

REACTION ENGINEERING METHODOLOGY AS AN EFFECTIVE APPROACH TO MODEL DRYING, BAKING AND WATER VAPOR SORPTION PROCESSES

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ABSTRACT

An effective model of simultaneous heat and mass transfer processes is useful to assist in process design, optimization of existing processes and monitoring product quality. Previously, the lumped reaction engineering approach (L-REA) has been shown to model the global drying rate of several heat and mass transfer processes very well. Here, the REA framework is implemented to model the local evaporation/condensation rate in drying of non-food materials, baking and water vapor sorption. The REA is combined with a set of equations of conservation of heat and mass transfer to yield the S-REA (spatial reaction engineering approach) to model these processes. For modeling each process, the activation energy is generated from one accurate run and evaluated according to environmental temperature and humidity. The relative activation energy implemented in the L-REA is implemented in the S-REA by applying local variables. The results indicate that the S-REA is accurate to describe baking, drying and water vapor sorption process, which shows the applicability of the REA to model the local evaporation/condensation rate of these processes. The S-REA is readily implemented to assist in process design, evaluation of existing processes and maintenance of product quality. In near future, by coupling with solid mechanics, the REA may be employed to predict material deformation and shape change during heat and mass transfer processes by coupling with solid mechanics. The development of the REA to describe migration of volatiles inside materials undergoing heat and mass transfer processes is also underway.

Keywords: reaction engineering approach, drying, baking, water vapor sorption, model

1. INTRODUCTION

Several heat and mass transfer processes including drying, baking and water vapor sorption are commonly applied in industry. For process design of new equipment and evaluation of current processes, a reliable mathematical model is useful. The model may also be used to predict product quality during the processes. The reaction engineering approach (REA), a

semi-empirical approach, was proposed in 1996 and initially used to model thin layer drying of food materials (Chen and Lin, 2005; Lin and Chen, 2006; 2007). The model accurately captures the major physics of drying. The relative activation energy, a material characteristic, basically expresses the difficulty to remove the moisture from the materials. The removal of both free and bound moisture is captured by the relative activation energy. The REA has advantages of simplicity, accuracy and effectiveness with respect to generating the drying parameters. Only one accurate drying run is required to generate the parameters (Chen, 2008). The REA in its lumped format, later called as the lumped reaction engineering approach (L-REA), has accurately modeled several challenging heat and mass transfer processes. In this study, the REA is combined with a set of equations of conservation of heat and mass transfer to yield the S-REA to model drying of non-food materials, baking and water vapor sorption. This study aims to develop S-REA and implement it in the study of several heat and mass transfer processes. Its accuracy is examined by benchmarking model results against high quality experimental data reported in the literature.

2. MATHEMATICAL MODELING

For drying, the applicability of the S-REA to describe the drying processes was benchmarked towards the experimental data of drying of honeycomb (Dhall et al, 2012) while for baking and water vapor sorption, the validity of the S-REA is tested towards Zhang and Chen (2014) and Li et al (2014), respectively. The S-REA consists of a set of equations of microscopic heat and mass balance in which the REA is used to describe the local evaporation/condensation rate. For drying of honeycomb (Dhall et al, 2012), the mass balance of liquid water in Lagrangian coordinate, which allows expansion and contraction of the matrix, is written as (Putranto and Chen, 2013a,b):

$$\frac{\partial(C_s X)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(D_w r \frac{\partial(C_s X)}{\partial r} \right) - \dot{I} \quad (1)$$

where D_w is the local surface diffusivity ($m^2 s^{-1}$), X is the concentration of liquid water ($kg H_2O kg dry solids^{-1}$), C_s is the solids concentration ($kg dry solids m^{-3}$)

which can change if the structure changes, is the evaporation or condensation rate (kg H₂O m⁻³ s⁻¹) and is positive when evaporation occurs locally.

The mass balance of water in the vapor phase (water vapor) in spherical coordinate system is expressed as (Putranto and Chen, 2013a,b):

$$\frac{\partial C_v}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (D_v r \frac{\partial C_v}{\partial r}) + \dot{I} \quad (2)$$

where D_v is the local effective vapor diffusivity (m² s⁻¹) and C_v is the concentration of water vapor (kg H₂O m⁻³).

The heat balance is represented by the following equation (Putranto and Chen, 2013^{a,b}):

$$\rho C_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (k r \frac{\partial T}{\partial r}) - \dot{I} \Delta H_v \quad (3)$$

where T is the sample temperature (K), k is the local thermal conductivity of sample (W m⁻¹ K⁻¹), ΔH_v is the water vaporization heat (J kg⁻¹), C_p is the local specific heat of sample (W m⁻¹ K⁻¹) and ρ is the local sample density (kg m⁻³).

The initial and boundary conditions for equations (1) to (3) are:

$$t=0, X=X_o, C_v=C_{v_o}, T=T_o \quad (4)$$

$$\begin{aligned} \frac{dX}{dr} = 0, \quad \frac{dC_v}{dr} = 0, \quad \frac{dT}{dr} = 0 \\ r=0, \\ r=R, \end{aligned} \quad (5)$$

$$-C_s D_w \frac{dX}{dr} = h_m \varepsilon_w \left(\frac{C_{v,s}}{\varepsilon} - \rho_{v,b} \right) \quad (7)$$

$$-D_v \frac{dC_v}{dr} = h_m \varepsilon_v \left(\frac{C_{v,s}}{\varepsilon} - \rho_{v,b} \right) \quad (8)$$

$$k \frac{dT}{dr} = h(T_b - T) \quad (9)$$

where R is the sample radius (m), h is the heat transfer coefficient (W.m⁻².K⁻¹), ε_w and ε_v are fraction of surface area influenced by liquid water and water vapor respectively.

\dot{I} is the local evaporation/condensation rate within the solid structure described as (Putranto and Chen, 2013a,b):

$$\dot{I} = h_{m,in} A_{in} (C_{v,s} - C_v) \quad (9)$$

where $h_{m,in}$ is the internal mass transfer coefficient (m.s⁻¹), A_{in} is the total internal surface area available for phase change (m².m⁻³), $C_{v,s}$ is the internal-solid-surface water vapor concentration (kg.m⁻³). Although the void space inside the samples may be large enough, the incorporation of the advection term in the S-REA is not necessary since its term has been captured by the local evaporation/condensation term as represented by equation (9).

By implementing the REA, the internal-surface water vapor concentration can be written as (Putranto and Chen, 2013a,b):

$$C_{v,s} = \exp\left(\frac{-\Delta E_v}{RT}\right) C_{v,sat} \quad (10)$$

where $C_{v,sat}$ is the internal-saturated water vapor concentration (kg m⁻³).

Therefore, the local evaporation rate can be expressed as (Putranto and Chen, 2013^{a,b}):

$$\dot{I} = h_{m,in} A_{in} \left[\exp\left(\frac{-\Delta E_v}{RT}\right) C_{v,sat} - C_v \right] \quad (11)$$

The relative activation energy of honeycombs is generated from one accurate drying run at temperature of 103 °C. The relationship between the relative activation energy and average moisture content is assumed to be represented by simple mathematical equation obtained by least square method using Microsoft Excel®. The relative activation energy was found to be suitably fitted as:

$$\begin{aligned} \frac{\Delta E_v}{\Delta E_{v,b}} = -138685(X - X_b)^5 + 50405(X - X_b)^4 \\ - 6953.5(X - X_b)^3 + 466.12(X - X_b)^2 \\ - 17.616(X - X_b) + 1.0053 \end{aligned} \quad (12)$$

For baking and water vapor sorption, the S-REA, similar to the ones written in equations (1) to (3) are setup and implemented. This is then combined with appropriate relative activation energies of dough during baking (Zhang and Chen, 2014) and silica gel during water vapor sorption (Li et al, 2007). The relative activation energy of dough can be written as:

$$\begin{aligned} \frac{\Delta E_v}{\Delta E_{v,b}} = -55.754(\bar{X} - X_b)^5 + 113.95(\bar{X} - X_b)^4 \\ - 96.768(\bar{X} - X_b)^3 + 40.609(\bar{X} - X_b)^2 \\ - 8.385(\bar{X} - X_b) + 1.006 \end{aligned} \quad (13)$$

While the relative activation energy of silica gel can be expressed as:

$$\begin{aligned} \frac{\Delta E_v}{\Delta E_{v,b}} = -4.19(\bar{X} - X_b)^4 - 15.66(\bar{X} - X_b)^3 \\ + 3.192(\bar{X} - X_b)^2 - 10.063(\bar{X} - X_b) + 1 \end{aligned} \quad (14)$$

In order to yield the spatial profiles of moisture content, concentration of water vapor and temperature, equations (1) to (3) are solved simultaneously in conjunction with the initial and boundary conditions (shown in equations (4) to (8) and the appropriate relative activation energy.

3. RESULTS AND DISCUSSION

For convective drying of honeycombs, as suggested by Dhall et al (2012), the liquid diffusivity of 10⁻¹⁰ m².s⁻¹ is used. Interestingly, as shown in Figure 1, the liquid

diffusivity of lower than $1 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$ does not result in any noticeable differences in the moisture content and temperature profiles. This may indicate that the modeling is independent on surface diffusivity and hence the surface diffusion term may be neglected in the modeling. Without incorporating the surface diffusion term, the results of modeling of drying of honeycombs at temperature of 103 and 137 °C are shown in Figures 2 and 3. A good agreement towards the experimental data is shown (R^2 of higher than 0.998 for moisture content and R^2 of higher than 0.993 for temperature). Benchmarks against the modeling implemented by Dhall et al (2012) shows that the S-REA yields closer agreement to the experimental data. The S-REA is accurate to model both moisture content and temperature profiles at drying air temperature of 103 and 137 °C.

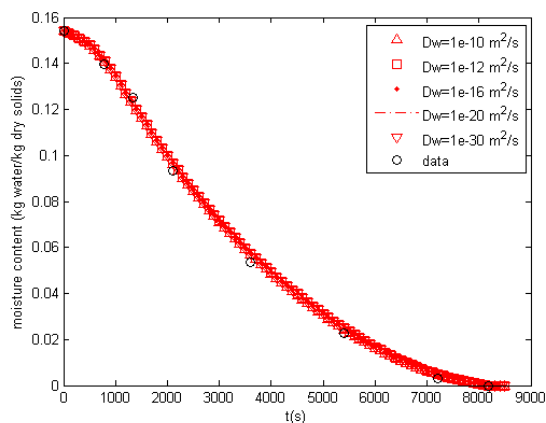


Figure 1. Sensitivity of effective liquid diffusivity towards profiles of moisture content during drying of honeycombs at temperature of 137 °C (Putranto and Chen, 2015)

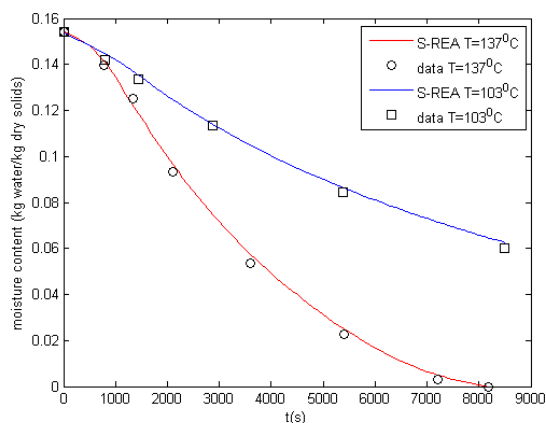


Figure 2. Profiles of moisture content during drying of honeycombs at temperature of 103 and 137 °C (Putranto and Chen, 2015)

For baking, the moisture content profiles during baking of 0.5 and 1 g bread are shown in Figure 4. A good agreement towards the experimental data is shown (R^2 of 0.992 and 0.988 for 0.5 and 1 g bread, respectively). Figure 5 shows the spatial profiles of moisture content

during baking of 1 g of bread at baking temperature of 235 °C. The profiles at the outer part of the samples are lower than those at the inner part which indicate that the moisture migrate outwards during baking. The profiles decrease during baking time since the moisture in the samples depletes as baking progresses. The S-REA models well the baking process which could be due to the applicability of the REA to represent the local evaporation/condensation rate during baking. The relative activation energy seems to be sufficiently accurate to capture the local evaporation/condensation inside the samples coupled with starch gelatinization, protein denaturation and browning.

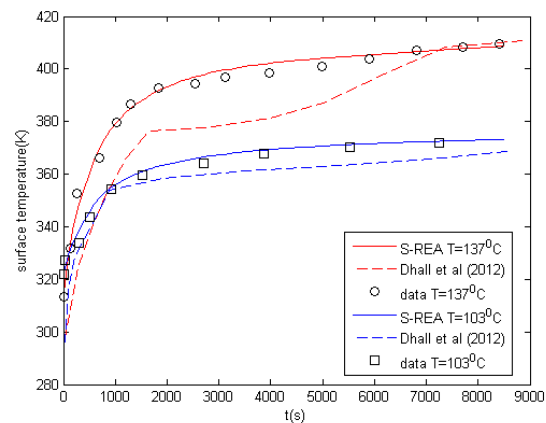


Figure 3. Profiles of surface temperature during drying of honeycombs at temperature of 103 and 137 °C (Putranto and Chen, 2015).

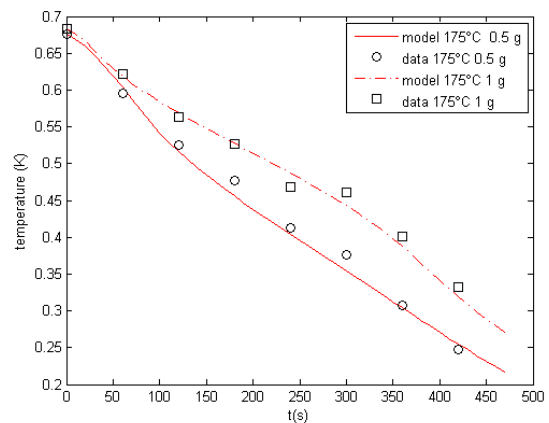


Figure 4. Profiles of average moisture content during baking of bread at baking temperature of 175 °C (Putranto and Chen, 2015)

For water vapor sorption, similar to the convective drying of honeycombs, the varied values of surface diffusivity do not give any noticeable differences in the profiles. Without using the surface diffusion term, the profiles of average moisture content are shown in Figure 6 while the profiles of spatial one are indicated in Figure 7. The S-REA models accurately the water vapor sorption which may be because the REA describes well the local condensation rate. The applicability of the REA indicates that the relative

activation energy used to model the global wetting rate (refer to equation (16)) (Putranto and Chen, 2014) is also applicable to model the local wetting rate of water vapor sorption.

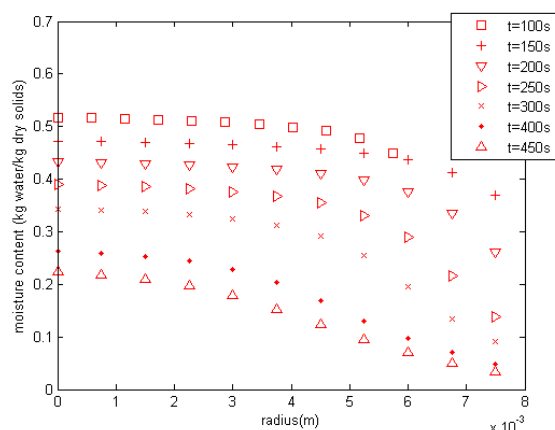


Figure 5. Spatial profiles of moisture content during bread baking of 1 g of bread at baking temperature of 235 °C (Putranto and Chen, 2015)

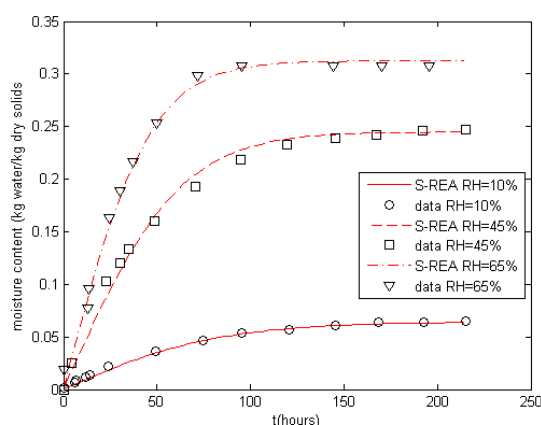


Figure 6. Profiles of moisture content during water vapor sorption at various relative humidity (Putranto and Chen, 2015)

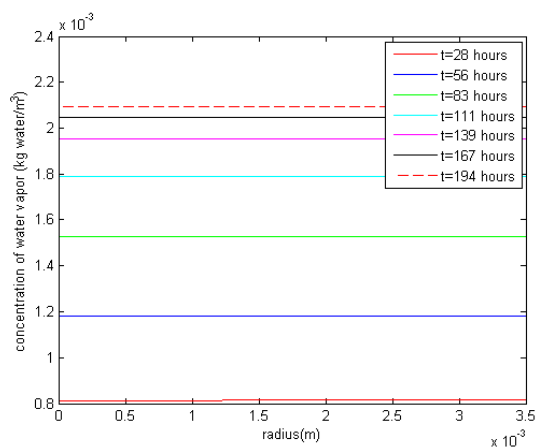


Figure 7. Spatial profiles of concentration of water vapor inside silica gel during water vapor sorption at relative humidity of 10% (Putranto and Chen, 2015)

4. CONCLUSIONS

In this study, the applicability of the S-REA to describe several simultaneous heat and mass transfer processes is demonstrated. The S-REA is accurate to model the convective drying, baking and water vapor sorption. This accuracy indicates that the REA is applicable to model the local evaporation/condensation rates during the processes. The combination of relative and equilibrium activation energy results in a unique relationship of activation energy which can describe the local structural changes during the simultaneous heat and mass transfer processes, as affected by the environmental conditions.

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Xiao Dong Chen was born in Beijing in 1965. BE in Engineering Mechanics from Tsinghua University (1987). PhD in Chemical and Process Engineering from Canterbury University in NZ (1991). MSc in Mathematics from University of New South Wales in Australia (2014). After working for Fonterra NZ for 2.5 years on food particle technology, he took up a lectureship at The University of Auckland, NZ. He was made a Personal Chair of Chemical Engineering in 2001 at The University of Auckland. In 2006, he was appointed to the Chair of Biotechnology and Professor of Chemical Engineering at Monash University, Melbourne, Australia. He has published over 440 refereed journal articles and 220 conference papers (over 30 were Keynote or Plenary Lectures), 3 books, 20 book chapters, and over 50 reports on industrial consulting projects. From early 2010 to the end of 2012, he held a 1000-Talent National Chair Professor of Chemical Engineering and the Executive Headship of Chemical and Biochemical Engineering at Xiamen University. He is an Elected Fellow of Royal Society of New Zealand since 2001 and an Elected Fellow of Australian Academy of Technological Sciences and Engineering since 2007, and is a Fellow of IChemE (UK) from 2001.

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