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Model reduction technique for faster simulation of drying of spherical solid foods

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ABSTRACT

To simulate drying of foods, the classical calculation based on finite differences, elements or volumes are quite time consuming, which may be an issue in an optimisation procedure where hundreds or thousands of simulations are necessary. A model with coupled heat and mass transfers, based on diffusion and convection, with non-linear properties and boundaries makes an accurate but slow simulator for drying of foodstuffs. In this work, it was shown that the model with coupled heat and mass transfer can be replaced by a simple and much faster, yet as accurate, two- or three-compartment model. Equivalent predictions of mean product temperature and moisture content are obtained by linking exchange coefficients (in compartmental model) to transfer coefficients (in diffusion convection model) and fine tuning the compartment volume sizes. The resulting simulations are very close with calculation time nearly a hundred times faster.

1. Introduction

Modelling of drying kinetics is essential in most agro-industrial simulations: sugar industry, biomass refinery, fodder processing etc. Commercially available simulation programmes are often limited to steady-state simulations, whereas dynamic simulations are based on a better understanding of the process hence lead to better plant optimisations. The classical dynamic simulation of drying makes heavy use of heat and mass transfer equations requiring both space and time discretisations. Discretisations are based on finite difference, finite volume or finite element methods (Puri and Anantheswaran, 1993). These numerical methods often require significant computing times to ensure stability and convergence, leading, e.g., to limited applicability in optimisation procedures. To overcome this computing time limitation, one may consider the work of Crank (1975) who developed several analytical solutions for regular shapes (sphere, cylinder and slab). Nevertheless, for most non linear ordinary differential equations, analytical solutions are not available. In that perspective, van der Sman (2003) proposed a simplified model by dividing the food body in a shell and a core which is similar to a compartmental approach. However, this model is designed to predict only the cooling of high-moisture cylindrical shaped foods. As a matter of fact, to simulate drying of foods, the coupling between heat and mass transfers must be taken into account explicitly. Furthermore, the fact that most product properties are depending on state variables (i.e. local product moisture content and temperature) is often responsible for the main nonlinearities of the model.

Predicting heat and mass transfers, during drying by compartment models, is far less demanding in calculation time than conventional numerical methods, such as finite differences, finite elements or finite volumes. It is applied successfully in many chemical engineering fields, such as spray fluidised bed agglomeration (Hussain et al., 2014), mechanical mixing (Delafosse et al., 2014) or liquid–liquid separation (Peng et al., 2012). In the drying domain, In the drying domain, a number of compartmental models are developed. These models can be divided into two categories: empirical and semi-theoretical models. So far, the diffusion mecanism, which includes both heat and mass transfers, is not taken into account by compartmental models. Empirical models require experimental drying data and a simple mathematical function (e.g. exponential, quadratic or logarithmic expressions). For instance, Sharma et al. (1982) used a two-compartment model

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Nomenclature

Roman capital letters

Bi_m	Biot number for mass transfer, dimensionless
Bi_{th}	Biot number for heat transfer, dimensionless
C	concentration of water vapour in air, kg m^{-3}
CV	control volume
Cp	specific heat capacity, J kg^{-1} K^{-1}
Cp_w	specific heat capacity of liquid water, J kg^{-1} K^{-1}
D	moisture diffusivity, m^2 s^{-1}
Fo	Fourier number, dimensionless
J	objective function fed to the simplex method, see Eq. (34)
M	Molar mass of water, 0.018 kg mol^{-1}
N	number of volumes of finite volume discretisation, dimensionless
ODE	ordinary differential equation
P_v	pressure of water vapour, Pa
R_G	gas constant, 8.314 J mol^{-1} K^{-1}
RH	relative humidity of air, decimal
$RMSE$	percentage of root-mean square error, %
S	surface area of an interface between compartments, m^2
T	temperature, K
U	enthalpy, J
V	volume, m^3
X	moisture content, dry basis

Roman small letters

a_w	water activity, dimensionless
dr	infinitesimal radius increment, m
h	convection heat transfer coefficient, W m^{-2} K^{-1}
i	i-th elementary volume/compartment
j	j-th drying time used to compare two models
k	convection mass transfer coefficient, m s^{-1}
$\dot{m}$	mass flux density at surface, kg s^{-1} m^{-2}
n	number of drying time used to compare two models
r	distance from the centre, m
t	time, s

Greek letters

α	thermal diffusivity, m^2 s^{-1}
β	root of the transcendental Eq. (32), dimensionless
Δr	thickness of a compartment/volume, m
ΔH_v	latent heat of water vaporization, J kg^{-1}
Δa_w	surface condition based on water isotherms, see Eq. (14)
ΔX	linear surface condition, see Eq. (30)
λ	thermal conductivity, W m^{-1} K^{-1}
ρ	density, kg m^{-3}
ξ	mass exchange coefficients at the interface between two adjacent compartments, m s^{-1}

Subscripts

1	relative to the first (central) *CV*
\	at the interface between two *CV*
2	relative to the second *CV*
3	relative to the third *CV*
∞	relative to the drying air
air	dry air
c	mean radius of a volume or of a compartment
dm	dry matter
$\vert_e$, *e*	east side face of the CV
eq	equilibrium, at end of drying
G	relative to R_G
i	i-th elementary volume/compartment
init	initial, just before drying starts
j	j-th drying time used to compare two models
m	see Bi_m
N	number of control volumes in finite volume method
$r = 0$	at centre of the particle
$r = R$	at outer surface of the particle
th	see Bi_{th}
v	water vapour
$\vert_w$, *w*	west side face of the CV (see also a_w and Cp_w).

Superscripts

¯	mean over the solid at a given time
1/2	square root
comp	predicted by a compartmental model
exact	exact algebraic calculation
finite volume	predicted by a finite volume method
sat	saturated water vapour

to predict drying rate of paddy rice. Costa et al. (1999) proposed an empirical relationship for the kinetics of fry-drying of potato slices by assuming that the product consists of two compartments. The same approach is used by Varadharaju et al. (2001) to model the drying of coffee cherry by a two-term exponential equation. These models require a lot of experimental data to be the best fit while providing minimal explanation for observed drying behaviours. On the contrary, semi-theoretical models are based on the principle of heat and mass balances. Toyoda (1988), Courtois et al. (1991) and Abud Archila et al. (2000), have used this approach with 2 or 3 compartments to model the drying of grains. In this approach, mass transfer, and possibly coupled heat and mass transfers within the drying particle, are considered to occur between separated compartments. Each compartment has its own moisture content and, possibly, its own temperature. Having only 2 or 3 compartments, the model results in a maximum of 6 ordinary differential equations to be solved. In addition, this restricted set of equations is observed to be numerically far more stable, allowing for faster numerical integration. On the other hand, such models are often considered as empirical ones due to the apparent lack of physical meaning of its coefficients. One may speak of exchange coefficients as opposed to well known transfer coefficients.

This works aims at bridging the gap between the two kinds of approaches in order to demonstrate that an optimised compartmental model can be far more efficient (e.g. 100 times faster computing time) than a finite volume model while keeping the advantage of meaningful parameters. A generic method was developed to deduce an equivalent compartmental model from a given diffusion convection model. The overall method is outlined in the Fig. 1 showing the hierarchy of model building. As will be explained further, to ensure the 2 (or 3) compartment model (noted $[2X{\cdot}2T{\cdot}\Delta a_w]$ and $[3X{\cdot}3T{\cdot}\Delta a_w]$ and their variants with non-limiting heat conduction $[2X{\cdot}1T{\cdot}\Delta a_w]$ and $[3X{\cdot}1T{\cdot}\Delta a_w]$) is numerically equivalent to the diffusion convection models (noted $[\nabla X{\cdot}\nabla T{\cdot}\Delta a_w]$