AERODYNAMIC MODELING OF EMISSIONS PASSAGE
IN THE NEUTRALIZATION PROCESS

Abstract. This paper discusses an approach to analyzing the aerodynamics of a catalytic converter body using the Boltzmann lattice method and cellular automata. The LBM (Lattice Boltzmann Method) method is based on discretization of the Boltzmann kinetic equation, which at the microscopic level corresponds to the diluted gas model (particle model), and at the macroscopic level asymptotically goes to the Navier-Stokes equation for liquids and gases. Numerical approximation is carried out on the basis of the standard Batnagar-Gross-Kruk model.

Key words: aerodynamics, lattice Boltzmann method, numerical simulation, neutralizer.

1. Introduction

Recently, the Boltzmann lattice method has begun to gain popularity among problems in the field of fluid dynamics [1-3], as well as special cases in modeling multiphase, multicomponent and porous media [4-6]. The main advantages of the method in comparison with standard algorithms for the numerical solution of CFD problems based on solving the Navier – Stokes equations by finite volume/element methods are the ease of implementation, good parallelization and high computation efficiency. Cellular automaton provides the ability to set simple rules for mixtures and phases, a small interdependence of calculations between the cells of the lattice, allowing unlimited scaling of the simulation area. The LBM (Lattice Boltzmann Method) method was developed in 1986 [7] as a result of attempts to optimize calculations for gas and liquids, it is relatively new. Modern models, able to operate stably at high speed can solve applied problems for aerodynamics, laws of quantum mechanical systems and shock waves.

2. Mathematical model

Numerical simulation of the gas transfer process is based on the Boltzmann kinetic equation. The main idea of Boltzmann is to represent the gas as interacting particles whose behavior can be described by the laws of classical mechanics. However, due very large number of particles, in practice, it is not possible. Boltzmann proposed a statistical formulation of the problem in which the state of the system under study can be described by some distribution function \( f^{(N)}(x_1, x_2, ..., x_N, p_1, p_2, ..., p_N, t) \), where \( N \) is a number of particles, \( x_i \) and \( p_i \) are coordinates and momentum of the i-th particle respectively. Consider the one-dimensional case. Let the probable number of molecules with coordinates in the interval \( x \pm dx \) and momentum in the interval \( p \pm dp \) be defined as \( f^{(1)}(x, p, t)dx dp \). Suppose that we have added some external force \( F \), which has a small magnitude in comparison with intermolecular forces. In case of the absence of collisions between molecules, the new positions of the molecules traveling from \( x \) at time \( t + dt \) will be equal to \( x = x + vdt = x + (p/m)dt = x + dx \), and the new impulses will be \( p = p + Fdt = p + (dp/dt)dt = p + dp \).
Therefore, if the positions and pulses at time $t$ are known, their increments allow us to determine the value of $f^{(i)}$ at time $t + dt$:

$$f^{(i)}(x + dx, p + dp, t + dt) dx dp = f^{(i)}(x, p, t) dx dp$$

(1)

Relation (1) describes the motion of particles without collisions. Collisions are taken into account by using the BGK model (Bhatnagar – Gross – Krook) - a classic choice among problems of physics:

$$f^{(i)}(x + dx, p + dp, t + dt) dx dp = f^{(i)}(x, p, t) dx dp + [\Gamma^{(+)} - \Gamma^{(-)}] dx dp dt$$

(2)

Here, the value of $\Gamma^{(+)} dx dp dt$ is equal to the number of molecules that did not arrive at the expected point of space with the coordinates $x + dx$ and momentum $p + dp$ due to collisions that occurred during time $dt$. The value of $\Gamma^{(-)} dx dp dt$ is equal to the number of molecules that began to move from points other than $x + dx$, but turned out to be in the region of space we are interested in due to collisions that occurred during time $dt$.

3. Boundary conditions

Usually during modeling the flow in channels or pipes using the LBM method, the channel walls are treated as a rigid boundary, from which particles are reflected, while periodic boundary conditions are applied to open channel sections [8].

In this case, the problem also has both types of boundary conditions. The computational domain (Fig. 1) consists of three boundaries - input, output and the rigid walls of the neutralizer. Reflection of particles will occur in a collision with the walls of the housing and the honeycombs of catalyst.

![Figure 1 - Computational domain of the problem, catalytic converter housing](image)

4. Numerical method

The method of lattice Boltzmann equations represents as a simplified implementation of the original Boltzmann idea through discretization of the equations. As a result, the number of particles, their possible velocities and positions in space is reduced. A uniform spatial grid called the Boltzmann lattice is built. Time is also discretized. Particles can be located only in the nodes of grid, the velocity of each particle can take a limited number of values, enough to reach the neighboring node during one time. Fig. 2 shows the lattice and directions of velocities $e_{a} B$, where $a = 0, \bar{8}$ is an index of the direction (at $e_{0} = 0$ particles are at rest).
The magnitude of the velocities $e_1, ..., e_8$ is 1 lattice unit in 1 time step, i.e. $lu \cdot ts^{-1}$. The magnitude of the velocities $e_{-1,0}, e_{0,-1}$ is $\sqrt{2} lu \cdot ts^{-1}$. Such choice of velocities is very convenient, since all their x- and y-components have values 0, 1 or -1 (Fig. 2). The value of $f_a$ determines the number of particles in a given node moving in the $e_a$ direction. The macroscopic density of gas in a given node is the sum of particles moving from a given node in all possible directions:

$$\rho = \sum_{a=0}^{8} f_a$$

In the simplest case the mass of all particles is the same and equal to one. The macroscopic velocity $u$ is the average of the microscopic velocities $e_a$, multiplied by the number of particles moving in a certain direction $f_a$:

$$u = \frac{1}{\rho} \sum_{a=0}^{8} e_a f_a$$

In the LBM representation, equation (2) will be:

$$f^\Delta_a (x + e_a \Delta t, t + \Delta t) = f_a (x, t) + \Omega_a (x, t)$$

The term $\Omega_a (x, t)$ describes the collision of particles. The authors of the model, Batnagar, Gross and Crook, suggested that if particles move without collisions, the system is in equilibrium. Any collision brings the system out of equilibrium. Then the iteration of the cellular automaton operating according to the LBM method will look as follows:

$$f^\Delta_a (x + e_a \Delta t, t + \Delta t) = f_a (x, t) - \frac{1}{\tau} [f_a (x, t) - f^{eq}_a (x, t)]$$

Where $f^{eq}_a (x, t)$ is an equilibrium function given by the formula:

$$f^{eq}_a (x, t) = w_a \rho (x) \left[ 1 + 3 \frac{e_a \cdot u}{c^2} + \frac{9 (e_a \cdot u)^2}{2 c^4} - \frac{3 u^2}{2 c^2} \right]$$

Where weight $w_a$ for particle at rest ($a = 0$) is equal to 4/9, for $a = 1, 2, 3, 4$ is 1/9 and for $a = 5, 6, 7, 8$ $w_a$ is 1/36; $c$ — the main velocity on lattice.
The model will qualitatively describe the flow at small values of the Mach number, and the kinematic viscosity depends on the relaxation time $\tau$: $\nu = (\tau - 0.5) c^2 dt$.

5. Results

In order to calculate the numerical approximation, a software complex for the universal Windows platform was developed. The program calculates aerodynamics, regime and design parameters of the process of emissions passage through the catalytic converter. Basing on results, it builds the geometry of the converter housing. The realization is done in Python, C#, Java languages.

Figures 2 - 4 present the results of the calculation of the aerodynamic characteristics of a single-component single-phase flow in a neutralizer with an optimal configuration and composition [9] at different incoming gas velocities.
6. Conclusions

The developed software complex for modeling the passage of emissions in the neutralization process, based on LMB method, has two key qualities - high speed of calculations, and the ability to model problems with complex boundary conditions. In this case, the complexity of the geometry lies in the structure of honeycomb catalyst, the main element of the catalytic converter. The lattice Boltzmann method and cellular automata allow one to simulate the gas dynamics using simple arithmetic expressions. The statistical approach to the numerical analysis of gas motion simplifies mathematical apparatus, thereby reducing the amount of computational costs. This mathematical model allows making modifications and subsequent additions, which will take into account the chemical composition and temperature [10-11] of waste gases in neutralizer.

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БЕЙТАРАПТАНДЫРУ ПРОЦЕССТЕГІ ПАЙДАЛАНЫЛГАН ГАЗДАР ШЫҒУДЫЗ ЭАРОДИНАМИКАЛЫҚ МОДЕЛДЕУ

Аннотация. Бұл мәкаләдә каталитикалық турлелдіріп корпусының аэродинамикасын өзгертетін тұрлелік төрлө дәлілсіз әуе әрікі арқылы тауалу дәлілі қарастырылды. LBM (Lattice Boltzmann Method) дәлілі мікроскопиялық дәнгейдегі құрылыстың ыңғайлығын (булдаксеретін моделі) бойынша келетін және сұйықтар мен газдарға арналған Навье–Стокс теңдеуіне бары-бар мікроскопиялық дәнгейлідегі ыңғайлық кинетикалық
АЭРОДИНАМИЧЕСКОЕ МОДЕЛИРОВАНИЕ ПРОХОЖДЕНИЯ ВЫБРОСОВ В ПРОЦЕССЕ НЕЙТРАЛИЗАЦИИ

Аннотация. В данной работе рассматривается подход к анализу аэродинамики корпуса каталитического нейтрализатора с применением решёточного метода Больцмана и клеточных автоматов. Метод LBM (Lattice Boltzmann Method) основан на дискретизации кинетического уравнения Больцмана, которое на микроскопическом уровне соответствует модели разреженных газов (модель частиц), а на макроскопическом уровне асимптотически переходит к уравнению Навье-Стокса для жидкостей и газов. Численное приближение осуществляется на основе стандартной модели Баттагара-Гросса-Крука.

Ключевые слова: аэродинамика, решеточный метод Больцмана, численное моделирование, нейтрализатор.

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