Supporting Information Appendix

Iterative procedure for adjusting data from the experiment in copper retention on composite gels:

Step 1. Determine an approximate value for the total number of free functional groups q as:

$$q = 2\left(Q_{alg} X_{alg} + Q_{edta} X_{edta} - (q_M)_{exp} - (q_{Ca})_{exp} - \frac{1}{2}(q_H)_{exp} \right) \qquad \text{(A1)}$$

where $(q_{Cu})_{exp}$, $(q_{Ca})_{exp}$ and $(q_H)_{exp}$ are the total amounts of copper, calcium, and protons in the gels, respectively, calculated from the data in the experiment according to the mass balances, referring to the total dry mass:

$$(q_{Cu})_{exp} = \left[(C_{Cu})_o - (C_{Cu})_f \right] \frac{V}{M_{tot}} \qquad \text{(A2)}$$

$$(q_{Ca})_{exp} = q^o_{Ca} - Y_{Ca} = \left[\left(q^o_{Ca} \right)_{alg} X_{alg} + Q_R X_R \right] - \frac{(C_{Ca})_f V}{M_{tot}} \qquad \text{(A3)}$$

$$(q_H)_{exp} = \left[(C_H)_o - (C_H)_f \right] \frac{V}{M_{tot}} = \left[10^{-pH_o} - 10^{-pH_f} \right] \frac{V}{M_{tot}} \qquad \text{(A4)}$$

Step 2. Substitute the values of q estimated according to equation (A1) in equation (7) and determine the values of the partition factor λ.

Step 3. Calculate the intraparticle concentrations via equation (5).

Step 4. Assume an initial value for $(K_{Ca1})_R$ and $(K_{Ca2})_R$, and calculate the values of q_{alg} and q_R.

Step 5. Determine the values of $(q_{Cu})_{alg}$ and $(q_{Cu})_R$ via equations (2) and (3), respectively.

Step 6. Calculate the total amount of copper chemically retained in gels via equation (1).

Step 7. Add the amount of copper enclosed in the gel fluid (due to the high content of water of these gels Γ_{Cu}, which is similar to that of single calcium alginate gels) and electrostatically bound to the polymer chains to the fraction of copper chemically retained q_{Cu},. This parameter is defined as:

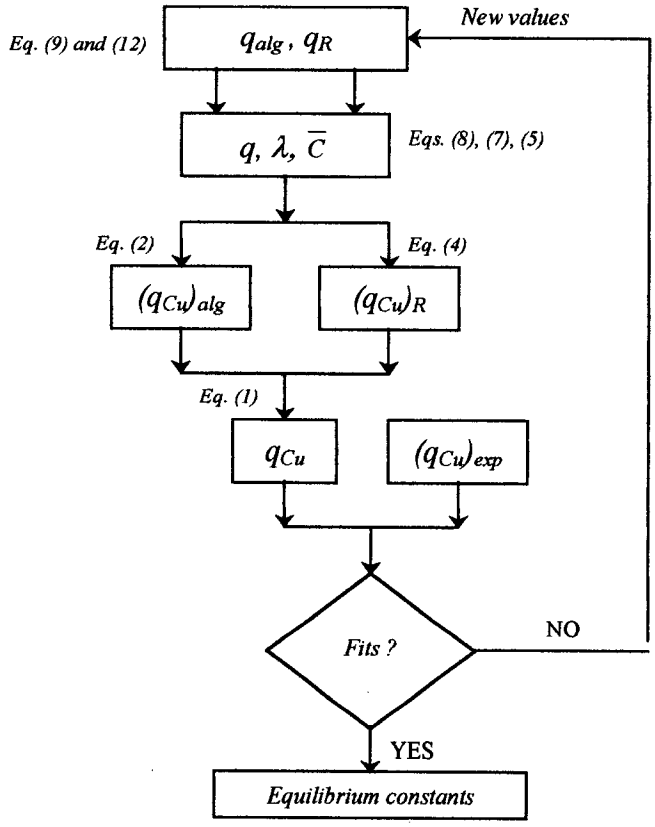
$$\Gamma_{Cu} = \overline{C}_{Cu} V_g / M_{tot} \qquad \text{(A5)}$$

In this way, a new value of $(q_{Cu})_{exp}$ is estimated.

Step 8. Compare this new value with the one from the experiment, checking the values of the equilibrium constants $(K_{Ca1})_R$ and $(K_{Ca2})_R$ which minimize the quadratic difference in the residuals between experimental and calculated values.

Step 9. With these values of the equilibrium constants, go back to step 4 and repeat the subsequent steps till the values of q remain constant.

FIGURE A1


Eq. (9) and (12)
q_{alg} , q_R
New values
q, λ, $\overline{C}$
Eqs. (8), (7), (5)
Eq. (2)
Eq. (4)
$(q_{Cu})_{alg}$
$(q_{Cu})_R$
Eq. (1)
q_{Cu}
$(q_{Cu})_{exp}$
Fits ?
NO
YES
Equilibrium constants