

A hybrid CFD-DSMC Method for Numerical Simulation of the Rotating Cylinder Flows

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ABSTRACT

In this work, we attempted to simulate UF₆ gas flow in the rarefied and continuum areas of the rotating cylinder. We used CFD, DSMC, and hybrid one-way and two-way CFD-DSMC methods. The results were verified by the DSMC method. Three goals were achieved using the two-way method. The first purpose was to simulate the flow in the rarefied area with the DSMC method, which was more valid than the CFD method. The second goal was to reduce the computational time of the continuum area simulation using the CFD method. The third goal was to investigate the effect of the rarefied solution on the continuum solution. Comparing the results with the DSMC method, it was found that the two-way CFD-DSMC method causes a difference of only 2% for the separation power, while the computational cost is reduced by 60%.

Keywords: Rarefied Area; Rotating Cylinder; Separation Power; CFD-DSMC; Coupled Method

1. Introductions

Continuum and rarefied regimes occur in many problems, e.g., cylinder, cavity, and rotating cylinder [1, 2, 3, 4]. In a rotating cylinder, the gas accumulates near the wall due to the centrifugal force. Thus, the gas flow near the wall is a continuum. At the same time, the central area of the rotating cylinder is rarefied (Fig. 1). If the Knudsen number is less than 0.05, the region is considered a continuum area

[5]. In this area, the Navier-Stokes equation is valid. The CFD method is utilized to solve these equations. In contrast, the Navier-Stokes equation is not valid in the rarefied zone. Thus, the DSMC technique simulates the gas flow in the rarefied area [6, 7, 8]. In other words, the CFD-DSMC method is the best technique to simulate the gas flow in rarefied and continuum problems.

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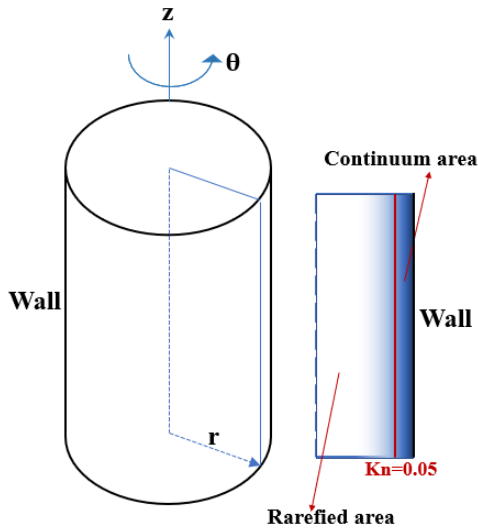


Fig. 1. Schematic of the Rarefied and continuum domain in a rotating cylinder.

In the last years, The CFD-DSMC method has been applied by researchers in several studies [11]. Wang and Boyd [9] investigated a coupled CFD-DSMC method to study non-equilibrium flows in 2D/axisymmetric states. Furthermore, Burt and Boyd [10] employed a CFD-DSMC scheme to simulate N_2 flow over a cylinder with Mach 6.0. The strongly hybrid two-way information transfer was applied in their study.

Many researchers have focused on simulating isotope separation in the rotating cylinder in the last years [12, 13, 14]. Roblin and Doneddu [15] studied the gas flow in the rarefied area of a rotating cylinder using the DSMC method. Jiang and Zeng [16] simulated a 3-D model of a feed jet using the CFD code in the rotating cylinder. It was shown that the numerical simulation results of a CFD code have errors in the rarefied area (near the axis of rotation). They suggested the DSMC simulation is a practical technique to solve this problem. Recently, Ghazanfari et al. [17] analyzed a gas flow in the rotating cylinder using an ICDB solver (Implicit Coupled Density-Based) in the OpenFOAM framework. Then, using a one-way CFD-DSMC method, the rarefied and continuum

area of the rotating cylinder was simulated separately with DSMC and CFD, respectively [4]. The results showed that the separation power of 9.5% and the separation factor of 6.5% differed.

In the present study, a hybrid two-way CFD-DSMC method is employed to analyze the UF_6 gas flow inside the rotating cylinder for the first time. This technique considers the effect of both rarefied and continuum areas on each other. In other words, after solving the rarefied area using the DSMC technique, the obtained results are used as a boundary condition for the CFD solution. Implicit Coupled Density-Based and dsmcFoam solvers in the OpenFOAM framework were employed for CFD and DSMC solutions, respectively.

2. Model Description

2.1. Fundamental Equations in the Continuum Area

The gas flow of UF_6 in the rotating cylinder is governed by mass, momentum, and energy conservation laws [18, 19]:

$$\frac{1}{r} \frac{\partial}{\partial r} (ru\rho) + \frac{\partial}{\partial z} (w\rho) = 0 \quad (1)$$

$$(2)$$

$$\begin{aligned} \rho \left(u \frac{\partial u}{\partial r} + w \frac{\partial u}{\partial z} - \frac{v^2}{r} \right) \\ = -\frac{\partial p}{\partial r} + \frac{\partial}{\partial r} \left[\mu \left(-\frac{2}{3} \nabla \cdot \bar{v} + 2 \frac{\partial u}{\partial r} \right) \right] \\ + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial r} \right) \right] + \frac{2\mu}{r} \left(\frac{\partial u}{\partial r} - \frac{u}{r} \right) \end{aligned} \quad (3)$$

$$\begin{aligned} \rho \left(u \frac{\partial v}{\partial r} + w \frac{\partial v}{\partial z} + \frac{uv}{r} \right) \\ = \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial v}{\partial z} \right) \right] + \frac{\partial}{\partial r} \left[\mu \left(\frac{\partial v}{\partial r} - \frac{v}{r} \right) \right] \\ + \frac{2\mu}{r} \left(\frac{\partial v}{\partial r} - \frac{v}{r} \right) \end{aligned} \quad (4)$$

$$\begin{aligned} \rho \left(u \frac{\partial w}{\partial r} + w \frac{\partial w}{\partial z} \right) = -\frac{\partial p}{\partial z} + \frac{\partial}{\partial z} \left[\mu \left(-\frac{2}{3} \nabla \cdot \bar{v} + 2 \frac{\partial w}{\partial z} \right) \right] \\ + \frac{\partial}{\partial r} \left[\mu \left(\frac{\partial w}{\partial r} + \frac{\partial w}{\partial z} \right) \right] + \frac{\mu}{r} \left[\frac{\partial u}{\partial z} + \frac{\partial w}{\partial r} \right] \end{aligned}$$

$$\begin{aligned}
 & \rho c_p \left(u \frac{\partial T}{\partial r} + w \frac{\partial T}{\partial z} \right) \\
 & = \frac{1}{r} \frac{\partial}{\partial r} \left(kr \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) \\
 & + \beta T \left[u \frac{\partial p}{\partial r} + w \frac{\partial p}{\partial z} \right] + \phi
 \end{aligned} \tag{5}$$

The state equation for an ideal gas is $p/\rho = \frac{R}{M}T$, M is the molar mass of the considered gas, R is the universal gas constant, and T is the temperature. Also, w , u , and v are the velocity in axial, radial, and azimuthal directions, respectively. p and ρ are the pressure and density, respectively.

To solve the hydrodynamic equations using the CFD technique, we use an Implicit Coupled Density-Based solver that has been employed by the present authors in the OpenFOAM framework [20]. OpenFOAM is an object-oriented C++ module for the solution of complex fluid flows [21]. Here, the residual of the energy equation is less than 10^{-7} , and residuals of the conservation of the mass and momentum equations are less than 10^{-6} . To calculate the separation performance, obtaining the concentration distribution for the uranium isotope in the rotating cylinder is necessary. For this purpose, the convection-diffusion equation of component A is employed as follows [22, 23]:

$$\begin{aligned}
 & \nabla \cdot [(-\rho D_{AB}) \nabla x_A] \\
 & + \frac{\Delta M}{R} \nabla \cdot \left[(-\rho D_{AB}) \left(\frac{x_A(1-x_A)}{\rho T} \nabla p \right) \right] \\
 & + \nabla \cdot [(-\rho D_{AB})(k_T \nabla \ln T)] + \nabla \cdot (\rho x_A \vec{V}) = M_{avg} S_A
 \end{aligned} \tag{6}$$

Where, R is the universal gas constant, x_A is the molar fraction of isotope A , the diffusion coefficient of isotope A in isotope B is D_{AB} , k_T is the thermal diffusion ratio, ΔM is (MB-MA), \vec{V} is the velocity vector, S_A is the source or sink term, and M_{ave} is the average molecular mass. This

study uses the Finite Volume Method (FVM) to solve the convection-diffusion equation.

2.2. Fundamental Equations in the Rarefied Area

DSMC is a random and particle-based technique that calculates and analyzes rarefied gas flows [24]. This is a relatively recently developed numerical model introduced in 1963 [25]. However, this technique has become one of the preferred methods for simulating non-equilibrium gas flows, which should consider the molecular nature of the gas [26].

Generally, the characteristics of dsmcFoam are entirely comparable with other well-known DSMC codes [27], such as MONACO [28] and Parallel Direct Simulation Monte Carlo (PDSC) [29].

2.3. Hybrid Procedure

In a hybrid procedure, one crucial question is determining the interface between two areas. The Gradient Length Local Knudsen number suggested by Wang and Boyd has been used in our study to illustrate the breakdown of the continuum hypothesis [9]. Transferring flow characteristics (temperature, pressure, and velocity) between these two areas is the second point. The CFD solution results, including velocity, temperature, and pressure, are used to compute the Gradient Length of Local Knudsen. The initial evaluation for specifying rarefied and continuum areas is $Kn=0.05$ [30].

The Gradient Length Local Knudsen is defined as follows [31]:

$$\begin{aligned}
 Kn_{GLL\phi} & = \frac{\lambda}{\phi} |\nabla \phi| \\
 & = \lambda \times \left[\max \left(\frac{|\nabla \rho|}{\rho}, \frac{|\nabla V|}{V}, \frac{|\nabla T|}{T} \right) \right], \lambda \\
 & = \frac{kT}{\sqrt{2\pi} D^2 p}
 \end{aligned} \tag{7}$$

Where the molecular mean free path is λ , the diameter of UF6 molecules is D , and k is Boltzmann's constant. In several works, the Gradient Length Local Knudsen number (has been employed to specify the interface location between rarefied and continuum areas [32, 33, 28, 9].

2.3.1. One-Way Hybrid Algorithm

In a one-way CFD-DSMC algorithm, only the results of the CFD technique are transported into the DSMC domain. In the one-way algorithm, hybrid simulation becomes more efficient and manageable while the results are sufficiently accurate. The application of one-way CFD-DSMC has been described to analyze the flow of high-altitude plumes [35]. In Fig. 2, the flowchart of the one-way hybrid algorithm is shown.

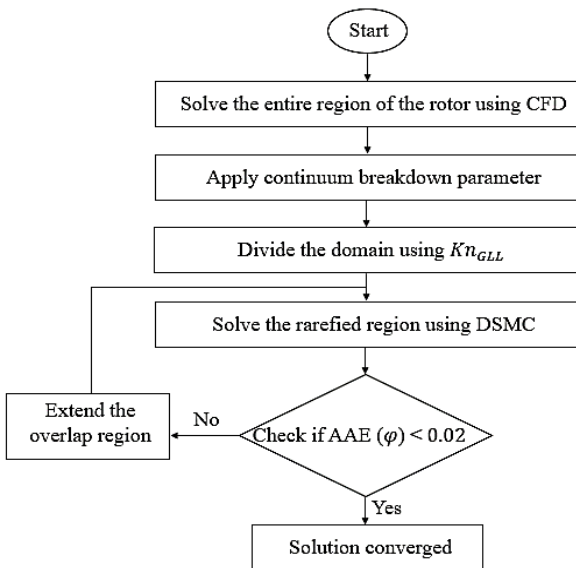


Fig. 2. Flowchart of the one-way hybrid [4].

This algorithm checks the convergence. criterion using AAE (ϕ) [21, 4].

(8)

$AAE(\phi)_{overlap\ outer\ boundary}$

$$= \left(\sum_{i=1}^{i=N_{cell}} \left| \frac{\phi_{CFD} - \phi_{DSMC}}{\phi_{DSMC}} \right| \right) < 0.02$$

2.3.2. Two-way hybrid algorithm

In a two-way hybrid algorithm, the obtained results from the CFD solution are employed as the boundary conditions for the DSMC solution. Next, the obtained results from the DSMC solution are used as the boundary conditions for the CFD solution [29]. To clarify, the effect of two rarefied and continuum areas on each other is considered. In Fig. 3, the flowchart of the two-way hybrid algorithm is shown. It consists of the following steps [29]:

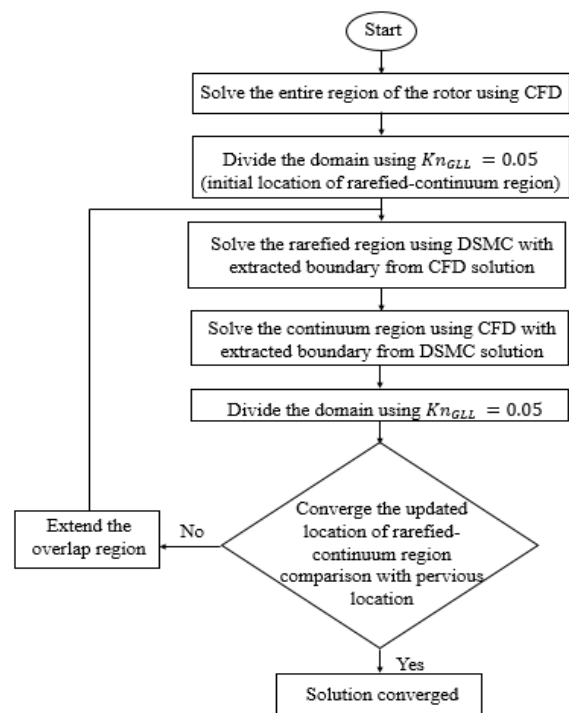


Fig. 3. Flowchart of the two-way hybrid [29].

Generally, less than four couplings are good enough to achieve a converged solution in two-way CFD-DSMC.

3. Modeling the Rotating Cylinder

The separation parameters are obtained from the calculated waste and product molar concentrations. The separation coefficients are presented as [17, 36]:

(9)

$$\alpha = \frac{\left(\frac{y_P}{1-y_P}\right)}{\left(\frac{x_W}{1-x_W}\right)}, \beta = \frac{\left(\frac{y_P}{1-y_P}\right)}{\left(\frac{z_F}{1-z_F}\right)}, \gamma = \frac{\left(\frac{z_F}{1-z_F}\right)}{\left(\frac{x_W}{1-x_W}\right)}$$

Where α is the overall separation factor, γ and β are tail and head separation factors, respectively. z_F , y_P , and x_W indicate the feed, product, and waste molar concentration, respectively. The cut coefficient is $\theta = P/F$ [37]. The separative power, δU , defined as the amount of useful work done by the rotating cylinder, is [38, 39]:

(10)

$$\begin{aligned} \delta U = & P(2y_P - 1) \ln \frac{y_P}{1-y_P} \\ & + W(2x_W - 1) \ln \frac{x_W}{1-x_W} \\ & - F(2z_F - 1) \ln \frac{z_F}{1-z_F} \end{aligned}$$

W , P , and F are the tailed, enriched, and feed flow rates in the separation unit, respectively.

Fig. 4 shows the rotating cylinder's schematic with the feed, baffle, and scoops. The finer mesh is used near the rotating cylinder wall due to the large gradient of the flow features (the smallest cell next to the wall is 1.0 μm). In the grid, the total number of cells is 255000. This cell number is adequate to have a grid independence study.

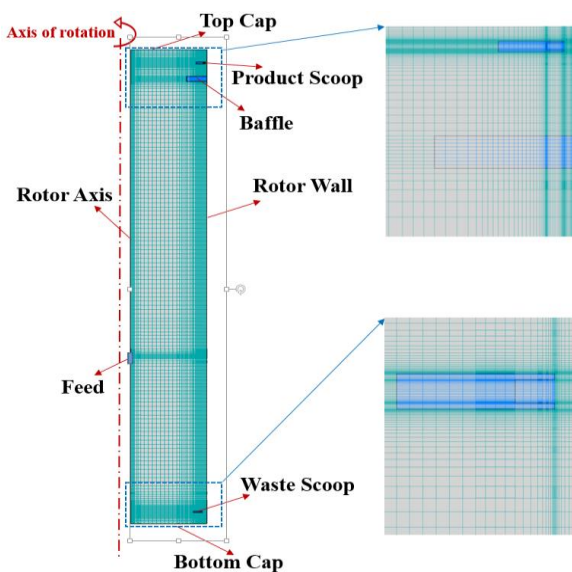


Fig. 4. The view of mesh in the fluid field of the rotating cylinder.

4. Results and Discussion

Here, the Knudsen number distribution is calculated to estimate the initial position of the boundary between the rarefied and continuum areas. This Knudsen number is obtained from the CFD solution in the total area of the rotating cylinder. Using the criterion $Kn=0.05$, the location of the interface between rarefied and continuum areas is in a radius of 0.0855 m. It should be noted that $AAE < 2\%$ is sufficient for the convergence criterion [4].

In the two-way algorithm, the radius of 0.0855 m is used as the interface between the continuum and rarefied areas. This radius is obtained using the results of pure CFD and Knudsen number. Four cell layers in the rarefied area in the overlapping area are employed to update the macroscopic flow characteristics from DSMC to CFD. Two cell layers in the overlapping area are employed in the continuum area to update the macroscopic flow characteristics from CFD to DSMC. The two-way procedure is repeated four times to get a converged solution. The final radius of 0.086 m is specified as the location of the interface between the continuum and rarefied areas.

Fig. 5 demonstrates the distributions of flow characteristics, including pressure, temperature, radial velocity, axial velocity, azimuthal velocity, and axial mass flux along the radial direction at $Z/H=0.5$. The pressure variation schemes on a logarithmic scale.

According to Fig. 5, the difference between the two-way method and the pure DSMC method is insignificant. Therefore, the two-way method has acceptable accuracy. Furthermore, it is observed that the results obtained from four methods in the continuum area (0.086) are consistent. In contrast, the CFD and one-way method results are different from the DSMC technique in the rarefied area.

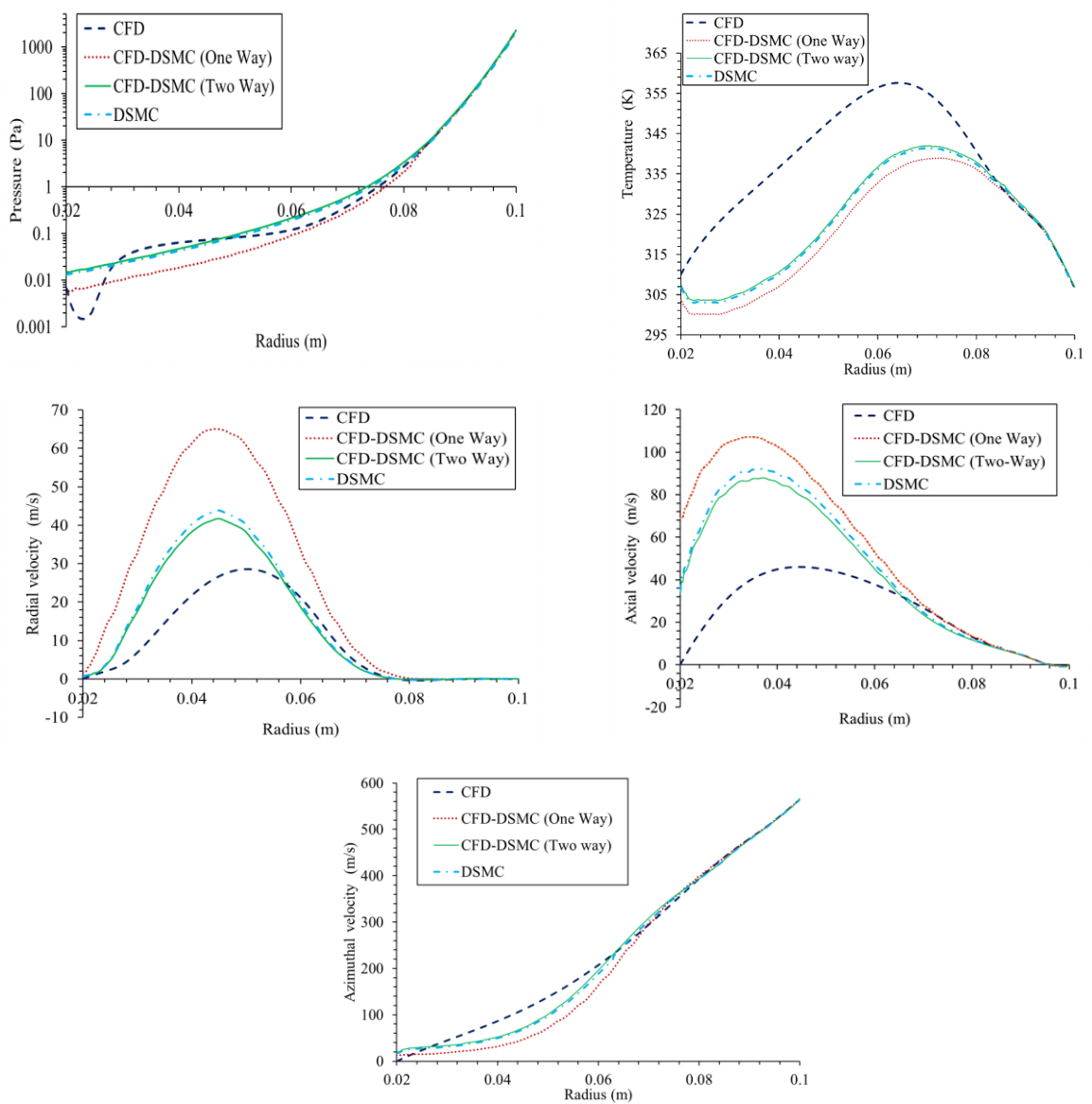


Fig. 5. The flow characteristics calculated by CFD [4], CFD-DSMC (one-way) [4], pure DSMC, and CFD-DSMC (two-way) methods.

Here, the concentration is calculated based on the flow hydrodynamic variables using the convective-diffusion equation's solution. Fig. In figure 6, the concentration of UF₆ (235) is calculated by the four techniques in r=0.096 m along the axial direction of the rotating cylinder. As can be seen, UF₆ (235) gas is enriched to about 0.0084 while depleted to about 0.0058.

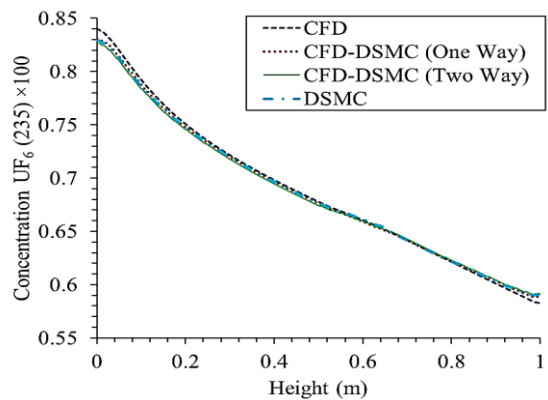


Fig. 6. The concentration of UF₆ (235) calculated by different methods.

Table 1. The separation performance of the rotating cylinder using different simulation schemes.

Case	Solution technique	Separation power (Kg (UF_6) SWU/year)	Separation factor	Enrichment factor	Stripping factor
1	CFD [4]	8.750	1.417	1.196	1.185
2	CFD-DSMC (One-way) [4]	8.001	1.341	1.161	1.155
3	CFD-DSMC (Two-way)	7.628	1.318	1.151	1.145
4	DSMC	7.451	1.322	1.153	1.147

The separation performance of the rotating cylinder is evaluated by calculating the separation power, separation, enrichment, and stripping factors (Table 1).

According to Table 1, the calculated separation power obtained from the pure CFD, one-way, two-way, and pure DSMC is 8.750, 8.001, 7.628, and 7.451, respectively. The results showed that separation power is about a 2% difference between two-way and pure DSMC solutions. Also, there is a 17.5% and 7% difference between the separation power of pure CFD and one-way solutions compared to pure DSMC solutions. According to the CFD-DSMC algorithm, the interaction between the DSMC and CFD method is considered in the two-way technique. Therefore, the two-way is more complex than the one-way technique, but the effect of the rarefied area can be better evaluated. Furthermore, it can be concluded that the significant difference between pure CFD and pure DSMC solutions is due to the generation errors due to using the CFD method in the rarefied area.

5. Conclusion

In the present study, using OpenFOAM software, the two-way CFD-DSMC technique was utilized to analyze the UF_6 gas flow inside a rotating cylinder. The results showed that the continuum area inside the rotating cylinder is about 18% of the total areas ($0.086 < r < 0.1$); Thus, the CFD method was valid only in this area. To investigate the effect of the

rarefied area, the one-way, two-way, and pure CFD were compared to the pure DSMC method. The one-way and pure CFD methods showed that if the rarefied area is simulated separately with DSMC methods, the difference in results will be reduced from 17.5% to 7%. If the two-way technique is used, the difference in results will be reduced to 2%. Comparing the one-way and two-way techniques showed that the effect of rarefied area solution on continuum area is about 5%. Finally, due to the features of the one-way and two-way techniques, it is recommended that the two-way technique be used to analyze the gas flow in the rotating cylinder.

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