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A Rule of Thumb for Binary Isotope Separations in a Gas Centrifuge

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Abstract

A simple hypothetical model of the binary isotope separation process in a modern countercurrent Gas Centrifuge is proposed. Like the usual Cohen-Onsager separation theory, internal fluid dynamics are obviously involved. But unlike that theory it *completely* obviates the flow integrals for Cohen's E, thereby allowing an immediate *estimate* of the flow efficiency of a given design by visual inspection of the flow field. At times this should be checked later by the usual analyses. To shed some light on this idea, derivations for two simple assumed idealized hydrodynamics are given, but a rigorous proof remains an open question. Then our hypothesis is tested against a battery of about 10 new "exact" formulas for E based upon analytical solutions to several variants of Onsager's pancake equation and is found to be "reasonably" accurate and surprisingly robust. Finally, some limitations of our rule are explored.

INTRODUCTION

Isotope separation theory is a fairly old subject, dating back to Onsager, Furry, Jones, Cohen, etc. (*1*), and has changed little over the intervening years. Many isotope separation theory papers on gas centrifuges (*2–4*) apply the integral formulas to assumed idealized flow profiles. Only recently have mathematically derived and physically reasonable profiles been introduced into the gas centrifuge separation theory, like the high speed thermal drive profile efficiency of $7.2/A^2$ due to

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Onsager (5). More recently Berger has analytically derived Cohen's integral separation parameters for numerous new countercurrent long bowl and 2-D flow fields, such as long bowl sources and sinks, thermal drive and sources and sinks for a long rotating annulus, a thermally driven tapered rotor, etc. At the other extreme, computational fluid dynamicists do a lot of expensive number crunching on big computers for the separative work units (SWUs) and/or Cohen's E and M, which might be appropriately called numerical isotope separation theory.

Such detailed analysis of the binary isotope separation process in a gas centrifuge really involves simulating the advective-diffusion equation (pde) with pressure diffusion for a prescribed internal flow field. Alternatively, one may simply solve the Cohen-Onsager gradient equation (ode). Then, from a mass balance and a value balance, the separative work can be calculated, but sometimes one may just want to determine the value of Cohen's flow profile efficiency. It is here that we can have the most dramatic effect.

Recall that in cylindrical coordinates Cohen's E and M for a countercurrent gas centrifuge are (4),

$$E = \frac{4\left(\int_0^{r_2} r\,dr \int_0^r r'cv\,dr'\right)^2}{cD_{AB}r_2^4 \int_0^{r_2} \frac{dr}{rcD_{AB}}\left(\int_0^r r'cv\,dr'\right)^2} \tag{1}$$

$$M = \frac{\int_0^{r_0} 2\pi rcv\,dr}{2\pi \int_0^{r_0} rcv\,dr \left[\frac{\int_0^{r_2} rcD_{AB}\,dr}{\frac{dr}{rcD_{AB}}\left(\int_0^r r'cv\,dr'\right)^2}\right]^{1/2}} \tag{2}$$

where r is the radical coordinate direction, r_2 is the bowl radius, c is the total molar concentration, v is the axial velocity, D_{AB} is the binary diffusion coefficient, and r_0 is the crossover point. E and M can be written nondimensionally as

$$E = \frac{4\,(I_2^*)^2}{I_3^*} \tag{3}$$

$$M = 2^{1/2}\mathrm{Pe}_{AB}(I_3^*(1))^{1/2} \tag{4}$$

where

$$I_1^*(x) \sim \frac{1}{2A^2}\int_x^\infty \rho_0 w dx' \tag{5}$$

$$I_2^* \sim \frac{1}{2A^2}\int_0^\infty I_1^*(x)dx \tag{6}$$

$$I_3^* \sim \frac{1}{2A^2}\int_0^\infty [I_1^*(x)]^2 dx \tag{7}$$

where curvature is neglected (i.e., pancaked) using (*6*) $x \approx 2A^2(1 - \eta)$.

Even in the pancake approximation, complex formulas for E and M usually result from exact integrations of separation theory for realistic flow fields. Obviously the situation for combined drives is much worse than for just pure drives. This author has often wished for a useful approximation to separation theory which went beyond simply pancaking. Undoubtedly it would be worth giving up some accuracy for more simplicity, especially since the first time the complete separation theory is applied to a new problem it is likely to contain mistakes. (This happens all too often to the author.) Perhaps one could approximate the required flow integrals by a simplified integration rule, e.g., method of steepest decent. Our prior attempts to truncate expressions for pure axial source/sink drives invariably led to artificial singularities and zeroes due to the terms thrown away. While considerable simplification is achieved for asymptotic approximations of sources and sinks, too much detail is lost in the process.

Recall that for the so-called "two-shell" profile (*7*) the optimal location of the return flow is .5335 times the machine radius, corresponding to $E = .815$. From the physics of the flow it seems reasonable that to improve the separative performance we must not only push the return flow high into the atmosphere but also push the velocity crossover point higher in the atmosphere. We take this notion as the crux of our hypothesis and note that the crossover point has some unusual properties. For example, a pure axial source/sink placed at the thermal drive crossover point produces zero flow profile efficiency and near zero flow, but until now x_0 has had little use in gas centrifuge separation theory. The only use known to the author is in computing the recirculation rate L (*4*).

$$L = 2\pi\int_0^{r_0} \rho_0 w r dr \tag{8}$$

where r_0 is the dimensional crossover point. Notice that this unnecessary usage gets into trouble when there are multiple crossover points, which is inevitable in the real world.

For any linear combination of drive perturbations, Cohen's E can be expressed as something over A^2, that is,

$$E \sim \frac{2\int_0^\infty [I_1^*(x)dx]^2}{A^2\int_0^\infty [I_1^*(x)]^2 dx} = \frac{K}{A^2} \tag{9}$$

where the constant K depends upon the type of drive(s). Olander (*8*) gives a similar formula in his own notation. The resulting problem is, of course, to estimate the single parameter K. Ordinarily one is interested in maximal SWUs but one may settle for some sort of approximation.

HYPOTHESIS

Consider the following simple rule to approximate the binary isotopic separation process in a high speed gas centrifuge and approximately solve the stated parameter estimation problem for K.

Rule of Thumb: For a single recirculating cell, in the absence of discontinuities, discrete sources and sinks, and negligible Ekman endcap boundary layers, the flow profile efficiency is directly proportional to the velocity crossover point at a fixed stratification. Or, more precisely,

$$E = \frac{\Upsilon x_0}{A^2} \tag{10}$$

where Υ is the separation "constant," x_0 is the hydrodynamical axial velocity crossover point due to a combination of drives, and A is the stratification parameter.

In cylindrical coordinates, Eq. (10) can be rewritten as

$$E = 2\Upsilon(1 - \eta_0) \tag{11}$$

where η_0 is the dimensionless radial crossover point.

Application of this rule to exceptional cases may of course lead to gross errors, but careful and judicious use of Eq. (10) might still be possible. For instance, treatment of multiple zeroes simply requires using the minimum x_0 in place of x_0, since flow fields with multiple zeroes often have near zero E due to remixing. Υ is defined by reference to a convenient solution, and since the thermal drive is of some historical significance (i.e., probably the first nonwheel flow hydrodynamical solution), we select it as the basis. But this is really arbitrary and doesn't matter much because any other reasonable reference would do more or less as well. So, using Onsager's thermal drive efficiency, one finds

$$\Upsilon \equiv \frac{7.2}{1.256} = 5.73 \tag{12}$$

where 1.256 is the nontrivial root of the thermal drive velocity profile,

$$(1 + 2x_0)e^{-x_0} - 1 = 0 \tag{13}$$

Then the usual optimization problem may be approximated as

$$\mathrm{MAX}_{A^2\text{fixed}} E \tag{14}$$

which is equivalent to

$$\mathrm{MAX}_{A^2\text{fixed}} x_0 \tag{15}$$

which *completely* eliminates the numerous separation integrals. Although x_0 is determined by the roots of a nonlinear, algebraic, transcendental equation, it is a much simpler numerics problem than we began with. Even constrained and unconstrained optimizations are possible, but CAVEAT CALCULATOR. It is strongly recommended that the resulting hydrodynamics be inspected for "reasonableness," and rigorous numerical or analytical calculation of E be made as a check. When this simple technique works it reduces the optimization problem to at most one or two detailed calculations of E. Because this is only a simple "rule of thumb," one *must* examine the final prediction for both validity and accuracy, as something may have gone wrong between beginning and end. Also, it is obvious that the integral calculation of Cohen's M remains, if one wants M. Of course, for optimal separations, $e_c = M^2/(M^2 + 1)$ is generally near unity.

DERIVATION

The following two simple derivations should shed some light on these ideas. I suppose that it might be possible to justify our hypothesis rigorously or something akin to it without assuming the profile vanishes beyond x_0. This is not an easy matter, so we leave this open question as an exercise for the interested reader. While these two derivations predict somewhat different values of K, the important point here is the appearance of x_0 in the formula.

Simple Derivation 1

Suppose

$$\rho_0 w = \begin{cases} 4A^4(1 - 2U(x - x_0)), & 0 \leqslant x \leqslant 2x_0 \\ 0, & 2x_0 \leqslant x \leqslant \infty \end{cases} \tag{16}$$

$$I_1^* = \frac{1}{2A^2}\int_x^\infty \rho_0 w\,dx' = -2A^2[-2x_0 - x(1 - 2U(x - x_0))] \tag{17}$$

$$I_2^* = \frac{1}{2A^2}\int_0^{2x_0} I_1^* dx = 3x_0^2 \tag{18}$$

$$I_3^* = \frac{1}{2A^2}\int_0^{2x_0} [I_1^*]^2 dx = \frac{52A^2}{3}x_0^3 \tag{19}$$

Thus,

$$E = \frac{27x_0}{13A^2} = \frac{2.08x_0}{A^2} \tag{20}$$

Simple Derivation 2 *(9)*

Suppose

$$\rho_0 w = \begin{cases} -4A^4 \sin\dfrac{\pi x}{x_0}, & 0 \leqslant x \leqslant 2x_0 \\ 0, & 2x_0 \leqslant x \leqslant \infty \end{cases} \tag{21}$$

$$I_1^* = \frac{-2A^2x_0}{\pi}\left[-1 + \cos\frac{\pi x}{x_0}\right] \tag{22}$$

$$I_2^* = \frac{2x_0^2}{\pi} \tag{23}$$

$$I_3^* = \frac{6A^2x_0^3}{\pi^2} \tag{24}$$

Thus E is

$$\frac{8x_0}{3A^2} = \frac{2.667x_0}{A^2} \tag{25}$$

TEST OF HYPOTHESIS

Tables 1–3 summarize some comparisons of our hypothesis with exact integrations of E for several quite different drive mechanisms. The fluid dynamics used here derive from the linearized Navier-Stokes equations and are exact solutions (sometimes in the perturbation sense) to Onsager's equation (*6*). For the most part they are taken from un-

TABLE 1
Hypothesis Test 1

Drive[a]	x_0	A^2E_T	A^2E_H	% Error
TD	1.256	7.2	7.2	—
W_{0_∞}	1.6	9	9.17	2
OPT(TD + W_{0_∞})	1.625	108/11 = 9.818	9.315	−5
U_{0_∞}[b]	1.6	9	9.17	2
$(T_0 - 2V_0)_\infty$	1.376	7.588	7.885	4
TR1	1.31	7.18	7.22	0.5
TR2	1.21	7.18	7.22	0.5

[a]TD = thermal drive; W_{0_∞} = uniform axial source/sink at $x = \infty$; U_{0_∞} = nonuniform radial source/sink at $x = \infty$; $(T_0 - 2V_0)_\infty$ = nonuniform heat and drag source/sink at $x = \infty$; TR1 = converging tapered rotor, $\varepsilon y = .05$, TD (*10*); TR2 = diverging tapered rotor, $\varepsilon y = -.05$, TD (*10*).

[b]$\rho_0 w_{W_{0_\infty}} = \rho_0 w_{U_{0_\infty}}$, see text discussion.

TABLE 2
Hypothesis Test 2: TD Rotating Annulus with No Slip at x_T

x_T	x_0	A^2E_T	A^2E_H	% Error
∞	1.256	7.2	7.2	0
8	1.1481	6.44	6.5815	2
6	1.1111	5.88	6.3694	8
4	1	4.61	5.7325	24

published works of the author. The subscript T indicates the so-called "exact" theoretical efficiency, while the subscript H indicates the hypothetical value. The notation for the drives is defined in the Table 1 footnotes.

These results are represented in a scatter graph, Fig. 1. In the range of validity, our rule has produced a maximum absolute relative error of about 8%. Surprisingly, the result that

$$E_{W_{0_\infty}} = E_{U_{0_\infty}} \tag{26}$$

was discovered using our simple rule. So based on these comparisons, we consider our rule to be "reasonably" accurate and surprisingly robust, but it is still just a rule and not a theory. As noted earlier, multiple crossovers present difficulties. For example, the profile for optimum $E \cdot e_C$ for combined thermal-1 axial source/sink drive has three nontrivial crossover points. So here our simple model is not of much use, but then, due to all the noise, who would guess that this profile is really very efficient ($E = 9.87/A^2$)? Alas, in such complex cases there is no substitute for a detailed analysis.

TABLE 3
Hypothesis Test 3: TD Rotating Annulus with Free Slip at x_T

x_T	x_0	A^2E_T	A^2E_H	% Error
∞	1.256	7.2	7.2	0
8	1.256	7.11	7.2	1
6	1.256	6.72	7.2	7

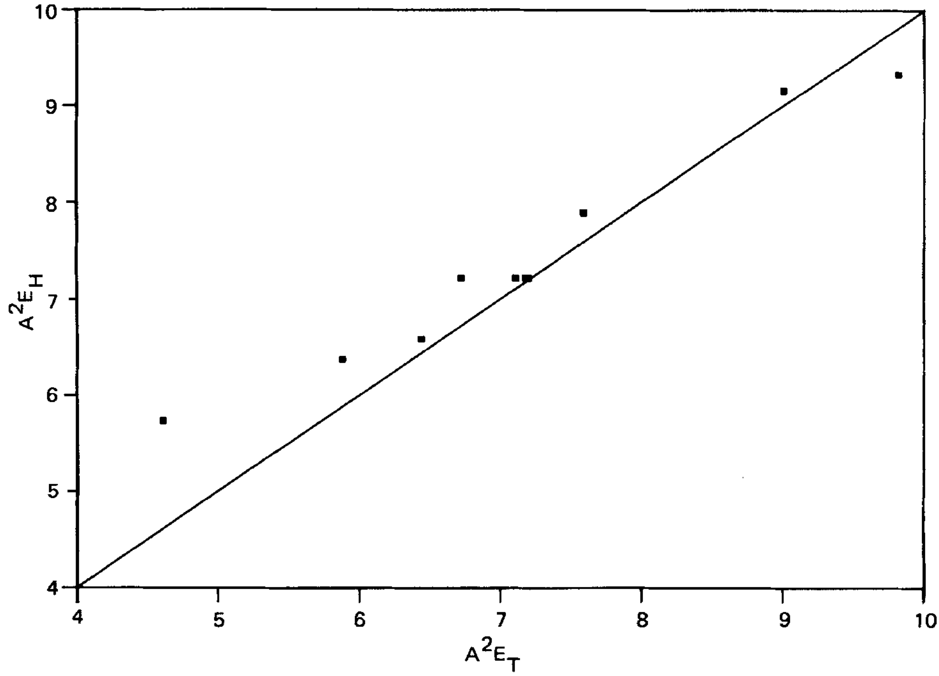

FIG. 1. Scatter graph.

SYMBOLS

A	stratification parameter $\left[\frac{MWV_w^2}{2RT_0}\right]^{1/2}$
a	rotor radius
D_{AB}	binary diffusion coefficient
E	Cohen's E
e_c	circulation efficiency, $M^2/(M^2 + 1)$
$I_1, I_2, I_3, I_1^*, I_2^*, I_3^*$	flow integrals
M	Cohen's M
MW	molecular weight
Pe_{AB}	Peclet number $\frac{\rho_0 V_w a}{\rho_0 D_{AB}}$
R	universal gas constant

r	radial coordinate
SWUs	separative work units
T_0	reference temperature
V_w	wall velocity
x	scale heights variable
x_T	annular gap width in scale heights
x_0, η_0	velocity crossover point
η	r/a
ρ_w	wall density
$\rho_0 w$	dimensionless axial mass velocity
Υ	separation "constant"
$\sim$	asymptotically equal

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