the inverse Fourier transform F^{-1}:

$$(\mathrm{K}(\theta)v)(x)=F^{-1}(R_\theta(k)\cdot F(v)(k))(x),\ \forall x\in \mathrm{D}, \quad (8)$$

where $R_\theta(k)=F(\kappa_\theta)(k)$ is the matrix of Fourier transform coefficients from κ_θ.

Thus, the layers of the Fourier operator will have the form:

$$L_l(v)(x)=\sigma(W_l v(x)+F^{-1}(R_l(k)\cdot F(v)(k))(x)). \quad (9)$$

The key difference between (9) and the traditional neural network architecture is the direct definition of all operations in feature space, which obviates a dependence on the discretization of the data.

We have developed a method for hydrodynamic modeling of UGS, consisting in a modified Fourier neural operator in which the layers of the neural operator include a convolution neural network U-Net operator to enhance expressiveness by processing high-frequency information that is not captured by the Fourier basis[3]. Such an algorithm involves the following three steps (Fig. 1):

1. Transformation of input data $a(x)$ into a hidden space of higher dimensionality $v_{l_0}=P(a(x))$;
2. Iterative application of Fourier layers and subsequent application of modified Fourier layers: $v_{l_0}\to\ldots\to v_{l_L}\to v_{m_0}\to\ldots\to v_{m_M}$, where v_{l_j} for $j=\overline{0,L}$ and v_{m_k} for $k=\overline{0,M}$;
3. Projection v_{m_M} from the hidden space into the original exit space $z(x)=Q(v_{m_M}(x))$.

The modified Fourier layer of the neural operator has the following form:

$$v_{m_{k+1}}(x)=\sigma(W(v_{m_k}(x))+ \\ +(Kv_{m_k})(x)+Uv_{m_k}(x)),\ \forall x\in \mathrm{D}, \quad (10)$$

where W is a linear operator; $Kv_{m_k}(x)=F^{-1}(R\cdot F(v_{m_k}))(x)$ is the integral transformation operator; U is the operator of the U-Net convolutional neural network.

It is important to note that the neural Fourier operator is an infinite-dimensional operator capable of generating invariant solutions regardless of the sampling grid on training and test samples. However, by adding a U-Net

[3] Wen G., Li Z., Azizzadenesheli K., et al. *U-FNO – An enhanced Fourier neural operator-based deep-learning model for multiphase flow*. 2022. http://arxiv.org/abs/2109.03697. Accessed April 25, 2023.

block, which inherently lacks the flexibility of training and testing at different sampling, the authors of the architecture sacrifice flexibility in favor of higher accuracy. This architecture is expected to provide acceptable accuracy even with a relatively small training sample.

Data configuration

In this work, the data from the HDM are used to form the dataset. The approximation period is chosen to be equal to the gas withdrawal season. The whole data set is formed from 70 different withdrawal scenarios with a time step of 10 days. The considered UGS has more than 100 active wells and a complex geometry.

The final dataset consists of 2850 input-output pairs. For training, 2250 images were allocated for the training sample and 300 each for the validation and test samples.

3. RESULTS

Relative error is used as a loss function

$$L(y,\hat{y}) = \frac{\| y - \hat{y} \|_2}{| y \|_2}, \qquad (11)$$

since formation pressure in UGS in different periods has a different scale; $\hat{y}$ is the value obtained from the model

During training, the initial learning rate coefficient, assumed to be 0.001, decreases gradually as the number of passed epochs increases. Training stops when the loss on the validation sample does not decrease any more (Fig. 2).

The quality of the trained model was evaluated on a test sample. Statistical parameters of model errors are as follows: mean = 0.006; standard deviation = 0.2.

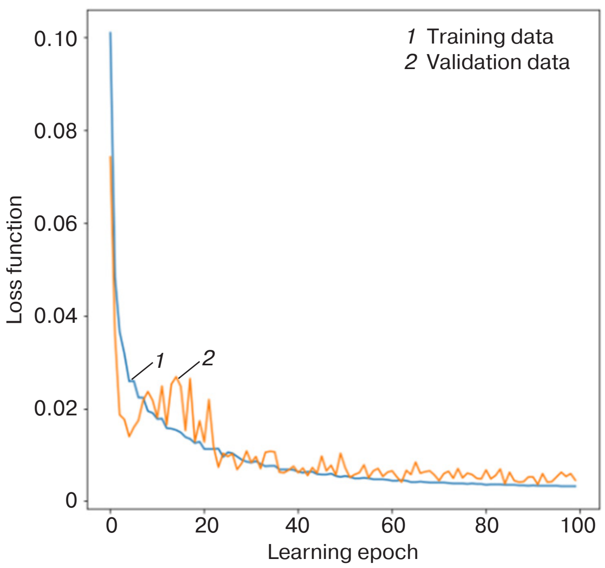

Fig. 2. Diagram of model error during the learning process

The trained model is able to reproduce the reservoir pressure dynamics for the period of sampling seasons to an acceptable degree of accuracy. Figure 3 shows the scatter diagram of normalized (scaled to the range from 0 to 1) formation pressure between the trained neural operator and the results of numerical simulations. The coefficient of determination $R^2 = 0.999$.

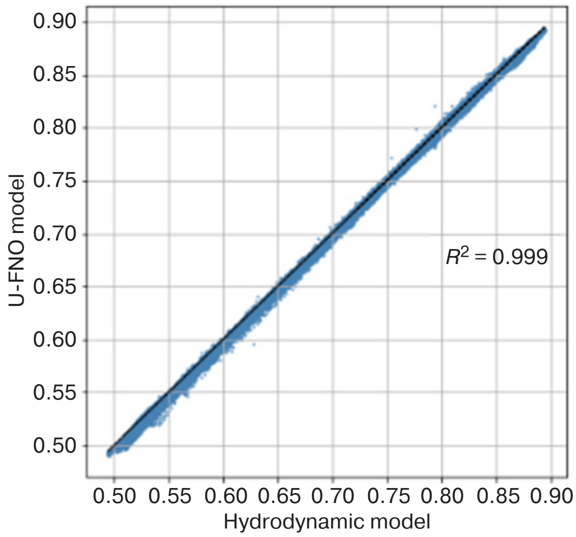

Fig. 3. Normalized reservoir pressure scatter diagram

Based on the scatter plot, it follows that the distribution generated by the neural operator on the test sample in each reservoir cell is very close to the distribution from the HDM.

A visualization of the comparison of simulation results of reservoir pressure field dynamics modeling by means of neural operator and HDM is presented in Figs. 4–6. The time step means the ordinal number of the ten-day period (decade) within the gas withdrawal season.

The trained neural operator demonstrated good performance on the test sample. Moreover, the obtained model calculates a given scenario in a fraction of a second, which is at least 10^6 times faster than a traditional numerical simulator.

In spite of the small number of PDE implementations in the training sample, we evaluated the generalization ability of the model on the example of reproducing the reservoir pressure dynamics in case of significant changes in the object itself involving variations in the number and location of wells. Since the use of the developed neural operator at this stage does not imply calculations or optimization of various well placement schemes, the scenario calculated on the operating HDM was taken as a reference scenario reproducing the situation with near-zero withdrawals from UGS during the entire period. Then, all wells were removed, 11 new production wells were placed in reservoir cells where they had never been before, and the scenario of forced gas withdrawals through these wells was modeled. The results are shown in Fig. 7.

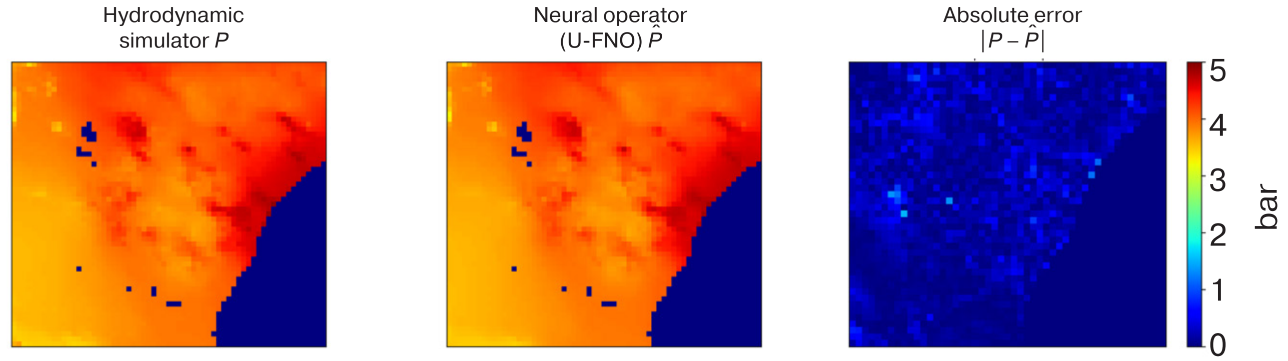

Fig. 4. Visualization of reservoir pressure from HDM, U-FNO model and absolute error on test sample (time step 4/16)

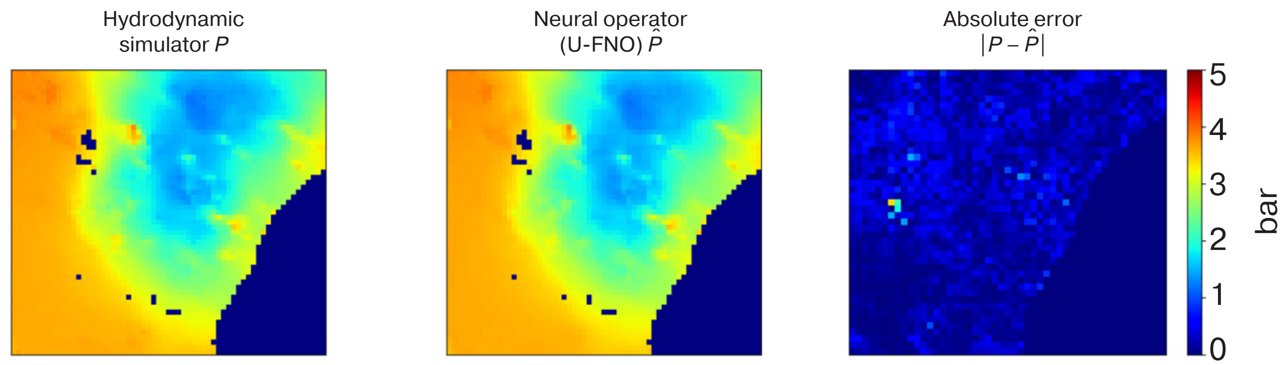

Fig. 5. Visualization of reservoir pressure from HDM, U-FNO model and absolute error on test sample (time step 10/16)

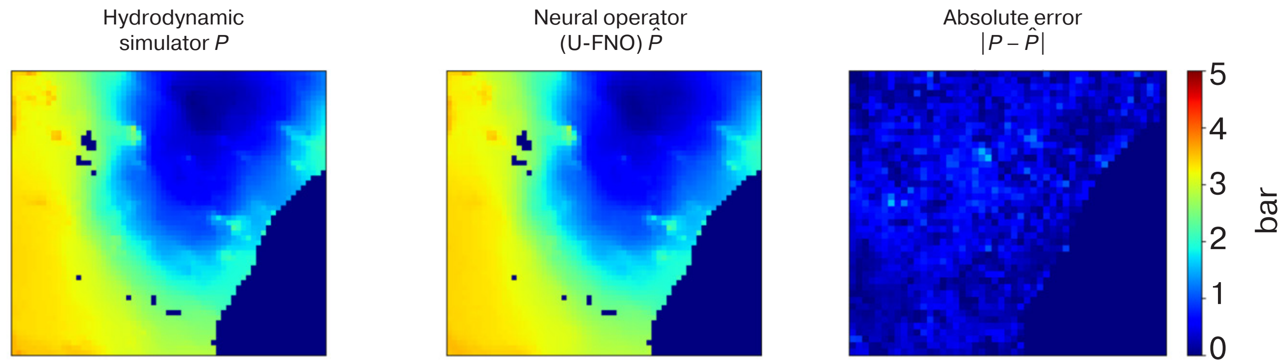

Fig. 6. Visualization of reservoir pressure from HDM, U-FNO model and absolute error on test sample (time step 16/16)

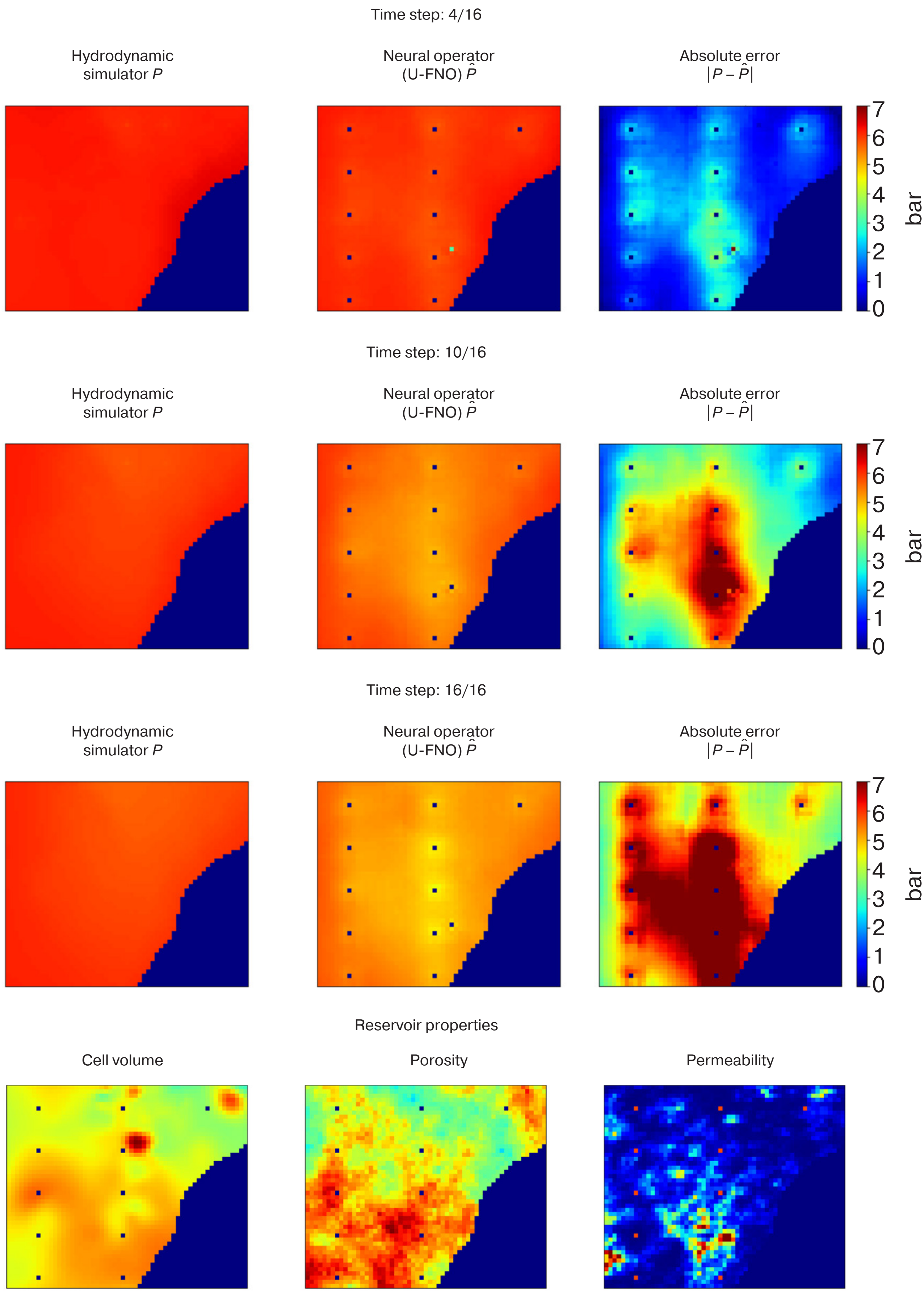

Fig. 7. Visualization of simulation results taking into account changes in well stock and visualization of formation properties (cells with placed wells are highlighted in color)

The lower part of Fig. 7 depicts visualizations of discretized reservoir cell volumes, porosity and permeability. Based on the obtained results, we conclude that the model responds adequately to such significant changes: the reservoir pressure field in the near-wellbore space changes taking into account the distribution of formation properties.

CONCLUSIONS

The reported study demonstrates the possibility of successfully applying the modified neural Fourier operator not only to the problems of modeling gas filtration in a cylindrical coordinate system with a single well, but also to the problems of three-dimensional gas filtration in a Cartesian coordinate system on objects with multiple wells. In addition, despite the use of the fast Fourier transform algorithm in the architecture, the developed model provides high quality modeling of objects with non-uniform sampling grid and complex geometry.

At the same time, the neural operator does not need a large training sample size to achieve high accuracy of approximation of PDE solutions, which is demonstrated not only on the test sample, but also on artificially generated scenarios involving significant changes in the structure of the modeled object. Based on the experiments, the trained neural operator simulates a given scenario in a fraction of a second, which is at least 10^6 times faster than a traditional numerical simulator. This makes the model suitable for application in tasks of planning and decision-making with respect to various aspects of UGS operation, such as optimal well utilization, pressure control and gas reserves management.

Authors' contributions

All authors equally contributed to the research work.

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