

# Determination of the optimal mesh parameters for Iguassu centrifuge flow and separation calculations

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**Abstract.** We present the method and the results of the determination for optimal computational mesh parameters for axisymmetric modeling of flow and separation in the Iguassu gas centrifuge. The aim of this work was to determine the mesh parameters which provide relatively low computational cost without loss of accuracy. We use direct search optimization algorithm to calculate optimal mesh parameters. Obtained parameters were tested by the calculation of the optimal working regime of the Iguassu GC. Separative power calculated using the optimal mesh parameters differs less than 0.5% from the result obtained on the detailed mesh. Presented method can be used to determine optimal mesh parameters of the Iguassu GC with different rotor speeds.

## 1. Introduction

Currently, the most effective method for the separation of a large number of isotope mixtures is the gas centrifuge (hereafter GC) [1]. Experimental investigation of flow and diffusion in a rotor of a gas centrifuge is a serious and unsolved problems due to the disturbances which are brought into a rotating flow by the measuring equipment. This makes the theoretical studies of the flow in the gas centrifuge an important tool for finding ways to improve the efficiency of centrifugal separation.

At present, the most effective approach to study high-speed centrifuges is a numerical solution of the system of differential equations describing the flow of gaseous mixture inside the rotor of GC. The accuracy of the results obtained by these calculations depends on the quality of the mesh [3]. To obtain reliable numerical solutions it is necessary to use a computational mesh with small spatial steps due to the complicated flow inside GC with large gradients of hydrodynamic parameters. This mesh discretization leads to compaction of the cells and increase the number of elements of the computational mesh. In this case significantly increases the computational cost and the duration of calculation of the given problem.

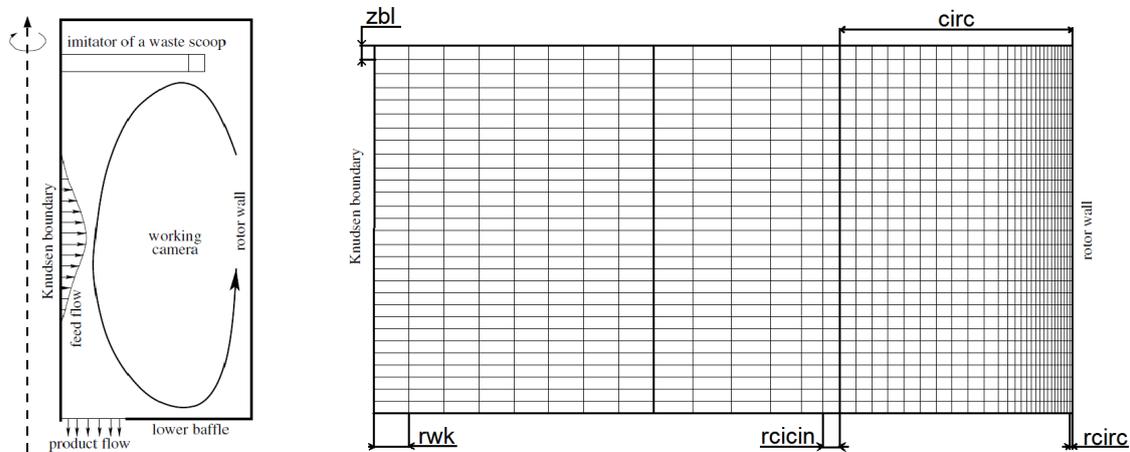
Studying the flow inside the rotor of a GC requires to carry out a large number of calculations. In particular, the determination of the most effective operating regime of a certain GC, one need to carry out up to several hundreds of simulations. Such calculations significantly increase time and computational cost of such investigations.

Thus, obtaining an optimal mesh to achieve high accuracy with an acceptable temporal and computational costs is an important issue. The aim of this study is to search for such a computational mesh that can provide reliable numerical solution that does not require much time and computational costs.



## 2. Model and mesh generation

We use a standard model of a Iguazu GC [7], which has a rotor diameter  $d=12$  cm and the rotor length  $L=1$  m. The modeling was performed in a rotating frame system in a two-dimensional axisymmetric approximation. The computational domain contains working camera and waste chambers located between two coaxial cylinders. The outer cylinder corresponds to the wall of the rotor. The inner cylinder corresponds to the boundary, where the hydrodynamic approximation is not valid [8]. Product chamber is not included in the computational domain. Its influence is simulated by imposing pressure on the wall of the rotor near the lower baffle of the working chamber. The effect of the waste scoop is modeled as a sources of mass, momentum and energy, distributed in small toroidal region [9]. The speed of rotation of the rotor in the range from 600m/s to 900m/s.



**Figure 1.** Scheme of the computational domain and part of mesh near lower baffle.

We use a mesh with a concentration of elements near the wall of the rotor to obtain a reliable solution in the boundary layer. Simultaneously, to ensure correct solutions and proper resolution of the gradients of the variables the refinement of the mesh is smooth, so that the sizes of neighboring cells differ not more than twice. This approach provides a reduction of errors of the interpolation scheme in case of the large gradients of density and pressure. In our problem, mesh is characterized by five parameters.

## 3. Optimization objective function

To find the optimal mesh parameters it is necessary to determine maximum of the objective function that reflects precision and computational cost of numerical solution. Since the main parameter characterizing the work of GC is separative power, we use the deviation of the separation power from the value obtained using the most detailed mesh as a criterion of accuracy. Computational cost is characterized by number of cells in the computational mesh. This value directly affects the duration of the calculation and the required computing resources. These considerations were drawn up the objective function of our problem:

$$f(x_i) = \frac{N_{eta} - N(x_i)}{N_{eta}} \cdot \frac{\delta U_{eta} - \delta U_{res}(x_i)}{\delta U_{eta}}, \quad (1)$$

where  $x_i$ - parameters describing the mesh,  $N(x_i)$ - the number of elements and  $\delta U_{res}(x_i)$ - the deviation from the reference values of the separative power,  $\delta U_{eta}$ - the reference value of the separative power,  $N_{eta}$ - the number of elements in the mesh for reference solution.

To determine the maximum of the objective function (1) we use BOBYQA [4] direct search method, which requires only calculations of the objective function at certain points [5]. This algorithm is included in a library of nonlinear optimization algorithms, NLOpt [6], freely distributed in the Internet.

#### 4. Results and discussion

To obtain the optimal mesh parameters we needed to minimize the number of elements and deviation from the reference values of the separation powers. The reference separative power value was obtained using the most detailed mesh, which apparently provides good accuracy. Reference separative power, mesh parameters and computational costs are shown in tab. 1.

**Table 1.** Reference separative power and mesh parameters.

$v$ , m/s	Mesh parameters					Number of cells	Time, s	Number of cores
	<i>circ</i>	<i>rwk</i>	<i>rcirc</i>	<i>rcircin</i>	<i>zbl</i>			
600	0.1	0.05	0.01	0.04	0.5	1268000	4545.0	72
900	0.1	0.05	0.01	0.02	0.5	625738	2622.7	72

**Table 2.** Calculations with optimal mesh parameters.

$v$ , m/s	Mesh parameters					Number of cells	Time, s	Number of cores
	<i>circ</i>	<i>rwk</i>	<i>rcirc</i>	<i>rcircin</i>	<i>zbl</i>			
600	0.1	0.7	0.01	0.06	6.0	56342	455.1	4
900	0.1	0.2	0.01	0.03	6.0	89080	459.8	9

Using the reference values shown in tab. 1 and the objective function (1) we determine the optimal mesh parameters. Results are shown in tab. 2. It is clear that the number of cells in the computational mesh as well as the number of cores and calculation time using the optimal mesh significantly decrease.

In order to test the accuracy of the calculations using the obtained mesh parameters, we perform the following procedure. On the first step, we determine the optimal separative power of the Iguasu GC using the mesh generated with the optimal parameters on each step of the optimization procedure. The results of the first step are shown in tab. 3. On the second step we calculate the separative power of Iguasu GC in the optimal regime using the most detailed mesh. The results of the second step are shown in tab. 4.

**Table 3.** The results of Iguasu GC optimization using the optimal mesh parameters.

$v$ , m/s	Operating parameters of GC Iguasu				$\delta U$ , c.u.
	$P$ , mmHg	$F$ , mg/s	$\delta T$ , K	$W_{torm}$ , W	
600	154.0	66.9	16.5	9.4	40.4
900	709.9	146.8	18.5	25.0	117.4

It is clear that the results on the most detailed mesh differ less than 0.5% from the results obtained on the optimal mesh. Thus, obtained optimal mesh parameters can be used in precise

**Table 4.** Verification of the optimum on the most detailed mesh.

$v$ , m/s	Number of elements	Calculation time, s	Operating parameters of GC Iguasu				$\delta U$ , c.u.
			$P$ , mm.Hg	$F$ , mg/s	$\delta T$ , K	$W_{torm}$ , W	
600	1268000	6480.6	154.0	66.9	16.5	9.4	40.4
900	625738	2622.7	709.9	146.8	18.5	25.0	116.9

calculations of the Iguasu GC separative power. Obtained parameters allows to reduce the computational costs of the separative power calculations and optimization procedure of the Iguasu GC.

## 5. Conclusions

The results of the optimal mesh parameters for Iguasu GC flow and separation calculations are presented. Optimal parameters were determined for two rotor speeds – 600 m/s and 900 m/s. Calculations using the optimal mesh require significantly less computational costs compared to the calculations on the detailed mesh without loss of accuracy. Obtained mesh parameters can be further used to study hydrodynamic flow inside the rotor to determine the most effective working regime of the Iguasu GC.

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