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Gel Extraction. The Main Equations

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ABSTRACT

Gel extraction is a new cyclic process of substances separation in solution according to their molecular size, which is based on phase transition in the swollen gel. In the article the equations of the process are obtained. The equations link the substance concentration in the concentrate and in the permeate, as well as the amount of these solutions, with the process parameters and the type of gel used in the process. It is assumed that all parameters of the process do not depend on the cycle number.

INTRODUCTION

The process of abrupt change in volume of swollen gels due to changes in external conditions has attracted much attention lately. These processes are interpreted as a phase transition (1–3).

Phase transition in the swollen gels makes possible the cyclic process of substances separation in solutions according to their molecular size. During the process low-molecular substances diffuse with solvent into a swollen gel and high-molecular ones are concentrated in the remaining solution. After the concentrate separation, regeneration of swollen gel is performed by gel compression (collapse) during phase transition (for example, by temperature change for a temperature-sensitive gel; by pH change for a poly-electrolyte or by change of solvent composition). The permeate—solution extracted from the swollen gel during collapse—is separated and the gel regenerated, the collapsed gel is inserted into a new portion of initial solution, and then the process is recycled.

This process has been patented by a number of authors (4–8) including Cussler (6–8), who has reported it in Ref. 9 and has named the process "gel-extraction." The new process has some advantages and may be considered as an alternative to the process of nanofiltration.

DERIVATION OF THE MAIN EQUATIONS

Stage of Concentrate Formation

A concentrate is formed in a process of partial extraction of solvent from initial solution by gel which is swelling in the solution. Gel used is obtained in the preceding cycle of separation after gel collapse and permeate removal. Gel contains M_g of dry gel, $M_g \cdot \Delta M_p$ of a "solution" with substance concentration $C_{g,p}$ and $M_g \cdot l_p$ of the permeate with substance concentration C_p. This gel is swelling in a solution whose initial amount is M_0 and initial substance concentration in the solution is C_0. During gel swelling, mass $M_g \cdot (\Delta M_c - \Delta M_p)$ of a solution converts into the gel. $M_0 + M_g \cdot l_p - M_g \cdot (\Delta M_c - \Delta M_p) = M_0 - M_g \cdot (\Delta M_c - \Delta M_p - l_p)$ is the amount of remaining solution; concentration of substance in "solution" inside a gel becomes $C_{g,c}$ and outside of gel $-$ C_c. The substances balance equation for this stage is:

$$M_0 \cdot C_0 + M_g \cdot \Delta M_p \cdot C_{g,p} + M_g \cdot l_p \cdot C_p = C_c \cdot [M_0 - M_g \cdot (\Delta M_c - \Delta M_p - l_p)] + M_g \cdot \Delta M_c \cdot C_{g,c} \quad (1)$$

From K_c definition it follows that $C_{g,c} = K_c \cdot C_c$ Taking this fact into account, eliminate $C_{g,c}$ from (1):

$$M_0 \cdot C_0 + M_g \cdot \Delta M_p \cdot C_{g,p} + M_g \cdot l_p \cdot C_p = C_c \cdot [M_0 - M_g \cdot (\Delta M_c - \Delta M_p - l_p)] + M_g \cdot \Delta M_c \cdot K_c \cdot C_c \quad (2)$$

The solution with concentration C_c is removed from the gel and $M_g \cdot l_c$ of the solution remains in the gel. The amount of removed concentrate is

$$M_c = M_0 - M_g \cdot (\Delta M_c - \Delta M_p - l_p + l_c) \quad (3)$$

Stage of Permeate Formation

A permeate is formed while the gel is collapsing. This gel remains after removal of concentrate. The collapse is induced by phase transition due to change in external conditions.

At the beginning of the stage, gel contains M_g of dry gel, $M_g \cdot \Delta M_c$ of "solution" with substance concentration $C_{g,c} = K_c \cdot C_c$ and $M_g \cdot l_c$ of concentrate, which is on the gel surface, with concentration C_c. As a result of the gel collapsing $M_g \cdot (\Delta M_c + l_c - \Delta M_p)$ of permeate is extracted with substance concentration C_p. $M_g \cdot \Delta M_p$ of the "solution" with substance concentration $C_{g,p}$ remains in the gel. The substances balance equation for this stage is:

$$M_g \cdot \Delta M_c \cdot K_c \cdot C_c + M_g \cdot l_c \cdot C_c = M_g \cdot (\Delta M_c + l_c - \Delta M_p) \cdot C_p + M_g \cdot \Delta M_p \cdot C_{g,p} \quad (4)$$

Taking into account that $C_{g,p} = K_p \cdot C_p$, the value $C_{g,p}$ may be eliminated from equation (4). Reducing both parts of equation (4) by M_g the following equation may be obtained:

$$\Delta M_c \cdot K_c \cdot C_c + l_c \cdot C_c = (\Delta M_c + l_c - \Delta M_p) \cdot C_p + \Delta M_p \cdot K_p \cdot C_p \quad (5)$$

The permeate with substance concentration C_p is removed from gel and $M_g \cdot l_p$ of the permeate remains on the gel. The amount of permeate removed is:

$$M_p = M_g \cdot (\Delta M_c - \Delta M_p + l_c - l_p) \quad (6)$$

Derivation of Formulae for C_c and C_p

These formulae are derived by combining equations (2) and (5). This method is correct because we analyze the steady-state process, so values of all variables in the equations (1)–(6) are independent on the cycle number.

The following formula for C_p may be derived from eq. (5):

$$C_p = \frac{\Delta M_c \cdot K_c \cdot C_c + l_c \cdot C_c}{\Delta M_c + l_c - \Delta M_p + \Delta M_p \cdot K_p} = \frac{C_c \cdot (\Delta M_c \cdot K_c + l_c)}{\Delta M_c + l_c - \Delta M_p \cdot (1 - K_p)} \quad (7)$$

Substitution of the value of C_p from (7) and expression $C_{g,p} = K_p \cdot C_p$ into equation (2) gives:

$$M_0 \cdot C_0 + \frac{M_g \cdot \Delta M_p \cdot C_c \cdot (\Delta M_c \cdot K_c + l_c) \cdot K_p}{\Delta M_c + l_c - \Delta M_p \cdot (1 - K_p)} + \frac{M_g \cdot l_p \cdot C_c \cdot (\Delta M_c \cdot K_c + l_c)}{\Delta M_c + l_c - \Delta M_p \cdot (1 - K_p)} = C_c \cdot [M_0 - M_g \cdot (\Delta M_c - \Delta M_p - l_p)] + M_g \cdot \Delta M_c \cdot K_c \cdot C_c \quad (8)$$

From equation (8), after identical algebraic transformations the formula for C_c is:

$$C_c = \frac{M_0 \cdot C_0 \cdot [\Delta M_c + l_c - \Delta M_p \cdot (1 - K_p)]}{\{M_0 + M_g \cdot [\Delta M_p + l_p - \Delta M_c \cdot (1 - K_c)]\} \cdot [\Delta M_c + l_c - \Delta M_p \cdot (1 - K_p)] - M_g \cdot (\Delta M_c \cdot K_c + l_c) \cdot (\Delta M_p \cdot K_p + l_p)} \quad (9)$$

As a result of substitution of equation (9) into equation (7), the formula for C_p is:

$$C_p = \frac{M_0 \cdot C_0 \cdot (\Delta M_c \cdot K_c + l_c)}{\{M_0 + M_g \cdot [\Delta M_p + l_p - \Delta M_c \cdot (1 - K_c)]\} \cdot [\Delta M_c + l_c - \Delta M_p \cdot (1 - K_p)] - M_g \cdot (\Delta M_c \cdot K_c + l_c) \cdot (\Delta M_p \cdot K_p + l_p)} \tag{10}$$

Formulae (3), (6), (9), and (10) indicate the amount of concentrate and permeate and substance concentration in the concentrate and the permeate in terms of process and gel parameters. These formulae are the ones commonly used for gel-extraction process.

Special Cases

1. Formulae (9) and (10) allow one to analyze the influence of l_c and l_p on process efficiency and to optimize these parameters by the greatest possible removal of solution from the gel particles surface after mass-exchange is finished. However, the amount of the solution on the surface and inside the gel particles is very difficult to determine. For practical purposes it is convenient to consider that l_c and l_p are equal to zero and to use the simpler equations (11) and (12), which are obtained from (9) and (10) by l_c and l_p elimination. However, it is necessary to point out that in this case the values ΔM_c, ΔM_p, K_c, and K_p will be not real but "effective." We denominate these "effective" values by (*). Naturally, in this case it is necessary to use "effective" values of ΔM in equations (3) and (6); l_c and l_p must be eliminated from these equations as well.

$$C_c = \frac{M_0 \cdot C_0 \cdot [\Delta M_c^* - \Delta M_p^* \cdot (1 - K_p^*)]}{\{M_0 + M_g \cdot [\Delta M_p^* - \Delta M_c^* \cdot (1 - K_c^*)]\} \cdot [\Delta M_c^* - \Delta M_p^* \cdot (1 - K_p^*)] - M_g \cdot \Delta M_c^* \cdot \Delta M_p^* \cdot K_c^* \cdot K_p^*} \tag{11}$$

$$C_p = \frac{M_0 \cdot C_0 \cdot \Delta M_c^* \cdot K_c^*}{\{M_0 + M_g \cdot [\Delta M_p^* - \Delta M_c^* \cdot (1 - K_c^*)]\} \cdot [\Delta M_c^* - \Delta M_p^* \cdot (1 - K_p^*)] - M_g \cdot \Delta M_c^* \cdot \Delta M_p^* \cdot K_c^* \cdot K_p^*} \tag{12}$$

(Conditions: $l_c = 0, l_p = 0$).

2. During permeate formation the amount of gel swelling is relatively small. Taking into account that value K is decreased with reduction of gel swelling, it is assumed that $K_p = 0$ for many practical cases. Then equations (11) and (12) are simplified substantially:

$$C_c = \frac{M_0 \cdot C_0}{M_0 + M_g \cdot [\Delta M_p^* - \Delta M_c^* \cdot (1 - K_c^*)]} \tag{13}$$

$$C_p = \frac{M_0 \cdot C_0 \cdot \Delta M_c^* \cdot K_c^*}{\{M_0 + M_g \cdot [\Delta M_p^* - \Delta M_c^* \cdot (1 - K_c^*)]\} \cdot (\Delta M_c^* - \Delta M_p^*)} \tag{14}$$

(Conditions: $l_c = 0$, $l_p = 0$, $K_p = 0$).

3. It is possible to obtain another simplified form of equations (9) and (10) taking into account the specific features of the gel used and the process performed. For example, if only a permeate is of interest and we extract a solvent from the redundant amount of solution, then the items with M_g can be neglected in equations (9) and (10). This leads to the formula:

$$C_c = C_0 \qquad C_p = \frac{C_0 \cdot (\Delta M_c \cdot K_c + l_c)}{\Delta M_c + l_c - \Delta M_p \cdot (1 - K_p)} \tag{15}$$

(Condition: $M_g \ll M_0$).

4. Let us consider the formula that can be used for experimental determination of value K_c. The experiment is carried out as follows:

—swelling of a weighted amount of dry gel is performed in the weighted amount of substance solution with known concentration;

—swollen gel is separated from the concentrate, and after drying by filter paper the gel is weighted;

—the substance concentration in obtained concentrate is determined.

These experimental conditions correspond to $l_c = 0$, $l_p = 0$ and $\Delta M_p = 0$. Formula (9) in this case becomes:

$$C_c = \frac{M_0 \cdot C_0}{M_0 - M_g \cdot \Delta M_c \cdot (1 - K_c)} \tag{16}$$

From equation (16) it is easy to obtain:

$$K_c = 1 - \frac{M_0 \cdot (C_c - C_0)}{M_g \cdot C_c \cdot \Delta M_c} \tag{17}$$

All values in (17) are determined in the experiment.

SYMBOLS

Process Parameters

M_g the amount of dry gel in the cycle

M_0 the amount of separated solution that is fed into the cycle

M_c	the amount of concentrated solution (concentrate) that is removed from the swollen gel
M_p	the amount of diluted solution (permeate) that is removed from the gel after it has collapsed
C_0	substance concentration in the initial separated solution
C_c	substance concentration in a concentrate
C_p	substance concentration in a permeate
$C_{g,c}$	substance concentration in a "solution" that exists in a swollen gel during the stage of concentrate formation
$C_{g,p}$	substance concentration in a "solution," that exists in a swollen gel during the stage of permeate formation

Gel Parameters

ΔM_c	gel swelling during the stage of concentrate formation
ΔM_p	gel swelling during the stage of permeate formation
l_c	the amount of solution that remains at the surface of swollen gel after concentrate has been removed
l_p	the amount of solution that remains at the surface of swollen gel after permeate has been removed
K_c	factor of substance distribution during the stage of concentrate formation

$$K_c = \frac{C_{g,c}}{C_c}$$

K_p	factor of substance distribution during the stage of permeate formation

$$K_p = \frac{C_{g,p}}{C_p}$$

Comments

1. Values ΔM and l are measured in per-units (relative to M_g).
2. C_g is calculated based on the amount of both substances penetrating the gel, a solute and a solvent, but without taking into account the amount of the gel.

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