Modelling and simulation of supercritical fluid extraction of volatile oils from aromatic plants

Rui M. Filipe[a,b]
rfilipe@isel.ipl.pt

José A. Coelho[a,c]
jcoelho@deq.isel.ipl.pt

[a] Área Departamental de Engenharia Química, Instituto Superior de Engenharia de Lisboa, Lisboa, Portugal
[b] Centro de Recursos Naturais e Ambiente, Instituto Superior Técnico, Lisboa, Portugal
[c] Centro de Química Estrutural, , Instituto Superior Técnico, Lisboa, Portugal

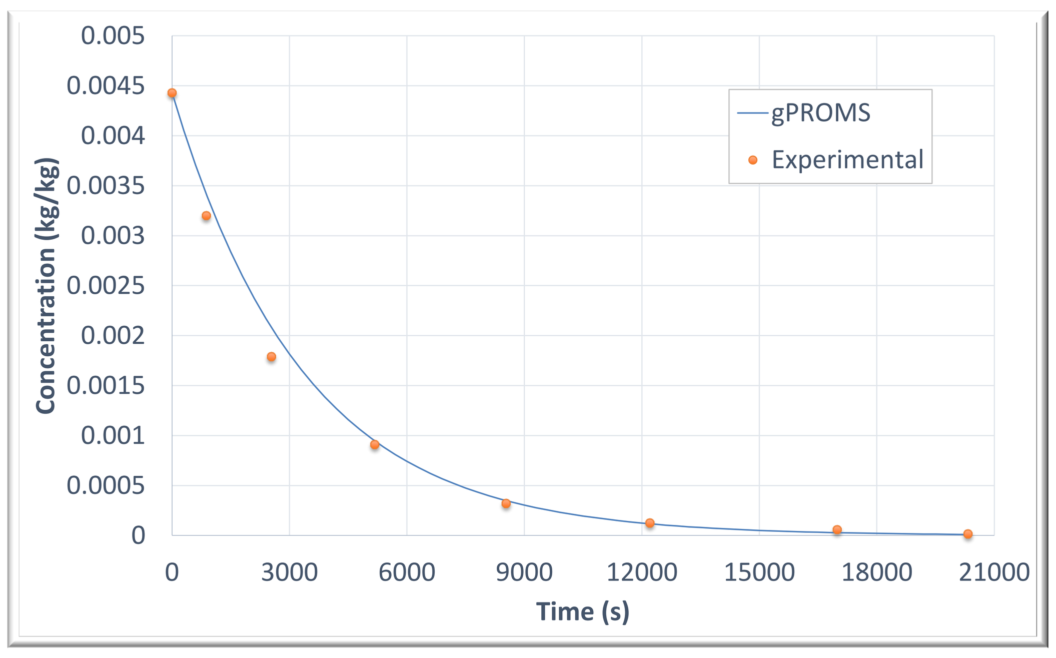
Dynamic models are a useful tool for the design, optimization and scale-up of supercritical fluid extraction processes, from laboratory to pilot and industrial scales. In particular, mass balance based models which include mass transfer coefficients in fluid and/or solid phases have a strong physical significance. They take into account the characteristics of the plant matrix, namely the particle size, the bed porosity and also the equilibrium relationships and mass transfer mechanisms. Although several models have been proposed in the literature, their solution is not always trivial and, additionally, the estimation of some parameters using experimental data is required. With this context, the opportunity to use new tools to model, simulate and perform parameter estimation seems promising.

Using gPROMS Model Builder, different models are applied to study the extraction of three different volatile oils from aromatic plants: **coriander** (c), **fennel** (f) and **savory** (s). The desorption model by Tan and Liou (1989) and the model proposed by Sovová (1994), both with and without axial dispersion are used. These models consider the variation of the concentration of the supercritical fluid as it flows along the extractor and, thus, include partial differential equations. Parameter estimation is used to determine the desorption rate constant (k_d), the internal and external mass transfer coefficient (k_s and k_f) and the axial dispersion coefficient (D_{ax}).

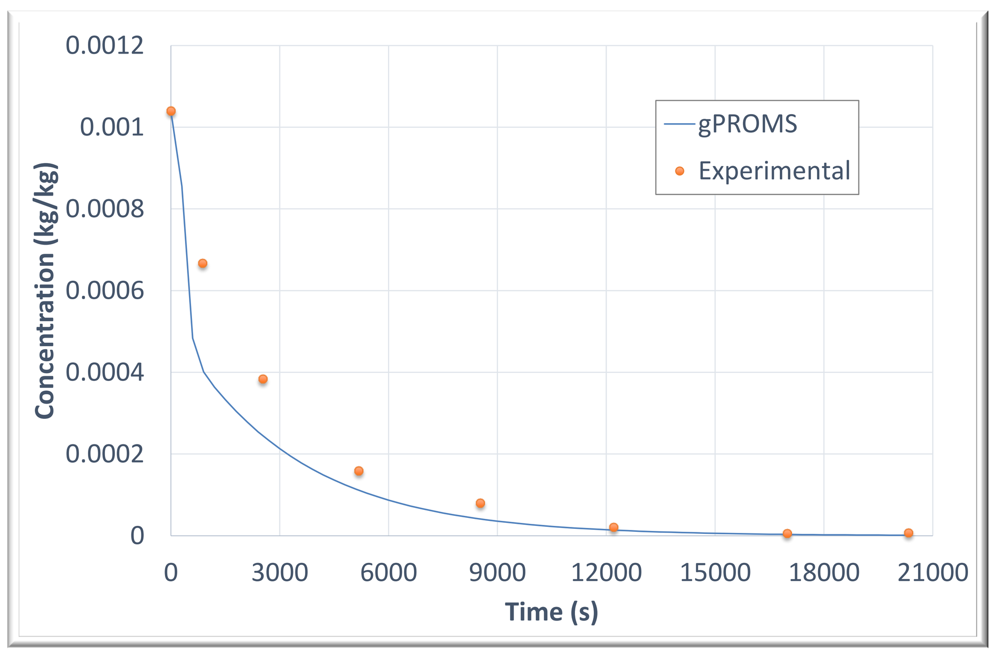
	Model			
Equations	1[iii]	2	3[ii]	4
$\frac{\partial C}{\partial t}+\frac{u}{\varepsilon}\frac{\partial C}{\partial h}+\frac{1-\varepsilon}{\varepsilon}\frac{\rho_s}{\rho_f}\frac{\partial q}{\partial t}=0$	✔		✔	
$\frac{\partial C}{\partial t}+\frac{u}{\varepsilon}\frac{\partial C}{\partial h}+\frac{1-\varepsilon}{\varepsilon}\frac{\rho_s}{\rho_f}\frac{\partial q}{\partial t}-D_{ax}\frac{\partial^2 C}{\partial h^2}=0$		✔		✔
$\frac{\partial q}{\partial t}=-k_d q$	✔	✔		
$\frac{\partial q}{\partial t}=-\frac{k_f a \rho_f}{\rho_s}(C_0-C)\,,\quad q\geq q_k$ $\frac{\partial q}{\partial t}=-k_s a q\,,\quad q<q_k$			✔	✔
I.C. $q(h,0)=q_0$ $C(h,0)=C_0$	✔	✔	✔	✔
B.C. 1 $C(0,t)=0$ $\frac{\partial C}{\partial h}=0\,,\quad h=L$	✔		✔	
B.C. 2 $\frac{u}{\varepsilon}C-D_{ax}\frac{\partial C}{\partial h}=0\,,\ h=0$ $\frac{\partial C}{\partial h}=0\,,\quad h=L$		✔		✔
Adjustable parameters	k_d	k_s, q_k, D_{ax}	k_s, k_f	k_s, k_f, D_{ax}

The yield of extraction is used as indicator for extractor efficiency:

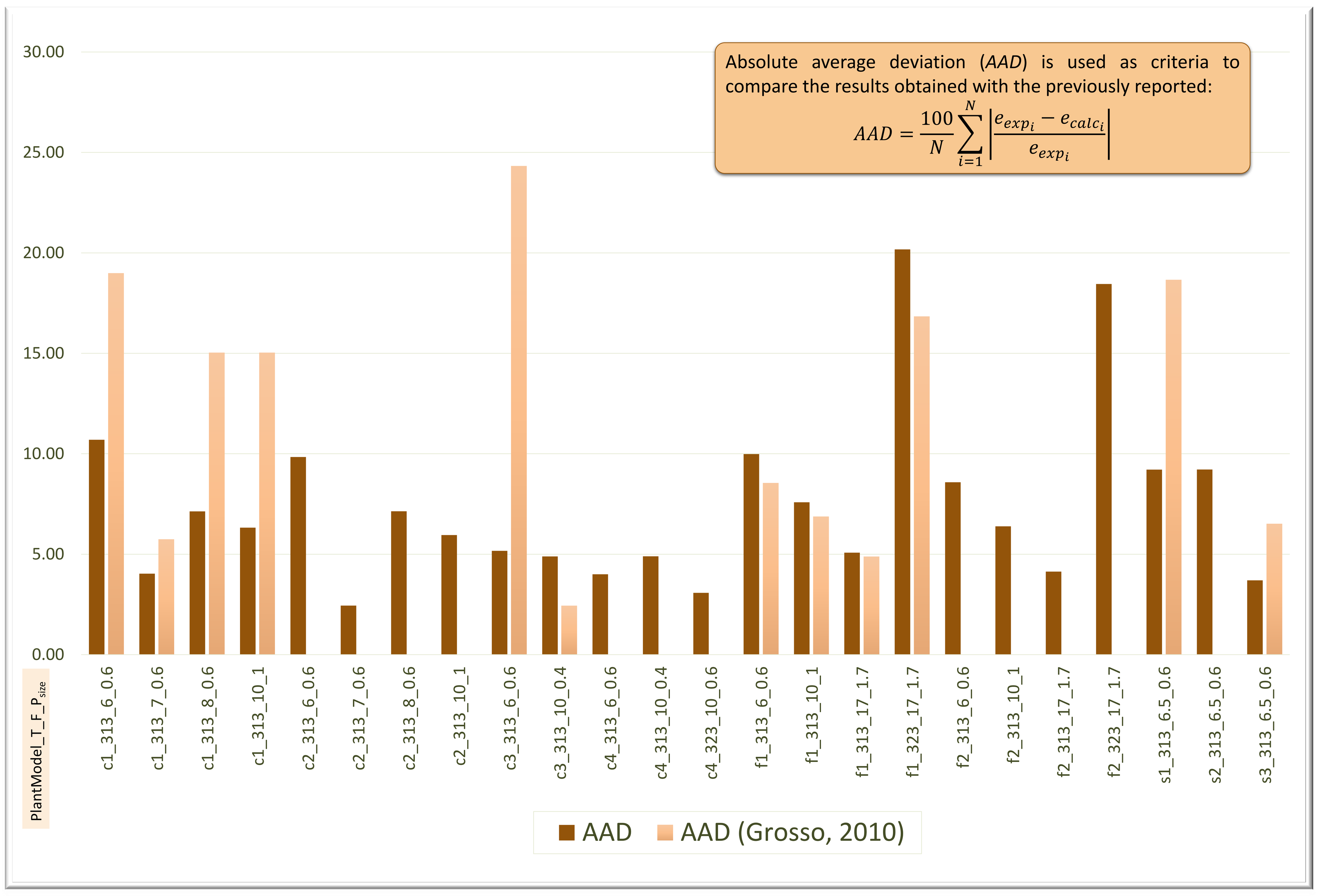
$$e=\frac{Q}{M_p}\int_0^t C(\mathrm{t},\mathrm{h}=\mathrm{L})\,dt$$



Concentration in the solid phase



Concentration in the fluid phase

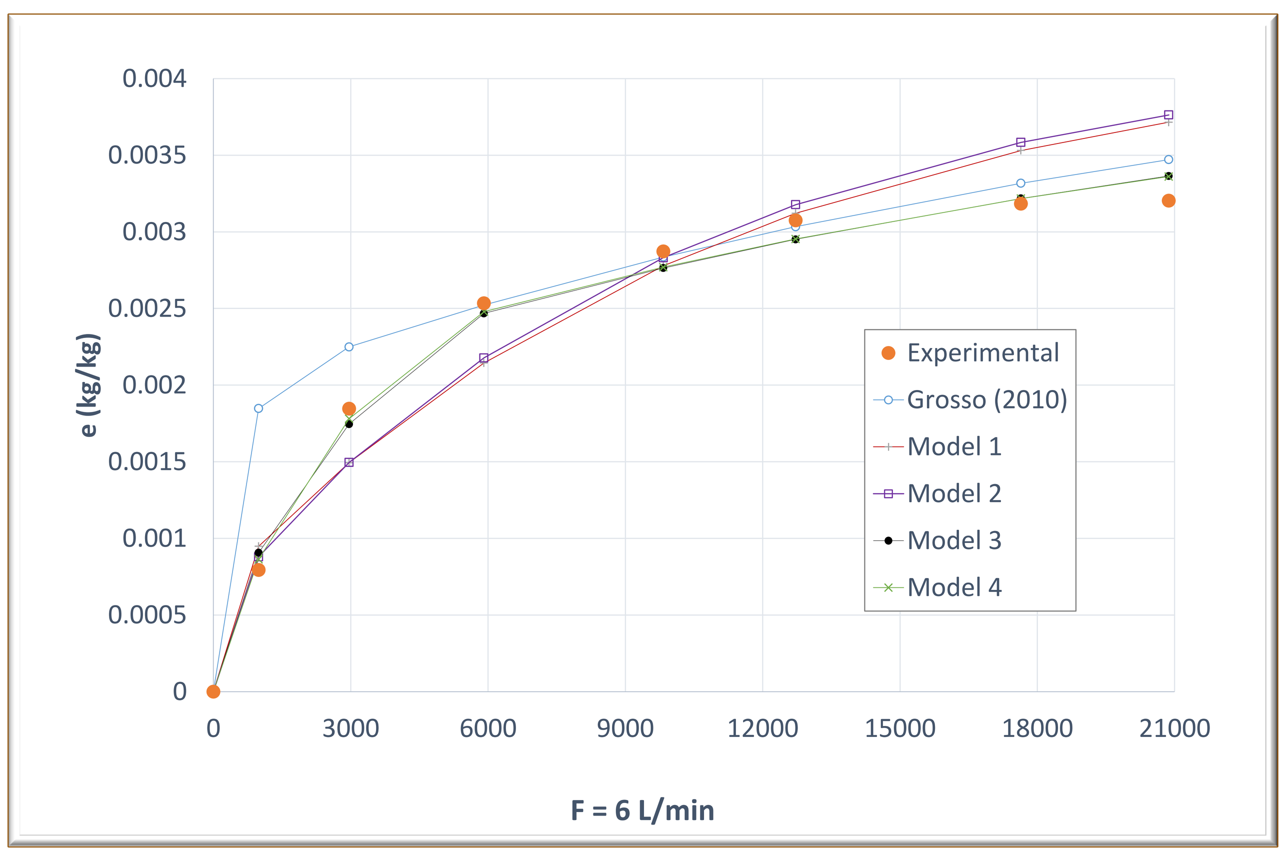


Absolute average deviation (*AAD*) is used as criteria to compare the results obtained with the previously reported:

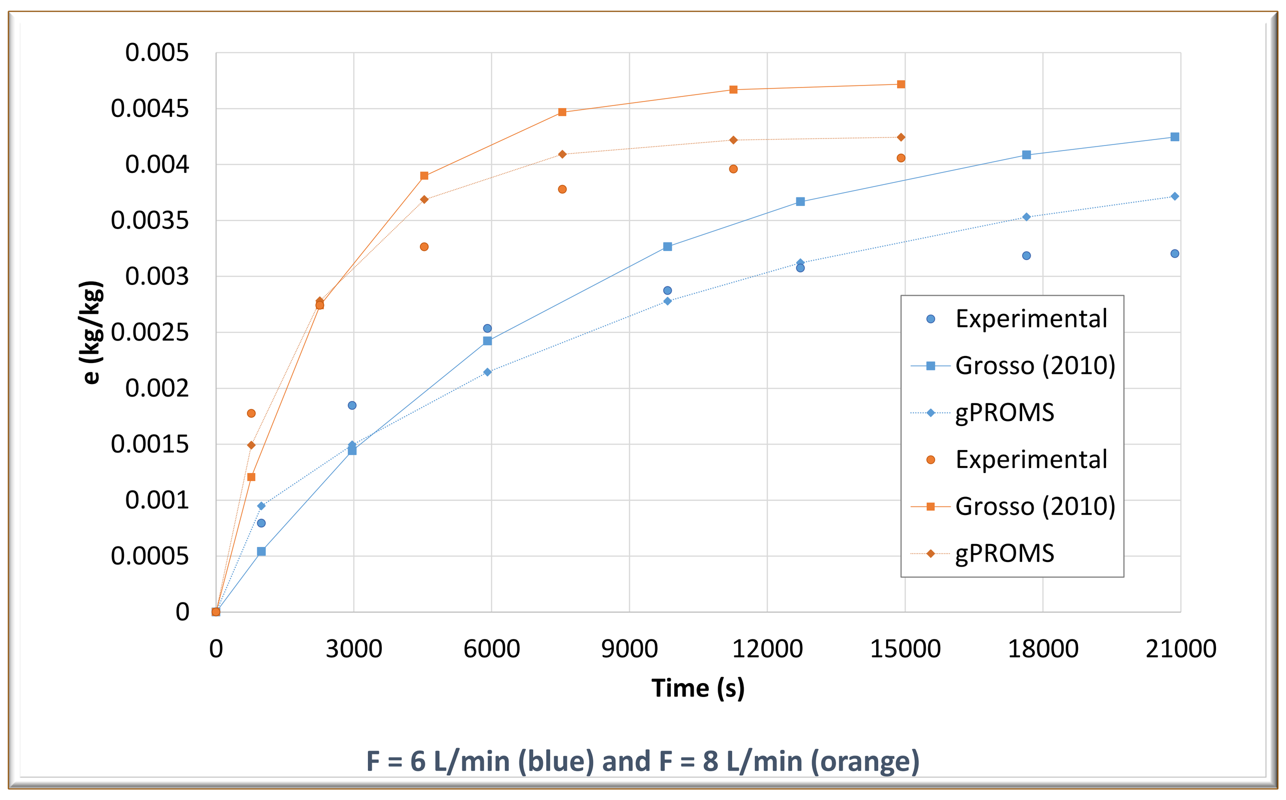
$$AAD=\frac{100}{N}\sum_{i=1}^{N}\left|\frac{e_{exp_i}-e_{calc_i}}{e_{exp_i}}\right|$$

Coriander

P = 9 MPa, T = 313.15 K, P_{size} = 0.6 mm



F = 6 L/min



F = 6 L/min (blue) and F = 8 L/min (orange)

Although some limitations were encountered due to the limited amount of data available for parameter estimation, the results obtained improved the ones previously reported (Grosso, 2010), assessed by the absolute deviation error.

gPROMS Model Builder appears as a good alternative as it integrates in a single environment features such as model development and parameter estimation.

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