Numerical Investigation of Unsteady Flow Dynamics in a Packed Bed

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Abstract. Numerical simulation of unsteady flow of a compressible fluid in a fixed bed filled with porous elements has been performed. The research was carried out via ANSYS Fluent software. The scientific substantiation and verification of the physical and mathematical approaches incorporated in ANSYS Fluent for the problem of unsteady flow in a fixed bed has been carried out. For the computational domain, the interfaces of the flow area and the surface of porous particles are coupled by combining the contacts into a component part. The numerical results were verified using experimental data. The study was carried out in the range of velocity from 0.25 to 3.25 m/s. An expression is proposed for determining the pressure drop in a fixed bed, in which the pressure drop depends on the velocity, flow properties and the linear coefficient of local resistance. The values of the linear coefficient of local resistance are determined for the most common nozzle shapes in the industry: cylinder, Raschig ring, convex cylinder with 7 holes, sphere with 7 holes. It was found that with an increase in velocity, the value of the linear coefficient of local resistance decreases.

1. Introduction

Devices with a fixed packed bed filled with elements of various shapes with different properties are widely used in industry: chemical engineering, power engineering, petrochemistry, etc. Devices with a fixed bed are used to improve the contact between two phases in the process of heat and mass transfer in chemical reactors [1], in adsorbers, thermochemical recuperators [2] and others [3]. In addition, the fixed bed can be used as a filter element in purification systems, as well as an element of a regenerative heat exchanger.

The calculation of such devices is an important engineering problem, since the fixed bed has significant flow dynamic resistance, the precise determination of which is the key to their efficient operation. The wide interest of researchers and engineers in this problem is explained not only by its practical importance, but by a wide variety of structures of fixed layers for various devices [4]. Variables that affect the pressure drop in a fixed bed can be divided into two groups: variables related to fluid properties (density, velocity, viscosity), and variables related to bed size, particle shape, porosity, filling structure, filled column geometry.

The traditional approach to the design of fixed bed devices is the use of the Ergun equation, which allows one to determine the pressure drop by linking the two groups of variables indicated above [5]. However, the versatility of this equation for calculating fixed layers of various geometry and structure has caused and still causes great criticism in the scientific literature. This is due to the fact that the
discrepancy between the calculated results and experimental data can reach several tens of percent. For this reason, there are many modifications of the Ergun equation, as well as empirical dependences [6].

In recent years, the widespread use of computational fluid dynamics (CFD-modeling) methods for engineering calculations has found application for calculating fixed beds. CFD modeling is performed both in special software, for example, ANSYS Fluent, Comsol Multiphysics, OpenFOAM, etc., and using custom programs written in C++, Pascal, etc. The existing publications on the numerical modeling of fixed layers mainly consider fillers as solid particles [7]. However, a large number of fixed bed apparatuses, in particular, reformer reactors, thermochemical recuperators, etc., use porous particles as fillers. It has been noted in a number of publications that the Ergun equation and CFD modeling for fixed layers in a wide range of Reynolds numbers give significant deviations from the experimental data if porous particles are used as packing [8]. In this regard, Monlet et al. Proposed introducing additional correlation coefficients into the Ergun equation [6].

The discrepancy between the results of numerical modeling and calculations by the Ergun equation for fixed layers filled with porous structures with experimental data can be caused by the following reasons. First, the Ergun equation does not take into account the porosity of particles that form a fixed bed. Second, CFD modeling is often performed for a stationary problem, where the Reynolds-averaged Navier-Stokes equations are solved. An example of the difference between the results of CFD modeling in the case of stationary and non-stationary formulation of the problem is the simulation of the Karman vortex street, which is observed only for the non-stationary formulation of the problem of an incident flow around a cylinder [9]. The search for a universal technique for calculating fixed layers of various geometries for a wide range of Reynolds numbers is an important task.

The aim of this study is to numerically simulate the unsteady flow of a compressible fluid in a fixed bed filled with porous packings of various shapes, in a wide range of Reynolds numbers. For numerical simulation, the software product ANSYS Fluent (version 18.2, license type Full Academic Research) was used.

2. CFD-modelling

2.1. Geometry and mesh

CFD modelling of flow dynamics in a fixed includes the following main stages:

- construction of a computational area that repeats the geometric characteristics of a real fixed layer as accurately as possible;
- generation of the computational grid for the computation area;
- development of a programmable algorithm (solver settings);
- validation and verification of results;
- processing and analysis of the results of a numerical experiment.

To verify the results of numerical modeling using a physical experiment, data sets on the gas-dynamic resistance of a fixed layer filled with porous particles were obtained. NIAP catalysts made in the form of cylinders and Raschig rings were used as porous packing. The porosity of the catalyst $\varepsilon_{\text{cat}}=0.41$. The catalyst particles were placed in a cylindrical tube 100 mm in diameter. The length (depth) of the fixed layer is 600 mm.

As a working substance, atmospheric air was used, the flow rate and speed of which is controlled by changing the number of fan revolutions on the dashboard (4). The pressure is measured using differential pressure gauges with digital indication of readings. To obtain stable values, the pressure measuring points before and after the fixed bed are located at a distance from the edge exceeding the diameter by 3 times.

The computational domain geometry is constructed in such a way that the real structure of the fixed layer is repeated as accurately as possible. The main criteria for the similarity between the calculated geometry and the real fixed bed are the number of catalyst particles and the depth (length) of the fixed
For all calculated geometries, the number of catalyst particles and the length of the fixed bed are equal to the values for the real object. For all forms of catalyst, the length and diameter of the reaction space are constant. An empty (not filled with porous catalyst) flow area is added to obtain a developed flow at the entrance to the fixed bed in laminar flow. A general view of the computational geometry for CFD modelling is shown in Fig. 1.

Figure 1. Computational domain for CFD modelling of gas dynamics in a fixed bed.

To generate the design geometry, the RBD algorithm (Rigid Body Dynamics) was used, which allows you to create chaotically filled areas of calculations. The RBD algorithm is often used in the field of graphic design and modelling [10]. The Maya Autodesk software is used as a platform for the RBD algorithm, in which the filling of a fixed layer is performed randomly based on Newton's laws of motion and Lagrange mechanics.

The computational mesh was generated in the ANSYS Meshing module. The total number of elements of the computational grid for all cases under study is about 20 million. The number of elements of the computational grid was determined after determining the grid convergence, where the pressure and flow rate at the exit from the fixed bed were chosen as a control parameter. The appearance of the grid of the catalyst bed and free space (flow area) is shown in Fig. 2. The unit cells of the catalyst layer are tetrahedrons. For the flow area near the catalyst walls, the mesh was refined to correctly model the boundary layer. For this, the inflation function was used with the number of layers equal to 5.

Figure 2. Mesh structure for the computational domain.
2.2. Governing equations
To simulate flow dynamics in a fixed bed, ANSYS Fluent solves a system of partial differential
equations describing the motion of a viscous Newtonian fluid, called the Navier-Stokes equations. In
general, the Navier-Stokes equations consist of the continuity equation (the law of conservation of
mass) and the equation of motion (the law of conservation of momentum) [11].

Based on the preliminary analysis and literature review, it was found that the gas-dynamic
resistance of the fixed bed will be significant; therefore, the Redlich–Kwong equation of state [11] is
used in the numerical model.

Taking into account the specifics and structure of the computational geometry, based on the
recommendations of [12-13], the time-averaged Navier-Stokes equations in the adopted model are
closed by the standard k-ε turbulence model (k-ε standard), which allows solving problems in a fairly
economical way for a wide range of Reynolds numbers.

The dynamics of the flow in a porous medium of catalyst particles is determined by the Ergun
equation through the determination of the coefficient of viscous resistance (α) and the coefficient of
inertial resistance (C₂):

$$\frac{\Delta P}{L} = \mu \frac{1}{\alpha} \frac{u}{2} \rho u^2$$

(1)

where \( \mu \) is the viscosity, \( L \) is the length of the porous element.

In equation (1), the viscous drag coefficient (α) and the inertial drag coefficient (C₂) depend on the
porosity of the particle filling the fixed layer:

$$\alpha = \frac{D_{cat}^2 e_{cat}^3}{150 (1 - e_{cat})^2}$$

(2)

$$C_2 = \frac{3.5}{D_{cat}} \frac{(1 - e_{cat})}{e_{cat}}$$

(3)

where \( D_{cat} \) is the diameter of a porous particle of a fixed bed, \( e_{cat} \) is the porosity of the catalyst.

The boundary conditions are set as follows:
- gas movement along the z axis;
- at the inlet (\( z = 0 \)), the flow is considered fully developed, while the profile of the developed flow
  at the inlet to the pipe is imported using the import profile procedure obtained in a separate calculation
  for a pipe without a catalyst, in which the length-to-diameter ratio is \( L/d = 15 \);
- standard conditions of sticking of a viscous liquid are used on the pipe walls;
- the flow rate at the inlet varies from 0.25 to 3.25 m/s, which corresponds to the technological
  modes of operation of most industrial installations with a fixed bed.

To solve the system of differential equations describing the dynamics of the gas flow, a second
order upwind scheme is used. The flow time for all investigated operating modes is 5 s. The time step
optimized for the Courant number is 0.01 s. The maximum number of iterations for each time step is
250. The criterion of convergence by the continuity equation is set at level \( 10^{-3} \).

3. Results and discussion
The computational experiment was performed on an HPC cluster (High Performance Computing),
consisting of two Intel Core i9 7960X LGA 2066 BOX processors with 96 GB of RAM. The average
duration of one calculation was about 55-60 minutes.

The main advantage of CFD modeling results is their clarity. In Fig. 3 shows the velocity contours
in a fixed bed filled with porous particles at an initial velocity \( v=1.5 \) m/s and a temperature \( t = 20 \) °C.
Using the above-described algorithm for conjugating the interfaces of the catalyst particle surface and
the flow area, the flow moves not only between the catalyst particles, but also in the interpore space of
the particles themselves.

Fig. 3 it can be seen that air moves not only in the flow area of the fixed bed between the catalyst
particles, but also in the porous catalyst particles. However, the speed of air movement between
particles the catalyst is much higher than the speed of air movement in the catalyst particles. This is
due to the fact that the porous medium of the catalyst particles also has aerodynamic drag determined
by the Ergun equation. In this regard, gas-dynamic resistance in a fixed bed is created not only by the
geometric shapes of the catalyst particles, but also by their porous structure. This can explain the
discrepancy between the experimental results and the results calculated using the Ergun equation (1)
observed by other researchers. According to the original source [5], the classical Ergun equation is
applicable for fixed layers filled with solid particles. While the investigated fixed bed is filled with
porous catalyst particles.

![Velocity contours in the axial and radial planes of a fixed bed filled with a cylindrical porous catalyst.](image)

Figure 3. Velocity contours in the axial and radial planes of a fixed bed filled with a cylindrical porous catalyst.

The pressure drop in the fixed bed, determined by experiment and CFD simulation, is shown in
Fig. 4. For clarity of results in the interval up to 1.5 m/s, the pressure drop values are transferred to the
logarithmic coordinate plane. Thus, Fig. 4a shows a linear coordinate plane, and Fig. 4b - a
logarithmic one. Typical quadratic dependences of the form $\Delta P = (v^2)$ are observed for all studied
variants. The mean square error for the interval 0.25 ... 3.25 m/s for the cylinder is 8.43%, for the
Raschig ring 6.12%.
Figure 4. Pressure drop in a fixed bed on a linear (a) and logarithmic (b) coordinate plane: hollow points - experimental data [14]; solid lines - CFD simulation results for a fixed bed filled with solids.

To evaluate the results of CFD modeling, they were compared with the results obtained for a fixed bed using the standard Ergun equation (1) and the Ergun equation, taking into account the shape of catalyst particles.

The results of comparing the value of the pressure drop in the fixed bed, obtained using CFD modeling and using equation (1), are shown in Fig. 4.

Figure 5. Comparison of the CFD simulation results for the pressure drop in a fixed bed filled with a porous cylindrical catalyst with the results obtained by Ergun's equation (1).

Fig. 5 shows significant (more than 50%) discrepancies between the experimental data and the results obtained by Ergun's equation (1), respectively. Similar dependences were obtained for the reaction space filled with catalysts in the form of Raschig rings. Significant discrepancies in the results experienced by many researchers [4, 6] led to the fact that researchers obtained many different forms of Ergun's equations, applicable for various structures of a fixed bed, taking into account the shape of particles, flow velocity, bed diameter, etc. [15-16]. At the same time, obtaining a universal equation that makes it possible to take into account the properties of the flow, its velocity and the structure of the fixed bed is still an unsolved problem. However, numerical modeling, in particular in the ANSYS
Fluent software product, makes it possible to take into account the real structure of the fixed bed, the porosity of the catalyst particles, the flow rate, etc.

The discrepancy between the results shown in Fig. 5 can be explained by the fact that the movement of gas through a fixed bed filled with a porous catalyst takes place not only in the flow region between the catalyst particles, but also in the interpore space of the particles themselves. In this case, the gas-dynamic resistance in a real fixed bed filled with a porous packing is of greater importance than the value calculated by Ergun’s equations.

Using CFD-modeling, it is possible to determine the pressure drop in a fixed bed filled with elements of various shapes and porosities. In addition, in practice, the fixed bed has a complex volumetric structure, while the Ergun equations allow one to determine the pressure drop per unit length of the fixed bed. Therefore, for engineering calculations of fixed layers, it is proposed to use the following expression:

\[ \frac{\Delta P}{V} = \xi_l \frac{\rho u^2}{2} \]  

(4)

where \( \xi_l \) is the coefficient of local resistance of 1m of the fixed bed.

In expression (4), the left term represents the specific pressure loss per 1m of the fixed bed. From expression (4) it can be seen that pressure losses in a fixed bed are determined only by the gas flow rate, its density and its volume, and the value of the local resistance coefficient of 1m can be determined both empirically and using the developed CFD model. Fig. 6 shows the dependence of the linear coefficient of local resistance \( \xi_l \) of a fixed bed on the flow rate for the most common forms of catalysts in industry: a cylinder, a Raschig ring, a convex cylinder with 7 holes, a sphere with 7 holes.

The dependences shown in Fig. 6 were obtained using numerical simulation, the algorithm of which is described above.

As can be seen from Fig. 6, the linear coefficient of local resistance changes significantly with a change in the flow velocity, especially in the range up to 1 m/s. Usually, when flowing around solid non-porous bodies, the coefficient of local drag depends weakly or does not depend at all on the speed of the incident flow in a narrow range of Reynolds numbers. This effect of velocity on the volumetric
Coefficient of local resistance can be explained by the fact that the CFD model takes into account not only the porosity of the fixed bed, but also the porosity of the catalyst particles themselves.

The ones shown in Fig. 6 are of great practical importance, since allow preliminary determination of the gas-dynamic resistance of a fixed bed for various conditions of its operation. To obtain the most accurate results of the pressure drop in a fixed bed, it is necessary to construct the CAD geometry of the object under study, filled with catalyst particles of a given shape, and, using the algorithm described above, determine the pressure drop values.

4. Conclusion

Numerical modelling of unsteady flow of a compressible fluid in a fixed bed filled with porous particles of various shapes was performed using the ANSYS Fluent software product. Using the interface of the computational geometry interfaces, it was possible, on the basis of the known physical and mathematical models embedded in the ANSYS Fluent program code, to obtain results close to the experimental data. Scientific substantiation and verification of the ANSYS Fluent approaches for the problem of modelling the flow of a compressible fluid in a fixed bed filled with porous nozzles has been carried out. It is shown that CFD modelling gives significantly more accurate results of pressure drop in a fixed bed in comparison with the values obtained by the Ergun equation. An expression is proposed for determining the pressure drop in a fixed bed having a complex geometry. Using numerical modelling, the value of the linear local resistance coefficients of 1 m of a fixed layer filled with elements in the form of a cylinder, a Raschig ring, a convex cylinder with 7 holes, a sphere with 7 holes was determined. It has been established that the linear coefficient of local resistance of 1 m of a fixed bed decreases significantly with an increase in the flow rate, especially in the range up to 1 m/s.

5. References

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