The computer simulation of 3d gas dynamics in a gas centrifuge

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Abstract. We argue on the basis of the results of 2D analysis of the gas flow in gas centrifuges that a reliable calculation of the circulation of the gas and gas content in the gas centrifuge is possible only in frameworks of 3D numerical simulation of gas dynamics in the gas centrifuge (hereafter GC). The group from National research nuclear university, MEPhI, has created a computer code for 3D simulation of the gas flow in GC. The results of the computer simulations of the gas flows in GC are presented. A model Iguassu centrifuge is explored for the simulations. A nonaxisymmetric gas flow is produced due to interaction of the hypersonic rotating flow with the scoops for extraction of the product and waste flows from the GC. The scoops produce shock waves penetrating into a working camera of the GC and form spiral waves there.

1. Introduction
Numerical simulation of the gas flow and diffusion of the mixture of isotopes is the most reliable tool to obtain information about processes in the gas centrifuges. Starting with the work [1], axisymmetric 2D models are widely explored for the numerical simulations. This model appears very useful as for academic study of the gas flow in the extremal conditions of hypersonic gas flow in GC as for engineering design of new GC’s. A range of works have been performed on the basis of this model [2, 3, 4, 5]. No doubts that this model will provide us more new information about the gas dynamics in GC in future. Nevertheless, there are processes in GC that have 3D geometry and it becomes more and more clear that essentially they effect on the gas dynamics in the GC. Engineering calculations of the gas dynamics in the GC are impossible without taking into account these processes.

In this work, we outline the basic results obtained in National Research Nuclear University, MEPhI on the numerical simulation of the gas dynamics in 2D and 3D models of GC.

2. The role of 3D flows in gas centrifuges
Strong centrifugal field is not the only factor which provides an efficient isotope separation in GC. A range of physical processes is explored to produce an additional axial circulation, which dramatically increases the efficiency of the isotope separation in the GC. This secondary circulation is one of the key features of the industrial GC.

Pair of scoops, located near the end caps of the GC, are used to extract enriched and depleted gas mixture from the GC. Simultaneously, they provide the additional axial circulation due to
the mechanical brake of the gas. Mach number of the gas in GC is of the order \( \sim 7 \). Interaction of the gas with the scoops is accompanied by formation of strong shock wave, which propagates along the rotational axis. The shock wave forms a spiral wave propagating from one end of the GC to another. It can reflect from the end caps of the GC forming waves running in both directions along the rotational axis. The amplitude of the shock waves is damped rather quickly. After the damping, they propagate in the working chamber of the GC in the form of small amplitude waves. Therefore, to understand the impact of the waves on the dynamics of the gas it is reasonable to start from study of the physics of the waves in the gas compressed by the strong centrifugal fields typical for the GC.

It is well known that the waves in an uniform gas can produce a flow due to their absorption [6]. These are so-called acoustic flows described by Lord Rayleigh [7, 8]. The acoustic flows are produced at the transfer of the energy and momentum from the waves to the gas due to the molecular viscosity.

The waves generated by the scoops and propagating along the axis of GC can also provide an additional mechanism of the secondary axial circulation in the GC due to their absorption. This mechanism can essentially differ from the conventional mechanism of the circulation generation. The waves can propagate and therefore transfer the breaking torque at larger distance from the scoops than it happens at the axisymmetric brake. Our recent numerical experiments confirm that the waves essentially changed the axial circulation [9].

There is another important motivation for study the role of the spiral waves on the gas flow in GC. It appears that the waves can essentially change the gas content in the GC due to modification of the gas flow through a hole connecting the working and waste camera of the GC. Numerical simulations show that the waves can change the gas content in the GC on 15-20% [10].

We are at the very beginning of the study of the role of the waves in the physics of GC. We already found some new physical phenomena due to the spiral waves and apparently, more effects will be found in future. Nevertheless, the impact of the waves on the axial circulation and gas content in GC give us convincing reasons to develop numerical technology for fully 3D simulation of the gas flow in GC. Comparison of the gas flow with and without waves is possible only in the 2D model. Nevertheless, the real waves in the GC, has 3D spiral shape. Therefore, the engineering calculation of the gas dynamics in the GC is possible only in 3D geometry.

3. The basic requests to the software for 3D simulation
The numerical simulation of the gas flow in the conditions of the GC by the conventional numerical codes is impossible because of extremal conditions in the GC. There are at least a few reasons requesting developing of specialized codes for simulation of the gas dynamics in the gas centrifuges. The most important among them are:

(i) Strong variation of density and pressure along radius. All the schemes based on the control volume method use interpolation schemes for calculation of the fluxes of mass, momentum and energy at the surfaces of the control volumes. Strong gradients of pressure give unrealistic fluxes, which produce unphysical solutions. Therefore, a specialized numerical scheme should be developed.

(ii) Velocities of the axial circulation are of the order of a few centimeters per second. They are small compared with the rotational velocity of the gas, which can achieve 600-700 m/s. Accurate calculation of the axial circulation of the axial circulation demands exploration of the rotational frame system. In this system, the rigid body rotation of the gas equals to zero. This is a conventional approach in the 2D axisymmetric models. The axial symmetry of the model is violated by the scoops in 3D models. The scoops rotate in the rotating frame. Therefore, one of the problems of the 3D numerical simulation is development of
the codes, which allow us to reveal axial circulation with accuracy better than $2 \cdot 10^{-5}$ at moderate mesh resolution in the laboratory frame system.

(iii) The scoops have rather complicated geometrical shape. Reproduction of the geometry of the scoops and other geometrical details of the GC is important for accuracy of the calculations. At present time, the universal technology for mesh generation around of the bodies with an arbitrary geometry is to use tetrahedral mesh. At the same time, this is not reasonable to use the tetrahedral mesh in the entire computational domain. This type of mesh creates too strong numerical diffusion. It is better to use hexahedral mesh in the largest part of the computational domain. Therefore, the numerical technology should include the mesh generation containing tetrahedral and hexahedral cells.

In addition, the 3D simulations demand huge memory and CPU time. They should be performed in multiprocessor regime. On these reasons the 3D simulations of the gas dynamics in GC has been performed in the very limited cases. As a rule, only fragments of the total flow have been modeled in 3D simulations before [11].

4. Computational Technology of National Research Nuclear University, MEPhI

For development of our original specialized numerical code, we used two schemes of interpolation. First one is the Rhie - Chow interpolation scheme proposed in [12]. Some details of modification of the scheme are presented in [13]. Second one is a second order Godunov interpolation scheme [14]. Our experience shows that the realization of the Godunov scheme is simpler and gives more stable code.

The problem of the gas flow in 3D geometry is solved as a steady state problem by the relaxation method starting from some initial state of gas. Implicit scheme is explored in all cases. The simulations have been performed on a computer cluster containing 525 nodes. Verification of the code has been performed with the special tasks developed by us specially for the verification of the numerical codes for simulation of the gas flows in strong centrifugal fields [15, 16].

The mesh generator exploring combined tetrahedral and hexahedral meshes has been developed. This generator allows us to reproduce the geometry of the scoops with high accuracy. The example of the mesh around one of the scoops is shown in fig.1.

![Figure 1. Mesh around a scoop. The mesh is combined of tetrahedral and hexahedral cells.](image)

We imposed the following boundary conditions at the boundaries of the computational domain:

(i) No slip walls were used at the walls of the rotor, walls of the scoops and baffles.

(ii) A temperature distribution is imposed at the walls of the rotor.
(iii) Zero thermal resistance is imposed at the walls of the scoops. The problem of the scoop heating is solved simultaneously with the hydro dynamical problem.

(iv) The computational domain is limited by an artificial inner wall located at the radius where the Knudsen number is close to 1. The hydro dynamical approximation is not valid at smaller radius. Free slip condition is imposed at this wall. The feed flux is also imposed on this wall as a boundary condition.

(v) A specified waste mass flow is imposed at the output from the upper (waste) scoop.

(vi) A small pressure is specified at the output from the lower (product) scoop.

**Figure 2.** The geometry of the computational model. The volume of the computational domain is located between the wall of the rotor and the inner wall located at the radius where the Knudsen number is close to 1. The location where the feed flux is imposed is shown in green at the inner wall. The volume of the computational domain is separated by the baffles (shown in blue) on 3 chambers connected by concentric holes. The scoops are located in the waste and product chambers at the right part of the figure.

Geometry of the computational domain is shown in fig. 2. The computational domain includes the volume of the rotor filled by the working gas $UF_6$, baffles, scoops and the artificial inner wall. The baffles divide the volume of the rotor into three chambers: working, waste and product chambers. Parameters of the rotor correspond to the parameters of the Iguasu centrifuge introduced in [17]. However, the length of the rotor is intentionally reduced to 20 cm to reduce the size of the mesh and computational time. The mesh generator produced the mesh containing $1.2 \cdot 10^7$ nodes.

**5. The basic results of the 3D simulations**

As it was expected, the numerical simulation has shown that the scoops produce strong shock waves. Fig. 3 demonstrates the velocity distribution of the gas on some cylindrical surface. The shock waves freely penetrate from the waste and product chambers into the working chamber.
Figure 3. Velocity distribution on a cylindrical surface located in the computational domain. The scoops are located on the left part of the figure. All the geometry is shown by the contour lines. The scoops produce the spiral shock waves penetrating into the working chamber, forming the spiral wave there. The amplitude of the spiral shock waves is reduced rather quickly. They transform into acoustic spiral waves propagating along the rotor.

Figure 4. Pressure distribution around the waste scoop in the plane cutting the scoop symmetrically perpendicular to the rotational axis.

The flow near the scoops has rather complicated structure. For example, the pressure distribution around the waste scoop is shown in fig. 4 in the plane perpendicular to the rotational axis cutting the scoop symmetrically. A bow shock is formed at the very nose of the scoop.

The flow through the concentric holes in the baffles separating the rotor on the chambers has essentially 3D character. Fig. 5 shows the flow through the hole in the waste baffle separating upper (waste) chamber from the working chamber. There is the flow from the waste chamber to the working chamber (down) and in the opposite direction (up). This strongly disagrees with the conventional 2D models, which demonstrate only the flow in one direction from the waste chamber. Nevertheless, the integral mass flow is directed from the waste chamber to the working
Figure 5. The flow of the gas through the hole in the waste baffle. The waves generated by the scoop produce rather complicated flow from the waste chamber to the working chamber and in the opposite direction. The integral flow is directed down.

Figure 6. The flow of the gas through the hole in the product baffle. The waves generated by the scoop produce the flow from the working chamber to the product chamber and in the opposite direction. The integral flow is directed down.

Almost the same picture we observe in fig. 6 for the flow through the hole in the lower (product) baffle. There are flows in opposite direction. Moreover, the largest velocity takes place for the flow directed from the product to the working camera (up). Nevertheless, the integral flow is directed from the working to the product chamber.

Fig. 3 demonstrates the shock wave propagation along the rotational axis. The shock waves are damped rather quickly and transform into the acoustic waves propagating in the gas subjected to the strong compression due to the centrifugal force. Fig. 7 shows that these waves can propagate along the entire working chamber without any visible damping. The waste and product chambers are removed from this figure because of strong pressure variation there.
6. Conclusions

The scoops of GC produce spiral waves, which can propagate in the axial direction along the rotor. These waves can be modeled numerically only in 3D model of GC. Our estimates on the basis of nonstationary flows in 2D models show that the waves can affect the axial circulation and gas content in the GC. Therefore, the engineering calculation of the gas flow in the GC with accuracy of the order of a few percents is possible only in 3D model. The conventional 2D models can give deviation from real optimized parameters on the level 20 – 30% due to the processes having essentially 3D character. Our experience shows that fully 3D simulation is possible with the existing software and hardware and is limited only by the memory and CPU time.

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