A homotopy algorithm to solve the problems of flows under strong rotation

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Abstract. A finite difference method for numerical simulation of a high speed rotating flow is improved by applying a homotopy algorithm. As a result a large-scale convergence algorithm is constructed to make numerical simulation of a rotating flow in the 2D axisymmetric model of a gas centrifuge for uranium enrichment. The computing code is verified and then applied for calculation of the flow field in a 2D GC operating in a total reflux mode. The peculiarities of an axial circulation flow in a working chamber of a GC are studied. The conclusion about the rate of attenuation of an axial circulation flow is made on the basis of the results obtained.

Keywords: Gas centrifuge; Homotopy algorithm; Finite difference method; Decay of circulation

1. Introduction
An extremely strong rotating flows are realized inside the modern gas centrifuge (GC) for uranium isotope separation. The pressure and density gradients of a process gas (UF₆) over a radial direction are very large and changing by 5-6 orders on 1 cm near the rotor side wall. It does not allow us to study properties of such flow fields experimentally. That is the reason why the flow field inside a GC is explored already more than 40 years by numerical simulation [1, 2].

The presence of static devices inside a GC, i.e. scoops for extraction of enriched and depleted in the target component fractions, demands the use of 3D modeling in the numerical study of a rotating flow in this apparatus. However, the 2D axisymmetric model is usually taken to study the general regularities of an internal flow structure in a GC to simplify the problem. Kai [3] has applied a staggered mesh finite difference scheme for numerical simulation of nonlinear flow field in a GC when a linear speed of GC rotation was about 500 m/s, whereas the modern GCs have the speed of rotation more than 800 m/s [3]. The studies [3-7] have demonstrated that with increase of a rotation velocity in a GC, the problems associated with the convergence of the obtained numerical solution is also increased.

In this paper it is presented the way to improve the traditional finite difference method (FDM) regularly applied to explore the 2D rotating flow in a GC by its combination with a homotopy method what results to a large-scale convergence algorithm suitable for numerical simulation of nonlinear flow field under strong perturbation.
2. Homotopy algorithm
A homotopy algorithm allows us to take into account the topology in the algebra fields. This makes it a large-scale convergence algorithm[6]. With the development of theory, a homotopy algorithm has been applied in such areas of human activities as economy, electronics, machinery, and many others. Now it became a powerful tool to solve various sets of nonlinear equations, fixed point problem, optimization problem, and so on. The main idea of this algorithm is to construct a homotopy mapping.

Assume that there is an $n$ order system of equations $F(x) = 0$ in the real number field $\mathbb{R}$, and the solutions of this system $x = x^* \in \mathbb{R}^n$ is unknown and to be solved. Then we have a mapping which is

$$F : \mathbb{R}^n \rightarrow \mathbb{R}^n.$$

If there is another $n$ order system of equations $G(x) = 0$ in the field $\mathbb{R}$, and the solutions of this system $x = x_0 \in \mathbb{R}^n$ is already known or easy to get, then we can construct another one mapping.

$$H : \mathbb{R}^n \times [0,1] \rightarrow \mathbb{R}^n$$

Additionally, we can make the new mapping meet the following conditions

$${}\begin{cases} H(x,0) = G(x) \\ H(x,1) = F(x) \end{cases} \tag{1}$$

We call the mapping $H : \mathbb{R}^n \times [0,1] \rightarrow \mathbb{R}^n$ as a homotopy mapping and the problem of solving the system of equations $F(x) = 0$ can be converted to solving the homotopy system of equations $H(x,\alpha) = 0, \alpha \in [0,1]$.

In fact, it is easy to construct a mapping meeting conditions (1). For example, we can construct the following kinds of mapping only from the mathematical point of view ignoring the physics.

$${}\begin{cases} H(x,\alpha) = (1-\alpha)F(x) + \alpha G(x) \\ H(x,\alpha) = \alpha F(x) + G(x) \\ \vdots \end{cases}$$

It is also easy to find that the solution of a homotopy system of equations is a function of a parameter $\alpha$, so a parameter $\alpha$ and the corresponding solution $x(\alpha)$ define a curve in the $n$ dimensional space $\mathbb{R}^n$, which is called a homotopy curve. Additionally, the start and end of a homotopy curve are $x(0)$ and $x(1)$ respectively. They will meet the following conditions

$${}\begin{cases} G(x(0)) = H(x(0),0) = 0 \\ F(x(1)) = H(x(1),1) = 0 \end{cases} \tag{2}$$

The conditions (2) show us that the start of a homotopy curve is the solution of $G(x) = 0$, and the end of a homotopy curve is the solutions of $F(x) = 0$. As we assumed above, the solution of $G(x) = 0$ is known or easy to get, which means that we will have known the start of homotopy curve once the homotopy mapping constructed. Therefore, if we can follow the curve from start to end, we will find the solution of $F(x) = 0$. 

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In sum, the main procedure of carry out a homotopy algorithm is to construct a proper homotopy mapping based on the problem and then to follow a homotopy curve to the end.

3. Homotopy algorithm based on the FDM

3.1. Kai’s FDM

Kai gave us a kind of a FDM with technique of the staggered meshes to solve the 2D axisymmetric Navier_Stokes equations in the paper \(^2\). The dimensionless 2D axisymmetric Navier-Stokes equations are given as follows

\[
\frac{1}{r} \frac{\partial}{\partial r} (r \rho \rho_0 u) + \frac{\partial}{\partial z} (\rho \rho_0 w) = 0, \tag{3}
\]

\[
\rho \frac{\partial u}{\partial r} + w \frac{\partial u}{\partial z} - (2 + \frac{v}{r})u = -[\rho r (T - 1) + \frac{1}{2A} \left( \rho \frac{\partial T}{\partial r} + T \frac{\partial \rho}{\partial r} \right)] + \frac{E}{\rho_0} \left[ \frac{4}{3} \frac{\partial^2 u}{\partial r^2} + \frac{2}{3} \frac{1}{r} \frac{\partial u}{\partial r} \frac{4}{3} \frac{u}{r^2} + \frac{\partial^2}{\partial z^2} \right], \tag{4}
\]

\[
\rho \frac{\partial v}{\partial r} + w \frac{\partial v}{\partial z} + (2 + \frac{v}{r})v = \frac{E}{\rho_0} \left[ \frac{\partial^2 v}{\partial r^2} + \frac{1}{r} \frac{\partial v}{\partial r} - \frac{v}{r^2} + \frac{\partial^2}{\partial z^2} \right], \tag{5}
\]

\[
\rho \frac{\partial w}{\partial r} + w \frac{\partial w}{\partial z} = -\frac{1}{2A} \left[ \rho \frac{\partial T}{\partial r} + T \frac{\partial \rho}{\partial r} \right] + \frac{E}{\rho_0} \left[ \frac{\partial^2 w}{\partial r^2} + \frac{1}{r} \frac{\partial w}{\partial r} + \frac{4}{3} \frac{\partial^2 w}{\partial z^2} \right] + \frac{1}{3} \frac{1}{r} \frac{\partial u}{\partial z} + \frac{1}{3} \frac{\partial^2 u}{\partial r \partial z}, \tag{6}
\]

\[
\rho \frac{\partial T}{\partial r} + w \frac{\partial T}{\partial z} = \frac{\gamma E}{\rho_0 \rho_0} \left[ \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right] - (\gamma - 1) \rho T \left( \frac{\partial u}{\partial r} + \frac{u}{r} + \frac{\partial w}{\partial z} \right) + (\gamma - 1)(2AE\Phi), \tag{7}
\]

where \( \rho_0 = \exp(A(r^2 - 1)) \) is the exponential distribution term, and \( \Phi \) in eq. (7) is the viscous dissipation term in form of

\[
\Phi = \frac{2}{3} \left( \frac{\partial u}{\partial r} + \frac{u}{r} + \frac{\partial w}{\partial z} \right)^2 + 2 \left( \frac{\partial u}{\partial r} + \frac{\partial w}{\partial z} \right)^2 + \left( \frac{\partial w}{\partial z} \right)^2 \tag{8}
\]

\[
+ \left[ \frac{\partial u}{\partial z} + \frac{\partial w}{\partial r} \right]^2 + \left( \frac{\partial v}{\partial z} \right)^2 + \left( \frac{\partial v}{\partial r} - \frac{v}{r} \right)^2.
\]

The dimensionless numbers in the above equations are defined below.
\[ A \equiv \frac{M \Omega^2 r_w^2}{2 R_c T_0}, \quad E \equiv \frac{\mu}{\rho_c r_w \Omega}, \quad Pr \equiv \frac{C_p \mu}{k}, \]

where \( R_0 \) is the universal gas constant, \( T_0 \) is the mean temperature in rotor which we can get from the preset conditions, \( \rho_w \) is a gas density near a rotor wall, \( r_w \) is a rotor radius, and \( \Omega \) is the angular velocity of a rotor. The ideal gas state equation should also be added to the Navier-Stokes equations to make the system be able to solve.

\[ pM = \rho R_c T \tag{9} \]

The reference values to do nondimensionalization are a radius of rotor \( r_w \), a linear speed of rotor rotation \( \omega r_w \), the density near a side wall \( \rho_w \) and the mean temperature in rotor \( T_0 \). The procedure of nondimensionalization is shown below. The variables with a hat symbol “\(^\wedge\)” represent the dimensional quantities.

\[ r = \hat{r} / r_w, \quad z = \hat{z} / r_w, \quad u = \hat{u} / (\omega r_w), \quad v = (\hat{v}_w - \omega r) / (\omega r_w), \quad w = \hat{v}_z / (\omega r_w) \quad \rho = \hat{\rho} / (\rho_w \rho_0) - 1, \quad T = \hat{T} / T_0 - 1 \]

The technique of a staggered mesh is used to discretize equations, and the position of original variables in cell \((i, j)\) is shown in Figure 1. Density \( \rho \) and temperature \( T \) are located in the center of cell, radial velocity \( u \) and angular velocity \( v \) are located in the center of left side of cell, and axial velocity \( w \) is located in the center of down side of cell.

![Figure 1. Schematic diagram of a staggered mesh](image)

The central difference scheme is used to discretize the equations (3-9), and to avoid errors caused by the large density gradient in the equation (3). This equation should be integrated in a cell.

\[
\int_{r_i}^{r_{i+1}} \int_{j}^{j+1} \left[ \frac{1}{r} \frac{\partial}{\partial r} (r \rho \rho_0 \mu u) + \frac{\partial}{\partial z} (\rho \rho_0 w) \right] r dr dz = 0.
\]

The density and temperature in the center of a cell, the radial and angular velocities in a center of the left side of a cell, and the axial velocity in a center of bottom side of a cell can be directly used during the discretization, while the variables in other location will be calculated by a linear interpolation procedure. If the discrete left hand side in the cell \((i, j)\) are represented by \( Y_{\rho u}, Y_{\rho v}, Y_{\rho w}, Y_{\rho T} \), respectively, then one can get the discrete algebra system of the equations below.
The system of equations above is a nonlinear one, and the Newton iteration method can be applied to solve it. If the Jacobian matrix is represented by \( J \), the iteration procedure can be written in a such way as follows.

\[
\begin{align*}
\{ x_0 &= \text{Initial Value} \\
x_{i+1} &= x_i - J^{-1}F(x_i), \ i = 0, 1, 2, \ldots
\end{align*}
\]

Consider a linear system of equations \( J\Delta x = F(x) \), the term \( J^{-1}F(x) \) in the procedure of the Newton iteration can be calculated by solving this system of equations, so there is no need to calculate the Jacobian one.

3.2. A homotopy algorithm based on FDM

The procedure of the Newton iteration in section 3.1 is extremely sensitive to the initial value and the iteration will be diverging when the initial value is much different from the solution. In order to solve this problem, one can improve the Kai’s FDM by using the idea of a homotopy algorithm to get a large-scale convergence tool.

For example, let us take a total reflux GC without upper and lower baffle, all disturbances are spread from the boundary. The disturbance term in the discrete boundary equations should appear. We use \( A(x) \) to represent these disturbance, and the flow field in a GC can be regarded as a superposition of the rigid body solution \( x_0 \) and the disturbance solution \( x_d \). Then we can construct a homotopy mapping as indicated below.

\[
H(x, \alpha) = F(x) + \alpha A(x), \ \alpha \in [0, 1]
\]

Besides, the homotopy mapping will meet a condition that when \( \alpha = 0 \), the solution of the homotopy equation is \( x = x_0 \), which is equal to the rigid body solution as is known, and when \( \alpha = 1 \), the solution of the homotopy equation is \( x = x^* \), which is exactly the solution of the flow field we need. Then, we can follow the homotopy curve from \( x = x_0 \) to the end and get the solution we need.

In order to follow the homotopy curve, we need to calculate the slope of the curve so that we can predict the next point on the curve from the point which is already known. After calculation of the total derivative of the homotopy equation one can get

\[
\frac{\partial H}{\partial \alpha} = \frac{\partial H}{\partial x} \frac{\partial x}{\partial \alpha}
\]  

(10)
The term \(\frac{\partial x}{\partial \alpha}\) is the slope we need and the equation (10) can be regarded as a linear system of equations in which the coefficient \(A = \partial H / \partial x = J\), the right-hand side is \(b = \partial H / \partial \alpha\) and the unknown number is \(z = \frac{\partial x}{\partial x}\).

Now we use the forward Euler interpolation method based on the slope to predict the next point, and after that we use the Newton iteration method to correct the point to the homotopy curve. The step length for the Euler interpolation is adaptable: if the predicted point can be corrected to the curve with the last step length \(d\alpha_{i+1}\), then the next step length will be \(d\alpha_{i+1} = 2d\alpha_{i}\), else the last step length will be reduced by half \(d\alpha_{i+1} = d\alpha_{i+1}/2\).

The pseudocode description of a homotopy algorithm based on a FDM is shown below.

1. Input the initial value \(x_0\), the initial step of the length \(d\alpha_0\) and set the parameter \(\alpha_0 = 0\);
2. Continue while \(\alpha < 1\).

**Prediction step**

Predict the next point by the forward Euler interpolation: \(x'_{i+1} = x_i + d\alpha_i \frac{\partial x}{\partial \alpha}\), and set the parameter \(\alpha_{i+1} = \alpha_i + d\alpha_i\).

**Correction step**

Solving the system of equations \(H(x, \alpha_{i+1}) = 0\) by the Newton iteration method with the initial value \(x'_{i+1}\), and the upper limit of a number of iterations is \(n_i\), and the upper limit of an error is \(\epsilon_i\).

If the iteration converged within the \(n_i\) iterations and get the point on the curve \(x_{i+1}\),

- calculate the next step length \(d\alpha_{i+1} = \min(2d\alpha_i, 1 - \alpha_{i+1})\), and do the next loop,
- else decrease the step length \(d\alpha_i = d\alpha_i / 2\), and do the loop again,
end.

3. Output the result \(x^*\).

4. Verification of a homotopy algorithm based on the FDM

For verification of a created computing code we consider a total reflux GC with a length of a rotor 1m and other parameters corresponding to the Iguassu GC model. The parameters of the model GC and the process gas are shown in Table 1 and Table 2.

The comparisons of results calculated in this paper and the data obtained by Bogovalov[11] playing a role of a benchmark for our code are shown in Figures from 2a, b to 6. It can be seen from the comparison that the constructed homotopy algorithm based on the FDM in this research can be used to simulate the flow field in GC.

| Table 1. Parameters of the Iguassu model GC |
|---------------------------------------------|
| Parameter                                    | Value   |
| \(V\), linear speed of rotor wall            | 600 m/s |
| \(P_w\), pressure near rotor wall            | 80 mmHg |
| \(T_o\), mean temperature in rotor           | 300 K   |
| \(R_{out}\), rotor radius                    | 0.06 m  |
| \(R_{in}\), inner boundary radius            | 0.048 m |
| \(\Delta T\), maximum of temperature disturbance | 0.3 K  |
Table 2. Parameters of the process gas

| Parameter        | Value                       |
|------------------|-----------------------------|
| $M$, molecular weight | 0.352 kg/mol                |
| $\mu$, dynamic viscosity | 1.83×10^{-5} Pa·s           |
| $k$, heat conductivity | 6.1×10^{-3} W/m/K          |
| $C_p$, specific heat | 372.84 J/kg/K              |
| $\gamma$, specific heat ratio | 1.068                 |

Figure 2. Comparison of the flow fields

(a) calculated in this paper.  
(b) calculated in the paper[1]

Figure 3. Comparison of disturbance for the radial velocity in the cross-section 1 in Figure 2b.

Figure 4. Comparison of the angular velocity disturbance in the cross-section 1 in Figure 2b.

Figure 5. Comparison of the axial velocity disturbance in the cross-section 2 in Figure 2.

Figure 6. Comparison of Temperature disturbance in the cross-section 1 in Figure 2.
5. Simulation of flow field in GC under strong disturbance

5.1. Introduction to the case
In this case, the total reflux GC without upper and lower baffle is used for research and all parameters of a GC correspond to the Iguassu model GC. The mechanical drive disturbance is located in the lower boundary, the end cap thermal drive disturbance is applied both in the upper and lower boundaries, and the side wall thermal drive disturbance is placed on a rotor wall boundary. The schematic diagram of the boundaries mentioned above is shown in Figure 7 and listed in Table 3.

The parameters of a process gas are the same as in Table 2. The inner boundary is free one and the boundary conditions on it are as follows

\[
\frac{\partial \rho}{\partial r} = 0, \quad u = 0, \quad \frac{\partial}{\partial r} \left( \frac{v}{r} \right) = 0, \quad \frac{\partial w}{\partial r} = 0, \quad \frac{\partial T}{\partial r} = 0
\]

Table 3. Parameters of a case under strong disturbance condition

| Parameter                        | Value     |
|----------------------------------|-----------|
| \(L\), length of rotor           | 0.48 m    |
| \(r_o\), radius of rotor         | 0.06 m    |
| \(r_{in}\), radius of inner boundary | 0.048 m  |
| \(V\), linear speed of rotor wall | 600 m/s   |
| \(P_w\), pressure near rotor wall | 100 mmHg  |
| \(T_0\), mean temperature in rotor | 300 K     |
| \(\Delta T_{up}\), temperature disturbance on upper endcap | -30 K     |
| \(\Delta T_{down}\), temperature disturbance on lower endcap | 30 K      |
| \(\Delta T_w\), temperature disturbance on rotor wall | -30 K – 30 K linear distribution |
| \(\Delta \Omega / \Omega\), mechanical disturbance on lower endcap | 40%       |

Note that the thermal and mechanical drives mentioned above are strong enough. The flow field is simulated by a homotopy algorithm based on the FDM and the iteration is convergent.

5.2. Results of numerical simulation results
Results of the density, velocity, temperature and stream lines distributions found in this research are presented in Figures from 8 to 13. It can be seen that the flow field in a total reflux GC without baffle under such disturbances is much different from the simple rigid body solution, the radial and axial velocities reach tens of meters, and this cannot be ignored comparing to the linear speed of the rotor wall. Because of the strong mechanical disturbance, the distribution of the angular velocity is also much different from the linear distribution in the rigid body solution.
Also, we use the maxima of the stream function in various cross-sections of a GC as the metrics of the axial circulation intensity. One can see in Figure 14, the dependence of the axial circulation intensity in the following cross-sections of a GC: 1/8, 2/8, 3/8, 4/8, 5/8, 6/8 and 7/8. The behavior of the axial circulation is shown in Figure 14. It can be seen that the circulation intensity under the condition of strong mechanical and thermal drives has a parabolic character.
6. Conclusions
1. It is demonstrated that the FDM can be radically improved by a homotopy algorithm what allows us to construct a large-scale convergence algorithm and on its basis a computing code.
2. The new algorithm is verified and proved to be valid using as a benchmark the data obtained for the model GC Iguassu by means of the independent algorithm.
3. Using the maxima of the stream function in various cross-sections of a total reflux GC as the metrics for the axial circulation intensity it is found that its damping along the axial coordinate has a parabolic character.

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