

## MATHEMATICAL MODELS FOR THE PREDICTION OF THE ENCAPSULATION BEHAVIOR IN FOOD SYSTEMS

**Iuliana Vintilă\***

*Dunarea de Jos University Galați,  
Food Science and Engineering Faculty,  
Domneasca 111, 800008 Galați, Romania*

\*Corresponding author: [vintilaiuliana@yahoo.com](mailto:vintilaiuliana@yahoo.com)

Received: February 10, 2010

Accepted: April 8, 2010

**Abstract:** The simulation of the encapsulation behavior in the multiphase complex system such food structure is based on the mathematical models constructed in respect with the Non-equilibrium thermodynamics Theory, Flory-Huggins Free Volume Theory (FHFV) and Complex Dispersed Systems (CDS).

The present research paper presents the differential equations describing the evolution in time of the multiphase dividing surfaces and the excess quantities such as surface density, surface momentum, surface energy and surface entropy associated with the dividing surfaces. The new completed theory of bio-polymers phase transitions co-jointed from Interfacial Transport Phenomena (ITP), FHFV and CDS will be validated with the inverse analysis method.

**Keywords:** *encapsulation, ITP, FHFV, CDS, bio-polymers*

## INTRODUCTION

Encapsulation is a process in which thin films, generally of polymeric materials, are applied to little solid particles, liquid or gases droplets. This method is used to trap active components and release them under controlled conditions. Several materials have been encapsulated in the food industry, among others, amino acids, vitamins, minerals, antioxidants, colorants, enzymes and sweeteners [1].

Encapsulation is used to protect compounds from oxidation, evaporation and off-flavor. The encapsulated compounds can be presented either with spherical geometry (single-particle structure) or with irregular geometry (aggregated structure) [2].

The most used mechanisms in encapsulation are extrusion, coacervation and complexation. Developing nanoencapsulation of multiple biologically active trace ions in a silica-based system for controlled-release is opening up application possibilities for regenerative biomedicine.

The quantitative macroscopic analysis of the complex food systems behavior in course of the encapsulation process is described in the scientific literature [1].

The mathematical models for the dynamics of the encapsulation process respect the non-equilibrium thermodynamics universal theory, in respect of stress-deformation behavior of the multi-phases interfaces.

Food systems with complex interfaces will be characterized with nonlinear constructive equations for stress-deformation behavior dependency.

The dynamic behavior of the complex encapsulation system is described based on the Interfacial Transport Phenomena [3].

Interfaces are modeled by the Gibbs' law dividing surface model and excess quantities such as surface density, surface momentum, surface energy and surface entropy are associated with the dividing surface [4].

The Flory-Higgins Free Volume (FHFV) theory is developed by Vrentas [5] and can predict the behavior of the synthetic polymers system in solution state.

The validation of the new mathematical model for description of the encapsulation dynamic process will be validated with the inverse analysis method [6].

## RESULTS AND DISCUSSIONS

The differential equations describing the evolution in time of the multiphase system interface and the excess quantities associated are as followings:

(1) Jump Mass Balance Equation:

$$\frac{ds\rho^s}{dt} + \rho^s \operatorname{div}_s v^s + \rho(v - v^s)\xi = 0 \quad (1)$$

(2) Jump Species Mass Balance:

$$\rho^s \frac{d_s \omega_i^s}{dt} + \operatorname{div}_s j_i^s + j_i \xi + \rho(\omega_i - \omega_i^s)(v - v^s)\xi = 0 \quad (2)$$

(3) Jump Momentum Balance:

$$\rho^s \frac{d_s v^s}{dt} - \operatorname{div}_s T^s - \sum_{i=1}^N \rho_i^s \tau_i^s + \rho(\omega_i - \omega_i^s)(v - v^s)\xi - T\xi = 0 \quad (3)$$

(4) Jump Energy Balance

$$\begin{aligned} \rho^s \frac{d_s E^s}{dt} = T^s : \nabla_s v^s + \sum_{i=1}^N j_i^s \tau_i^s - \text{div}_s q^s + \rho^s Q^s \\ - \rho(E - E^s) + \frac{1}{2} |v - v^s| (v - v^s) \xi - (v - v^s) T \xi + q \xi \end{aligned} \quad (4)$$

(5) Jump Entropy Balance

$$\rho^s \frac{dS^s}{dt} + \text{div}_s \left( \frac{\phi^s}{T^s} \right) - \rho^s \frac{Q^s}{T^s} + \rho(S - S^s)(v - v^s) \xi + T^{-1} \phi \xi \geq 0 \quad (5)$$

where:

- $v^s$  - the surface velocity;
- $\rho$  - the phases density;
- $\xi$  - the surface normal vector;
- $\omega_i^s$  - the mass fraction of  $i$  species;
- $j_i$  - the mass flux vector of  $i$  species;
- $T^s$  - the surface stress tensor and T stress tensor of phases;
- $\tau_i^s$  - the force per unit mass acting on the  $i$  interface species;
- $E^s$  - the surface energy per unit mass;
- $q^s$  - the surface energy flux vector;
- $Q^s$  - the rate of radiant energy transfer per unit mass;
- $\phi^s$  - the surface thermal energy flux vector;
- $S^s$  - the surface entropy per unit mass;
- $T^s$  - the interface temperature.

The boldface bracket represents the transfer of mass, momentum, energy and entropy from the bulk phase to the interface (6).

$$[\psi \xi] = \psi^{(1)} \xi^{(1)} + \psi^{(2)} \xi^{(2)} \quad (6)$$

where  $\psi^{(1)}$  and  $\psi^{(2)}$  are the values of the  $\psi$  described as the unit mass, momentum, energy and entropy of the adjoining bulk phases (1) and (2) in the ITP.

The deformation behavior in the encapsulation process of the W/W emulsions depends on 6 factors:

- (1) mass transfer coefficient across the interfaces ;
- (2) interfaces surface tension (Helfrich expansion);
- (3) interfaces bending rigidities;
- (4) interfacial permeability;
- (5) interfaces dilatational coefficient;
- (6) surface rheological parameters.

The rheological behavior of an emulsion interface stabilized with low molecular peptides is described by the Boussinesq law [2]. The alignments of the particles at the interfaces affect the interfacial rheological parameters. The increasing of the deformation rate decreases the shear viscosity and surface dilatational viscosity.

The surface chemical potential  $\mu_i^S$  of species  $i$  depend on total surface Helmholtz free energy  $F^S$  (7):

$$\mu_i^S = \left( \frac{\partial F^S}{\partial \rho_i} \right)_{T^S, \rho_j^S}, j \neq i \quad (7)$$

$$F^S = \int F^S(\rho_1^S, \dots, \rho_N^S) di$$

The Flory-Higgins Free Volume (FHFV) theory is developed by Vrentas [5] and can predict the behavior of the synthetic polymers system in solution state.

Based on the FHFV theory expressed in equation (8), we can design the phase diagram in the transition state of all types of bio-polymers as a dependency of water activity vs. temperature.

$$\frac{\mu_w}{RT} = \ln(1 - \phi) + \left(1 - \frac{1}{N}\right)\phi + \lambda\phi^2 + F(\phi) \quad (8)$$

where:

$\mu_w$  - is the activity of water absorbed in the bio-polymer structure;

$T$  - is the absolute temperature;

$\phi$  - is the volume fraction of dissolved bio-polymer/fraction of bio-polymer;

$F(\phi)$  - is the free volume term;

$N$  - is the ratio of the molar volume of solvate bio-polymer and water.

In addition, the state diagram can be completed with the Complex Dispersed System data in order to investigate the different transition states of the bio-polymers in the encapsulation process.

We propose also the evaluation of the encapsulation performance index (9) with the following expression:

$$Encapsulation\ Performance\ Index\ (\%) = \left( C_i \cdot V_i - \frac{F_i \cdot W_i}{C_i \cdot V_i} \right) \times 100 \quad (9)$$

where:

$C_i$  - the concentration of  $i$  compound from the initial nanoparticle extract;

$W_i$  - the theoretical amount of  $i$  compound added;

$V_i$  - the volume of compound  $i$  from the nanoparticle extract;

$F_i$  - the concentration of compound  $i$  in the un-encapsulated portion.

We propose the validation of the new complex mathematical model for the describing of the encapsulation dynamics to be realized with the inverse analysis method (Figure 1).

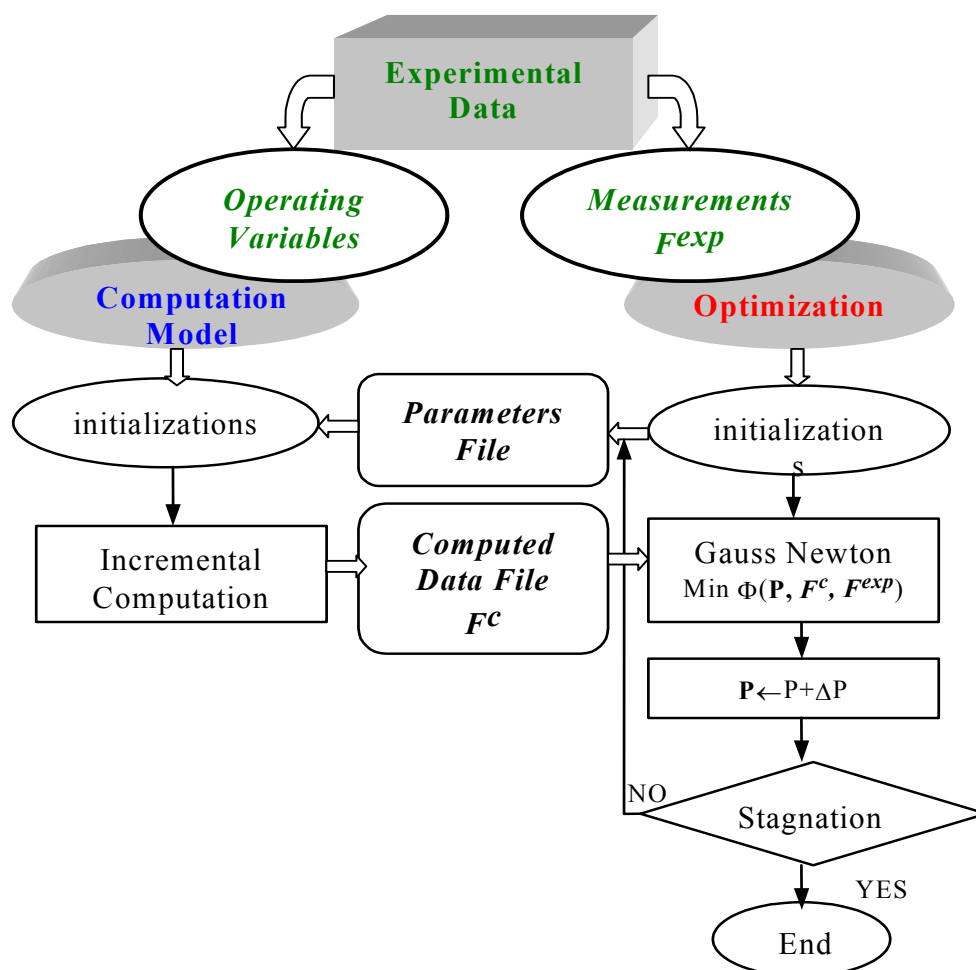


Figure 1. The principle of inverse analyses method [6]

## CONCLUSIONS

The encapsulation phases' transitions can be described with the thermodynamics equations and the chemical potential of the coexisting phases. The complete model of the encapsulation dynamics can also predict the phase transitions with the construction of a state diagram. The state diagram allows the selecting of the optimum processing system in order to create a certain food structure.

## REFERENCES

1. Shahida, F., Han, X: Encapsulation of food ingredients, *Critical Reviews in Food Science and Nutrition*, **1993**, 33, 501–547;
2. Pedrolas, I.R.: Alimentos microencapsulados. Particularidades de procesos para la microencapsulacion de alimentos para larvas de especies acuicolas, in: *VI International Symposium of Aquatic Nutrition*. (Editors: Cruz Suarez, L.E., Ricque-Marie, D., Tapia-Salazar, M., Gaxiola-Cortes, M.G., Simies N.), Mexico, **2002**, 103-109;
3. Sagis, L.M.C.: Dynamics of controlled release systems based on water-in-water emulsions: A general theory, *J. Controlled Release*, **2008**, 131 (1), 5-13;

4. Slattery, S.C., Sagis, L.M.C.: *Interfacial Transport Phenomena*, Springer, New York, **2007**;
5. Vrentas, J.S., Vrentas C.M.: Evaluation of the sorption equation for polymer-solvent system, *Journal of Applied Polymer System*, **1994**, **51** (10), 1791-1794;
6. Gavrus, A: *Identification des paramètres rhéologiques par analyse inverse*. In: Ph.D. Thesis, Paris, **1996**.