iJRASET
International Journal For Research in
Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 8 **Issue:** XII **Month of publication:** December 2020

DOI: https://doi.org/10.22214/ijraset.2020.32496

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 8 Issue XII Dec 2020- Available at www.ijraset.com

CFD Simulation of Compressible Flow inside a Gas Centrifuge using OpenFOAM

Harshawardhan Kulkarni
Institute of Chemical Technology, India

Abstract: Gas Centrifuge is an equipment used for separation of isotopes like UF6, SF6 or separation of CO_2-CH_4 mixture from natural gas reservoirs consist of annular region scoops for enriched and depleted isotopes. Baffle is creating vertical structure in the vessel. The simulations are carried out to capture the shock wave near the scoop region which is used for collection of enriched uranium. This region has very high Mach number. This work is providing insight of how to simulate high speed flow with the help of rhoCentralFoam in OpenFoam. SnappyHexMesh utility from OpenFOAM is used for meshing this kind of geometry where parts of geometries intersecting as well as Swak4Foam utility is used to give profile for the internal field and to boundary condition.

Keywords: Gas Centrifuge, SnappyHexMesh, Swak4Foam, Oblique shock

I. INTRODUCTION

A large part of natural gas reservoirs discovered till date are not available for production because these reservoirs contains more than 10% CO2 and more than 1% H_2S. The removal of CO_2/H_2S from gas streams can be achieved by a number of separation techniques including absorption into aqueous solutions of alkano-amines, adsorption onto a solid, permeation through membranes. At lower level of contamination, amine based separation technique is economically feasible. Amine based technology has disadvantages such as high energy requirement, pre-heater to regenerate the amine. Another disadvantage is that waste gases are produced at atmospheric pressure. These gases thus need to be compressed for reinjection in reservoirs. Thus, amine based technology is not economically viable for the gas field containing >10% CO_2 and > 1% H_2S due to high solvent requirement and solvent regeneration cost. To overcome these disadvantages gas centrifuge technology can be used to extract the gas from these reservoirs. The Gas Centrifuge is high speed rotating device with compressible flow inside consist of following parts an annulus, scoop and baffle. Annular region consists of two concentric cylinder with outer is rotating with the velocity in the range of 100-600 m/s. Scoop in this region is used for collection of products as well as helps in creation of circulation of the gas in the annular region. Various groups have explored the application of Gas centrifuge for separation of isotopes used in nuclear engineering as well as applications such as separation of CO_2-CH_4 mixture. The next section describes the previous work on Gas centrifuge technology.

II. PREVIOUS WORK

The Onsagar pancake model is used to calculate separative performance of single stage Gas Centrifuge. This Cohen Onsagar pancake model is the solution for counter current flow. This counter current flow is important for centrifuge design consideratio[1]. Rebecca Bourn solved the new sixth order partial differential equation obtained from differential formulation by using Eigen value expansion and finite element method. The solution was compared with Eigen function solution of original sixth order onsager pancake model[2]. Wood et al. developed a method based on Onsager Pancake Equation, diffusion equation for each isotope and optimization routine. Onsager Pancake approach was adapted for multi isotope separation. Diffusion equation is developed for each isotope. This PDE is converted to ODE by radial averaging method. This ODE is linked to solution of Onsager equation and was solved iteratively[3]. Optimization routine is used to find the parameter for optimal counter current parameter. This methodology is applied to long and high speed GC. For short and low speed GC, complete solution was obtained[4]. Donald Olander et al. used the method developed by Wood models for coupling the flow models in the rotor wall and end cap boundary layers to complete the hydrodynamic analysis of the centrifuge[5]. Stadler and Chand solved sixth ordet PDE onsager pancake by converting equivalent coupled system of three equations. Simple Analytical solution is provided for verification of numerical codes for modelling of unsteady gas flows in GC. In this solution, it is assumed that rotor is infinite, and force required for rotation varies harmonically along the axial coordinate. This causes unsteady problem to be reduced to a system of ordinary differential equations. The periodicity of the solution is prescribed at the end face of rotor. Semi analytical method allows determining for optimal mesh resolution and accuracy of the calculation[6]. S.V.

Bogovalov developed an analytical equation to calculate separative power for an arbitrary binary mixture of isotopes. The flow of the gas was assumed with an exponential profile of the density along the radius in the concurrent centrifuge. The equation derived is from first principle and well agreed with empirical data[7,8]. Matsuda et al. carried out 3D axis symmetric simulation of inviscid gas flow around past scoop in a gas centrifuge. In his simulations, Euler's equation is solved by using explicit Second Order accurate Roe upwind TVD scheme. Cylindrical and wing shaped scoop were used for his simulation. Detached Bow shock is formed in front of the scoop in case of cylindrical scoop while oblique shock is produced in case of wing shape scoop. For cylindrical scoop strong radial inward gas motion is produced behind the shock. A strong radial inward motion of gas produced a counter current flow which results in production of vortex in front of the scoop. In case of wing shape scoop, shock formed is not as strong as cylindrical shape scoop. Algebraic method and Multi-block transformation technique is used for grid generation. Tran-finite interpolation method used for the surface volume grid generation. At the top boundary counter current is not uniform in azimuthul direction. Due to vortex column in front of the scoop inner gas rotate in the opposite direction of the rotar motion. For wing shape scoop no vortex column is formed in front of the scoop[9]. Tsnunetoshi Kai et al. (10) studied isotope separation for SF_6 gas centrifuge. They reported 37% separation efficiency. Motion of gases can be obtained by solving Navier Stokes Equation. Since they solved for axi-symmetric case, azimuthal derivative vanishes in the equation. The Gas is assumed to bean ideal gas and in a steady state. The separation efficiency and throughput are inversely related. Ralph van Wissen et al. (11) studied CO_2-CH_4 separation using gas centrifuge. They studied maximum achievable separation for decontamination using Gas Centrifuge. The result obtained from study shows that it has good separative strength but it's throughput is limited. The centrifuge with length of 5 m and peripheral velocity 800 m/s would have throughput of 0.57 mol/sec and product flow 0.17 mol/sec. Production rate is a function of internal circulation, product, product-feed ratio, peripheral velocity and centrifugal velocity and radius. Bogovalvo et al. (12) carried of numerical simulation performed for different lengths of rotor. Results showed that separative power of GC reduced with the length of the rotor. Reduction of the specific separtive power is connected with growth of the pressure in the optimal regime and corresponding growth of the temperature. In this work parameters of the flow and GC have been optimized to obtain the maximum value of the separative power. They reported that pressure at the wall of the rotor should be less than the pressure of sublimation of the working gas. S.V. Bogovalvo(13) carried out simulation of 2D axis symmetric transient flow induced by a pulse breaking force. The computational domain consists of three sections: top, working and bottom. Transient case is compared with stationary case where the flow is generated by a stationary breaking force. The product flux in case of the transient case is 15 % exceeds that in stationary case for same temperature and pressure. In the steady state regime the pressure in the working camera of the transient case is expected to be lower than the pressure in stationary case. Brouwers (14) studied axis symmetric flow of a perfect gas in GC by applying a linearised analysis to a small perturbation about rigid body rotation. In this study special attention was given on effect of length to radius ratio and effect of a strong radial density gradient on isothermal rigid rotation. Ekman number, *E* based on the small radial density scale and the density at the cylinder wall is taken to be small. Flow outside Ekman boundary layer consists of the three types. The inviscid flow of a limited thickness near cylinder wall is found. Due to strong radial density gradient, radial diffusion is not confined to Stewartson layer and it extends to core (14). Ribando (15) used finite difference method for computing secondary flow in gas GC. Time marching technique was used to solve linearized axi-symetricNavier Stokes equation,analytical Matching condition which has same effect as that of thermal and hydraulic boundary condition. The algorithm is used is based on eigen function. In this study source and sink and non linear terms were not included. Pascal Omnes (16) compared two models used to compute internal hydrodynamics of Gas Centrifuge. Numerical Method used is Finite Volume Method on staggered grid and fixed point iteration. In the first model boundary conditions are applied on the flow entering in the bowl and in second model on sink and drag force in chamber. First model correctly predicted separative power on coarser grid while second model correctly predicted drag force and return flow on finer grid. In his study he concluded that linear computation on rough grid for prediction separation is more and non linear computation on finer grid used for studying the physical parameter like return flow rate, heating up of gas. De Andrade (17) integrated thermal and hydrodynamic model to obtain realistic separative power. He carried out simulation of gas inside a rotor with arbitrary thermal boundary condition. Then structural thermal boundary Kai (18) numerically determine flow field inside a centrifuge by solving flow equation for a compressible gas in a strong rotation. Diffusion equation is solved for obtaining molar concentration of a lighter isotope in a flow field. A modified Newton raphson Method used to obtained solution for non linear equation. Jiang (19) use vector splitting method of finite volume method for solving finite volume method, result shows that strong detached shock wave in front of scoop, as the radial position increase shock become stronger. In this case oblique shock is formed between scoop and centrifugal wall. Because of pressure gradient and centrifugal force radial inward flow of gas is produced behind the shock.

Brouwers (20)carried out linear analysis of conservative equation of mass, momentum and energy to obtained different region along the radius. Near wall region Stewartson layer then inviscid layer and inner layer to diffusion controlled centre region. Due to axial motion in these layer region is short circuited in Ekman layers at the end. The solution of the flow field used to calculate separtive power. Auvil (21) developed the operating theory for both steady and unsteady sate of gas centrifuge. The counter current flow developed enhances the possible separation. Self diffusion is more in low molecular weight gas while less significant with heavy gas. Kai (22-23) used modified Newton's method to evaluate steady state motion in a rotating cylinder without the use of time consuming marching process with respect to time for solving Navier stokes equation and convection diffusion equation. The approach included gauss elimination procedure which consist of the transformation jacobian matrix to a triangular matrix then followed by backward substitution. Bogovalvo (24) used two camera models to explore the impact of pulse breaking force on the axial gas circulation in gas centrifuge. This force causes generation of wave which propagates along the length of the rotor. Pulasting force increased the mass flux almost twice in comparison with stationary breaking force. Borisevich (25)used Dirac's law to compute separative power. Separtive power of a gas centrifuge depends on geometric parameter and position of a bellows on the rotor wall as well as the effect of the scoop drag and feed flow. Finite difference technique has been used to solve Navier Stokes and Convection-diffusion equation. They claimed 24% increase in separative power by optimizing the location of bellows. Cracknell and Golombok used monte carlo method for prediction of dew pontingas a function of radial pressure gradient. Previously radial pressure was first calculated and then it is used in a separate equation to find out whether condensation will occur or not. In this study, potential energy along with molecular interaction term is used. they developed the model for separation of hydrogen sulphide from methane. The heavier component has strong molecular interaction than lighter component and therefore it augments the operation of the centrifuge and helped in finding out where the condensation will occur. Isotope enrichment is a result from superposition of the elementary separation effect due to the centrifugal field in the gas and its internal circulation is analyzed by the Onsager-Cohen theory. The performance function representing the optimized separative power of a centrifuge as a function of throughput and cut is calculated for several simplified internal flow models. The use of asymmetric ideal cascades to exploit the distinctive features of centrifuge performance functions is described (26). Soubramayar and Billet (27) developed boundary conditions in terms of controllable function to optimize gas centrifuge. These controlled function expansion in a finite base this convert to minimization problem and then solved by using simplex method. Numerical code developed gives operational condition to optimize separative power and used to calculate rotation speed parameter A^2.

III. METHODOLOGY

A. *OpenFOAM capabllity*

The aim of this work is to capture shock wave generated at scoop and is to verify OpenFOAM solver capability. The actual geometric configuration is as shown in figure 3.1 bellow. The length of gas centrifuge is 1000 mm and this is in annular in shape with inner and outer radius are 120 and 150 mm respectively. For the simulation purpose we consider a scaled down model of Geometry of actual geometry having length of 1000 mm. Figure 7.1 shows the pictorial representation of the geometry. This gas centrifuge has annular geometry with inner radius of 120 mm and outer radius of 150 mm. The scoop used for extraction of isotopes is having cylindrical in shape with radius 3mm. For spatial discretization of the geometry we used snappyHexMesh utility in OpenFoam. The density based solver, rhoCentralFoam was used for solving the governing equations since the flow inside gas centrifuge chamber is compressible with Mach number greater than 3.

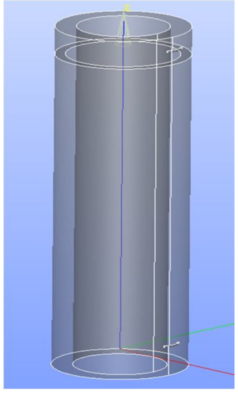


Figure 3.1: Geometry of Gas Centrifuge used in the current study

The geometry consider is 1/10th of the actual geometry Figure 3.2 shows the snapshots of the geometry and meshing. Intersecting bodies cannot easily mesh with simple discritization with proper hexahedral cell division hence blocking concept is used from snappyHexMesh utility in OpenFOAM where the thickness of first cell from inner and outer wall is 10 micrometer and 25 layers are added from both sides to capture gradient of pressure and velocity. To resolve shock near scoop, this region has to refined more. Numerical Methods in rhoCentralFoam

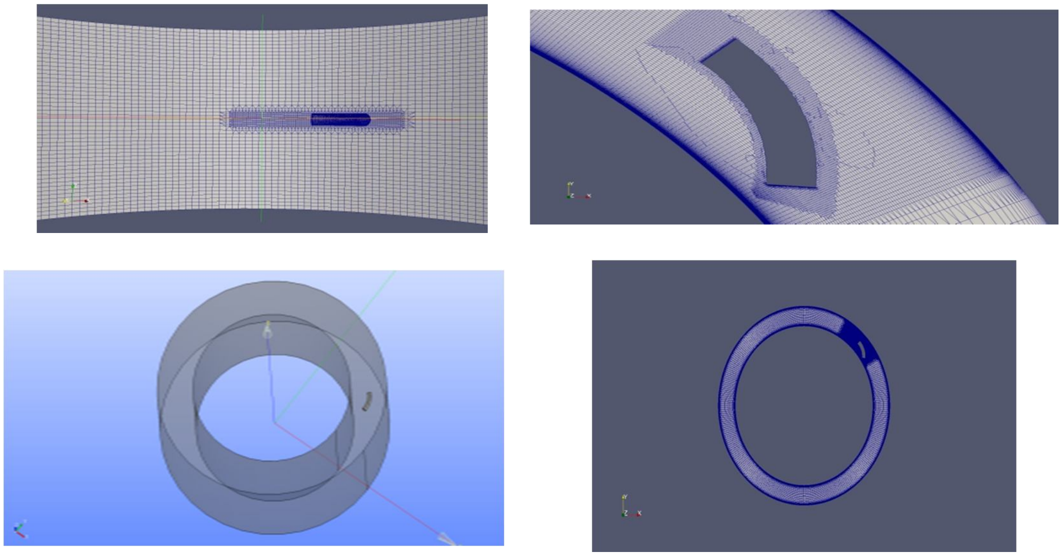


Figure 3.2: Details of mesh configuration

Flow field Initialization is important thing in flow modelling to reduce time that takes for obtaining fully develop profile of flow field was done using swak4foam utility. The arbitrary radial profiles of pressure and velocity have been given at the stage of initialization. The grid refinement in adaptive meshing technique was controlled using pressure gradient.

B. Model Equations used in rhoCentralFoam

The solver is solving each of the governing compressible equation separately. First the continuity equation is solved, providing a new value for ρ. Thereafter the momentum equation is solved in two steps where the first inviscid part is calculated and the values updated and afterworld the viscid part is added. The energy equation is first solved without diffusive flux of heat, which is later added when the updated temperature is calculated.

The continuity Equation is solved with the previous time velocity values.

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x_i}(u_i\rho) \qquad (3.1)$$

For convention purpose $\hat{u}_i = \rho u_i$ and $\hat{E} = \rho E$. After the continuity is solved the inviscid momentum equation is solved.

$$\left(\frac{\partial \hat{u}i}{\partial t}\right)_I+\frac{\partial}{\partial x_j}(u_i\hat{u}_j)+\frac{\partial\rho}{\partial x_i}=0 \qquad (3.2)$$

Equation 3.2 explicitly calculates $\hat{u}_i$ and thus no linear solver is needed. The time derivative $\left(\frac{\partial}{\partial t}\right)_I$ is only the inviscid contributions. The new velocity u_i is updated by using the uploaded density, thus $u_{i=}$ $\hat{u}_{i\,/}$ ρ. The diffusion correction equation is now solved for $u_{i,}$ where the viscous terms are added.

$$\left(\frac{\partial(\rho u_i)}{\partial t}\right)_V-\frac{\partial}{\partial x_j}-\left(\mu\frac{\partial u_i}{\partial x_j}\right)-\frac{\partial}{\partial x_j}\mu\left(\frac{\partial u_j^{exp}}{\partial x_i}-\frac{2}{3}\frac{\partial u_k^{exp}}{\partial x_k}\delta_{ij}\right)=0 \qquad (3.3)$$

In the equation the time derivative $\left(\frac{\partial}{\partial t}\right)_V$ is the contribution of diffusion and viscous forces. The velocities u_i^{exp} are taken from the solution of the inviscid equation (3.3).

The laplacian terms is added implicitly in u_i and solved for with a linear solver available in OpenFOAM.

A similar procedure is done for the energy equation. First Ê at the new time step is found explicitly from the equation,

$$\left(\frac{\partial \hat{E}}{\partial t}\right)_I + \frac{\partial}{\partial x_k}\left[u_k\left(\hat{E} + p\right)\right] - \frac{\partial}{\partial x_i}\mu u_j\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) = 0 \qquad (3.4)$$

From Ê the temperature T is calculated through,

$$T = \frac{1}{C_v}\left(\frac{\hat{E}}{\rho} - \frac{u_k u_k}{2}\right) \qquad (3.5)$$

Then a diffusion correction equation for T is solved to include the dissuasive terms

$$\left(\frac{\partial(\rho C_v T)}{\partial t}\right)_v - \frac{\partial}{\partial x_k}\left(k\frac{\partial T}{\partial x_k}\right) = 0 \qquad (3.6)$$

The diffusion correction equation for T is carried our implicitly, thus the laplacian of T is taken at new time step. An iterative solver of choice is used to solve this system of equations. After the temperature is calculated the temperature dependent quantities k and μ are evaluated at the new temperature T. Also the pressure p = ρRT is updated. The variables k, μ, p are held constant through each iteration and only updated at the end of it.

IV. RESULTS AND DISCUSSION

The high rotational field in the domain creates motion of gas phase and the tangential velocities are generated in the system. The tangential flow field gets redirected in radial and axial directions due to the presence of stationary body. This stationary body acts as an outflow for the gas components and is also known as scoop. The pressure profile in domain follows exponential form. The pressure on the wall is very high compared to in the central region. The stagnation point near the scoop surface has very high pressure compared to the rest of the domain (Figure 4.1). The flow pattern is quite complex and boundary layer separation takes place. High Mach number flow gets creates at the edge of upstream of scoop. The high Mach number shock wave propagates the wall of the domain and reflects back (Figure 4.2). This complex flow pattern and axial mixing due to high mach number region can impact the separation efficiency. The axial mixing reduces with increase in the peripheral velocity; however, due to very high stagnation pressure as well as high Mach number flow in the scoop region, temperature rises due to viscous dissipation. This can also have an impact on the separation. Hence it is necessary to predict pressure, Mach number and temperature profiles in the domain to optimize the performance of gas centrifuge.

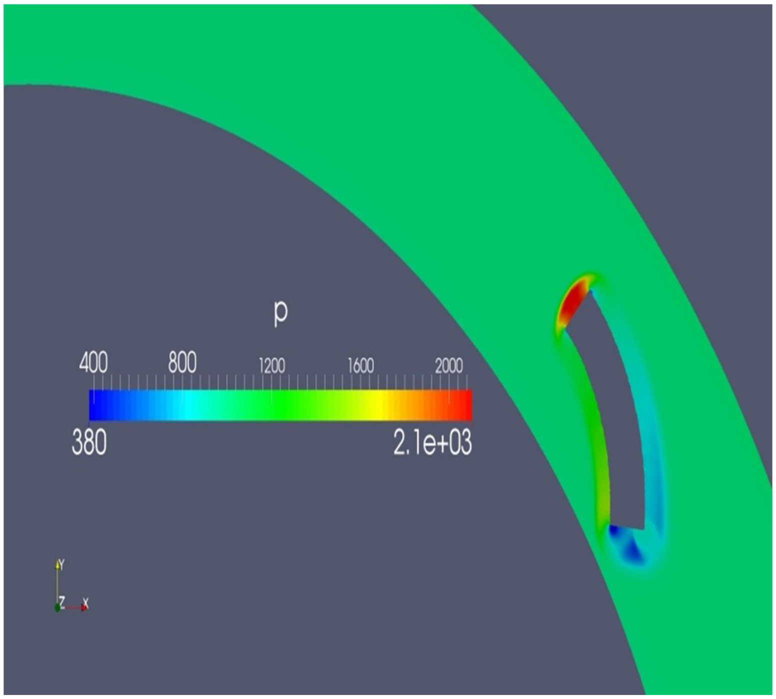


Figure 4.1: pressure profile in annulus region

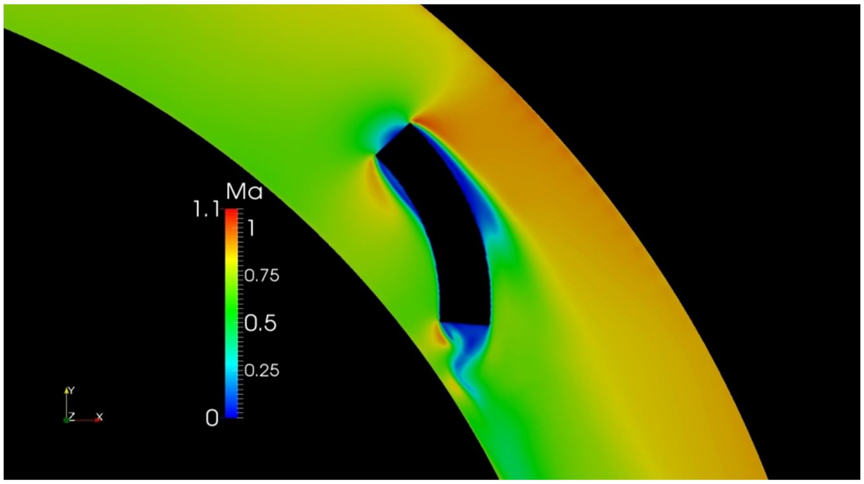


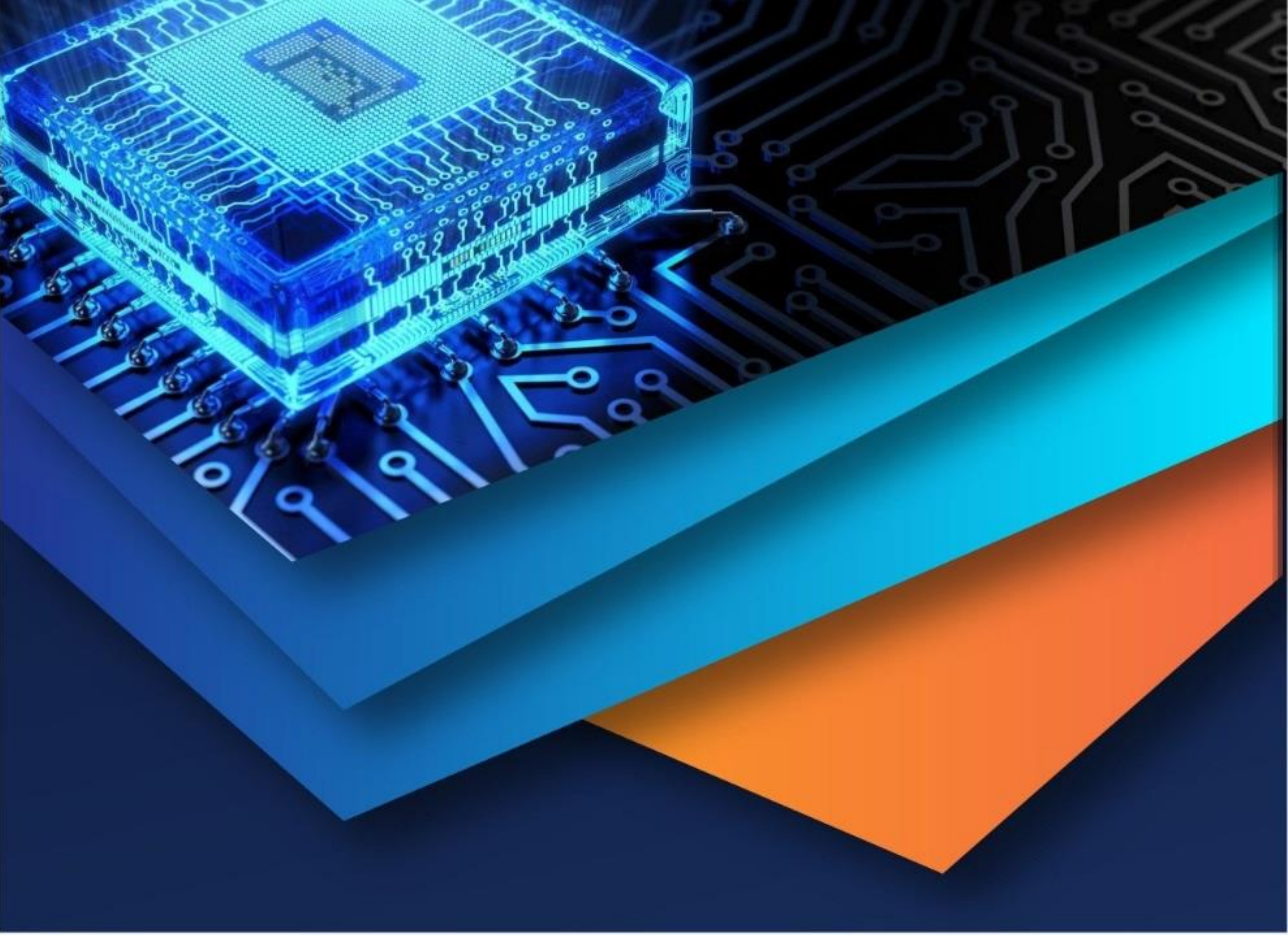
Figure 4.2: Mach number profile

V. CONCLUSION

Numerical solutions of pressure and Mach number profiles were obtained for 3-dimensional flow in gas centrifuge. The outflow through the centrifuge is controlled through stationary scoops and the scoops also offer significant pressure gradient and produce high Mach number. OpenFOAM's meshing utility snappyHexmesh used to mesh complex domain, check it's capablity to simulate compressible flow and swak4foam utility to create boundary conditions and to initialize flow fields. With the help of CFD, we can predict pressure and mach number profile in rotating compressible flow.

REFERENCES

[1] Houston G. Wood III, Analysis of Feed Effects on a Single-Stage Gas Centrifuge Cascade, Separation Science and Technology Volume 30, 1995,13 .
[2] Houston G. Wood, Solution of the pancake model for flow in a gas centrifuge by means of a temperature potential, Computer Methods in Applied Mechanics and Engineering, Volume 178, Issues 1–2, July 1999, Pages 183-197.
[3] Houston G. Wood, Multi-Isotope Separation in a Gas Centrifuge Using Onsager's Pancake Model, Separation Science and Technology Volume 31, 1996 - Issue 9 , Pages 1185-1213.
[4] Donald R. Olander, The Theory of Uranium Enrichment by Gas Centrifuge, Progress in Nuclear Energy, Progress in Nuclear EnergyVolume 8, Issue 1, 1981, Pages 1-33.
[5] M. B. de Stadler and K. K. Chand. A Finite-Difference Numerical Method for Onsager's Pancake Approximation for Fluid Flow in Gas Centrifuges. UCRL-TR-236581, Lawrence Livermore National Laboratory, 2007
[6] S.V. Bogovalov, Method of Verification of Numerical Code for Modeling of Flows in Gas Centrifuge,Physics Procedia 72 (2015) 305 – 309.
[7] S.V.Bogovalov, Isotopes Separation in Concurrent Gas Centrifuge, Physics Procedia 72 (2015) 297 – 304.
[8] Takuya Matsuda, Three-dimensional numerical simulation of flows past scoops in a gas centrifuge, J . Fluid Mech. (1989), vol. 201, p p . 203-221.
[9] Tsunetoshi KAI, Numerical Calculation of Flow and Isotope Separation for SF6 Gas Centrifuge, Journal of Nuclear Science and Technology, vol (32).No.2, p. 153-165, Feb2000.
[10] Ralph van Wissen et al. Gas centrifugation with wall condensation, AIChE Journal 52(3):1271 – 1274, March 2006
[11] S.V. Bogovalov, Numerical Modeling of dependence of Separation Power of the Gas centrifuge on the length of Rotor, Physics Procedia 72 (2015) 283 – 286.
[12] S.V. Bogovalov, Modeling of Waves in Iguasu Gas Centrifuge, Physics Procedia 72 (2015) 287 – 291.
[13] J. J. H. Brouwers, On compressible flow in a rotating cylinder, Journal of Engineering Mathematics, Vol. 12, No. 3, July 1978.
[14] R . J. Ribando, A finite-difference model for flow solution of onsager's in a gas centrifuge, Computers & Fluid~ Vol. 12, No. 3, pp. 235-252, 1984.
[15] Pascal Omnes, Numerical and physical comparisons of two models of a gas centrifuge,Computers& Fluids 36 (2007) 1028–1039.
[16] S.V.Bogovalov, Method Verification of numerical codes for modeling of the flow and isotope separation in gas centrifuges, Physics Procedia 72 (2015) 305 – 309.
[17] Tsunetoshi KAI, Theoretical Research on Gas-Centrifugal Separation for Uranium Enrichment, Journal of Nuclear Science and Technology, 26[1], pp. 157-160 (January 1989).
[18] Jiang Dongjun, CFD Simulation of 3d Flowfield In A Gas Centrifuge, Proceedings of ICONE14 International Conference on Nuclear Engineering July17-20
[19] J. J. H. Brouwers, On Compressible Flow in a gas Centrifuge and its effect on maximum separative power.
[20] Steven R. Auvil, The Steady and Unsteady State Analysis of a Simple Gas Centrifuge, AlChE Journal (Val. 22, No. 3), 564-568
[21] Tsunetoshi KAI, Basic Characteristics of Centrifuges (III), Journal of Nuclear Science and Technology,14[4], 1977, pp 267-281.
[22] Tsunetoshi KAI, Basic Characteristics of Centrifuges (IV), Journal of Nuclear Science and Technology, 14(7), 1977, pp. 506-518.
[23] S.V. Bogovalov, Impact of the pulsed braking force on the axial circulation in a gas centrifuge, Applied Mathematics and Computation, Volume 272, Part 3, 1 January 2016, Pages 670-675.
[24] V.D.Borisevich, Numerical simulation of bellows effect on flow and separation of uranium isotopes in a supercritical gas centrifuge, Physics Procedia 72 (2015) 283 – 286.
[25] Cracknell et al.Monte-Carlo Simulations of Centrifugal Gas Separation, Molecular Simulation, Vol. 30 (8), 15 July 2004, pp. 501–506.
[26] Donald R. Olander, The Theory Of Uranium Enrichment By The Gas Centrifuge, Progress in Nuclear Eneroy, Vol. 8. pp. 1-33.
[27] Soubbaram Ayer, A Numerical Method For Optimizing The Gas Flow Field In A Centrifuge, Computer Methods In Applied Mechanics, 24 (1980) 165-185.



10.22214/IJRASET

45.98

IMPACT FACTOR: 7.129

IMPACT FACTOR: 7.429

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY