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Optimization Studies for Gas Centrifuges

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ABSTRACT

In this paper we give a brief introduction to the Onsager pancake model for the fluid dynamics of a gas centrifuge and a history of the pancake computer code. We then present a comprehensive study of separative performance using the hypothetical gas centrifuge parameters of the so-called "Iguaçu machine." In particular, we present: (a) the optimal parameters (feed, wall pressure, temperature profile, scoop drive, position of product and waste orifices) for the maximum separative power for UF_6; (b) study of the sensitivity for this machine of all these parameters around the optimum; (c) modeling of the scoop chamber (waste scoop) by a countercurrent flow through the chamber rather than sources/sinks; (d) general laws describing optimal parameters, such the wall pressure or position of product orifice, as functions of the speed, radius, and length; and (e) a general law for the optimum separative work. These results provide a benchmark for comparing the predictions of the pancake model with the predictions of other models.

I. INTRODUCTION

The late Nobel laureate, Lars Onsager, developed a mathematical model that describes the internal flow along the sidewall in a gas centrifuge. The model was presented to the US Atomic Energy Commission in an unpublished report

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(1965). In another unpublished report, Carrier and Maslen (1966) studied the Ekman boundary layers on the end caps of the centrifuge. Wood and Morton (1) used these results to produce a model of the complete centrifuge flow field and implemented this mathematical model in the pancake computer program.

Subsequently, Wood developed a complementary computer code to solve the binary concentration gradient equation of Cohen (2) and Onsager, and to optimize the separative work as a function of the magnitudes of the various countercurrent drives. The first version of the pancake code was developed to run on a mainframe computer, and an early PC version was developed by Gary Sanders at Oak Ridge Gaseous Diffusion Plant circa 1985. A modern PC version was completed by Mason at the University of Virginia in 1995, and the program to solve the concentration gradient equation was extended to the case of multicomponent mixtures. This work was reported by Wood et al. (3). Since that time, one of the present authors (P.R.) has made extensive modifications to this computer model to make it easier to use and to allow for more complete optimization of the parameters.

In this paper we use the gas centrifuge parameters of the Iguaçu machine (4) to optimize the performance for the binary separation of UF_6. We also study the multicomponent separation of spent uranium fuel from power reactors.

Parametric studies are presented here that examine the sensitivity of the separative performance with respect to each of the controllable parameters: feed rate, temperature difference, and scoop drive using two different models to simulate the action of the waste removal scoop. In these calculations we use a wall pressure of 60 torr (8×10^3 Pa) to ensure that the UF_6 will remain a gas at the average temperature of 300 K. The general law of the similarity parameter $H = B/(L/a)$ (where B is the parameter of the pancake equation defined in the next section, L is the separative length of the centrifuge, and a is its radius) is demonstrated. It is shown that for lengths of 1 to 5 meters and peripheral speeds of 500 to 800 m/s, the optimum value of separative performance in a binary mixture of UF_6 occurs at a value of the similarity parameter of $H \approx 10$.

In the next section the pancake model is described as well as the method of simulating the introduction of feed and removal by scoop of the waste stream. In Section III. the optimization of binary and spent fuel mixtures is presented, and parametric studies are presented in Section IV. The conclusions are given in the final section.

II. PANCAKE MODEL

II.1. Onsager Pancake Equation

The derivation and solution of the equations has been reported (1, 5). In this model the solution to the equations of motion for a viscous heat-conducting compressible ideal fluid is represented as a first-order perturbation about solid

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body isothermal flow in a right circular cylinder. The perturbation equations can be combined into a single sixth-order, linear partial differential equation

$$(e^x(e^x\chi_{xx})_{xx})_{xx} + B^2\chi_{yy} = F(x, y) \quad (1)$$

where χ is a master potential from which the physical variables can be extracted. The independent variable $x = A^2[1 - (r/a)^2]$ is the radial scale height or e-folding distance for the density, and $y = z/a$ is the axial position z nondimensionalized by a. The variable $B^2 = \mathrm{Re}^2S/16A^{12}$ is a parameter containing the physical description of the particular rotor and operating parameters. In particular $\mathrm{Re} = \rho_w\Omega a^2/\mu$, where ρ_w is the density at the wall, Ω is the frequency of rotation, and μ is the viscosity where the bulk viscosity has been taken to be 0. The quantity $S = 1 + [\mu(\Omega a)^2/4KT_0]$ is a thermodynamic variable where K is the thermal conductivity of the gas. The speed parameter is $A^2 = \Omega^2a^2/2RT_0$ where T_0 is the average temperature of the gas and R is the specific gas constant.

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The nonhomogeneous term $F(x, y)$ arises from internal sources or sinks of mass, momentum, or energy which are used to model the introduction of feed gas from the axis and the removal of angular momentum by the stationary scoop and is written

$$F(x,y) = \frac{\mathrm{Re}}{32A^{10}}\left[\int_x^{x_T}(Z_y - 2V_y)dx' - [(e^xU_y)_x + (e^xW)_{xx}]\right] - \frac{B^2}{4A^4}\int_x^{x_T}\int_0^{x'} M_y dx''dx' \quad (2)$$

x_T is the x position of the inner boundary, or top of the atmosphere, where conditions of no shear and no heat flux are imposed. Numerical experiments have shown that $x_T = 15$ is large enough to ensure that the solution is independent of the choice of x_T. Here M, U, V, W, and Z are dimensionless quantities which represent source terms in the conservation equations for mass, momentum, and energy. In terms of the dimensional physical variables, the mass source (per unit time and volume) is M_s, and the sources of momentum and energy, with no feed origin, are respectively $\vec{F} = (F_r, F_\theta, F_z)$ and R_s. The mass is introduced at $r = r_s$ with a velocity $\vec{V}_s = (V_r, V_\theta, V_z)$. The local velocity of the rotating gas is assumed to be given by solid body rotation $\vec{q} = (0, \Omega r_s, 0)$ with local density and pressure ρ and p. The total specific internal energy is called E (subscript s for source). The quantities in Eq. (2) are related to these physical variables as follows:

$$M = M_s/\rho_w\Omega \quad (3a)$$

$$U = (M_sV_r + F_r)/\rho_w\Omega^2 a \quad (3b)$$

$$V = (\mathrm{Re}/4A^4)[M_s(V_\theta - \Omega r_s) + F_\theta]/\rho_w\Omega^2 a \quad (3c)$$

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$$W = 2A^2\,[M_sV_z + F_z]/\rho_w\Omega^2 a \tag{3d}$$

$$Z = (1/4A^4)\left[R_s + (E_s - E) + \frac{1}{2}M_s(\vec{V}_s - \vec{q})^2 - (p/\rho)\right] \tag{3e}$$

When the axial variable z is scaled by the separative length, $\zeta = z/L$, the computational domain of the Pancake model is $(x,\zeta) \in [0,\infty] \times [0,1]$, and is not machine dependent. Defining $H = Ba/L$ as the ratio of B by the aspect ratio L/a, we obtain

$$(e^x(e^x\chi_{xx})_{xx})_{xx} + H^2\chi_{\zeta\zeta} = F(x,\zeta) \tag{4}$$

For simplicity, assume that all perturbations are modeled by boundary conditions, with no volume source. Then Eq. (4) is homonegeous, and two machines characterized by the same H parameter and the same locations of the perturbations on the boundaries in the (x,ζ) plane are modeled by the same Eq. (4) with the same boundary conditions. Thus, the two machines lead to the same solution of Eq. (4). H appears to be the similarity parameter of the homogeneous part of Eq. (4).

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II.2. Feed Model

At high rates of rotation, the gas is compressed into a narrow annular region near the cylinder wall and a very good vacuum is established in the center region of the centrifuge. The feed gas is introduced from a hole in the pipe which is located along the axis of rotation. We will simplify the study of the test case, assuming no energy or momentum exchange. Therefore the source terms for our feed model are

$$M = M_s/\rho_w\Omega \tag{5a}$$

$$U = V = W = Z = 0 \tag{5b}$$

This feed model is, in fact, close to the one called F1 by Wood (6), where only mass is introduced at a radial location $x = x_T$. We suppose here that after gas expansion, the mass is introduced in the dense region of the rotating gas. The radial position r_s (x_s for x position) is where the mean free path $\lambda(r_s)$ is equal to a local density scale height. So

$$\lambda(r_s) = \left(\frac{1}{\rho}\frac{\partial\rho}{\partial r}\right)^{-1}_{r=r_s} \qquad \text{with } \rho = \rho(x=0)e^{-x} \tag{6}$$

II.3. Mechanical Countercurrent

II.3(1). With Scoop in the Fluid

The mass that is introduced by the feed F is removed through two boundaries for product P and waste W. Referring to Fig. 1, the bottom scoop is sup-

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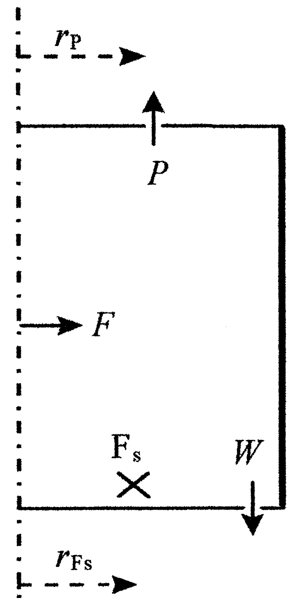

FIG. 1 Scheme of the model with scoop in fluid. The scoop drag is a Dirac delta function: $F_s = \delta(r - r_{Fs}, y)$.

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posed to be at the extremity of the centrifuge of length L and in $r = r_{F_s}$. This scoop is stationary and acts as a source (a sink) of angular momentum. Therefore, $\vec{F} = (0, F_\theta, 0)$, where F_θ is the source of angular momentum exerted by the scoop on the fluid. The source model for the scoop is then

$$M = U = W = Z = 0 \tag{7a}$$

$$V = (\mathrm{Re}/4A^4)F_\theta/\rho_w\Omega^2 a \tag{7b}$$

After integration of F_θ over the volume, we obtain the drag force F_s (which has a negative value). In practice, we locate F_s at the bottom of the centrifuge ($y = 0$), and take a Dirac delta function: $F_s = \delta(r - r_{Fs}, y)$.

II.3(2). With Scoop in the Chamber

An alternate way to model the action of the scoop is to model the return flow from the chamber R_c as shown in Fig. 2. In this case the modeled part of the centrifuge does not include the chamber, and the scoop effects are taken into account only through the return flow R_c. Then there is no source term (Eq. 4) for the scoop, and we must determine the magnitude of the return flow rather than the magnitude of the scoop drag. The results presented in the next section show that the same value of the maximum performance is found with both methods of modeling the mechanical countercurrent drive of the scoop.

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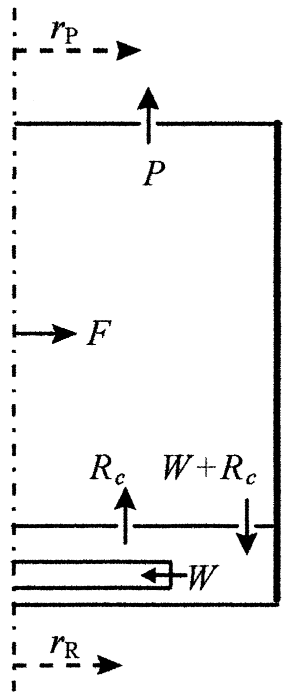

FIG. 2 Scheme of the model with scoop in the chamber. The scoop effects are taken into account through the return flow R_c; the modeled part of the centrifuge does not include the scoop chamber.

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II.4. Optimization of Centrifuge Parameters

II.4(1). Scheme for Hydrodynamic Parameters

The geometry of the centrifuge plays an important role in determining the hydrodynamic flows in the centrifuge. The geometric parameters that are considered in the scheme are: 1) the radial location of the product and waste removal holes r_p and r_w; 2) the radial location of the scoop source terms r_{F_s} (location of the Dirac source of momentum) or the radial location of the scoop chamber return flow r_R; 3) separative length L and radius a of the centrifuge; and 4) axial location of the feed introduction z_F. Other parameters that determine the hydrodynamic flows for a specific process gas are: 1) peripheral speed v_p; 2) wall pressure p_w which is proportional to the gas content in the centrifuge; and 3) average gas temperature T_0. These parameters are systematically varied over a range to provide the basis for the determination of an optimal set of these parameters.

II.4(2). Controllable Variables (hydrodynamic perturbations)

For each combination of geometry and gas parameters, the internal countercurrent flow driven is calculated by four fundamental drives, considered as

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perturbations around the rigid-body rotation: 1) feed F with a cut θ (product to feed ratio) of unity; 2) feed with a cut of zero; 3) temperature difference ΔT between the two endcaps; and 4) scoop drive (either by source of drag or return flow from chamber). The values of feed rate, cut, temperature difference, and scoop drive are determined to produce the maximum separative performance for each geometry and set of process gas parameters. Product flow P, waste flow W, temperature difference ΔT, and flow R_c or scoop force F_s constitute the weights of each corresponding stream function to finally give the optimal stream function. For a given flow the diffusion equation is solved in 1-D and gives the radial mean concentrations of desired isotopes. We can therefore evaluate the separative performance of the centrifuge as a function of the four drive forces. The separation performance is then optimized by using a method of maximization of multidimensional functions. This optimization is realized by a Monte-Carlo method or by the simplex method due to Nelder and Mead (7); both method give the same results.

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II.4(3). Criterion for the Optimization

For a given set of hydrodynamic parameters and controllable variables, the Onsager equation is solved, and the resultant flow field values are used as entries in the diffusion equations. These are ordinary differential equations (ODEs) when the radial averaging method due to Cohen (2) is used. For multicomponent mixtures, the ODEs are coupled by the averaged weight of the mixture, and an iterative method is used to solve them (3). At each step the axial profile of the averaged weight is calculated with the concentration profiles of the preceding step, and iterations are performed until all the concentration profiles are stabilized.

For separation of a binary mixture such as natural uranium, the value function is used to calculate the separative work ΔU, and the parameters described above are varied to find the optimum value. For a multicomponent mixture such as spent reactor fuel, the standard value function does not exist. While generalized value functions have been suggested [see, for example, Wood et al. (8)], we used a more classical criterion (3), the maximum ^{235}U concentration of the product (for a given feed).

III. IGUAÇU MACHINE

III.1. Optimization for Binary Mixture

The Iguaçu machine was suggested by V. D. Borisevich (4) as "a hypothetical machine which allowed scientists to have a non classified set of parameters which could be used for comparing the numerical predictions of the different models for the flow and separation in the gas centrifuge." The Iguaçu machine is described by the parameters given in Table 1.

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TABLE 1
Characteristics of the Iguaçu Machine

Centrifuge parameters	Notation	Value
Radius	a	0.06 m
Length	L	0.48 m
Peripheral speed	$v_p = \Omega a$	600 m/s
Cut	θ	0.5
Axial position of feed	z_F	$L/2$
Temperature	T_0	300 K

The gas that we decided to study is nevertheless UF_6 and not SF_6 as first proposed. Indeed, with SF_6 the A^2 parameter is about 10 and gives no assurance of the validity of the pancake model. To avoid the problem of crystallization, we must take care with the wall pressure. For the nominal temperature the solidification pressure is about 125 torr. We have studied the influence of wall pressure on the performance in the binary case (two isotopes ^{235}U and ^{238}U). For each pressure all the perturbations are optimized and the other hydrodynamic parameters used for these calculations are fixed to their optimum. Because the temperature difference is about 10 K for a wall pressure between 50 and 120 torr, we decided to choose a pressure less than the solidification pressure at $T_0 - \Delta T/2$.

So we have chosen to perform our calculations at a value of 60 torr (8×10^3 Pa), which safely ensures that the UF_6 is in the gaseous state (Fig. 3).

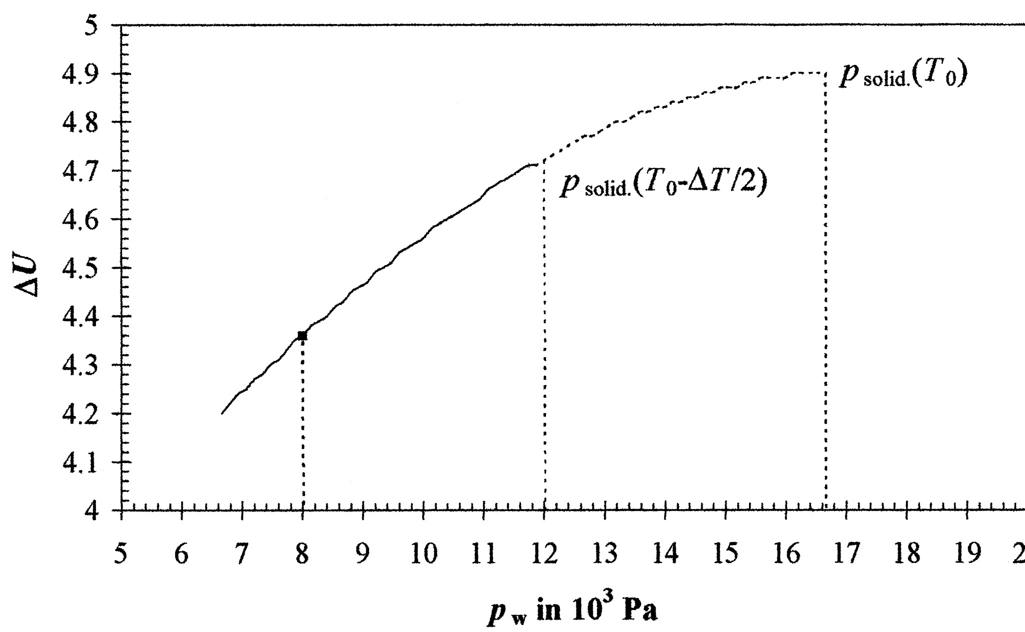

FIG. 3 Influence of the wall pressure on the performance.

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TABLE 2
Iguaçu Machine. Results of the Optimization (all the hydrodynamic parameters and the controllable variables are optimized, apart from the cut which is fixed: $\theta = 0.5$)

	With scoop in fluid	With scoop in chamber
p_w (Pa)	8×10^3	8×10^3
r_p/a	0.81	0.81
$\mathbf{F}$ (kg/s)	30×10^{-6}	30×10^{-6}
ΔT	11	10
F_s (N)	7×10^{-3}	—
r_{F_s}/a	0.75	—
R_c (kg/s)	—	60×10^{-6}
r_R/a	—	0.81
α	1.1167	1.1167
β	0.8835	0.8835
ΔU (SWU/y)	**4.4**	**4.4**

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For this set of conditions the scoop was modeled in the two ways described earlier, and the results of these optimizations are given in Table 2. We chose a linear profile for the wall temperature. Application of Eq. (6) gives a radial location x_s of the feed gas introduction of about 10. The position of the waste hole r_w is taken the closest to the wall. In fact, the model does not give sensible variation of performance with the size of the removal holes and also with the feed profile (for its axial extent that used 0.02 m). The separation factors for U^{235}, α and β, are defined respectively as $\alpha = [c_p/(1 - c_p)]/[c_F/(1 - c_F)]$ and $\beta = [c_w/(1 - c_w)]/[c_F/(1 - c_F)]$, where c_p, c_w, and c_F are the concentration of the product, the waste, and the feed, respectively.

To the accuracy of the model, these two scoop models yield the same optimum separative work of 4.4 SWU/y, so there is an efficiency of about 26%, and the optimal parameters of feed rate and temperature difference are the same.

Figure 4 shows the streamlines for these two cases, and it provides further confirmation of the equivalence of the scoop models. Note that the optimum values of r_p and r_R are equal for the return flow model.

III.1(1). Sensitivity to Controllable (hydrodynamic) Parameters

Figures 5 and 6 show the sensitivity of the separative work to the feed rate and temperature difference, respectively. To produce each of these curves, all parameters were set to their respective optimal values and only the one variable was changed. The same sensitivity curves are obtained with both scoop models. The figures show the optimal feed rate to be 30 mg/s and the optimal temperature difference to be 10 K.

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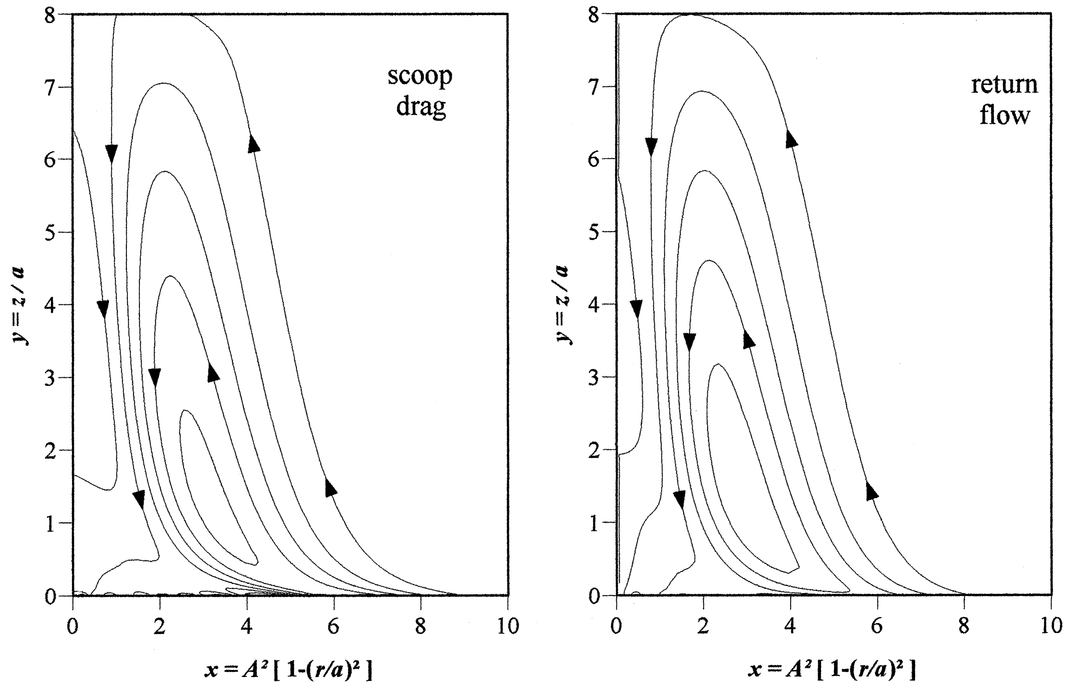

FIG. 4 Stream functions for scoop drag and return flow ($F = 0$, $\Delta T = 0$, $p_w = 8 \times 10^3$ Pa).

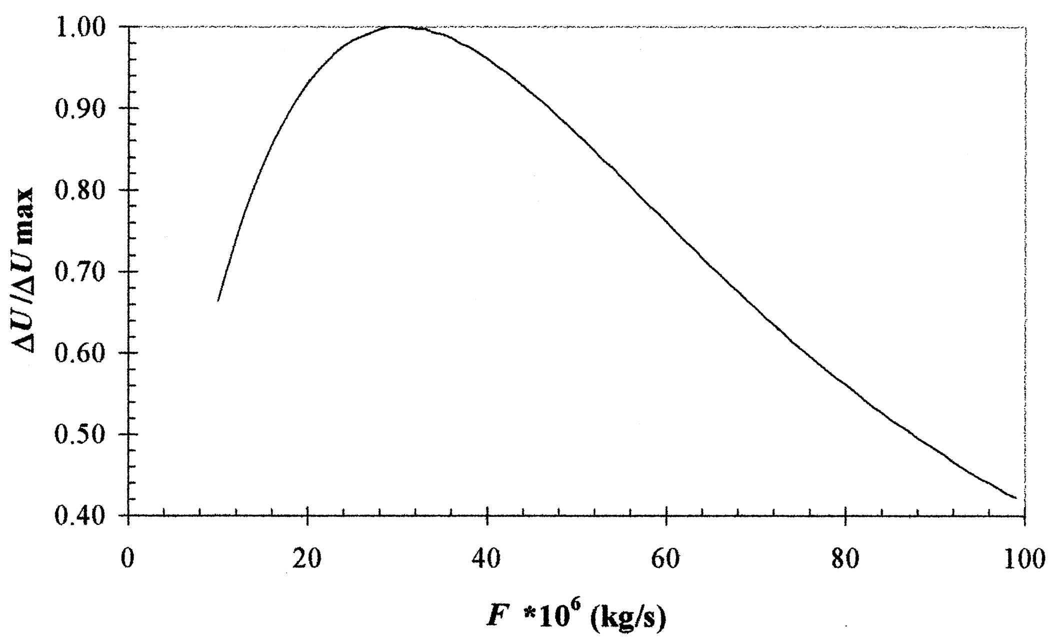

FIG. 5 Sensitivity of performance to feed rate.

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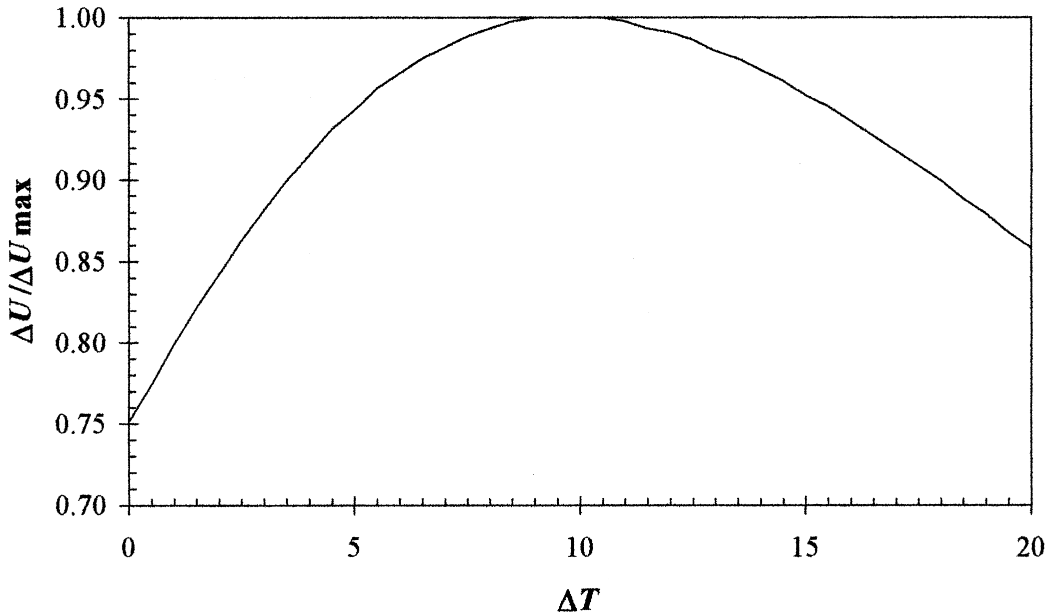

FIG. 6 Sensitivity of performance to ΔT.

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Figures 7 and 8 demonstrate the sensitivity of separative work to the scoop drag force and scoop return flow, respectively. These optimal values are 7×10^{-3} N and 60 mg/s. We note that these curves are relatively flat around the optimum. Indeed, a variation of 15 and 25% around the optimum of F and ΔT, respectively, leads to a variation of about 1% on ΔU.

III.2. Optimization for a Spent Fuel Mixture

A multicomponent mixture of spent reactor fuel was next considered. The isotopic fractions are 1×10^{-11}, 2×10^{-4}, 9×10^{-3}, and 4×10^{-3} for ^{232}U, ^{234}U, ^{235}U, and ^{236}U, respectively. The separation factors α^i and β^i, defined for isotopes i, were calculated. These factors are shown in Fig. 9 as functions of the feed rate where the concentration of ^{235}U has been maximized with respect to the wall temperature drive and the scoop drive (the values of r_R, r_p, and p_w are those of Table 2). Selectivities of ^{232}U, ^{234}U, and ^{236}U can be calculated as

$$\frac{\alpha^{232}-1}{\alpha^{235}-1} = 1.97, \qquad \frac{\alpha^{234}-1}{\alpha^{235}-1} = 1.32, \qquad \frac{\alpha^{236}-1}{\alpha^{235}-1} = 0.66$$

The values of these quantities were found to vary by less than 1% as the feed rate was varied from 1 to 100 mg/s. We can also verify on these numerical results that $\alpha^i - 1$ is proportional to ΔM^i, the difference between the mass of isotope i and those of ^{238}U (averaged mass), since we would have found 2, $\frac{4}{3}$, and $\frac{2}{3}$, respectively.

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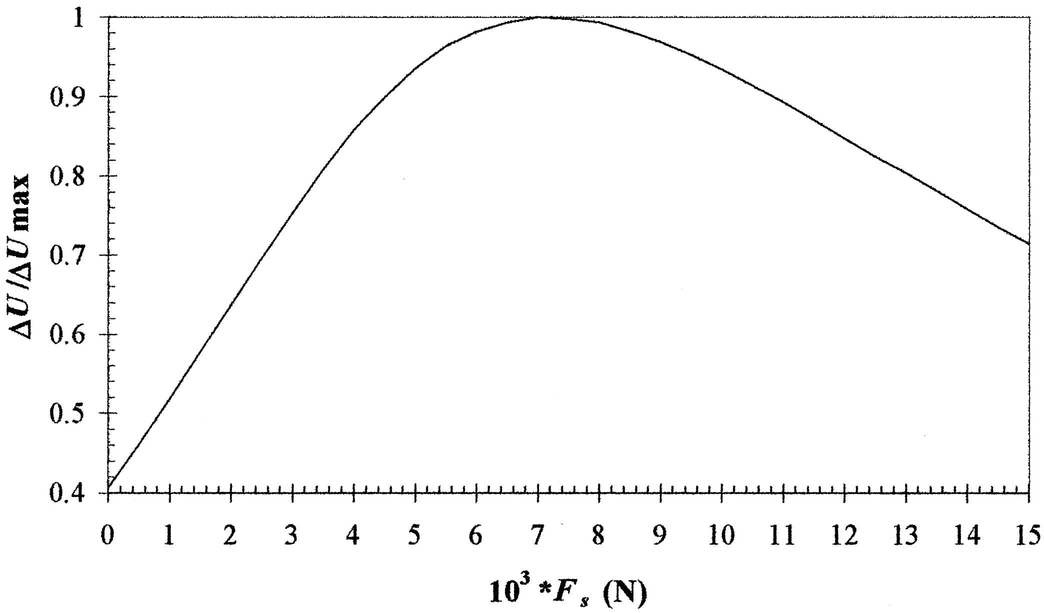

FIG. 7 Sensitivity of performance to scoop drag force.

For this particular multicomponent separation the optimal parameters for the binary separation are the same as those for the multicomponent case with the ^{235}U concentration optimized.

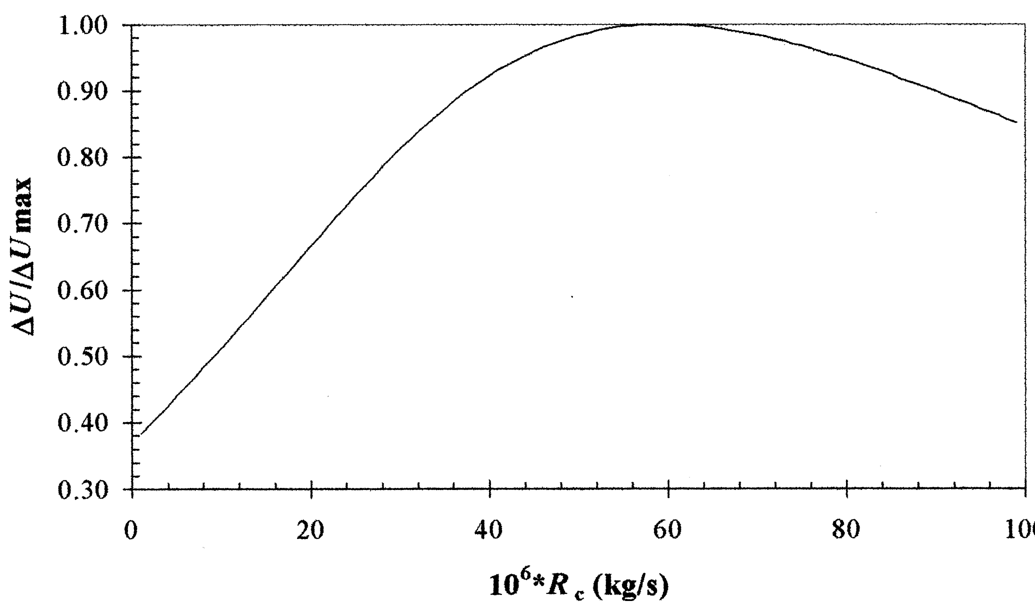

FIG. 8 Sensitivity of performance to scoop return flow.

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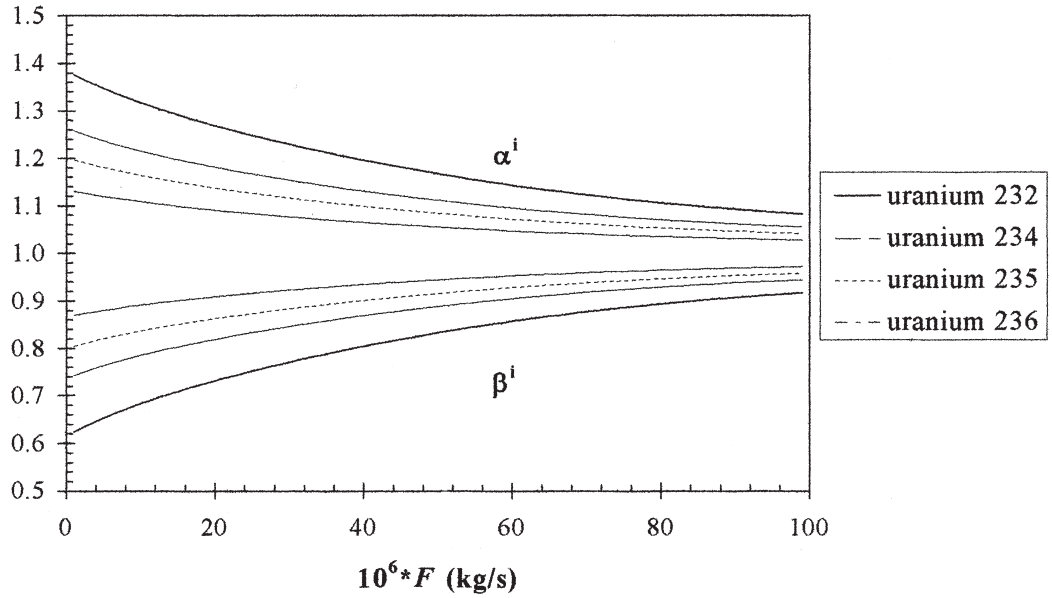

FIG. 9 Influence of feed rate on separation factors.

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IV. PARAMETRIC STUDY

Thanks to a procedure that allows us to automatically run cases in series while varying all the hydrodynamic parameters, we could optimize centrifuges of different speeds, lengths, and radii. For each, the position of product hole, the wall pressure, and position of scoop force could vary over an adopted range. The perturbations were systematically optimized.

We showed that for lengths of 1 to 5 meters, radii between 6 and 10 cm, and peripheral speeds of 500 to 800 m/s, the optimum value of separative performance in a binary mixture of UF_6 occurs at a value of H between 9 and 11. So we consider that the general law is $H^* \approx 10$. In this parametric study we did not pay attention to the possible solidification of UF_6. Hence, in spite of high wall pressure, we kept a fixed gas temperature of 330 K. From these calculations we see that an optimum fixed value of H leads to the expression $p_w^* a^2/L$ as an increasing function of v_p, where p_w^* is the optimal wall pressure:

$$p_w^* = \mu(8RT_0)^{1/2}\, H^* \, \frac{L}{a^2} \, \frac{A^5}{\left(1 + \dfrac{\mu R}{2K} A^2\right)^{1/2}}, \tag{8}$$

$$\text{with } H^* = 10 \text{ and } A = v_p/(2RT_0)^{1/2}$$

So the optimal wall pressure increases with speed and length and decreases with the radius. For very high speed or length, this formula can lead to very

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high wall pressures with no physical sense, because the maximum gas temperature is the real constraint. The numerical application for the Iguaçu machine gives an optimum wall pressure of 105 torr (which gives in reality 97% of the maximum of ΔU, see Fig. 3).

We also noted that the x position of the product hole was approximately constant with a value of about 8 in our parametric study. Moreover, the optimal position of scoop chamber return flow r_R^* is shown to be equal to the optimal product hole position r_p^*. That leads to the following formula:

$$r_p^*/a = r_R^*/a = (1 - 8/A^2)^{1/2} \tag{9}$$

Application of Eq. (9) for the Iguaçu machine gives r_p/a equal to 0.82, which is close to the 0.81 value obtained by our particular optimization (Table 2).

Finally, with a linear fit of our results, we obtained a law for the optimal separative performance, ΔU^* (SWU/y), function of length L(m), and peripheral speed v_p (m/s):

$$\Delta U^*/L = 0.038 v_p - 11.5 \tag{10}$$

Equation (10) is an approximation in the considered range of peripheral speeds (500–800 m/s) and leads to errors of about 10% compared to computed points.

A fit of the same results with a formula of the form $\Delta U^*/L = \alpha v_p^{\beta(v_p)}$ gives $\alpha = 9 \times 10^{-8}$ and $\beta = 3.038 - 2.19 \times 10^{-4}\ v_p$. This last fit leads to errors of the same order as Eq. (10).

Note that ΔU^* (Eq. 10) is obtained with the set of optimal parameters. But we did not take into account solidification phenomena for Eqs. (8) and (10). Nevertheless, the separative performance has to be optimized under crystallization constraint. So if p_w^* given by Eq. (8) is greater than the solidification pressure, the optimum ΔU will be less than ΔU^* of Eq. (10). For example, Eq. (10) leads to $\Delta U^* = 5.4$ SWU/y for the Iguaçu machine, with $p_w^* = 100$ torr (1.4×10^4 Pa), while with the solidification constraint, as taken into account in Section III.1, leads to $\Delta U = 4.4$ SWU/y (with $p_w = 8 \times 10^3$ Pa).

V. CONCLUSIONS

In this paper we have discussed the results of many new calculations that have led us to a wide variety of conclusions. For example, we have applied the pancake theory for the first time to a set of parameters defining a much smaller centrifuge than those of previous studies, and the results appear to be quite reasonable. It is intended that these calculations will serve as benchmarks for other codes based on models that have fewer approximations. We have shown the equivalence of two methods of modeling the flows produced by the action of the scoop. One of these is based on internal sources and the other on the re-

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turn flow from a chamber. For the multicomponent separation considered here, the optimal parameters have been shown to agree with those of the binary case. The calculations have also shown the selectivities to be constant over a wide range of feed rates.

The optimization studies have included not only the strengths of the various countercurrent drives. The optimization process we utilized allows for the automatic optimization of many parameters including the location of withdrawal holes, wall pressure, etc. A fit of our calculation results provides a simple formula for the optimal position of the product hole and scoop return flow, and also for the optimal separative power. The utility of the similarity parameter *H* has been demonstrated to provide guidance in selecting the design parameters for centrifuges, and in particular for the optimum wall pressure.

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