A discontinuous Galerkin method for mathematical simulating of gas-liquid mixture flows

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Abstract. We present mathematical simulating results of a gas-liquid mixture flow in a cylindrical pipe. The gas-liquid mixture consists of the mineralized water and propane gas. To analyze the mineral composition of the fluid, a sensor is mounted in the pipe. The sensor affects the topology of the flow velocity vector field. The gas-liquid mixture flow is described by the unsteady Navier-Stokes equations. When the flow rate of gas-liquid mixtures exceeds 20 m/s, eddy flows occur in the pipe with obstacles. A method of discretization should take into account the problem specifics: rapidly changing gradients, the prevalence of the convective term in the Navier-Stokes equations. A computational scheme of discontinuous Galerkin method has the local conservative property and is best suited for solving such singularly perturbed problems. To perform a spatial discretization, a computational scheme of the discontinuous Galerkin method in the function spaces $H(\text{div})$ and $L^2$ is used. Application of the multiscale approach allows breaking down the solution of the simulation problem into several smaller ones that can be solved using parallel computations. Mathematical modeling results of the gas-liquid mixture flow in the pipe with different options for the sensor location are presented.

1. Introduction

There are three groups of numerical methods for mathematical simulating of gas-liquid mixture flows: meshfree, meshfree-mesh-based, and mesh-based methods.

Meshfree methods include discrete element methods, particle methods, and its variations [1, 2]. An implementation of meshfree methods is associated with the development of effective parallel algorithms on powerful computer architectures since one requires solving a large number of equations describing the motion of particles.

Meshfree finite element methods, natural neighbor methods, lattice Boltzmann methods, and its modifications are considered as meshfree-mesh-based methods [3, 4]. Meshfree-mesh-based methods make it possible to construct a solution to a problem using interpolation on Voronoi's cells. For each space point, a shape function is determined in accordance with Galerkin’s method. The efficiency of applying the meshfree-mesh-based methods is completely determined by the tessellation algorithm of space by Voronoi's cells.

Computational schemes of finite element methods (FEM), finite difference methods (FDM), finite volume methods (FVM), and boundary element methods (BEM) are pure mesh-based methods.
The classical FEM is not locally conservative. Its use for solving problems with a prevailing convective effect leads to physically irrelevant results. The prevailing convective effect is the property for the Navier-Stokes equations in simulating of gas-liquid mixture flows.

To increase the stability of classical FEM computational schemes, special stabilizing terms are introduced into variational formulations. Stabilized finite element methods are based on the numerical solution residual analysis. The most popular stabilized finite element method are upwind computational schemes of the Petrov-Galerkin method [5, 6].

For hydrodynamics problems with discontinuous solutions or rapidly changing solution gradients in the near-wall areas, computational schemes based on the discontinuous Galerkin method (DG) are used. DG-methods belong to the family of nonconforming finite element methods.

The DG-method has the local conservative property and combines the efficiency of the finite volume methods and the computational flexibility of the finite element methods [7]. To discretize the Navier-Stokes equations, the discontinuous Galerkin method is used in the concept of mixed finite element methods [8 – 11].

Recently, the virtual finite element method (VFEM) has been gaining popularity. VFEM is a generalization of the FEM and allows the use of polytopic meshes with hanging nodes and non-convex elements. As noted in [12], this method is effective for modeling flows in complex media, since it allows taking into account the internal boundaries with high accuracy. VFEM uses special virtual-space projection operators and stabilizing bilinear forms. Moreover, the form functions are not explicitly calculated. The application of virtual elements for solving the Stokes problem can be found in [13, 14].

There are special methods for solving hydrodynamics problems in media with deforming boundaries. These methods allow not to rebuild finite element meshes. The idea of the extended finite element method (XFEM) is based on the introduction of additional degrees of freedom near deformation zones (pores, cracks, or cohesive zones). It is worth noting, for solving the Navier-Stokes equations, the XFEM technology has been currently developed for a very limited set of applied problems [15].

There are alternative approaches that are similar to the discontinuous Galerkin method. To solve the hydrodynamics problems, domain decomposition methods (DD) with the Mortar or Trefftz methods are used. DD technologies allow building a parallel solution procedure in inconsistent subdomains. The Mortar and Trefftz methods expand the capabilities of the classical FEM and allow taking into account discontinuities of solutions at the inter-element boundary [16 – 19].

2. Problem definition

We consider a problem of a gas-liquid mixture flow in a pipe of cylindrical form. The gas-liquid mixture consists of the mineralized water and propane gas. For analyzing the mineral composition of the fluid, a sensor can be located both inside the pipe (figure 1a) and in the recess of the wall pipe (figure 1b).

![Figure 1. Sample: a – sensor inside the pipe; b – sensor in the recess of the pipe wall.](image)

The length of the pipe is 2 m, the radius is 0.1 m. The sensor has a cylindrical shape, the height of the sensor is 1 cm and the radius is 1 cm. The velocity of the gas-liquid mixture does not exceed 20 m/s. The roughness of the pipe wall is not taken into account.

The gas-liquid mixture consists of mineralized water and propane gas. The density and viscosity of the gas-liquid mixture are considered constant: 0.0214 MPa*s and 451 kg/m³, respectively. The diffusion coefficient of the gas-liquid mixture is 0.51 cm²/s. Equilibrium density is 990 kg/m³.
3. Mathematical model

The mathematical model of the gas-liquid mixture isothermal flow is described by the Navier-Stokes equations in the field of gravity

\[ \rho_0 \left( \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) + \nabla p = \nabla \cdot (\mu \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^\top \right)) + \mathbf{g} (\rho - \rho_0), \quad (1) \]

\[ \frac{\partial p_0}{\partial t} + \text{div}(\rho_0 \mathbf{v}) = 0, \quad (2) \]

where \( \rho \) is the equilibrium density (kg/m\(^3\)), \( \rho_0 \) is the density of the gas-liquid mixture (kg/m\(^3\)), \( \mathbf{v} \) is the flow velocity of the gas-liquid mixture (m/s), \( p \) is the dynamic pressure (Pa), \( \mu \) is the dynamic viscosity (Pa\(\cdot\)s), \( \mathbf{g} \) is the acceleration of gravity (m/s\(^2\)).

Equations (1) – (2) are supplemented by the equation for the mass concentration of the impurity

\[ \frac{\partial s}{\partial t} + (\mathbf{v} \cdot \nabla) s + f = \nabla \cdot \mathbf{D} \nabla s, \quad (3) \]

where \( s \) is the mass concentration of the impurity (kg/m\(^3\)), \( \mathbf{D} \) is the diffusion coefficient (m\(^2\)/s), \( f \) is the source (kg/m\(^2\)/s).

The initial conditions for the velocity vector and mass concentration of the impurity have the form

\[ \mathbf{v}|_{t=0} = \mathbf{v}_0, \quad s|_{t=0} = s_0. \quad (4) \]

On the impermeable side surface of the pipe \( S_1 \), the non-leakage condition (wall) of the gas-liquid mixture is formulated for the velocity normal component

\[ \mathbf{v} \cdot \mathbf{n}|_{S_1} = 0, \quad (5) \]

where \( \mathbf{n} \) is the normal vector.

At the inflow boundary \( \Gamma_1 \), the normal component of the flow velocity \( v_1 \leq 20 \) is specified as

\[ \mathbf{v} \cdot \mathbf{n}|_{\Gamma_1} = v_1. \quad (6) \]

On the outflow boundary \( \Gamma_2 \) homogeneous conditions are set for the normal component of the stress tensor

\[ \mathbf{\sigma} \cdot \mathbf{n}|_{\Gamma_2} = -(p \mathbf{I}) \cdot \mathbf{n} + \mu \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^\top \right) \cdot \mathbf{n} = \mathbf{t} = \mathbf{0}. \quad (7) \]

The change in the concentration of the mixture occurs due to the point source \( f \). We assume on all pipe walls that

\[ \nabla s \cdot \mathbf{n} = 0. \quad (8) \]

For \( \rho_0 = \text{const} \), the system of equations (1) – (2) is solved with conditions (4) – (7). For the calculated velocity vector, equation (3) is solved with conditions (4) and (8). We can solve these problems in parallel.

4. Variational formulation of the DG-method for the gas-liquid mixture flow problem

Let \( \Xi_n(\Omega) \) be a partition into disjoint sets \( \Omega_k \). Let \( \Gamma = \bigcup_k \partial \Omega_k \) be the set of the boundaries, \( \Gamma_0 = \Gamma \setminus \partial \Omega \) be the set of the inner boundaries, and \( T(\Gamma) = \prod_{\Omega_k \in \Xi_n(\Omega)} L^2(\partial \Omega_k) \) be the trace space. We introduce finite-dimensional subspaces on the set \( \Xi_n(\Omega) \) as

\[ P^k = \left\{ p \mid p \in L^2(\Omega) : p \in \mathcal{J}_n(K) \forall K \in \Xi_n(\Omega) \right\}, \quad (9) \]

\[ V^k = \left\{ v \mid v \in H(\text{div}, \Omega) : v \in \left[ \mathcal{J}_n(K) \right]^3 \forall K \in \Xi_n(\Omega) \right\}, \quad (10) \]

where \( \mathcal{J}_n(K) \) is a polynomial space of degree \( m \).

For building the trace operator on the inter-element boundaries, we consider the average \( [\cdot] \) and jump \( [\cdot] \). For the functions \( v \in [T(\Gamma)]^3 \) and \( p \in T(\Gamma) \) at the external boundary \( \partial \Omega \) we can write [7]
\[
\begin{align*}
\|v\|_\Omega &= v \otimes n, \quad \| \nu \|_\Omega = v \cdot n, \quad \|v\|_\partial\Omega = v, \\
\|p\|_\Omega &= p n, \quad \|p\|_\partial\Omega = p,
\end{align*}
\] (11)

at the inner boundary \( \Gamma = \partial \Omega \cap \partial \Omega \) between elements \( \Omega \) and \( \Omega \), we have [7]
\[
\begin{align*}
\|v\|_\Gamma &= v_i \otimes n_i + v_k \otimes n_k, \quad \| \nu \|_\Gamma = v_i \cdot n_i + v_k \cdot n_k, \quad \|v\|_\partial\Gamma = (v_i + v_k)/2, \\
\|p\|_\Gamma &= p_i n_i + p_n n_n, \quad \|p\|_\partial\Gamma = (p_i + p_n)/2,
\end{align*}
\] (12)

where the index indicates belonging to \( \Omega \).

The variational formulation for the Navier-Stokes problem based on the IP-DG-method is: find such \( v^h \in V^h \times [0,T] \), \( p^h \in P^h \times [0,T] \) that \( \forall w^h \in V^h \) \& \( q^h \in P^h \) [17, 18]
\[
\begin{align*}
a(v^h, v^h) + c(v^h, w^h, v^h) + b_1(w^h, p^h) &= (w^h, F), \\
b_2(v^h, q^h) + d(q^h, p^h) &= 0,
\end{align*}
\] (13)

\[
\begin{align*}
&= -\int_{\Gamma} \mu \nabla \nu \cdot \nu d\Gamma + \int \mu (\nabla \nu^h + \nabla^T \nu^h) \cdot \nabla \nu d\Omega - \int_{\Gamma} \mu \left( \nabla \nu^h + (\nabla \nu^h)^T \right) : \left[ \nu^h \right] - \tau^{DG} \left[ \nu^h \right] : \left[ \nu^h \right] d\Sigma, \\
&= -\int_{\Gamma} \nu \cdot \nu^h d\Gamma + \left[ q^h \right] \left[ v^h \right] d\Sigma,
\end{align*}
\] (14)

\[
\begin{align*}
c(a; v^h, v^h) &= -\int \rho_0 \nabla \nu^h \cdot a \cdot v^h d\Omega + \int \rho_0 \left( \left[ \nu^h \right] \cdot a \right) \left( \left[ \nu^h \right] \cdot n \right) d\Sigma, \\
b_2(v^h, q^h) &= -\int \rho_0 \nabla \nu^h \cdot q^h d\Omega + \int \rho_0 \left( \left[ q^h \right] \right) \left[ v^h \right] d\Sigma, \\
&= \int (\rho - \rho_0) g : w^h d\Omega + \int t \cdot w^h d\Sigma + \\
&+ \int \mu (\nabla \nu^h + \nabla^T \nu^h) \cdot (u_i \otimes n) - \tau^{DG} (u_i \otimes n) : (w^h \otimes n) d\Sigma, \\
d(q^h, p^h) &= -\int_{\Gamma} \frac{\partial \rho}{\partial t} q^h d\Gamma + \tau^{DG} \int_{\Gamma} \left[ q^h \right] \left[ p^h \right] d\Sigma.
\end{align*}
\] (19)

The variational formulation for the diffusion problem based on the IP-DG-method is: find \( s^h \in P^h \times [0,T] \) that \( q^h \in P^h \) [7]
\[
\begin{align*}
a(q^h, s^h) + c(q^h, s^h) &= (q^h, f), \\
a(q^h, s^h) &= \int \nabla s^h \cdot \nabla q^h d\Omega - \int \left[ \nabla \cdot \nabla s^h \right] \left[ q^h \right] d\Sigma - \int \left[ \nabla \cdot \nabla q^h \right] \left[ s^h \right] - \tau^{DG} \left[ s^h \right] \left[ q^h \right] d\Sigma. \\
c(q^h, s^h) &= -\int \nu \mathbf{v} \cdot s^h q^h d\Omega + \int \left[ q^h \right] \left[ \nu \mathbf{v} \cdot s^h \right] d\Sigma, \\
&= \int f q^h d\Omega.
\end{align*}
\] (20)

We use the stabilizing parameter \( \tau^{DG} > 1 \) [20]. The uniqueness of the solution of the Navier-Stokes problem is determined by the fulfillment of the inf-sup conditions [18]
\[
\inf_{p^h \in P^h} \sup_{v^h \in \mathcal{V}^h} \frac{(\nabla \cdot \nu^h, p^h)_{\Omega,\partial\Omega}}{\|\nabla \nu^h\|_{\Omega,\partial\Omega}^2} \geq \alpha > 0,
\] (24)

where \( \alpha \) is independent of the finite element mesh size.
5. Experimental results
Computational experiments were performed for two positions of the sensor: inside the pipe in the form of a cylindrical protrusion and in the recess of the lower pipe wall.

1. Sensor is located inside the pipe (1 cm protrusion)
Figure 2 shows the finite element tetrahedral mesh of the computational domain.

![Finite element tetrahedral mesh](image1)

Figure 2. Finite element tetrahedral mesh: 21720 tetrahedra.

The normal component of the velocity vector at the inflow boundary is 20 m/s. Figures 3–5 show the dynamic pressure fields and the modulus of the velocity vector of the gas-liquid mixture at different times. For the numerical solution, we used the finite element basis on tetrahedra, Crouzeix-Raviart elements, time discretization step $\Delta t = 0.01$ s.

![Dynamic pressure and velocity module](image2)

Figure 3. Dynamic pressure (a) and vector velocity module of the gas-liquid mixture flow (b) in time $t = 0.1$ s.
Figure 4. Dynamic pressure (a) and vector velocity module of the gas-liquid mixture flow (b) in time $t = 0.5$ s.

Figure 5. Dynamic pressure (a) and vector velocity module of the gas-liquid mixture flow (b) in time $t = 2$ s.
2. Sensor is located in a recess (depth 1 cm)

Figure 6 shows the finite element tetrahedral mesh of the computational domain.

![Finite element tetrahedral mesh: 18344 tetrahedra.](image)

The normal component of the velocity vector at the inflow boundary is 20 m/s. Figures 7–9 show the dynamic pressure fields and the modulus of the velocity vector of the gas-liquid mixture at different thickness of the liquid phase. For the numerical solution, we used the finite element basis on tetrahedra, Crouzeix-Raviart elements, time discretization step $\Delta t = 0.01$ s.

![Dynamic pressure (a) and vector velocity module of the gas-liquid mixture flow (b), the liquid phase thickness is 1 cm.](image)

6. Conclusion

For mathematical simulating of the gas-liquid mixture flow process, a computational scheme based on the discontinuous Galerkin method using the function spaces $L_2$ and $H(\text{div})$ was developed and implemented.

At the gas-liquid mixture velocity of 20 m/s, vortex flows arise. If the sensor location is above the pipe wall, stagnation zones arise in front of and after the sensor. In this case, it is impossible to guarantee in real-time the physically relevant measurement result and the correctness of the data on the mineralogical composition of the fluid.

The result analysis allows concluding that the most suitable sensor location is a recess in the pipe wall since with this configuration the vortex flows does not form stagnant zones.
Figure 8. Dynamic pressure (a) and vector velocity module of the gas-liquid mixture flow (b), the liquid phase thickness is 0.5 cm.

Figure 9. Dynamic pressure (a) and vector velocity module of the gas-liquid mixture flow (b), the liquid phase thickness is 0.1 cm.

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