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IChemE



## From laboratory to scale-up by modelling in two cases of $\beta$ -carotene extraction from vegetable products

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### A B S T R A C T

The laboratory investigation of  $\beta$ -carotene separation from rose hip fruits (RHF) powder and carrot noodles (CN) was analyzed by means of mathematical modelling, in order to develop models for process scale-up. The developed models contain parameters characterizing species transport inside and outside of vegetal material particle as well as species interphase equilibrium distribution. The model parameters were estimated by experimental data capitalization. The solvent type, liquid–solid ratio and extraction temperature were selected as process factors in  $\beta$ -carotene extraction. Having a significant influence on the process yield, these factors determined the values of model parameters. A model based on process control by external diffusion of extracted species and particle swelling was adopted for  $\beta$ -carotene extraction from RHF, whereas an internal diffusion one was chosen to describe the process in the case of  $\beta$ -carotene extraction from CN. The model parameters were identified by least squares method using theoretical and experimental data characterizing the dynamics of species extraction yield. The scale-up of counter current multistage extraction was performed through analysis of the processes studied at laboratory level.

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**Keywords:**  $\beta$ -Carotene; Solid–liquid extraction; Extraction modelling; Parameters identification; Scale-up; Multistage extraction

### 1. Introduction

The scale-up of a process involves the development of a suitable mathematical model, enabling the process design for a fixed production capacity, as well as the model simulation in order to establish the production capacity of an existing plant (Dobre and Sanchez, 2007; Donati and Paludetto, 1997). Usually, the laboratory research in herbal extraction field does not deeply focus on models building for design and simulation of a real separation. From this point of view, the present study tries to be a step forward. The paper focuses on  $\beta$ -carotene extraction from two sources, i.e. fine

ground rose hip fruits and carrot noodles. It is known that these sources are characterized by significant carotenoids content. The carotenoids have important applications in food and pharmaceutical industry, especially  $\beta$ -carotene, known as E160a additive (Milne, 2005). Various  $\beta$ -carotene enriched food or medicines are used today for prevention and control of some affections, e.g. cancer, cardiovascular and degenerative diseases (Ashurst, 1999; Carter et al., 2004; Delgado-Vargas and Paredes-Lopez, 2003; Wenzig et al., 2008; Yuan et al., 2008). Increasing demand for  $\beta$ -carotene has resulted in a growing interest in its extraction from different natural resources, e.g. vegetable and fruit wastes, using different solvents, including

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### Nomenclature

$A_p$	article interphase transfer surface area ( $m^2$ )
$c_l$	species concentration in the liquid phase ( $kg/kg_l$ )
$c_s$	species concentration in the solid phase ( $kg/kg_s$ )
$c_{se}$	species specific mass in the liquid phase ( $kg/kg_s$ )
$D_{ef}$	effective diffusion coefficient ( $m^2/s$ )
$D_m$	molecular diffusion coefficient in the liquid phase ( $m^2/s$ )
$d_p$	particle diameter (m)
$k$	mass transfer coefficient (m/s)
$k_{de}$	species interphase distribution coefficient ( $kg_l/kg_s$ )
$k_{dis}$	species interphase distribution coefficient, $k_{dis} = 1/k_{de}$ ( $kg_s/kg_l$ )
$k'_{dis}$	corrected interphase distribution coefficient ( $kg_s/kg_l$ )
$K_v$	volumetric mass transfer coefficient ( $s^{-1}$ )
$l$	carrot noodle width (m)
$L$	carrot noodle length (m)
$m_l$	liquid mass ( $kg_l$ )
$m_p$	particle mass ( $kg_s$ )
$m_s$	solid mass ( $kg_s$ )
$M_\tau$	species mass transferred at $\tau$ moment (kg)
$n$	exponent in Eq. (10)
$r_{ls}$	liquid–solid ratio ( $kg_l/kg_s$ )
$t$	temperature ( $^\circ C$ )
$x$	axial coordinate (m)

### Greek letters

$\beta$	swelling speed constant ( $s^{-n}$ )
$\delta$	carrot noodle thickness (m)
$\varepsilon$	particle porosity
$\gamma$	particle erosion speed (m/s)
$\eta$	species extraction yield
$\rho$	density ( $kg/m^3$ )
$\sigma_m$	specific interphase transfer surface area ( $m^2/kg_s$ )
$\tau$	time (s)
$\xi$	tortuosity

### Subscripts

calc	calculated
exp	experimental
l	liquid
min	minimal
p	particle
ref	reference
s	solid
sat	saturation
0	initial
$\infty$	long contacting time

### Superscripts

*	equilibrium
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carotenes extractions (Bashipour and Ghoreishi, 2012; Doker et al., 2004).

The scale-up of an extraction procedure, by means of experimental data capitalization, can be performed according either to the investigated procedure or to a different one. For instance, characteristic experimental data of single stage extraction can be used to scale up the multistage countercurrent extraction. Accordingly, based on experimental results obtained in a single stage procedure, kinetic models characterizing the transfer of extractable species at particle level have been developed (Ho et al., 2005; Minkov et al., 1996; Thomas et al., 2007). These kinetic models coupled with characteristic models of contacting procedure can be applied for process scale-up (Dobre et al., 2010; Simeonov et al., 2004).

A classification of the models used to describe the species transfer at particle level is presented in Fig. 1. It has been considered that the particle of vegetal material (PS) has the capacity to change its dimension (WCD) or, alternately, to keep its initial one (NCD). The WCD case characterizes the pure swelling and swelling with surface erosion. The species mass transfer (MT) can be classified as: (i) extraction with process control inside the particle (IMT abbreviation for internal mass transfer); (ii) extraction with process control outside the particle (EMT abbreviation for external mass transfer). The internal diffusion in particles beds (PB) can be predicted by a shrinking core model (SCM) or an integral diffusion model (IDM) (Goto et al., 1996; Monnerat et al., 2006; Seikova et al., 2004). Depending on operation conditions, two types of boundary conditions have been identified for particle surface species transfer: type 1 (CL1), taking into account a constant species concentration and type 3 (CL3), considering species flux given by convective mass transfer, respectively. According to the mentioned abbreviations, the names of the models can be easily established. For instance, the model coded as SCMMFE/CL3 corresponds to a shrinking core model (SCM) with erosion (E) at mobile frontier (MF) and type 3 boundary conditions (CL3).

As shown in Fig. 1 the number of parameters characterizing the models for species transfer at particle level can range from 2 to 6 (Goto et al., 1996; Martinez-Vera et al., 2010; Simeonov et al., 1999). When a single type of experimental data is available, it is recommended to identify only one or two parameters (Cacace and Mazza, 2003).

This paper focuses on application of mathematical models in order to describe the extraction of  $\beta$ -carotene from rose hip fruits (RHF) powder as well as from carrot noodles (CN) and to estimate the model parameters, which can be further used for process scale-up. Like in most experimental cases, we used a single type of data, consisting of results on dynamics of  $\beta$ -carotene extraction yield from RHF powder and CN for batch extraction procedure under various extraction conditions (liquid–solid ratio and operation temperature). In the case of  $\beta$ -carotene extraction from RHF powder, a model of external diffusion with particle mobile frontier (EDMF) was selected to predict the process at particle level. This selection was based on a small diffusion length inside the fine particle with an equivalent diameter less than 0.3 mm. Accordingly, the internal mass transfer resistance was neglected and the external diffusion in a liquid film surrounding the particle was assumed as a rate-limiting step. Another assumption taken into account was the particles swelling during the extraction process, so that the transfer surface varied in time. Based on particle geometry and contacting procedure, an internal diffusion model with type 1 boundary conditions (IDM/CL1) was adopted to describe  $\beta$ -carotene extraction from CN.

supercritical carbon dioxide (Favati et al., 1988; Fikselová et al., 2008; Spanos et al., 1993; Sturzoiu et al., 2011; Vega et al., 1996). More simple or complex models have been developed in order to explain experimental data in some

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