CONCENTRATION DEPENDENT DIFFUSION COEFFICIENT ESTIMATION IN DRYING CONSIDERING SHRINKAGE- AN OBSERVER APPROACH

C. Martínez Vera, M. G. Vizcarra Mendoza

Departamento de Ingeniería de Procesos e Hidráulica, Universidad Autónoma Metropolitana-Iztapalapa.
Apartado Postal 55-534, México D.F., 09340, México, e-mail: cmv@xanum.uam.mx

Abstract: The estimation of the diffusion coefficient from experimental data in cases in which this coefficient is concentration dependent and taking in account the shrinkage associated to the moisture lost during drying is a problem not so well studied and which does not admit a unique solution. In this work we present a methodology for estimating concentration dependent diffusion coefficients in drying processes taking in account the associated shrinkage.

Keywords: drying and shrinking, diffusion coefficient estimation

INTRODUCTION

The solution of the mathematical model of the drying process considering shrinkage, the direct problem, is a problem that has been treated in the literature (for example in Aguerre et al., 2008). However, the inverse problem, the estimation of the diffusion coefficient from experimental data in cases in which this coefficient is concentration dependent and taking in account the shrinkage associated to the moisture lost during drying is a problem not so well studied and which does not admit a unique solution. In this work we present a methodology for estimating concentration dependent diffusion coefficients in drying processes taking in account the associated shrinkage. The methodology has been previously applied for estimating diffusion coefficients in cases in which there are not volume changes associated to the mass transfer process (Martínez et al., 2009; Martínez et al., 2010) and here is extended to cases in which shrinkage is appreciable. For this purpose we simulate the drying of a shrinking solid under isothermal conditions based in the work presented by Aguerre et al. (2008). The average moisture profiles as well as the radius profile are obtained and are taken as the available information for reconstructing the diffusion concentration dependent coefficient by means of a non linear filter consisting of a reduced order model of the process plus an innovation term driven by the data. In a final step the diffusion model, obtained wit an approximated numerical solution of the diffusion equation and, therefore, imprecise, is refined in a final optimization step. It should be remarked that inverse problems does not have a unique solution and as a consequence it should not be expected that the numerical coefficients of the diffusion coefficient model obtained coincide with those with which the data were generated. However it should be expected that the profiles taken as data (information fed to the estimator) and those obtained with the diffusion model estimated should be similar. This is shown with the results obtained in this work.

METHODOLOGY

Assuming that the drying process is described by the diffusion equation and that the solid volume reduction is proportional to the volume of water lost by the solid we describe the drying and shrinking of a solid particle under isothermal conditions following the work of Aguerre et al. (2008). The moving boundary problem is transformed in a fix boundary problem through a variable change in order to have variations of the dimensionless spatial variable between 0 and 1. The isothermicity condition leads to a constant condition at the border and the consideration of a spherical particle leads to a symmetry condition at the center of the particle. The resulting equations are

\[
\frac{dc}{dt} = \frac{1}{(x \cdot R)^2} \frac{\partial}{\partial x} \left( \frac{x^2 \cdot D \cdot \frac{dc}{dx}}{R} \right) + \frac{z \cdot dc}{R} \frac{dR}{dt} \quad 0 \leq z \leq 1, \quad t > 0 \quad (1a)
\]

\[
\frac{dc}{dz} = 0 \quad \text{for} \quad z = 0, \forall t \quad (1b)
\]

\[
c = c_{eq} \quad \text{for} \quad z = 0, \forall t \quad (1c)
\]

\[
c = c_0 \quad \text{for} \quad 0 \leq z \leq 1, t = 0 \quad (1d)
\]
With the diffusion coefficient given by

\[
D = D_0 \exp \left( \frac{\rho_p R_c u c_{eq}}{2 R_0^2} \right) \tag{2a}
\]

\[
\lambda(T) = 3423.8 - 5.237 + 9.66 \cdot 10^{-3} T^2 - 1.13 \cdot 10^{-5} T^3 \tag{2b}
\]

With \( u = c/c_B \), \( D_0 = 3.44 \times 10^{-4} \text{ m}^2 \text{s}^{-1} \); \( K_1 = 9.03 \text{ K} \); \( K_2 = 0.274 \); \( u_{sw} = 0.072 \text{ kg kg}^{-1} \); \( T = 60 \text{ °C} \); \( R_p = 3.588 \text{ mm} \); \( C_0 = 864.8 \text{ kg m}^{-3} \); \( C_{eq} = 137.9 \text{ kg m}^{-3} \).

The solid properties assumed here are those given in the work of Aguerre et al. (2008). The above given equations are solved discretizing the spatial variable by finite differences and the system of nonlinear ordinary differential equations together with the differential equation that describes the radius evolution are integrated by a proper method for stiff equations (Rosenbrock method). The spatial concentration profiles are numerically averaged at each time step for obtaining the average moisture profile. Exponential functions are fitted to the average moisture content profile and to the radius variation profile as functions of time in order to have the values of these variables available at any time.

The diffusion coefficient estimation algorithm consists of a model of the system plus an innovation term that takes into account the difference between the estimated concentration and the experimental value (in our case the value obtained by a rigorous simulation). The model of the drying process for the estimation algorithm consists of a one point collocation solution to the problem (1) that satisfies the boundary conditions. The solution proposed is

\[
c(z, t) = (1 - z^2) \cdot A(t) + c_{eq} \tag{3}
\]

We propose the following model for the diffusion coefficient dependence on concentration

\[
D(c) = d_1 e^{d_2 c} \tag{4}
\]

Based on this solution given by equation (3), taking \( z = 1/2 \) as the collocation point the concentration dependence of the diffusion equation given by equation (4) and taking \( d_0 \) as a known value (in the order of the expected magnitude of the diffusion coefficient) the estimation algorithm is given by the following set of equations

\[
A(t) = -\frac{6D \cdot A(t)}{R^2 (1 - z^2)} + \frac{4z^2 \cdot A^2(t) d_1 \cdot D}{R^2 (1 - z^2)} \frac{2z^2 \cdot A(t)}{R (1 - z^2)} \frac{dR}{dt} + \omega_1 \left( \frac{c_{exp}(t) - c_{eq}}{1 - z^2} - A(t) \right) \tag{5a}
\]

\[
\dot{d}_1 = -\omega_2 \left( \frac{c_{exp}(t) - c_{eq}}{1 - z^2} - A(t) \right) \tag{5b}
\]

In which the last equation expresses the assumption of the constancy of \( d_1 \) and where \( \omega_1, \omega_2 \) are the filter gains whose values are \( \omega_1 = \omega_2 = 15 \) for the estimator runs shown in the figures below.

Fig. 1. Concentration data fed to the estimator and concentration estimated at the collocation point.

Fig. 2. Estimated diffusion coefficient versus time starting from two different initial conditions.

RESULTS

As can be seen in Fig. (1) the estimator converges very fast with the filter gains reported above to the concentration profile fed to the estimator. The convergence time is about 100 s. The diffusion coefficient variations with time predicted by the estimator are also shown in figure (2). From the concentration-time data and the diffusion-time data a relationship between diffusion coefficient and concentration can be obtained. Without considering the learning time of the estimator a model for the diffusion dependence on concentration can be obtained by fitting a model to the corresponding
diffusion-concentration values. The chosen model and its parameters are

\[ D(c) = a_0 + a_1 e^{c/b} \]  

\( a_0 = 2.62947 \times 10^{-10}, \quad a_1 = 3.45919 \times 10^{-11}, \quad b = 290.07863 \) with \( R^2 = 0.996 \).

Introducing this diffusion-concentration model to the program with which the data were generated instead of the model given by equation (2) is obtained the concentration profile shown in figure (3). In this figure is also shown the data profile that we are trying to approach. Even though the profile shown with the continuous line in this figure could be acceptable we improve it through an optimization step. The optimized parameters for the D-c model given by equation (6) are

\( a_0 = 2.82596 \times 10^{-10}, \quad a_1 = 3.15947 \times 10^{-11}, \quad b = 288.267 \)

The profile obtained with this set of parameters is shown in figure (4) in which it is possible to appreciate the improvement in the approximation to the original profile.

The data sets obtained solving equation (1) and (2), taken here as if were experimental values, are the base for a dynamic optimization process for the parameters values, reported above, of the diffusion-concentration model (6). The objective function to be minimized in this process is the absolute value of the difference between the average concentration value fed at the estimator and the average concentration value obtained solving equation (1) with diffusion model (6). It should be expected a small difference between the optimized and the non optimized values because the diffusion values before optimization are matched to the concentrations at the collocation points and those after optimization are matched to the average concentration at each time step. The shrinking rates obtained with model (2) and with the optimized model (6) are nearly identical.

CONCLUSIONS

A methodology previously published for estimating diffusion coefficients in mass transfer processes in which shrinkage can be neglected is extended here to cases in which shrinkage is appreciable and cannot be neglected. The methodology is based in a high gain filter. The shrinking rate is given as an information input to the estimation algorithm. The effectiveness of the methodology is tested here with a simulated case. The results are quite acceptable as can be seen in the graphs shown confirming the bondage and the applicability of the method.

NOMENCLATURE

\( c \) volumetric concentration  \( \text{kg/m}^3 \)
\( \bar{c} \) average volumetric concentration  \( \text{kg/m}^3 \)
\( c_{eq} \) equilibrium concentration  \( \text{kg/m}^3 \)
\( c_0 \) initial concentration  \( \text{kg/m}^3 \)
\( R \) radius of the equivalent sphere  \( \text{m} \)
\( r \) radial distance  \( \text{m} \)
\( t \) time  \( \text{s} \)

REFERENCES

