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Prediction of the pressure, velocity and axial mass flux profiles within a high-speed rotating cylinder in total reflux condition *via* modified dsmcFoam solver

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A modified version of the dsmcFoam solver was extended for molecular simulation of high-speed rotating geometries. Rotary machines' advantages have made them appealing to various applications such as laboratory centrifuges, analytical ultracentrifuges, haematocrit centrifuges and gas centrifuges. So, simulating the content inside the rotating machines can be important. The dsmcFoam solver has some shortcomings in the rotary machines gas flow modeling. Weakness to model the internal flows with pressure gradient characteristic creating a temperature gradient as a boundary condition and use of Adaptive Mesh Refinement (AMR) are some of them. We selected dsmcFoam as the base solver and tried to troubleshoot all of the above-mentioned faults. Through fixing these shortcomings, the Wide Application Dsmc SIMulation (WADSIM_1) software is introduced that is capable to simulate a wide range of internal flow problems with high-speed rotation. It was used to simulate the gas flow inside the rotating cylinder. Then the pressure, velocity and axial mass flux profiles inside it for light and heavy gases were calculated. Next, the results were compared with the DSMC code for axially symmetric flows. Finally, the compression ratio of a Holweck-type molecular pump (as a complex geometry with the presence of a rotating rotor inside it) obtained from WADSIM_1 was validated with the experimental results. The achieved results illustrated that the WADSIM_1 software has the capability to simulate a wide range of rotating geometries with high precision.

Keywords: dsmcFoam solver; WADSIM_1; Rotating rotor; Helix grooves.

Article Highlights: WADSIM_1 solver is able to simulate all two- and three-dimensional geometries with high-speed rotation; WADSIM_1 solver is able to use Adaptive Mesh Refinement (AMR) and gradient boundary conditions; Inside a rotating cylinder, the amount of light gases present in the cylinder's axis is higher than that of heavy gases.

INTRODUCTION

There are intensive changes in the density of gases within rotating cylinders due to a strong centrifugal force field. The force field causes the formation of different types of flow regimes inside the cylinder, extending from molecular ($kn > 0.1$) to continuous ($kn < 0.1$) regime.

In rotating cylinders, the Navier-Stokes equations are used to model the flow in a continuous domain. Generally, analytical solution of these equations is impossible and their numerical solutions require significant amounts of cost and time. Since the mid-1950s, a method has been developed to solve the Navier-Stokes equations based on simplifying and linearizing by appropriate assumptions. In this method, the six governing equations, i.e. conservation of mass, momentum (radial, tangential and axial components), energy and the state equation are combined to form a six-order PDE equation called the Onsager equation [1]. The main reasons for using this method are its high speed comparing to other methods and lack of requirement for high computational facilities. By developing the computational systems, the Onsager method has been replaced by CFD methods. Other modern methods are Lagrangian methods, especially DSMC, which has the ability to simulate systems with a large number of molecules for all flow regimes by representative particle selection [2, 3]. In recent years, the use of DSMC for simulating the flow inside a rotating cylinder has been widely extended. For instance, Pradhan and Kumaran, in 2011 and 2016, studied and analyzed the axial mass flux based on the dimensionless term in a radial direction using the DSMC method. They compared their results with the generalized Onsager model and achieved similar results [4, 5]. Inside a rotating cylinder, by moving radially forward into the continuous region, and thus, reducing the Knudsen number (Kn), the amount of calculations for the DSMC method increases, causing its implementation for the single core to be time-consuming.

Hence, researchers have recently started using some pieces of software and codes capable to run *via* multiple cores in parallel. In addition to commercial

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software such as Fluent and CFX for solving the fluid flow by numerical methods, open-source softwares are also provided in this branch, with the most important advantage of having access to code text. As a result, the considered solver and the boundary conditions can be changed according to the problem, and the closest simulation conditions can be achieved for the desired geometry. One of the most important open-source softwares is *OpenFoam*, which is able to solve a wide range of physical phenomena such as compressible and incompressible flows, molecular-based flows, two-phase flows, flows in porous materials, dynamics of gases, combustion, turbo machines, etc. The main strength of *OpenFoam* is its ingenious utilization of C++ programming language abilities, which provides an arranged structure of classes, libraries and objects due to its object-oriented nature [6]. The dsmcFoam solver is usually used for external flows. To our knowledge the gas flows inside a rotating cylinder with a dsmcFoam solver have not been studied so far. In 2013, for the first time, Gutt *et al.* used the internal flow through this solver for a PVD chamber [7]. In 2015, White applied an Adaptive Mesh Refinement (AMR) technique for an arbitrary geometry by modifying its Knudsen number for a modified dsmcFoam solver and achieved good results [8].

John *et al.* investigated in 2015 the high-speed rarefied flow past both stationary and rotating cylinders using the direct simulation Monte Carlo (DSMC) method. The DSMC simulations had been carried out using dsmcFoam solver. They compared various aerodynamic characteristics such as coefficients of lift and drag, pressure, skin friction, and heat transfer for stationary and rotating cylinder [9]. John *et al.* investigated in 2016 the flow past a rotating cylinder over a wide range of flows rarefied from the early slip through to the free molecular regime using dsmcFoam solver. They focused on high-speed flow conditions and considered a wide range of Mach numbers near the high subsonic, transonic, and supersonic regimes [10]. Dongari *et al.* evaluated the effect of curvature on rarefied gas flows between rotating concentric cylinders. They found that non-equilibrium effects were not only dependent on Knudsen number and accommodation coefficient but were also significantly affected by the surface curvature [11]. Kumar *et al.* developed a new multi-species, polyatomic, parallel, three-dimensional Direct Simulation Monte-Carlo (DSMC) solver for external flow problems. The main features of this solver include its ability to handle multi-species, polyatomic gases for 2D/3D steady and transient nature of flow problems over arbitrary geometries, with a density-based grid adaptation technique. Furthermore, 3D surface refinement (for accurate calculation of surface properties) and 3D gas-surface interaction was implemented in a very efficient manner in the solver [12]. The gas inside the high-speed rotating cylinders has a very high pressure gradient, so the size of each grid can change over time. For this problems the *AMR* technique should be used. The method for modeling the gas inside the rotating cylinder is a hybrid method. The molecular region (near the axis) can be simulated using the DSMC method, and then the results can be transferred as a mass source/sink to the numerical solution of the continuum region equations (the area next to the wall) [13]. Due to the problems of transferring information from one region to another in this method, the DSMC method is chosen as another method to simulate the total gas inside the rotating cylinder. In this paper, the *dsmcFoam* solver has been selected as DSMC molecular-based solver. This solver has previously been rigorously validated for a variety of benchmark cases [14,15]. The dsmcFoam solver, despite having many advantages like the high speed of its execution due to highly optimized codes and the possibility of using parallel runs with unlimited cores, has some defects in modeling the gas inside the rotating cylinders. In the present study, by correcting the temperature and velocity gradient boundary conditions for the dsmcFoam solver as well as applying an internal flow and using the *AMR* technique, a new software called *WADSIM_1* is introduced, which is capable to simulate the different gases inside the high-speed rotating cylinders. Due to the lack of experimental test results for the flow inside the rotating cylinders, simulation of a Holweck-type molecular pump was used to validate the *WADSIM_1* software. Finally, the value of the compression ratio obtained from the simulation was validated by the experimental compression ratio of the molecular pump. Holweck-type molecular pump has a complex geometry where gas molecules move through the grooves to the top of the grooves by hitting the rotating rotor [16].

THEORY

DSMC Method

From the Lagrangian point of view, DSMC is a fluidized simulation method in which a large number of simulated molecules are followed simultaneously, and in addition to colliding the molecules with a surface, the intermolecular collisions are also calculated. DSMC algorithm is shown in Fig. 1.

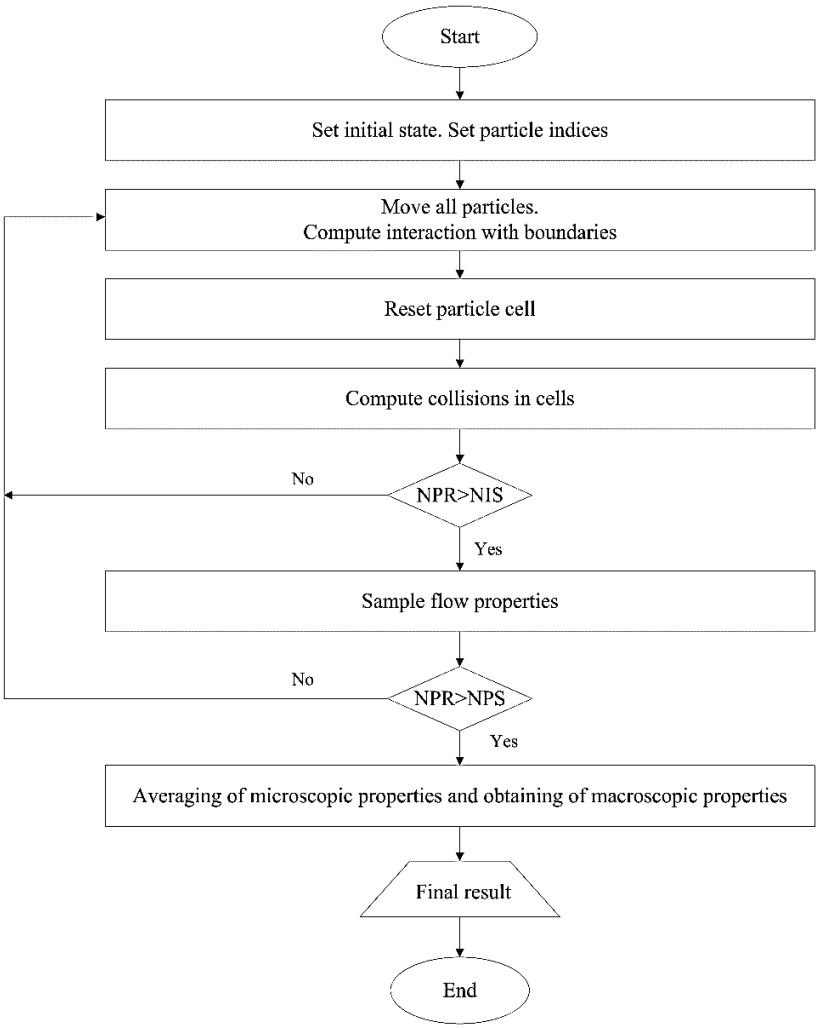

Fig. 1. DSMC algorithm

In this algorithm, the NPR, NIS, and NSP quantities represent the number of repetitions for obtaining the output file, the number of time steps between the samples, and the number of samples between the restart and output file updates, respectively [2].

Different collision models can be used at the collision step of particles. The easiest one is the Hard Sphere (HS) model in which the value of the collision cross-section is constant and does not change with the relative velocity whereas the actual cross-section should be decreased due to increasing the relative velocity.

This model has the advantage of easily calculating the collision mechanics because of the isotropic scattering in the center of the mass frame of reference. However, as its disadvantage, this scattering law is not realistic and the cross-section is independent of the relative translational energy in the collision. In this model, the temperature exponent of the coefficient of viscosity (ω) is equal to 0.5.

The Variable Hard Sphere (VHS) model is a hard sphere model in which the diameter is a function of relative velocity. The cross-section of the VHS model is determined from the viscosity coefficient, but the ratio of momentum to the viscosity cross-section follows the hard sphere value, which is a deficiency in the model. Therefore, the viscosity and the thermal conductivity coefficients are well calculated, but the Schmidt number, which depends on the diffusion coefficient, does not conform to the behavior of a real gas. The Variable Soft Sphere (VSS) model relates the probabilistic relationships to the type of gas used by an exponent in the VSS molecular model (α). As a result, the VSS model involves an empirical modification of the isotropic scattering law and the basic HS collision mechanics.

The Generalized Hard Sphere (GHS) model is an extension of the VHS and VSS models. It bears the same relationship to the Lenard-Jones class of models as the conventional VHS or VSS model bear to the inverse power law model. The Larsen-Borgnakke Variable Hard Sphere model (LBVHS)

is also proposed when the objective is to calculate the internal energy of the particles after their inelastic collision. A general Larsen-Borgnakke distribution function for the division of energy between the translational and internal modes between molecules, and between internal modes in each molecule may be defined such that it includes all the distribution functions of the preceding sections as special cases. At the step of the particles' collision with the wall and their reflection (boundary conditions), the five conditions (i.e. periodic, specular, diffusion, Maxwell, and Cercignani-Lampis-Lord) can be used. In fact, at this step, the particles collide with the wall, and then, based on the boundary conditions, the new values of their velocity and positions are set. In the periodic boundary condition, by changing the location of the particles, their location is set to the opposite side of the wall. In the specular boundary condition, the molecular velocity component normal to the surface is reversed, while the velocity components parallel to the surface remain unaffected. In the Diffuse boundary condition, the velocity of each molecule after reflection is independent of its velocity before reflection. However, the velocities of the reflected molecules as a whole are distributed in accordance with the half-range Maxwellian equilibrium for the molecules that are directed away from the surface. The diffuse reflection model is a suitable model for engineering problems and has a good accuracy. In the Maxwell boundary condition, two types of specular and diffuse interactions are considered together so that the specular interaction is reflected with an angle equal to the angle of impact and the interaction of the diffuse with a random angle. Given that the probability of a collision for a pair of molecules is proportional to the product of the cross-section and the relative velocity in the Maxwell's collision model, the collision probability for a particular molecule is independent of velocity. Also, in this model, the viscosity coefficient is linearly related to temperature, which is unrealistic for real gases. In fact, in this model, the collision probability for all molecules is the same. The Cercignani-Lampis-Lord (CLL) boundary condition model, as shown in Fig. 2, is defined based on the coefficients σ_n and σ_t, which represent the accumulation coefficients for the kinetic energy related with the normal and tangential components of the velocity. The model assumes that there is no coupling between the normal and tangential components of the velocity during the reflection process. Set v_r to be the normal component of the molecular velocity normalized to the most probable molecular speed at the surface temperature, and v_θ and v_z to be the similarly normalized tangential components. Furthermore, the deflection angle is always a function of the incident particle angle [2, 17].

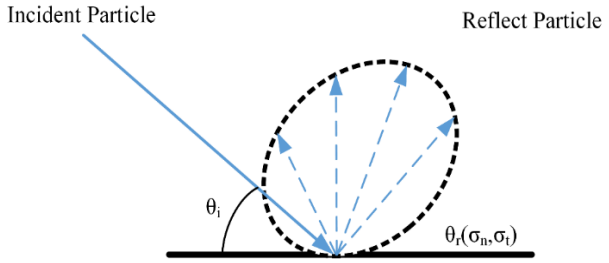

Fig. 2. Incident and reflected particle scheme in the Cercignani-Lampis-Lord model

In geometries with repetitive and symmetric physics, the boundary condition of the periodic can be used instead of the boundary condition of the wall type.

This boundary condition is applied to reduce the computational volume so that when a particle passes through one side of the unit cell of a periodic boundary, it re-appears on the opposite side with the same velocity. The large systems approximated by PBCs consist of an infinite number of unit cells. Consequently, instead of the whole geometry modeling, it is enough to model the repeating element. Fig. 3 illustrates part of a circle sector in which two boundary conditions, PB1 and PB2, have been used.

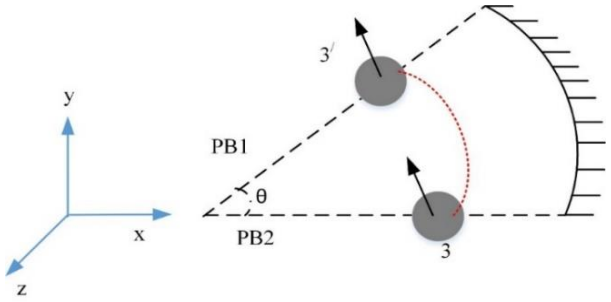

Fig. 3. A schematic of a periodic boundary condition in a rotational transform

Calculation of the position in a rotational transform

The center of a particle (e. g. $3^{/}$ in $z_3'\ y_3'\ x_3'$) from the periodic boundary condition of 1 to the periodic boundary condition of 2 can be moved using the following equations:

$$x = x'\cos\alpha + y'\sin\alpha$$
$$y = -x'\sin\alpha + y'\cos\alpha$$
$$z = z' \qquad (1)$$

where, α is the rotation angle, α = -θ defines the rotation in the clockwise direction, α = θ defines the

counterclockwise rotation, and θ is the sector angle of the model.

Calculation of the velocity in a rotational transform

When the particle is in its new position, its dynamic characteristics, which may affect the subsequent time step calculations (especially speed), should also be transformed. The velocity of a particle will be kept constant if its value is returned at a rotation angle of α according to the following relations:

$$v_x = v_x' \cos\alpha + v_y' \sin\alpha$$
$$v_y = -v_x' \sin\alpha + v_y' \cos\alpha \; v_z = v_z' \quad (2)$$

where, v_x،v_y and v_z are the velocities of the particles in the three directions, x, y and z, respectively.

WADSIM_1 Software

The dsmcFoam solver is one of OpenFOAM's solvers developed under OpenFOAM Version 1.5 by Macpherson and Scanlon at the University of Strathclyde. In spite of its high abilities, it has weaknesses for modeling of the gas inside the rotating cylinder. The WADSIM_1 software is developed to cover a wider range of issues. Table 1 compares the WADSIM_1 software and the dsmcFoam solver. The steps arrangement of the WADSIM_1 software algorithm is similar to the dsmcFoam solver. This implies that it also includes the steps of movement, indexing, collision, reflection from the wall and sampling of the results.

Table 2 shows the types of models of particles collision with each other and the particles collision with the wall used in WADSIM_1 software. In WADSIM_1, the NTC technique is used to calculate the maximum number of collisions in a cell. In the following sections, it will be briefly outlined how to apply Adaptive Mesh Refinement, gradient boundary conditions, and to use the appropriate boundary condition for creating an internal flow in the WADSIM_1.

Applying Adaptive Mesh Refinement (AMR) for WADSIM_1. An intensive change occurs in the radial direction due to the effect of centrifugal force inside a rotating rotor. The criteria for a good DSMC calculation are that, at every location in the flow, the time step should be smaller than the mean collision time and the cell size should be smaller than the mean free path. It is impossible to meet these conditions in the flows involving large changes in the flow properties unless the time step varies across the flow field, and the cell size must also be adapted to the local flow density. Therefore, the cell used in its geometry simulation should be transformed into a changeable cell over the λ density variations.

Table 1. Comparison of dsmcFoam and WADSIM_1 capabilities

Feature	dsmcFoam	WADSIM-1
Steady / transient solutions	✓	✓
Arbitrary 2D/3D geometries	✓	✓
Arbitrary number of gas species	✓	✓
Rotational energy	✓	✓
Unlimited parallel processing capability	✓	✓
Robust open source solver and utility executables	✓	✓
Periodic boundary condition	✓	✓
Possibility to solve issues with high wall speed	✓	✓
Suitable for the internal flows with strong gradient of variables the characteristic length	×	✓
Suitable for external flow	✓	✓
Gradient boundary conditions	×	✓
Adaptive Mesh Refinement	×	✓

Table 2. WADSIM_1 capability in the models of particle- particle and particle-wall collisions

Interaction Models	WADSIM _1	Reflection Models	WADSIM _1
HS	✓	Periodic	✓
VHS	✓	Diffusion	✓
VSS	×	Specular	✓
GHS	×	Cercignani -Lampis- Lord	✓
LSVHS	✓	Maxwell	✓

In fact, in an AMR, the mean free path in each cell is calculated and compared with the largest cell size, Δx_{max}. The ratio $\lambda/\Delta x_{max}$ should be greater than

one; then, the cell size value is smaller than the mean free path [8,18]. The correction of AMR in CFD has been widely used since about 30 years ago. It is practically used to regulate cells in the areas with a high gradient such as shock waves. These areas with a high flow gradient in CFD could have the same concept as a strong difference in the mean free path of DSMC. An AMR for the WADSIM_1 open source solver has been used to provide more accurate results in this research, especially in the areas where changes in the mean free path exist. One of the main advantages of OpenFOAM is its ability to modulation. AMR libraries are available in some continuous flow regime solvers such as multiphase solver (interFoam) that can correct the cell at the connecting point of two fluids and also the rhoCentralDyMFoam solver for compressible gas flows [8]. These solvers use a library called dynamicFvMesh to adapt the cell. The dsmcFoam solver uses the fvMesh cell library, in which the cell does not change over time. In this paper, dsmcFoam connects to a dynamicFvMesh library so that cells could be corrected dynamically and adaptively with the simulation time forward. The steps required to create adaptive cells are mentioned in the following sections. The first step in connecting the library is to create a constructor for the DSMC code with the dynamicFvMesh library instead of fvMesh. The users are supposed to go to the following address at first:

OpenFoam2.1.x/src/lagrangian/dsmc/clouds/
Templates/dsmcCloud

and then find the following commands:

```
Foam::dsmcCloud::dsmcCloud
(
Time   & t,
Const    word&   cloudName,
Const    fvMesh& mesh,
bool     readFields
)
```

and replace them with the following commands:

```
Foam::dsmcCloud::dsmcCloud
(
Time&  t,
Const      word&   cloudName,
Const      dynamicFvMesh& mesh,
bool       readFields
)
```

At the beginning, it should call the proper header file for the dynamicFvMesh library. This is done in three files including dsmcCloud.C, dsmcCloud.H, and dsmcCloudl.C. Then, the dynamicFvMesh folder in the Src file should be inserted at the following directory:

OpenFoam2.1.x/src/lagrangian/dsmc

Next, the user can go to the above-mentioned directory and enter “wclean” followed by “wmake”. If the command “is to update” came up at the end of the task, it could be concluded that the applied changes are correct. Afterwards, the following directory should be entered:

OpenFoam2.1.x/applications/solvers/
discreteMethods/dsmc/dsmcFoam

And then, the following changes to the dsmcFoam solver should be applied:

```
# include  “fvCFD.H”
# include  “dynamicFvMesh.H”
# include  “dsmcCloud.H”
Int  main (int  arc,char   *argv[])
{
# include  “setRootcaseD.H”
# include  “createTime.H”
# include  “createDynamicFvMesh.H”
While   (runtime.loop())
{
Scalar
timeBeforeMeshUpdate=runtime.elapsedCPUTi
me();
{
Mesh.update();
}
If (mesh.changing())
{
Info<<”Execution time for mesh.update()=”
<< runtime.elapsedCPUTime()-
timeBeforeMeshUpdate
<< “s”  <<endl;
}
```

Afterwards, "wclean" and "wmake" should be entered in the terminal, and finally, the user should see the message “is to update”. Now the user can use a dynamic cell in dsmcFoam. The same process could be performed to obtain a variable time step which has not yet been implemented in the dsmcFoam solver.

Creating the internal flow. The definition of geometry is the first step in simulating with the OpenFoam. Given that most open-source softwares define geometry in three dimensions, OpenFOAM is no exception to this. The geometry in this simulation is a wedge from a cylinder with a 5-degree angle, in which one cyclic patch is linked to another through a neighbor Patch keyword in the boundary file.

Due to the symmetry in the geometry, calculations could be made only for the desired wedge greatly reducing the volume of computations. The simulated geometry is shown in Fig. 4.

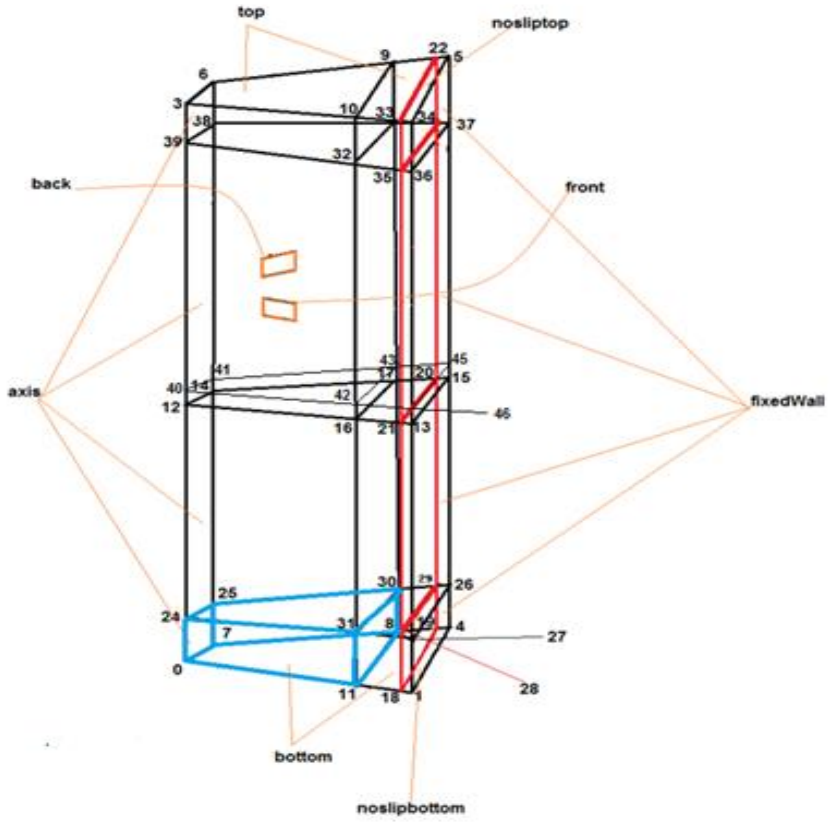

Fig. 4. The simulated geometry and its elements and boundaries

To create an internal flow in the WIDSIM_1 software for rotating cylinder simulation in the total reflux condition, the "Inflow Boundary Model" type should be selected in the "dsmc Properties" folder as "none" meaning that there is no free entrance and exit or free flow in the simulation. In other words, flow is confirmed in the simulation geometry.

Furthermore, in the geometry definition, the type of all boundary conditions must be set to the type "wall". For an internal flow of a geometry with a rotating boundary condition, the following code should be used in the folder "boundary U":

```
rotorWall
      {
Type        rotatingWallVelocity;
axis        (0 0 1);
origin      (0 0 0);
omega       ω;
```

Creating gradient boundary conditions. The GroovyBC library could be used to create gradient boundary conditions in OpenFoam. It is noteworthy that these boundary conditions are not applicable to the dsmcFoam solver because the library is not defined for this solver. Therefore, the user should use the proper coding to create such gradient on the wall.

To create a linear gradient on the wall (points 1-4-5-34), the user can apply the following code in the boundaryT folder:

```
rotorWall
      {
Type        fixedValue;
Value       uniform List<scalar>
Number  Cell
(
Temperature Gradient
)
}
```

In the above command, the "Temperature Gradient" is equivalent to the temperature corresponding to the cells along the rotor length.

Calculating the initial parameters required by WADSIM_1

The following two conditions should be met in a proper simulation with the DSMC method [19]:

- ✓ The time step Δt must be smaller than the mean collision time (τ).
- ✓ The size of each cell (Δx) should be smaller than the mean free path (λ).

The method to calculate the number of cells, the number of simulation particles, the scaling factor

(number of real molecules represented by a single DSMC molecule) and the time step for starting the simulation with the WADSIM_1 solver is described in the following sections.

If the Knudsen number or the pressure of a problem was known, the value of the number density could be calculated as follows:

$$Kn = \frac{\lambda}{L}$$
$$\lambda = \frac{k_B T}{\sqrt{2}\pi d^2 p}$$
$$p = nk_B T \quad (3)$$

where, p is the pressure, λ is the average distance between two collisions of particles with each other, L is the characteristic length of the system, n is the number density of the particles (the number of particles per volume unit), and d is the diameter of the molecule. To determine the local Knudsen number in a field with a strong gradient of variables, the characteristic length should be determined as follows [18]:

$$Kn_{GL} = \max(Kn_{GL-\rho}, Kn_{GL-T}, Kn_{GL-|v|}) \quad (4)$$

where,

$$Kn_{GL-Q} = \frac{\lambda}{|Q_{Local}|}|\nabla Q| \quad (5)$$

In Eq. (5), Q represents fluid density, velocity or temperature. By calculating the mean free path, the length of each cell to change the intensity of the density could be calculated as below:

$$\Delta x, \Delta y, \Delta z \simeq \frac{\lambda}{3-5} \quad (6)$$

Figure 5 shows the simulated geometry and meshing for a rotating cylinder.

By calculating the number density of the simulation environment, the actual number of molecules can be calculated as follows:

$$n = \frac{N}{V} \rightarrow \quad N_{Real} = nV \quad (7)$$

The number of cells in each direction is determined by the following equations:

$$N_x = \frac{L_x}{\Delta x}, N_y = \frac{L_y}{\Delta y}, N_z = \frac{L_z}{\Delta z} \quad (8)$$

As a result, the total number of cells required for simulation is obtained as follows:

$$N = N_x \times N_y \times N_z \quad (9)$$

If the number of simulated particles in each cell was equal to NPPC, then the number of simulated particles N_s will be:

$$N_S = N \times NPPC \quad (10)$$

Now, the number of real molecules represented by a single DSMC molecule in WADSIM_1 can be calculated as follows:

$$F_N = \frac{N_{Real}}{N_S} \quad (11)$$

The mean collision time and time step can be obtained as follows:

$$\tau = \frac{\pi\mu}{4nk_B T} \quad (12)$$

At the end, the time step could be calculated by calculating the mean collision time. In any time step, to prevent losing any collision that occurs in the mean collision time, the time step is chosen to be smaller than the time between collisions:

$$\Delta t = \frac{\tau}{3-5} \quad (13)$$

Note that the viscosity coefficient has been given as an input parameter by the user, although it is not in the list of inputs required by the gas properties. In fact, the gas viscosity coefficient is dependent on the gas molecular diameter parameter. The diameter, given by the user as input in this solver, is indeed the reference diameter which must be calculated from the reference temperature and reference viscosity coefficient. The reference diameter and then the effective diameter of each species can be calculated using Eqs. (14) and (15), respectively [2]:

$$d_{ref} = \left(\frac{5(\alpha+1)(\alpha+2)\left(mkT_{ref}/\pi\right)^{1/2}}{4\alpha(5-2\omega)(7-2\omega)\mu_{ref}}\right)^{1/2} \quad (14)$$

$$d_{eff} = d_{pq} = \left(d_{ref}\right)\left[\frac{\left\{2k(T_{ref})_{pq}/(m_r c_r^2)\right\}^{\omega-1/2}}{\Gamma\left(\frac{5}{2}-\omega_{pq}\right)}\right]^{1/2} \quad (15)$$

As seen in Eq. (15), if the HS model is used to collide two particles together (ω = 0.5), it is observed that by inserting the value ω = 0.5 in Eq. (15), the nominator and denominator of the fraction would be equal to one ($\Gamma(n) = (n-1)!$). This indicates that for the HS model, the effective diameter and reference are equal, in other words, the diameter is independent of the relative velocity in the HS model.

When describing the VHS and VSS models, the diameter of the particles varies with inversing the relative velocity between the two particles. This expression is well seen in Eq. (15) so that the effective diameter has an inverse relation with the relative velocity.

The overall structure of WADSIM_1 software is presented in Fig. 6. The software has three main folders: applications, utilities, and dsmc. The particle' collision and reflection are included in the "submodel" folder.

RESULTS

DSMC code validation for comparison with WADSIM_1 software

The DSMC code is written in FORTRAN programming language in 2-D to validate the results obtained from the WADSIM_1 software, and all the boundary conditions used in the WADSIM_1 software are applied to the DSMC code. The DSMC code for a solid body rotation cylinder with a speed of 500 meters per second was validated with a one-dimensional code written by Bird [3]. The combination of the same percentages of helium, argon, and xenon gases inside the rotating cylinder is simulated by the DSMC method, and at the end, the radial changes of each gas component are shown in Fig. 7. As can be seen, the results obtained from both codes agree with each other.

Simulation of the rotating cylinder in the total reflux mode

In this paper, uranium hexafluoride (as a heavy gas) and air (as a light gas) were separately simulated based on the same input conditions. The purpose was to investigate the effect of the distribution of particles within the rotor based on the molecular mass of the gas. The number of iterations to reach the final results is about 50,000,000, which was executed in a cluster in a parallel mode (MPI) with 31 threads. The physical properties of the studied gases and the required inputs for the open source WADSIM_1 software and DSMC code are presented in Tables 3 and 4.

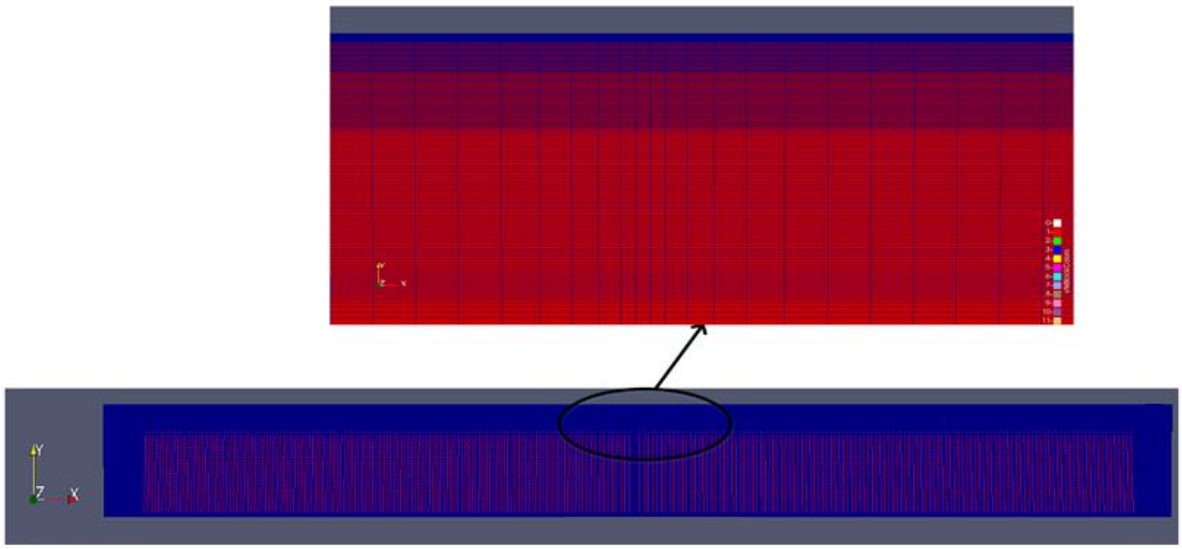

Fig. 5. Example of geometry and meshing of a simulated rotating cylinder.

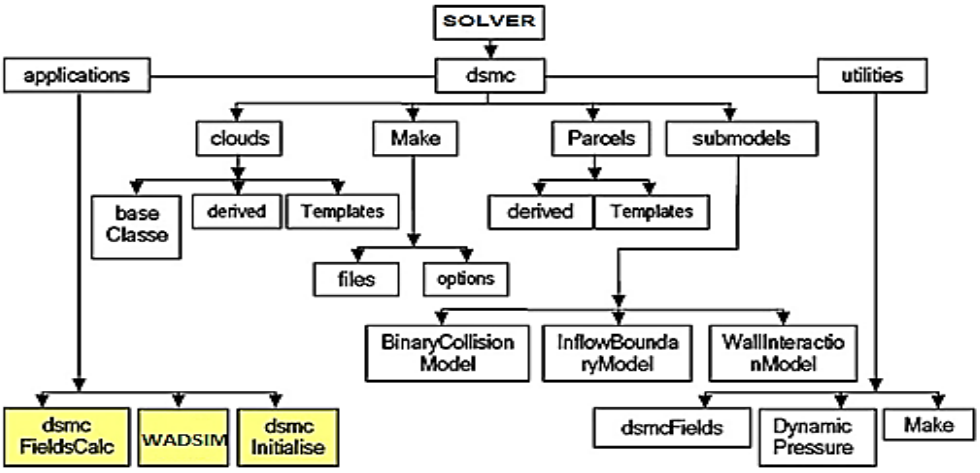

Fig. 6. Directory structure of WADSIM_1

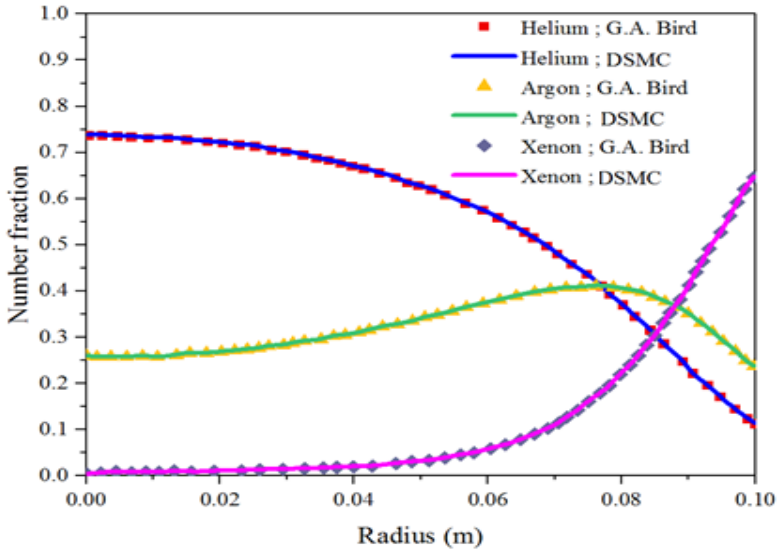

Fig. 7. Comparison of the number density profiles obtained from the two-dimensional DSMC code and the one-dimensional code of Bird [3].

Table 3. The data required to implement the VHS model

Gas	Diameter at 273 K ($\times 10^{-10}$ m)	Molecular Mass ($\times 10^{-27}$ kg)
UF_6	6.0	$^{238}UF_6$ 584.51011 $^{235}UF_6$ 579.5284
Air	N_2 4.17 O_2 4.07	N_2 46.5 O_2 53.12

Table 4. Characteristics of the hypothetical gas centrifuge

Number density of gases	Azimuthal velocity (m/s)	Number cells
7.729×10^{21}	500	500×1000
Interaction model	Time step	Wall thermal gradient
VHS	1×10^{-7}	20
Gas-Surface interactions	End caps temperature (K)	Dimension of the rotor (m)
Diffuse reflection	300-320	0.1×0.5

The pressure contour resulting from the simulation of air and uranium hexafluoride is shown in Fig. 8.

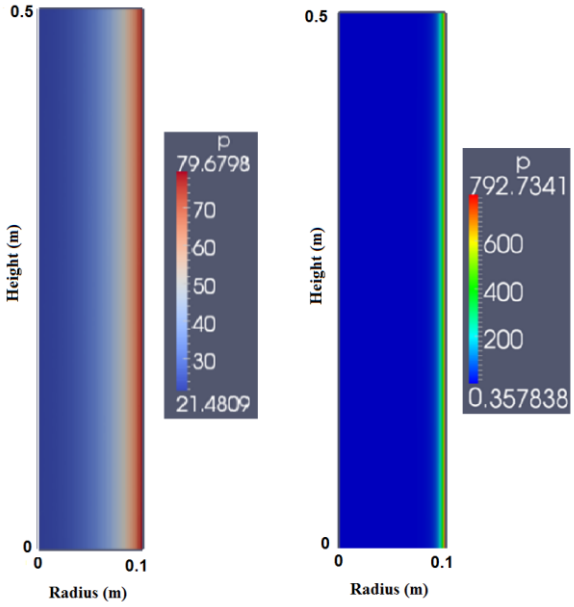

Fig. 8. Contours pressure for air and UF_6

As seen, for the light gas, the pressure at the rotor axis is much higher than that for the heavy gas, and on the wall, it is lower than that for the heavy gas, which is due to the low molecular mass of the light gases. This shows that even with the same amount of inputs and the same number density, for the gases with different molecular masses, different pressure contours could be obtained. The pressure changes inside the rotor for light (air) and heavy (uranium hexafluoride) gases are shown in Fig. 9.

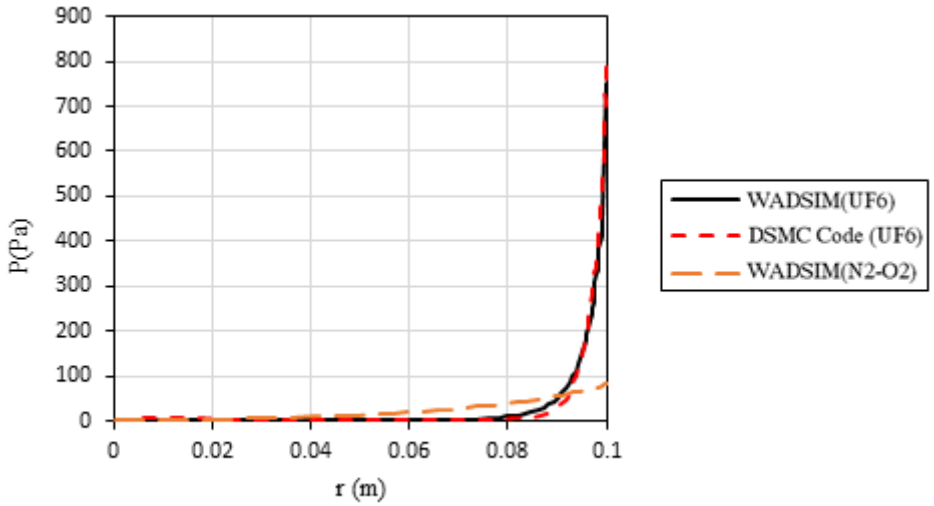

Fig. 9. The radial pressure distribution for air and UF_6 using WADSIM_1 software and DSMC code.

One of the most important contours is the radial velocity. As shown in Fig. 10, the particles take the radial velocity alongside the top and bottom caps due to the collision of the particles with the wall. Thus, the radial velocity in these regions is not equal to zero. It is to be noted that if air is used in the simulation, the maximum radial velocity between the two caps will be lower than when using uranium hexafluoride, because the pressure of light gases is higher than that of heavy gases in the center of the rotor. Hence, the collided particles with the top and bottom caps take the velocity proportional to the radius. In addition, when they want to rebounce from the wall, they collide with the particles on their faces and, in turn, their radial velocity will be reduced; however, in case of using a heavy gas, due to the sharp decrease in pressure within the center of the rotor, the particles would take azimuthal velocity proportional to the radius after colliding with the two caps. As a result, their velocity would be less slowed down due to the very low presence of particles in front of them at the time of return and a low number of molecular collisions between them. The radial velocity drops drastically due to the collision with the background gas. The gas in the total reflux mode is sufficiently compressed to the wall; thus, it does not allow the movement unless in the form of diffusion. Azimuthal velocity graphs are also very important in a machine. The linear behavior of the rotational velocity graph is completely pressure-dependent. As shown in Fig. 11, when uranium hexafluoride is used in the simulation, the azimuthal velocity changes linearly because of the high pressure near the wall; however, with the decrease of pressure in the radial direction, the azimuthal velocity of particles also decreases nonlinearly.

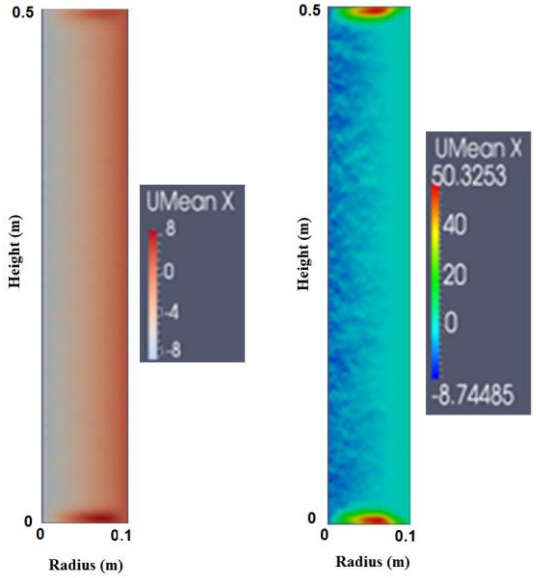

Fig. 10. Radial velocity contour for air and UF_6

Since the pressure variation is roughly uniform along the rotor's radius, if air is used, the change in the azimuthal velocity of the particles also occurs linearly. The steady state of the flow is similar to a "solid body" rotation with azimuthal velocity proportional to the radius.

To convert radial flow to axial one and to increase the gas separation within the rotor, different types of drives can be used in a rotating cylinder. Each driving mechanism drives axial velocity in the rotor. It is possible to use thermal drives of the rotor wall and the caps to create a secondary flow inside the rotor to model and simulate the gas flow in the rotor *via* total reflux mode. Due to the presence of drives, an axial velocity is generated in the entire rotor. The dominant mass lies in the Stwartsons layer (near the rotor wall) due to the centrifugal force effect.

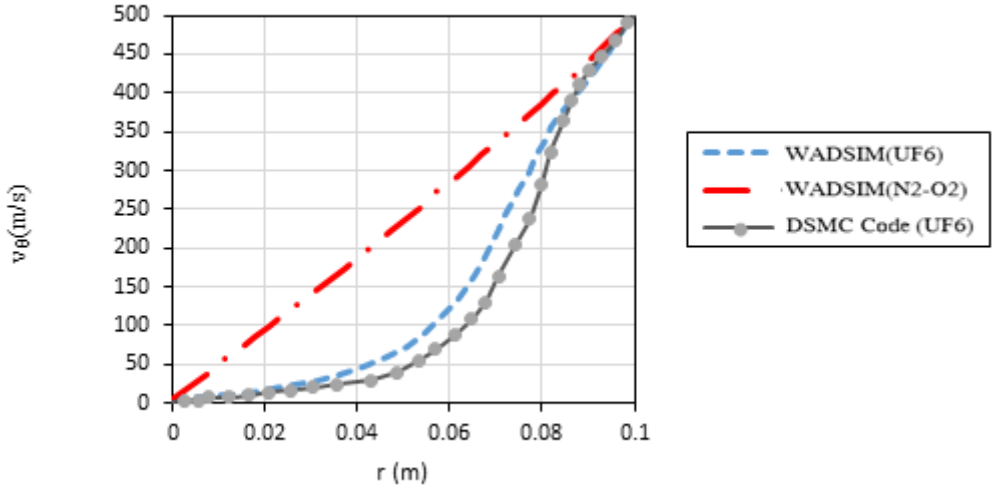

Fig. 11. Azimuthal velocity of air and UF_6 using WADSIM_1 software and DSMC code

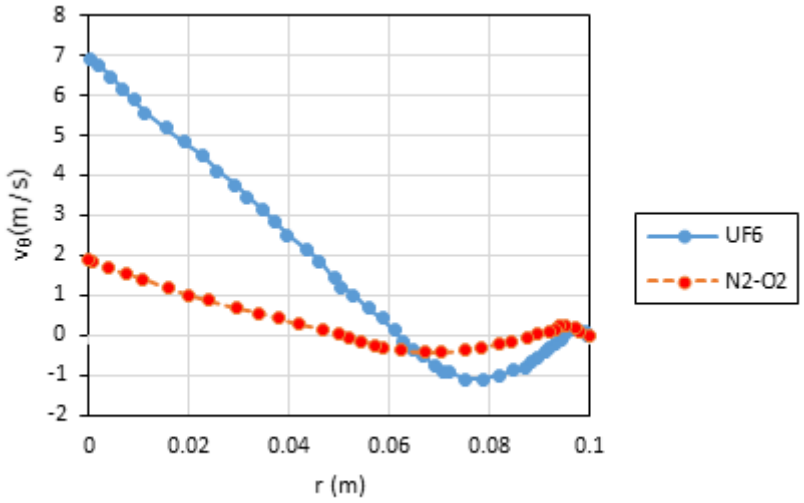

Fig. 12. Axial velocities of air and UF_6

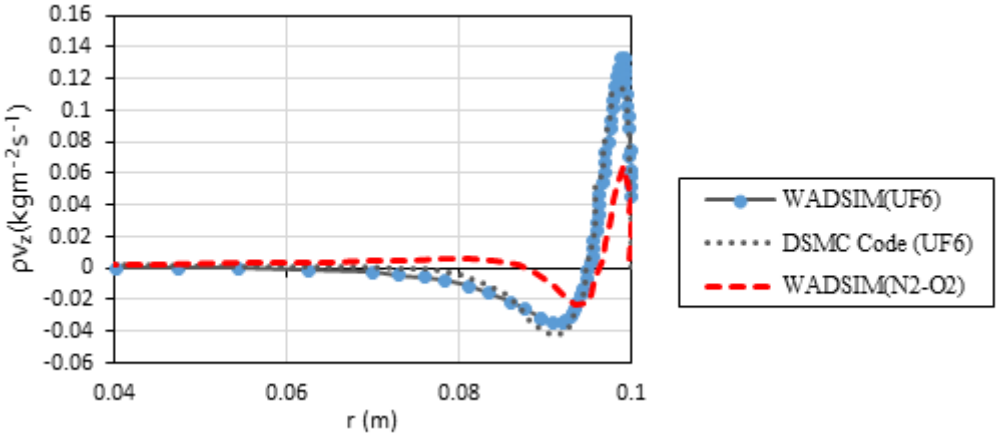

Fig. 13. Axial mass fluxes of air and UF_6 using the WADSIM_1 software and DSMC code

It is worth noting that v_z is created even in the molecular domain of the rotor and has a high value. The axial mass flux (ρv_z) could be calculated by evaluating the axial velocity inside the rotor. Indeed, due to the secondary flow, it is expected that the resulting axial mass flux has a positive region due to

the upstream flow and a negative region due to the downward flow. The axial velocity diagrams for two different gases are shown in Fig. 12. The axial mass flux diagram in the center of the rotor for uranium hexafluoride gas is plotted in Fig. 13; as shown, it is similar to the results of the DSMC code.

Simulation of the helix groove using the WADSIM_1 software

To demonstrate the ability of the WADSIM_1 software, this section simulates the gas flow within a helix groove as a complex geometry. The molecular pump is located in the upper part of a centrifuge in the space between the rotor and the casing, with the main task of maintaining a vacuum in this region. This pump is made up of a number of grooves, and the wall opposite each groove has a high rotating speed so that the gas molecules collide with this rotating wall and lead to the groove output.

In this simulation, a groove and a periodic boundary condition for it have been used to repeat its geometry to complete the molecular pump's geometry. The pressure gradient with exponential growth will be created along the length of the groove because of the presence of a rotating wall with a high rotation speed. The complex geometry of the mentioned groove was simulated using WADSIM_1 software (see Fig. 14).

The geometrical and operational characteristics of the studied molecular pump, as well as the values of the compression ratio obtained from the simulation and experimental test are given in Table 5.

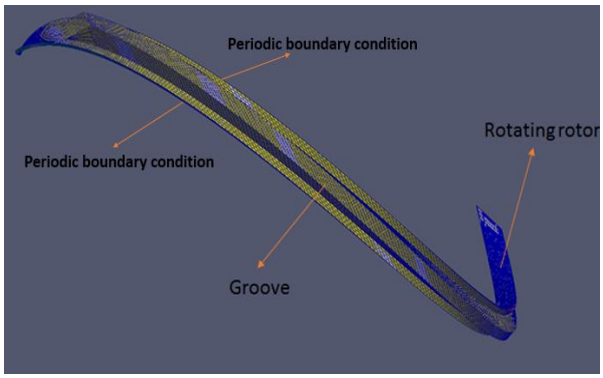

Fig. 14. Geometry and mesh of helix groove

The contour of pressure variations along the groove length is shown in Fig. 15.

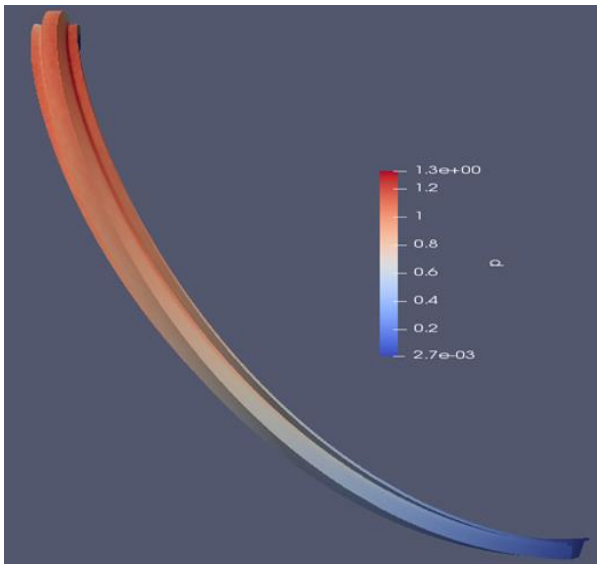

Fig. 15. The contour of pressure variations (Pa) along the groove length using WADSIM_1 software

Table 5. Compression ratio of molecular pump obtained using WADSIM_1 software and experimental test.

Gas	Top width of groove (mm)	Bottom width of groove (mm)	Clearance (mm)	Rotor velocity (m/s)	Length of pump (mm)	Shape of groove
Air	13.8	6.4	1.2	560	170	trapezoidal
Compression ratio of the WADSIM_1 software				Compression ratio of experimental test		
481				470		

CONCLUSION

Since molecular methods have the capability of modeling all flow regimes (molecular and continuous region) and because of the strong pressure stratification, continuous-fluid equations are not valid in the whole cylinder, with or without linearization of the model. In the present work, the molecular-based dsmcFoam solver for investigating the total gas flow in the rotor was chosen from the OpenFoam software. Then it was modified to simulate the gas flow inside a rotating cylinder and introduced as WADSIM_1 software. The capabilities of the software include the possibility of investigating the gas flow inside a rotating cylinder with high-speed rotation, applying a thermal gradient boundary condition for the rotor wall, and

employing the Adaptive Mesh Refinement (AMR) technique due to the strong gradient of flow in the rotor's radial direction.

The simulation results indicated the significant effect of the molecular mass of a gas on the formation of pressure, velocity, and axial mass flux profiles within the rotor after 5 seconds of real time. By changing the gas type, the pressure on the rotor axis was changed significantly so that when a light gas was used in a rotating cylinder, the amount of pressure in the rotor's axis was higher than when a heavy gas was used. As the pressure on the rotor's axis increased, the pressure in the space above the molecular pump increased; as a result, the molecular pump's performance was affected.

Furthermore, comparing the results of DSMC code with the results obtained from the WADSIM_1 software showed that besides having the right precision, the calculation speed was multiplied due to the use of WADSIM_1 software from the MPI parallelization tools with unlimited cores. For example, using a 31-thread cluster, the computing time was ten times lower than with single-core DSMC implementation. At the end, it is concluded that this software, in addition to having the right precision, has a very high speed for simulating the gas flow for all regions (molecular and continuous regimes) within the rotor. In the future works, its development for simulation of the gas inside the rotor under actual conditions is proposed by applying all drives (feed, scoop and baffle drives).

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