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Separation of Close Species by Displacement Development on Ion Exchangers. II. Band Production

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Abstract

Computer simulation shows that in displacement development the marginal enrichment depends only on the total enrichment, not on the isochrone shape. This allows simple calculation of the semicontinuous production by a knowledge of the enrichment variation along the displacement.

INTRODUCTION

Displacement development of a mixture of close species produces a rich mixture of the less retained substance in front of the band and a rich mixture of the more retained substance at the rear of the band.

When the equilibrium constant is close to 1, we pointed out (*1*) that it was impossible to obtain a complete separation of the mixture but that a limited state could be reached, the so-called stationary state, where the displacement isochrone (which expresses the repartition of species all along the band) is a part of a bilogarithmic curve.

If we take a given quantity of the mixture at the front and at the rear of a band in a stationary or nonstationary state (in such a manner that the average composition remains unchanged) and we introduce the whole quantity at the point of the band corresponding to the original composi-

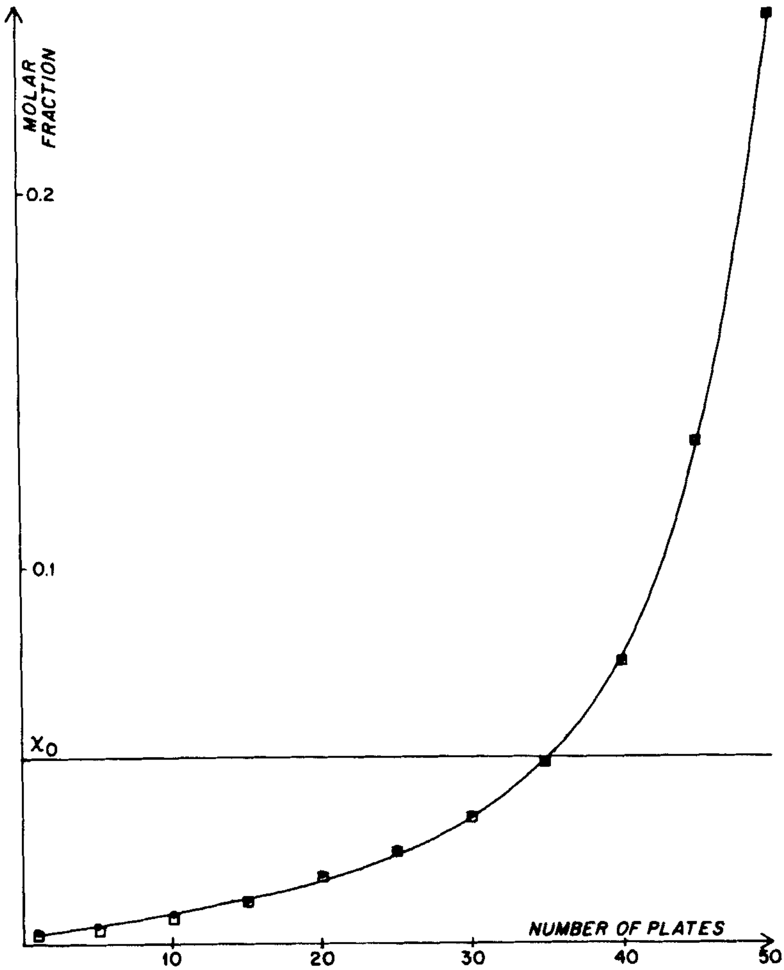

FIG. 1. Displacement of a 50-plate band, $k = 1.1$; $x_0 = 0.05$. (1) Isochrone after a 300-plate displacement, or 6 band lengths. (2) After the same displacement, sampling of 5 rich plates and 17 poor plates, injection of 22 plates having the initial composition, and displacement of 218 plates.

tion, it is possible to find the original shape after a certain displacement. This is demonstrated by simulation of the phenomenon on a computer as illustrated on Fig. 1.

By repeating the sampling–injecting–displacing cycle, important quantities of the richer (or poorer) mixture can be produced in a semicontinuous manner.

We intend to solve the problem of determining the displacement necessary to find, after sampling and injecting, the original enrichment and predicting the isochrone shape after this cycle.

Of course, complete simulation on a computer (*2*) can given an answer to both problems, but we shall show that they can be directly solved in a satisfactory way by a simple hypothesis.

DEFINITIONS AND NOTATIONS

Let x be the molar fraction of the ion more retained by the resin in any plate and x_0 its molar fraction in the original mixture. *Absolute enrichment* is the difference $x - x_0$ in the plate considered. *Relative enrichment* is defined as $(x - x_0)/x_0$.

Reduced relative enrichment. The relative enrichment has two disadvantages. On the one hand, if a given separation has been studied completely, the study of another separation carried out under the same experimental conditions, but with a slightly different exchange constant k, can be deduced by pointing out that enrichments are proportional to $\epsilon = k - 1$ in a given zone. It is then interesting to introduce the quantity

$$(x - x_0)/x_0\epsilon$$

But, on the other hand, this expression depends on the chosen substance. For example, if a mixture where $x_0 = 0.2$ is considered, the molar fraction y of the other ion will be $y_0 = 1 - 0.2. = 0.8$.

If the absolute enrichment is 0.1, then the relative enrichment will be, according to the ion considered

$$(x - x_0)/x_0 = 0.5 \qquad \text{or} \qquad (y - y_0)/y_0 = 0.125$$

The different values of the relative enrichment, however, express the same phenomenon, so we shall introduce the notion of a reduced relative enrichment independent of the ion considered and defined by

$$E = \frac{x - x_0}{x_0(1 - x_0)\epsilon}$$

Henceforth this quantity will simply be called enrichment. For an ion with a molar fraction represented by x, it is equivalent to expressing the enrichment as a function of $\epsilon' = \epsilon(1 - x_0)$, a factor which was introduced in the study of the stationary state repartition (*1*).

Total Enrichment. Enrichment as defined above, is related to one plate, and the total enrichment of a P-plate zone will be called

$$E_P = \sum_P \frac{x - x_0}{x_0(1 - x_0)\epsilon}$$

Marginal Enrichment. The evolution of enrichment all along the development will be characterized by the marginal enrichment, defined as the enrichment variation of the richer zone when the band is moved one plate; if t represents the band displacement, expressed by the number of plates, the marginal enrichment is the mean value of dE/dt, when t varies by one unit.

HYPOTHESIS

First we shall make an assumption which will be shown to allow a simple calculation of production. Then we shall justify the validity of this hypothesis.

For a band of a given length, we shall assume that the marginal enrichment depends only on the total enrichment; not on the isochrone shape.

Enrichment of an artificially constituted band with very rich front plates, very poor rear plates, and an important zone of x_0 composition will evolve in a same way as a band of the same length displaced in order to have a total enrichment equal to that of the artificial one (Fig. 2).

Figure 3 represents the evolution of the total enrichment of the rich zone of a band as a function of displacement t. The shape we give to the curve $E = f(t)$ has been suggested by computer simulation. Let P be the total number of plates of the band. At a given moment the state of the band is represented by Point A (t_0, E_0). Then p_1 and p_2 plates are picked-up, respectively, in the rich and the poor part (so that the mean composition remains x_0). The p_1 extracted plates correspond to a total enrichment E_2. The band then involved with $P - (p_1 + p_2)$ plates has the enrichment $E_1 = E_0 - E_2$. If we inject $(p_1 + p_2)$ plates of x_0 composition at the part of this band where we find the original molar fraction x_0, the

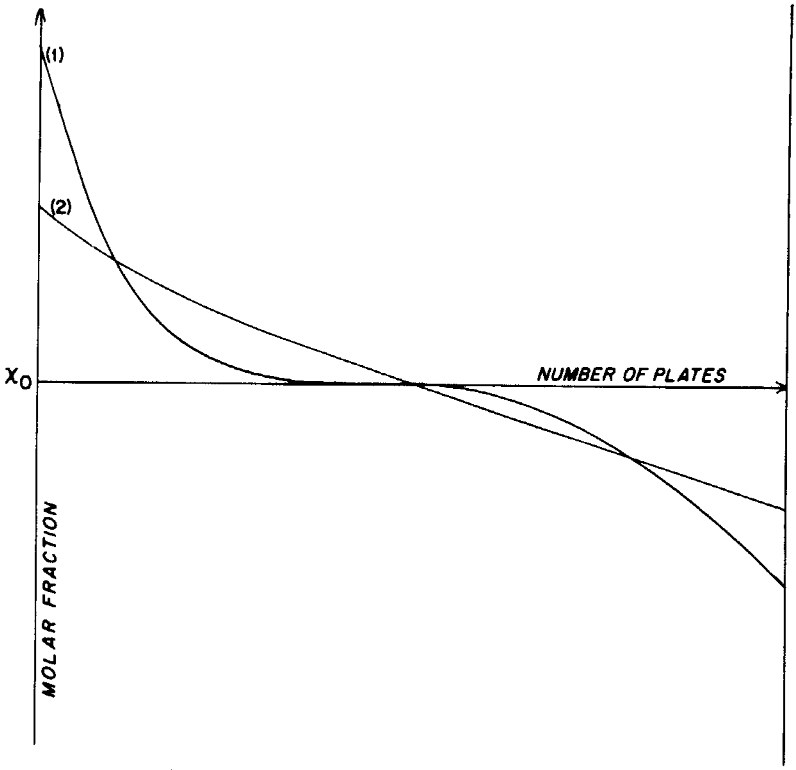

FIG. 2. Isochrones corresponding to two bands having the same enrichment. Band 1 is artificially made with a very poor mixture, a very rich mixture, and an important zone having the x_0 initial composition. Band 2 has the same enrichment as Band 1 but has been made by a suitable displacement.

total enrichment is unchanged and we artificially make P plates band with total enrichment E_1 (corresponding to Point B on Fig. 3).

The assumption we made allows us to say that this band will recover its original enrichment E_0 if it is displaced by $t_2 = t_0 - t_1$ plates.

As for the shape of fronts, Fig. 1 shows in a particular case that, when starting from a very classically displaced band, we are brought back to the same shape by the sampling–injecting–displacing cycle. This phenomenon, checked on numerous examples, is very general and could indeed be predicted.

In fact, the perturbation is much stronger as sample enrichment is in-

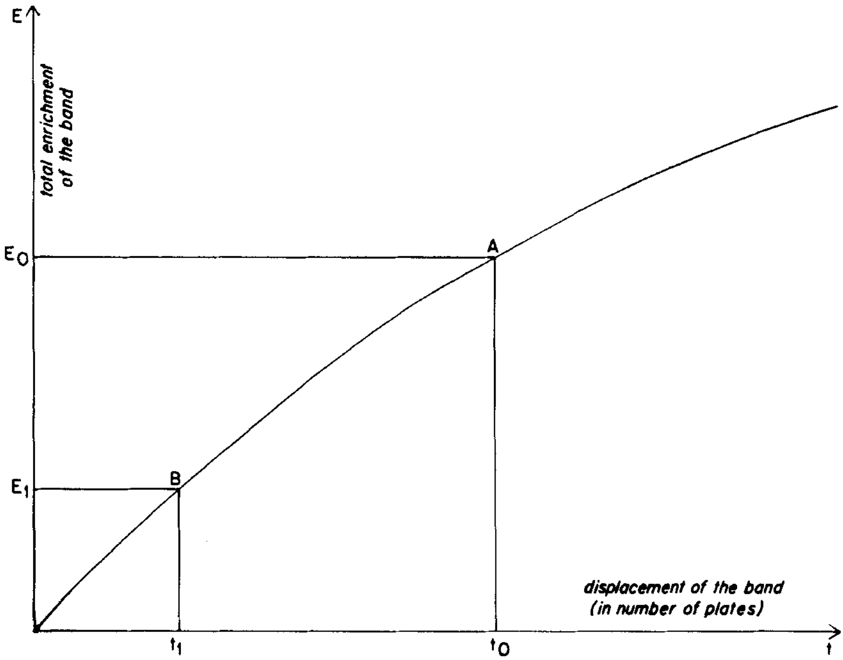

FIG. 3. Enrichment evolution vs. displacement for the general case. Graphic study of the production.

creased (corresponding to the injection in the band of a large number of plates with an original molar fraction x_0). But, to recover the original enrichment, a long displacement which will allow the disappearance of perturbation effects will be necessary.

Figure 4 summarizes the rest of the operation undertaken along a cycle.

CHECKING THE HYPOTHESIS BY COMPUTER SIMULATION

In Table 1 we present the results of numerous displacements prepared by computer simulation (this simulation allows us to know the isochrone for any t value of the number of plates corresponding to the displacement of the band).

In each case we give the enrichment obtained after the $t_0 - t_1$ displacement of a band displaced of t_0 plates for which a given number of plates has been sampled at the front and at the rear and a corresponding quantity of the original mixture x_0 has been injected, and the displacement necessary to find the enrichment E_0 before sampling.

We also give the composition in front of the band after the theoretical displacement (corresponding to the zone which would be taken in a further cycle).

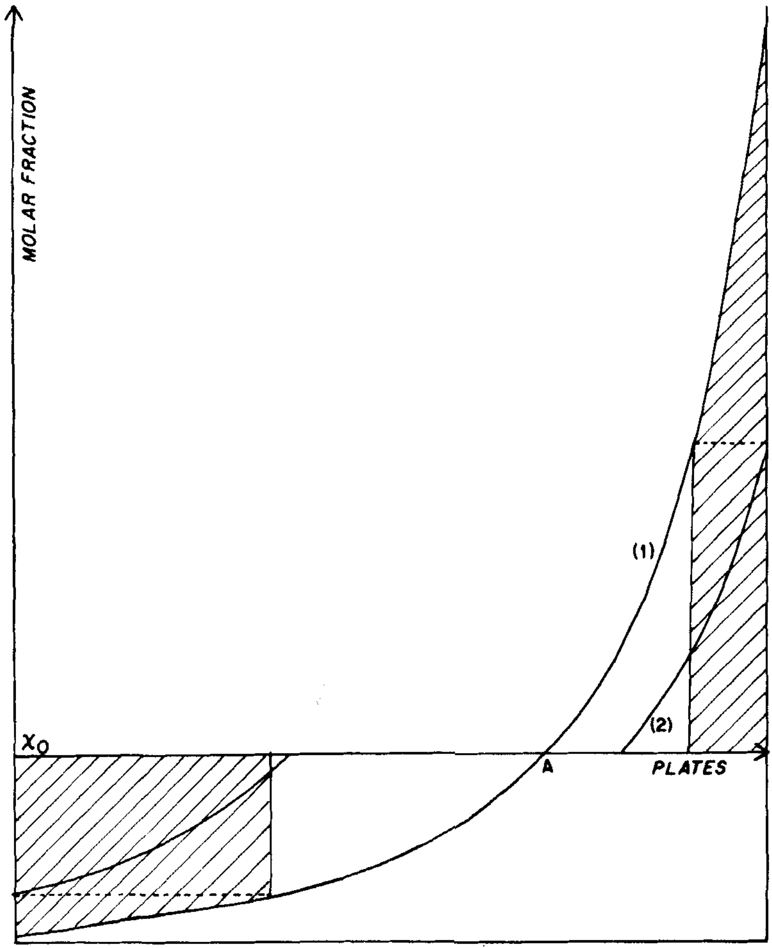

FIG. 4. Production mechanism. After sampling poor and rich fractions on Isochrone 1 (hatched zones of equal areas) and injecting the same quantity of initial mixture at Point A, the band to be displaced corresponds to Isochrone 2.

The necessity of sampling an integer number of plates in the poor zone only approximately balances sampling in the rich zone. This introduces slight fluctuations in the average composition of the band, which explains the difference sometimes observed between theoretical enrichment after $t_0 - t_1$ and the one calculated by complete simulation.

TABLE 1

Simulation on a Computer of Displacement Development of 6 Bands (I to VI) under Various Conditions

Band number	I	II	III	IV	V	VI
Number of band plates	20	20	50	21	50	100
k	1.01	1.01	1.01	1.1	1.1	1.001
x_0	0.2	0.8	0.2	0.25	0.05	0.01
Displacement t_0	100	100	550	63	300	998
Total enrichment E_0	66	66	387	47.5	230.5	900
Marginal enrichment	0.32	0.34	0.34	0.5	0.5	0.83
Front:						
Number of sampled plates	2	2	5	4	5	10
$E_0 - E_1$	25	24	156	34	156	394
Mean composition of the sample (molar fraction)	0.22	0.819	0.250	0.408	0.198	0.0104
Rear:						
Number of sampled plates	2	2	6	5	17	10
Mean composition of the sample (molar fraction)	0.18	0.791	0.156	0.127	0.001	0.096
E_1 total enrichment of the band after sampling	41	42	231	14	75	506
t_1 corresponding displacement	47	49	258	15	82	523
Left to displace, $t_0 - t_1$	53	51	192	48	218	475
Enrichment after displacement, $t_0 - t_1$	67	68	395	47.5	230	900
Front composition for $t_0 - t_1$ (molar fraction)	0.22	0.819	0.250	0.409	0.198	0.0104
Displacement really necessary to obtain E_0 again	50	47	272	48	219	475

TABLE 2

Comparison between the Mean Parameters Calculated According to the Simple Hypothesis and Those Obtained by Simulation on a Computer (Values Reported from Table 1)

Theoretical displacement $t_0 - t_1$	53	51	292	48	218	475
Displacement really necessary to obtain E_0 again	50	47	272	48	219	475
E_0	66	66	387	47.5	230.5	900
E after the $t_0 - t_1$ displacement	67	68	395	47.5	230	900
Front composition, in %	22	81.9	25	40.8	19.8	1.04
Front composition for $t_0 - t_1$, in %	22	81.9	25	40.9	19.8	1.04

Table 2 is a simplified table which, by summarizing the values of Table 1, makes easier the comparison between various parameters calculated according to our hypothesis and those obtained by direct simulation. Taking into account the above-mentioned approximations, the simple hypothesis used can be considered a very good approach to the actual results.

CONCLUSION

We have shown that, thanks to a simple hypothesis, prediction of conditions for semicontinuous production in displacement–development is possible by knowledge of the enrichment variation along the displacement $E = f(t)$. The displacement simulation on a computer gives the shape of the isochrone at any moment of the displacement, the curve $E = f(t)$ then being immediately deduced. The assumption allows prediction of production and its optimization without doing a computer simulation for each sampling ratio and for each enrichment value corresponding to this sampling.

We now intend to determine the mathematical equation of curve $E = f(t)$.

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