Homotopic method applied to solving the flow field in a gas centrifuge

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Abstract. To investigate the flow field in a hyper-speed gas centrifuge, a hybrid difference scheme is used to discretize the axisymmetric Navier-Stokes equation. Source terms are included to simulate the injection and extraction of gas, also the mechanical drive of the scoops. The nonlinearity is obvious as the drive is strong. A Newton iteration used to solve the equation system becomes sensitive to the initial guess of the solution, which makes it difficult to converge. A homotopic method with self-adaptive steps is adopted to cope with this problem and to accelerate the iteration process. Numerical experiments simulating different strengths of scoop drive prove the effectiveness of the algorithm.

1. Introduction
Hyper-speed gas centrifuges are elementary devices to separate isotope mixtures. The injection and extraction of working gas, the temperature distribution on the rotor wall of a centrifuge and the drag effect exerted by the extraction scoops stimulate a complex secondary flow inside the rotor, which has very important influences on the separation power of the centrifuge. Due to the high speed of present centrifuges (over 600m/s), it is very difficult to study the flow field experimentally. As a result, numerical study is more preferable.

A traditional way of numerically simulating a centrifuge flow field is to use linearized N-S equations, e.g., work by Cloutman [1], Dickinson [2], Kozlov [3]. However, only when the effects stimulating the secondary flow (drive effects) are not strong, the linearized models can give reasonable predictions. More precise models use the nonlinear N-S equations. Typical works include Lahargue [4], Harada [5], Kirkpatrick [6], Kai [7][8][9], and Omnes [10], etc. To solve the resulting nonlinear algebraic equation system, usually an iterative method, for example a Newton iteration, is applied. In the case of strong drives, the flow field presents strong nonlinearity and the iteration process becomes sensitive to initial solution, making it difficult to converge or divergent. Therefore, the stability and speed of an iteration method is very important for successful numerical simulation of a gas centrifuge flow field.

Here we present a predictor-corrector homotopic method to accelerate Newton iteration for solving centrifuge flow field. A self-adaptive step strategy is used to obtain fast and robust convergence. To show the effectiveness of the method, simulation of the flow field in an Iguassu model centrifuge is performed. Different drive effects are considered, and the mechanical drive of scoops is adjusted to simulate the disturbances of the flow field with different strengths. Numerical experiment results prove the robustness of the method. A simple separation analysis is also carried out to show the flexibility and success of the method in dealing with different combinations of drive effects.
2. Computational Model

Here the axisymmetric N-S equations in cylindrical coordinates are used to describe the flow field inside a gas centrifuge rotor. The characteristic quantities \( a \) (radius of the rotor), \( \omega a \) (rotor peripheral speed), \( p_w \) (pressure on rotor wall at rigid body rotation) and \( T_0 \) (average temperature along rotor wall) are used to nondimensionalize the equation system:

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \rho \rho w u \right) + \frac{\partial}{\partial z} (\rho \rho w w) = \dot{m}
\]

(1)

\[
\rho \rho w \left[ u \frac{\partial w}{\partial r} + w \frac{\partial u}{\partial z} - \frac{(r + v)^2}{r} \right] + \frac{1}{2A} \frac{\partial}{\partial r} (\rho_w p) = F_i + E_G i + \dot{m}(u_m - u)
\]

(2)

\[
\rho \rho w \left[ u \frac{\partial v}{\partial r} + w \frac{\partial v}{\partial z} + u \left( 2 + \frac{v}{r} \right) \right] = F_0 + E_G w + \dot{m}(v_m - v)
\]

(3)

\[
\rho \rho w \left[ u \frac{\partial w}{\partial r} + w \frac{\partial w}{\partial z} \right] + \frac{1}{2A} \rho_w \frac{\partial p}{\partial z} = F_z + E_G z + \dot{m}(w_m - w)
\]

(4)

\[
\rho \rho w \left[ u \frac{\partial T}{\partial r} + w \frac{\partial T}{\partial z} \right] + (\gamma - 1) \rho \rho w \left[ \frac{\partial u}{\partial r} + u \frac{\partial v}{\partial z} \right] = (\gamma - 1) \left( 2AE \Phi + \dot{\theta} \right) + \frac{2E}{Pr} G_t
\]

\(+ \dot{m} \left( (T_m - T) + (\gamma - 1) A \left[ (u_m - u)^2 + (v_m - v)^2 + (w_m - w)^2 \right] \right) \]

(5)

where \( \gamma \), \( A \), \( E \) and \( Pr \) are the specific heat ratio, speed factor, Ekman number and Prandtl number respectively. The source terms \( \dot{m} \), \( F = (F_i, F_w, F_e) \) and \( \dot{\theta} \) are included to simulate the gas injection (or extraction), mechanical drives and heat production in the rotor.

Variables \( \rho \), \( T \) and \( \mathbf{V} = (u, v, w)^T \) in the equations represent the deviations of the gas density, temperature and velocity from the rigid body rotation state, whose density variation is exponential:

\[
\rho_0 = \exp \left[ A \left( r^2 - 1 \right) \right]
\]

(6)

so the dimensionless density and temperature of the flow field is \( \rho \rho_0 \) and \( T \), and the dimensionless velocity field is \( \dot{u}, r + v, w \).

For simplicity, we use symbols \( G_i \), \( G_w \), \( G_z \) and \( \Phi \) to represent the dissipative terms in the momentum equations and energy equation, \( G_t \) to represent the thermal diffusion term in the energy equation, which have the following forms, respectively:

\[
G_i = \frac{4}{3} \left( \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} - \frac{u}{r^2} \right) + \frac{\partial^2 w}{\partial z^2} + \frac{1}{3} \frac{\partial^2 w}{\partial r \partial z}
\]

(7)

\[
G_w = \frac{\partial^2 v}{\partial r^2} + \frac{1}{r} \frac{\partial v}{\partial r} - \frac{v}{r^2} + \frac{\partial^2 v}{\partial z^2}
\]

(8)

\[
G_z = \frac{\partial^2 w}{\partial r^2} + \frac{1}{r} \frac{\partial w}{\partial r} + \frac{4}{3} \frac{\partial^2 w}{\partial z^2} + \frac{1}{3} \frac{\partial u}{\partial z} + \frac{1}{3} \frac{\partial^2 u}{\partial r \partial z}
\]

(9)
\[ G_r = \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \]  \tag{10}

\[ \Phi = -\frac{2}{3} \left( \frac{\partial u}{\partial r} + \frac{u}{r} + \frac{\partial w}{\partial z} \right)^2 + 2 \left[ \left( \frac{\partial u}{\partial r} \right)^2 + \left( \frac{\partial w}{\partial z} \right)^2 + \left( \frac{u}{r} \right)^2 \right] + \left[ \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial r} \right)^2 + \left( \frac{\partial v}{\partial z} \right)^2 + \left( \frac{\partial v}{\partial r} - \frac{v}{r} \right)^2 \right] \]  \tag{11}

In addition, the perfect gas assumption is used and the dimensionless state equation is given below:

\[ p = \rho T \]  \tag{12}

To determine the solution to this system, we adopt the following boundary conditions:

On solid walls:

\[ \mathbf{v}_b = 0, \quad \left( \frac{\partial \rho}{\partial n} \right)_b = 0, \quad T_b = T_{\text{wall}} \]  \tag{13}

On the vacuum core boundary (at the radius position \( r_{in} \)):

\[ \left( \frac{\partial \rho}{\partial r} \right)_{in} = \left( \frac{\partial T}{\partial r} \right)_{in} = \left( \frac{\partial w}{\partial r} \right)_{in} = 0 \]  \tag{14}

\[ u = 0 \]  \tag{15}

\[ \left( \frac{\partial (v/r)}{\partial r} \right)_{in} = 0 \]  \tag{16}

As the above boundary conditions impose no restriction on the gas content in the rotor, a subsidiary condition restricting the holdup \( H \) of the centrifuge should be provided:

\[ \iiint_V \rho d\tau = H \]  \tag{17}

The integration here is carried out over the volume of the centrifuge considered.

3. Numerical Method

The N-S equations are discretized on a staggered grid [7][10]. To suppress non-physical oscillations in advection dominating grid cells, a hybrid scheme is used to discretize the convection terms. If the grid Reynolds number \( R_\Delta \) is less than 2, a second-order central difference scheme is used, otherwise a first-order upwind scheme is adopted.

To solve the resulting discretized nonlinear equation system, usually iterative methods are applied. A widely used method is the Newton iteration. However, achieving convergence is not always an easy task if the system has a strong nonlinearity. In this circumstance, the iteration process can be sensitive to the initial guess: if the initial guess is not close enough to the real solution, the iteration may converge very slowly or even diverge.

In computations of various areas, employing the continuation technique or homotopic method is a strategy to tackle such a problem [11]. We will demonstrate in the following how to use it to accelerate and stabilize the iteration process in solving the N-S equations.
3.1. Concept and implementation of homotopic method

Here we briefly introduce the basic concept of homotopic method. As our target is to apply the technique to the problem of solving centrifuge flow field, no detailed mathematical discussion is given. Readers with interest are referred to reference [11].

Suppose the nonlinear equation system to be solved is denoted as a $\mathbb{R}^n \mapsto \mathbb{R}^n$ mapping:

$$ F(X) = 0 $$

Let us define another $\mathbb{R}^{n+1} \mapsto \mathbb{R}^n$ mapping called $H(X, \alpha)$, which satisfies the following conditions:

$$
\begin{align*}
H(X, 0) &= G(X) \\
H(X, 1) &= F(X)
\end{align*}
$$

where $G(X)$ is a function with known zeros.

The solution set of system $H(X, \alpha) = 0$ forms a curve $c(\alpha)$ in $\mathbb{R}^{n+1}$ with $\alpha$ as its parameter. Curve $c$ connects $X_0$, the solution of $G(X) = 0$, with the final solution $X^*$. If we can trace this curve, the final solution can be achieved. Since $c$ is called a homotopic curve, this solution technique is known as homotopic method.

According to the definition of homotopic curve:

$$ H(c(\alpha), \alpha) = 0 $$

Differentiating the equation with respect to $\alpha$:

$$ H'(c)c'(\alpha) = 0 $$

where $H'(c) = (\partial H / \partial X)$ and $c'(\alpha) = dc / d\alpha$, then we have an initial value problem as follows:

$$ H'(c)c'(\alpha) = 0 $$

$$ c(0) = X_0 $$

This problem can be solved by many numerical methods, such as Euler method, Runge-Kutta method, etc. Here we present a predictor-corrector homotopic method:

**Algorithm A**

1. Assign the starting point $c(0) = X_0$ and step length $h$. Let $\alpha_0 = 0$ and $n = 0$.
2. Solve the linear equation system (22) and obtain the solution $c'(\alpha_n)$.
3. Calculate the predictor $\tilde{c}(\alpha_n) = c(\alpha_n) + hc'(\alpha_n)$. Let $\alpha_{n+1} = \alpha_n + h$.
4. Solve the nonlinear equation system $H(c(\alpha_{n+1}), \alpha_{n+1}) = 0$ with $\tilde{c}(\alpha_n)$ as the initial guess.
5. If $\alpha_{n+1} = 1$, then $X^* = c(\alpha_{n+1})$ is the final solution, or otherwise let $n := n + 1$ and go to (2).

In Algorithm A the predictor step (3) uses Euler method to trace the next point on the curve. The corrector step (4) uses a nonlinear solver to correct the prediction. As our aim is to get the final solution $X^*$, i.e., the end of curve $c$, the precision requirement for the intermediate tracing points can be relaxed to save computation cost. Therefore, a Newton method as the corrector step’s nonlinear solver is sufficient. A convergence requirement $\varepsilon_1$ controls the solver precision.
Note that Algorithm A uses a constant step length, which may be costly because \( h \) should be small for the first few steps and larger for the rest steps. So Algorithm A is modified by using a self-adaptive step strategy as follows:

Algorithm B

(1) Assign the starting point \( c(0) = X_0 \) and step length \( h \). Let \( \alpha_0 = 0 \) and \( n = 0 \).

(2) Solve the linear equation system (22) and get the solution \( c'(\alpha_n) \).

(3) Calculate the predictor \( \hat{c}(\alpha_n) = c(\alpha_n) + h c'(\alpha_n) \). Let \( \alpha_{n+1} = \alpha_n + h \).

(4) Solve the nonlinear equation system \( H(c(\alpha_{n+1}), \alpha_{n+1}) = 0 \) with \( \hat{c}(\alpha_n) \) as the initial guess. The convergence requirement is \( \| H(c(\alpha_{n+1}), \alpha_{n+1}) \| < \varepsilon_1 \). If convergent within \( N \) steps, go to (5), or otherwise, let \( h := h/2 \) and go to (3).

(5) If \( \alpha_{n+1} = 1 \), solve the nonlinear system \( H(X^*, 1) = 0 \) with \( c(\alpha_{n+1}) \) as the initial guess, or otherwise let \( h := 2h \), \( n := n + 1 \) and go to (2).

3.2. Homotopic mapping for GC N-S equations

In this section we will illustrate the way to construct the homotopic mapping \( H \) for the N-S equations in a gas centrifuge. Previous study shows the main factors to cause large disturbances in the rotor are the gas injection of the feed flow and mechanical drive exerted by the extraction scoops. In our model, these effects are simulated by the N-S equation system with source terms:

\[
F(X) = G(X) + S(X) = 0
\]  

(24)

where \( G(X) \) is the discretized N-S equation system without source terms and \( S(X) \) is an \( \mathbb{R}^n \) vector for the source terms.

We suggest constructing \( H \) as the following:

\[
H(X, \alpha) = G(X) + \alpha S(X)
\]  

(25)

The equation system \( G(X) = 0 \) is relatively easy to solve because there are no large disturbances introduced in the flow field, as in the case of the rigid body rotation. With this solution as the initial guess \( X_0 \), the homotopic method in above sections can be performed.

4. Numerical experiments and discussion

In this part we present some results of numerical experiments to show the effectiveness of the homotopic method. The simulated model centrifuge is an Iguassu model. Table 1 presents the main working parameters of the centrifuge.

To simulate the flow field with different strengths of disturbances, we adjust the strength of the momentum source terms \( F \). In the previous studies, different methods simulated the influence of scoops, such as those in [5][6][9][10]. An intuitive model is to use a disk rotating at a different speed from the rotor [5][6]. We imitate this model to set the strength of \( F \) as in equation (26).

\[
F_\theta = \frac{4\pi}{3\delta_h} E \left( \frac{\Delta \Omega}{\Omega} \right) \left( \frac{r_2^3 - r_1^3}{V} \right)
\]  

(26)

where \([r_1, r_2]\) is the radial range of the source; \( \Delta V \) is the volume of the source; \( \delta_h \) and \( \Delta \Omega/\Omega \) are, respectively, an estimate of the thickness and the relative difference of the rotation speed of the disk.
model. In this way, the retardation effect of the angular momentum source term is approximately the same as a disk model with a $\Delta \Omega$ difference in the rotation speed.

### Table 1. Main working parameters for the Iguassu model centrifuge

| parameter                      | value     |
|-------------------------------|-----------|
| angular speed $\Omega$ (rad/s)| $1.0 \times 10^4$ |
| mean temperature $T_0$ (K)    | 300       |
| waste end temperature $T_{\text{bot}}$ (K) | 300.5 |
| product end temperature $T_{\text{top}}$ (K) | 299.5 |
| wall pressure $p_w$ (kPa)      | 13.33     |
| feed flow rate $F$ (mg/s)      | 12        |
| flow cut $\theta$             | 0.5       |

A $116 \times 256$ mesh is used to discretize the equations. Five cases with different strengths of scoop drive are considered. A direct Newton method, Algorithms A and B are tested on these cases. The Newton method fails in all cases, and the comparison between the two homotopic methods are shown in table 2, where CT is the number of total P-C steps used and IT is the total Newton iteration count. The maximum allowed IT is 150.

From table 2 we see the maximum $\Delta \Omega / \Omega$ reaches 100%, which means that the retardation effect of the angular momentum sink approximates a still disk in the gas. In these cases, the flow field definitely deviates from the rigid body rotation state, especially in the extraction chambers. Consequently, the direct Newton method fails to converge. Algorithm A fails in the last 2 cases because the step length must keep small enough, resulting in too large a total number of iterations. In contrast, Algorithm B adjusts its step lengths whenever needed and the computation cost can be reduced significantly.

### Table 2. Comparison between two homotopic algorithms

| case | $\Delta \Omega / \Omega$ (%) | Algorithm A | Algorithm B |
|------|-----------------------------|-------------|-------------|
|      |                             | CT | IT | CT | IT |
| 1    | 10                          | 15 | 38 | 7  | 49 |
| 2    | 20                          | 28 | 66 | 8  | 54 |
| 3    | 40                          | 37 | 96 | 10 | 72 |
| 4    | 80                          |    |    | 11 | 84 |
| 5    | 100                         |    |    | 11 | 100|

In figure 1 stream lines with $\Delta \Omega / \Omega = 0$ and 10% are shown. The stream lines are derived from the stream function defined as below [12]:

$$
\frac{\partial \psi}{\partial r} = r \rho \rho \psi, \quad \frac{\partial \psi}{\partial z} = -r \rho \rho \mu - \int r \hat{m}^* \, dr^* 
$$

After the introduction of mechanical drive, the stream lines change a lot. Without any mechanical drive, the thermal drive along the rotor wall forms a circulation near the wall. The feed flow drives two reverse small circulations, which have an adverse effect on the separation process. In the case with
a 10% mechanical drive, the thermally driven circulation has a larger range: the gas flows from the inner hole of the waste baffle, reflects on the product baffle, and returns to the waste chamber through the outer hole of the waste baffle. However, there is still a strong reverse circulation stimulated by the product scoop. This is probably because the product mechanical drive is too strong. In order to achieve a satisfactory separation efficiency the strength of the mechanical drive should be optimized.

Figure 1. Stream lines with different strengths of mechanical drives

Figure 2 shows the angular velocity perturbation in the radial direction at \( z = 0.2 \) in the waste chamber. It is clear that in some areas of the rotor, the gas slows down, exceeding over 50% of the peripheral speed. This is by any means not a small perturbation, and, therefore, a linear model cannot and should not be used to simulate flow in these regions.

Figure 2. Angular velocity perturbation on cross section \( z = 0.2 \)
5. Conclusion
A hybrid difference scheme is used to discretize N-S equations in a gas centrifuge. In cases with large perturbations, solving the resulting nonlinear equation system is difficult because of the sensitivity to initial solution by using a traditional iterative method. A predictor-corrector homotopic method with adaptive steps is applied to solve this problem. Basic concept and also implementation procedure are presented.

Numerical experiments computing the flow fields of the Iguassu model centrifuge with different strengths of scoop mechanical drive verify the effectiveness of the proposed method. The results also show the strong nonlinearity in the extraction chambers of the gas centrifuge, which prove the necessity of using a nonlinear model in simulating the flows in these regions.

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