



HEAT AND MASS TRANSPORT MECHANISMS IN 3D CAPILLARY MEDIUM

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Abstract. *Multidimensional dimensionless Luikov problem in capillary porous media is analytically solved by the GITT (Generalised Integral Transform Technique) formalisms for the associated temperature and moisture potentials behaviour. Linear transport coefficients, three-dimensional geometry and automatic global error control are employed to obtain the solution of the coupled partial differential equations. The description of the simultaneous heat and mass transfer phenomena is analysed through the aspects of Lu thermophysical parameter variation and graphic illustration.*

Keywords:

Drying in porous media, Thermophysics, Heat and mass transfer and Integral transform method

1. INTRODUCTION

The simultaneous heat and mass transfer in capillary porous media is especially important in the current technological development. In recent years, the GITT (Generalised Integral Transform Technique), associated with analytical-numerical hybrid methods, became possible to alternatively obtain better solutions to some convection and diffusion-convection advanced problems (Cotta, 1993, 1998; Cotta & Mikhailov, 1998; Ribeiro et al., 1993; Duarte et al., 1998). If compared to methods denominated purely numeric, like the Finite Element Method and Finite Difference Method, the GITT presents some advantages, such as: relevant reduction of CPU time; no use of meshes (factor that is accentuated in multidimensional problems); automatic error control; direct numeric determination of the function in a point without need of numeric processing of previous states and versatility of the method in hybridisation with others. As disadvantages it is mentioned the limited number of users, complex boundary surfaces and hyperbolic problems

Without loss of generality, the GITT formalisms consist of adopting a transform-inverse pair, being assumed a group of associated auxiliary problems of Sturm-Liouville type. The original partial differential equation (PDE or system of equations) is transformed to an ordinary differential system of ODE's. This eliminates all spatial dependence from original co-ordinates. The computational effort will only be necessary to solve an 1D problem.

The drying Luikov problem on his original form is expressed by a coupled parabolic system for different combinations of boundary conditions, including complex cases (Ribeiro et al., 1993; Cotta, 1993 and Luikov, 1980). Typical examples are the drying of wood, ceramics, pharmaceutical and agriculture products, and also the moisture transfer through components of building materials and soils (Ribeiro et al., 1998). Historically, (Ribeiro et al., 1993 and 1995) observed that some authors pointed out some numerical difficulties associated to the solution aspects found on variations of Luikov problems, caused by analytical coupling characteristics or a non-easy calculus of complex eigenvalues and consequently named them as a non-attractive problem class. The analytical-numerical characteristics of GITT permitted alternative solutions to the Luikov problems. For this mentioned non-attractive cases (Ribeiro et al., 1993 and 1995; Duarte, 1998; Cotta, 1993 and Duarte et al., 1997) presented a general approach using the GITT formalisms when it was assumed decoupled associated auxiliary problems of Sturm-Liouville type. So, it was definitively possible to avoid complex eigenvalues, to adopt a prescribed error and to obtain a stable and systematic solution. Recently, (Pandey et al., 1998) using Laplace transform technique alternatively presented an exact solution to a linear variant of Luikov problem in a spherical co-ordinate system and critically commented the influence of complex eigenvalues on the temperature and moisture distributions.

In the next section, as an application of the mentioned GITT formalisms, it will be presented a three-dimensional Luikov variant problem, with prescribed potentials at the boundaries. Without loss of generality, the principal solution steps are pointed out.

2. ANALYSIS

Without loss of generality and according to the GITT formalisms extended to the Luikov problem (Ribeiro et al., 1993 and 1995; Duarte, 1998; Cotta, 1993 and Duarte et al., 1997), let the particular case of the Luikov dimensionless equations over the region \mathbf{V} , ($\mathbf{X} \in \mathbf{V}$) \Rightarrow ($0 < X < 1$, $0 < Y < 1$, $0 < Z < 1$), and the boundary surface \mathbf{S} , that is mathematically rearranged and presented as follows (Duarte et al., 1997; Duarte, 1998 and Lewis, 1996):

$$\frac{\partial \Theta_1(X, Y, Z, \tau)}{\partial \tau} = \alpha \nabla^2 \Theta_1(X, Y, Z, \tau) - \beta \nabla^2 \Theta_2(X, Y, Z, \tau); \quad \text{on } \mathbf{V}; \tau > 0 \quad (1.a)$$

$$\frac{\partial \Theta_2(X, Y, Z, \tau)}{\partial \tau} = Lu \nabla^2 \Theta_2(X, Y, Z, \tau) - Lu Pn \nabla^2 \Theta_1(X, Y, Z, \tau); \quad \text{on } \mathbf{V}; \tau > 0 \quad (1.b)$$

the initial and mathematically rearranged boundary conditions are,

$$\Theta_1(X, Y, Z, 0) = \Theta_2(X, Y, Z, 0) = 0; \quad \text{on } \mathbf{V} \quad (2.a,b)$$

$$\frac{\partial \Theta_1(0,Y,Z,\tau)}{\partial X} = 0; \quad \frac{\partial \Theta_1(X,0,Z,\tau)}{\partial Y} = 0; \quad \frac{\partial \Theta_1(X,Y,0,\tau)}{\partial Z} = 0; \quad \tau > 0 \quad (3.a,b,c)$$

$$\frac{\partial \Theta_2(0,Y,Z,\tau)}{\partial X} - Pn \frac{\partial \Theta_1(0,Y,Z,\tau)}{\partial X} = 0; \quad \tau > 0 \quad (4.a)$$

$$\frac{\partial \Theta_2(X,0,Z,\tau)}{\partial Y} - Pn \frac{\partial \Theta_1(X,0,Z,\tau)}{\partial Y} = 0; \quad \tau > 0 \quad (4.b)$$

$$\frac{\partial \Theta_2(X,Y,0,\tau)}{\partial Z} - Pn \frac{\partial \Theta_1(X,Y,0,\tau)}{\partial Z} = 0; \quad \tau > 0 \quad (4.c)$$

$$\Theta_1(1,Y,Z,\tau) = \Theta_2(1,Y,Z,\tau) = 1; \quad \tau > 0 \quad (5.a,b)$$

$$\Theta_1(X,1,Z,\tau) = \Theta_2(X,1,Z,\tau) = 1; \quad \tau > 0 \quad (6.a,b)$$

$$\Theta_1(X,Y,1,\tau) = \Theta_2(X,Y,1,\tau) = 1; \quad \tau > 0 \quad (7.a,b)$$

$$\alpha = 1 + \varepsilon Ko Lu Pn; \quad \beta = \varepsilon Ko Lu \quad (8.a,b)$$

Lu expresses the Luikov number (ratio between the mass and thermal diffusivities in the porous medium), **Pn** is the Posnov number (the relative decrease on moisture potential, caused by a certain temperature gradient via the thermogradient effect), **Ko** is the Kossovitch number (ratio between the amount of heat needed for the vaporisation of all liquid in the porous media and the energy necessary to heat the humid body), **ε** is the phase-change criterion (if **ε** = 0 means that all moisture in the porous body is on a liquid phase, if **ε** = 1, all moisture is on a vapour phase). $K_{XY} = l_y/l_x$ and $K_{XZ} = l_z/l_x$ are the aspect ratio for the porous media and l_y , l_x and l_z are their correspondent characteristic lengths.

Physically, the Luikov number expresses the rate between the mechanisms of mass to heat transport in the porous body. Therefore, as **Lu** is made larger, the growth of the characteristic velocity of mass transfer becomes more significant than the corresponding variation for the characteristic velocity of heat transfer. If Luikov is smaller, the inverse effect is expected.

According to the GITT formalisms, to accelerate the convergence rate, this mathematical problem could be decoupled in a particular and homogeneous parts (Cotta, 1993; Duarte & Ribeiro 1997, 1998 and Ribeiro et al., 1993, 1995). The particular component, Θ_{ks} , is easily calculated and its solution has the following form ($k=1,2$ for temperature and moisture):

$$\Theta_{ks}(X,Y,Z) = 1 \quad (9.a,b)$$

The homogeneous part, Θ_{kh} , would be now easy and exactly solved, since the solutions of the following three pairs of available classical decoupled eigenfunction problems of Sturm-Liouville type are available:

$$\frac{d^2\Psi_{ki}(X)}{dX^2} + \mu_{ki}^2\Psi_{ki}(X) = 0, \quad X \in \mathbf{V} \quad (10.a,b)$$

$$\frac{d\Psi_{ki}(0)}{dX} = 0, \quad \Psi_{ki}(1) = 0 \quad X \in \mathbf{S} \quad (11.a,b;12.a,b)$$

$$\frac{d^2\Gamma_{kj}(Y)}{dY^2} + \lambda_{kj}^2\Gamma_{kj}(Y) = 0, \quad Y \in \mathbf{V} \quad (13.a,b)$$

$$\frac{d\Gamma_{kj}(0)}{dY} = 0, \quad \Gamma_{kj}(1) = 0, \quad Y \in \mathbf{S} \quad (14.a,b;15.a,b)$$

$$\frac{d^2\Phi_{kl}(Z)}{dZ^2} + \sigma_{kl}^2\Phi_{kl}(Z) = 0, \quad Z \in \mathbf{V} \quad (16.a,b)$$

$$\frac{d\Phi_{kl}(0)}{dZ} = 0, \quad \Phi_{kl}(1) = 0, \quad Z \in \mathbf{S} \quad (17.a,b;18.a,b)$$

where the subscripts i,j,l characterise the number of eigenfunctions necessary to achieve the prescribed numerical error in the inverse formula, that are presented in the next equations. Elementary sinus or cosines formula express the correspondent eigenvalues for this focused Sturm-Liouville problems

These auxiliary problems allow the definition of the following integral transform pairs, necessary for the solution of the homogeneous problem ($k=1,2$):

Inverse,

$$\Theta_{kh}(X,Y,Z,\tau) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \sum_{l=1}^{\infty} \frac{1}{N_{ki}^{1/2} M_{kj}^{1/2} P_{kl}^{1/2}} \Psi_{ki}(X) \Gamma_{kj}(Y) \Phi_{kl}(Z) \bar{\Theta}_{kijl}(\tau) \quad (19.a,b)$$

Transform,

$$\bar{\Theta}_{kijl}(\tau) = \int_0^1 \int_0^1 \int_0^1 \frac{\Psi_{ki}(X) \Gamma_{kj}(Y) \Phi_{kl}(Z)}{N_{ki}^{1/2} M_{kj}^{1/2} P_{kl}^{1/2}} \Theta_{kh}(X,Y,Z,\tau) dXdYdZ \quad (20.a,b)$$

The normalisation integrals are,

$$N_{ki} = \int_0^1 \Psi_{ki}^2(X) dX \quad (21.a,b)$$

$$M_{kj} = \int_0^1 \Gamma_{kj}^2(Y) dY \quad (22.a,b)$$

$$P_{kl} = \int_0^1 \Phi_{kl}^2(Z) dZ \quad (23.a,b)$$

Eigenvalues and eigenfunctions are easily numerically calculated. Using the “transform” concept over the Luikov equation system and the auxiliary problems and, after truncation to a sufficient order N , for a prescribed convergence, it results a transform constant coefficient ordinary differential equations system:

$$\frac{dY(\tau)}{d\tau} + A_{2N,2N} Y(\tau) = 0_{2N,1} \quad (24.a)$$

where,

$$Y(\tau) = \{\bar{\Theta}_{11}(\tau) \dots \bar{\Theta}_{1N}(\tau) \quad \bar{\Theta}_{21}(\tau) \dots \bar{\Theta}_{2N}(\tau)\}^T \quad (24.b)$$

Now applying the GITT formalism to the initial conditions on the homogeneous problem, it is possible to obtain the initial transform conditions, as follows:

$$Y(0) = \bar{F}(\tau) \quad (25)$$

Equations (24.a,b) and (25) can now be easily numerically solved through matrix eigenvalue analysis or well-established algorithms (Cotta, 1993; Duarte, 1998; Ribeiro et al., 1995; IMSL, 1994; Wolfran, 1998 and Fortran PowerStation, 1995). After this, temperature and moisture potentials are computed from Eqns. (9.a,b) and (19.a,b).

3. RESULTS

The main required computational effort for this 3D problem is to solve a ordinary differential equations system (initial value problem, Eqns. (24) and (25)). In other words, this calculus basically depends of “ τ ”, the independent variable and the other calculations represents less than 1% of CPU time. Observe that there no mash generation for the spatial variables (x,y,z). If it was adopted the Finite Element Method or Finite Difference Method, computationally it would be necessary to solve the problem in all the space domain (x,y,z) at each time step, to perform a 3D mash generation and its control. This factors increase the CPU time and algorithm implementation. By other hand, in the case of GITT choice, to solve 1D, 2D or 3D Luikov problems and compare their CPU time, there is a small CPU increase (Duarte, 1998), with a variation between 5% to 10%. This effect can be predict analysing Eqn. (19.a or 19.b): notice that for each respective solution, to express the associated analytical formula of inversion (non expanded formulae), are necessary 1, 2 or 3 eigenfunctions (it was discussed that the main requested computational effort is to solve the initial value problem, expressed by Eqns. (24) and (25)). As consequence, this CPU characteristic is very promising in the case of the solution of other multidimensional problems.

To exemplify, it is chosen a relative error target of 10^{-4} and the compiler Fortran PowerStation 4.0. To achieve the prescribed numerical error the generated system is truncated with $N \leq 72$, for each expansion required. The thermophysical parameters used are listed in the Table below:

Table 1. Numerical values of the parameters.

Ko	7,009
Pn	5,556
ε	0,3
<i>l_x</i>	100 mm
<i>l_y</i>	25 mm
<i>l_z</i>	30 mm

For this parameters and agreement with a convenient graphic visualisation of the problem, a typical run took less than 30 sec. in a Pentium 233 CPU with 128 Mb of RAM memory and for the following dimensionless time, τ ($\tau = 5,0$; $\tau = 14,0$). Figures (1) and (2) show the variations on the dimensionless temperature (Θ_1) and moisture (Θ_2) potential distributions for $Y=0,0$, $Z=0,0$ and at different values of ***Lu*** parameter (***Lu***=0,0030, ***Lu***=0,0035, ***Lu***=0,0040). It should be observed that the Luikov is approximately 10^{-3} . Consequently, the mass transfer process is more inertial than the associated heat transfer process, as it can be observed by the time variation behaviour of dimensionless moisture and temperature distributions in Figs. (2) and (1). For the same dimensionless time, if ***Lu*** is made larger, the drying effect in porous media becomes more significant, and also as time is made larger, the temperature potential on the body decreases. Physically, this behaviour is expected, because a certain amount of energy is requested to the liquid-vapour phase-change process and mass diffusion in the porous body, consequently causing the decrease of temperature in the medium.

In summary, one can conclude that larger ***Lu*** thermophysical values induce a faster drying behaviour and this characteristic is economically more attractive for some industrial purposes.

In recent years there is a new tendency of programming using analytical-numerical approaches combined with declarative symbolic computation (Wolfran, 1998), this was recently named as hybrid computation (Cotta & Mikhailov, 1998 and Duarte et al., 1998). Intelligent and interactive characteristics can be utilised to implement the algorithms through functional programming and rule based programming (Gray, 1998 and Hughes, 1989), permitting to the programmer create rules that automatically generate steps of programming, that permit, for instance, the manipulation of extensive and or repetitive analytical advanced calculus. This is not possible using procedural programming (C or Fortran). The combination of this tools open a new scenario of advanced programming and approximate more and more the code of the reality contained in the original analytical problem. As consequence, it is expected that in the future that the programmer can improve convergence problems, generate code more intelligent, interactive and easily modifiable.

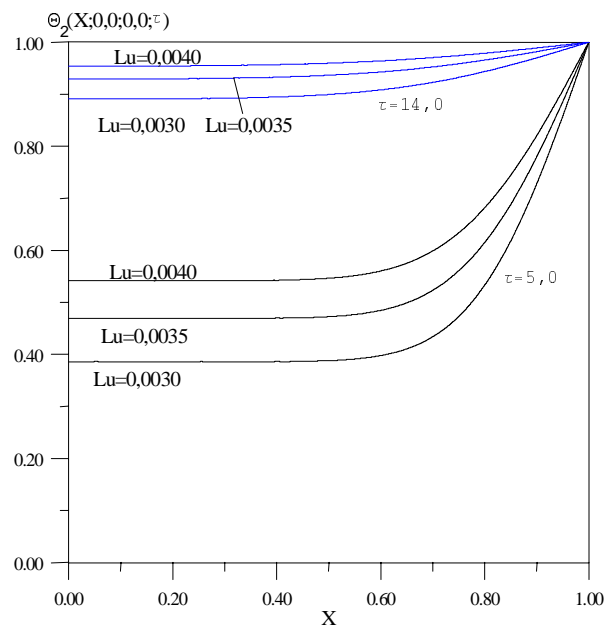
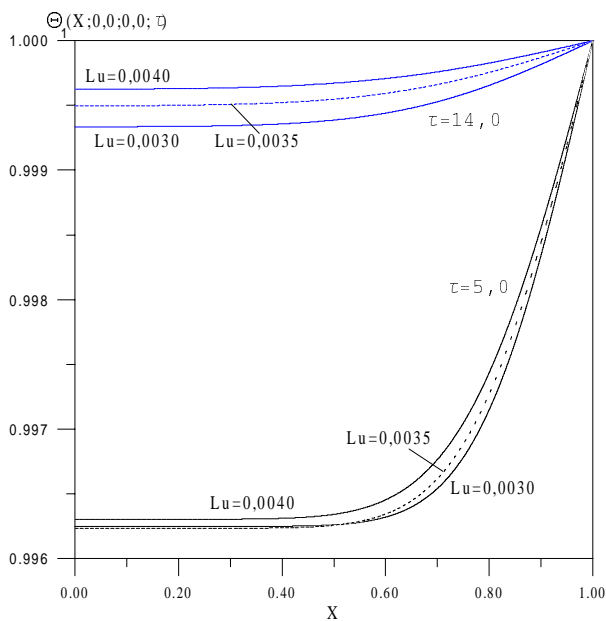


Figure 1 - Evolution of temperature profiles during drying process. $Pn=5.556$, $Ko=7.009$, $\epsilon=0,3$. Figure 2 - Same as left, for moisture profiles.

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