Proceedings of CHT-17
ICHMT International Symposium on Advances in Computational Heat Transfer

May 28-June 1, 2017, Napoli, Italy

CHT-17-xxx

ANEW APPROACH FOR THE DIFFUSION OF A SINGLE CLASS OF PARTICLES UNDER TWO DISTINCT ENERGY STATES

Luiz Bevilacqua[*§], Maosheng Jiang[*], Antonio Silva Neto[**], Diego Knupp[**], Augusto C. N. R. Galeão[***]
[*] A. L. Coimbra Institute, Graduate Course in Engineering, Federal University of Rio de Janeiro, Brazil
[**] Polytechnique Institute, State University of Rio de Janeiro, Brazil
[***] National Laboratory for Scientific Computation, Brazil
[§] Correspondence author. Fax: (0-55-21)3938-8464 Email: bevilacqua@coc.ufrj.br

ABSTRACT The main aim of this paper is to introduce the behavior of a new class of diffusion process consisting of a set of particles split into two partitions β and (1−β) corresponding to two distinct energy states generating two different fluxes. The set corresponding to the partition β moves according to the classical flux potential as function of the diffusion coefficient D and the complementary set moves according to a new potential which is function of β and a new coefficient R, that we call reactivity coefficient. This new flux is subsidiary to the principal, classical flux, meaning that it exists if and only if the main flux is activated. The new governing equation is a fourth order PDE. The two streams may be in the same or in opposite directions. Therefore it is admissible to have in a given spatial domain, increasing density, rarefaction or stagnation depending on the inflow/outflow ratio. This flexibility to model the dynamics of motion allows for a better representation of the effect of external fields on the moving particles. This is particularly important for temperature sensitive particles scattering on substrata subjected to non-uniform temperature fields. It was clearly shown through the solution of the inverse problem that it is expected a relation of the form β=F(R). As a consequence of the introduction of the second potential the solutions of a large class of problems show that the concentration tends to grow in regions where *R* is large. Therefore secondary flux plays an important role on the concentration distribution. Some examples are presented to illustrate the peculiar evolution processes obtained with this theory.

THE BASIC THEORY

Mathematical modeling of natural phenomena has been extensively used particularly due to the extraordinary advancements of computational techniques. Mass and energy transfer, dispersion of microorganism, motion of invading species are some examples where mathematical and computational modeling have been successfully applied. It has been confirmed that diffusion models match overall experimental data for a large number of physical-chemical observations. The classical model uses the well known diffusion equation that for isolated systems diffusing in isotropic media can be written as:

$$C\frac{\partial q}{\partial t} = D\frac{\partial^2 q}{\partial x^2}$$

This equation is related to a single potential that triggers the flux $\mathbf{\Psi}_1 = (-D\,\partial q/\partial x)\,\mathbf{n}$. We claim that this equation is limited to processes where all particles are similar and move in a single energy state that decays with increasing time. Consider for instance a set of n particles moving with the total translational kinetic energy $K_{tot} = (K_T)_1 = n\,p_1^2/2m$. This energy state that we call E_1 is correlated to the classical diffusion process. Now after passing an energy field a subset n_2 acquires rotational energy that is subtracted from the translational energy such that we have now a subset of particles n_2 moving with same total kinetic energy, except that it is divided into two varieties:

$(K_T)_2 = n_2\,p_2^2/2m$ and $(K_L)_2 = n_2\,L_2^2/2I$ and therefore

$$K_{tot} = (K_T)_1 + (K_T)_2 = n_1\,p_1^2/2m + n_2\,p_2^2/2m + n_2\,L_2^2/2I$$

Since the flux potential is derived from the translational kinetic energy the new process consists of two sets, the set (1) composed by n_1 particles diffusing according to the potential $\mathbf{\Psi}_1$ and n_2=n-n_1 particles diffusing according to a new potential $\mathbf{\Psi}_2$.

The purpose of this paper is to propose a method to derive the new potential $\mathbf{\Psi}_2$ consistent with the conservation principles. A simple way is to consider a string of cells containing some material that is distributed to the adjacent cells, left and right, according to a given rule. Consider a string of adjacent cells as shown in Figure 1. A fraction β of the contents q_n of a given cell "n" is transferred in equal proportions to the left and to the right neighboring cells at time t. The remaining fraction (1−β) is temporarily retained in the original cell "n". The process is easily represented by the equations (1-a) and (1-b) defining the distribution law at time t and t+Δt.

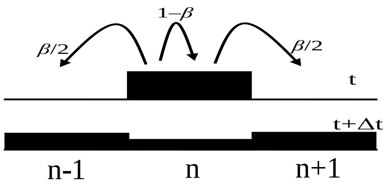

Fig.1. Particles distribution process in a given time interval Δt. The fraction (1−β) is temporarily retained at cell n

$$q_n^t = (1-\beta)\,q_n^{t-1} + \frac{1}{2}\beta q_{n-1}^{t-1} + \frac{1}{2}\beta q_{n+1}^{t-1} \qquad (1\text{-a})$$

$$q_n^{t+1} = (1-\beta)\,q_n^{t} + \frac{1}{2}\beta q_{n-1}^{t} + \frac{1}{2}\beta q_{n+1}^{t} \qquad (1\text{-b})$$

After straightforward but relatively lengthy algebraic operations it is possible to show that for $q(x,t)$ sufficiently smooth a fourth order PDE is obtained:

$$\frac{\partial q}{\partial t} = \beta D\frac{\partial^2 q}{\partial x^2} - (1-\beta)\beta R\frac{\partial^4 q}{\partial x^4}$$

Detailed derivation may be found in Bevilacqua [2013]. This equation shows that the new process is composed by two sets of particles corresponding to the fractions β and (1−β) associated respectively to two distinct fluxes, the first corresponding to the classical flux $\mathbf{\Psi}_1$ and the second to a new law $\mathbf{\Psi}_2$. For isotropic media it is easy to see that $\mathbf{\Psi}_2 = \left(\beta R\,\partial^3 q/\partial x^3\right)\mathbf{n}$. For anisotropic media however three possible definitions may apply. Besides the previous one where β and R are functions of x it is also plausible to admit the following definitions: $\mathbf{\Psi}_2^* = \left(R\,\partial\left(\beta\,\partial^2 q/\partial x^2\right)/\partial x\right)\mathbf{n}$ and $\mathbf{\Psi}_2^{**} = \left(R\,\partial^2\left(\beta\,\partial q/\partial x\right)/\partial x^2\right)\mathbf{n}$ with R(x) and β(x). The behavior of the solution depends strongly from the definition taken for the secondary flux. It was also shown in Silva [2014] that there is strong evidence that the partition β is function of R. Extension of the theory to a two dimensional domain presents no particular difficulty. The new equation reads:

$$\frac{\partial q}{\partial t} = \nabla\cdot\left(\beta D\nabla q\right) - \nabla\cdot\left((1-\beta)R\nabla\left(\beta\Delta q\right)\right) \quad \text{with} \quad \mathbf{\Psi}_2^* = \left[R(x,y)\nabla\left(\beta\Delta q(x,y,t)\right)\right]\left[\mathbf{e}_x,\mathbf{e}_y\right]^T \qquad (2\text{-a})$$

$$\frac{\partial q}{\partial t} = \nabla\cdot\left(\beta D\nabla q\right) - \nabla\cdot\left((1-\beta)R\nabla\left(\nabla\cdot\left(\beta\nabla q\right)\right)\right) \quad \text{with} \quad \mathbf{\Psi}_2^{**} = \left[R(x,y)\Delta\left(\beta\nabla q(x,y,t)\right)\right]\left[\mathbf{e}_x,\mathbf{e}_y\right]^T \qquad (2\text{-b})$$

APPLICATION

Consider a two dimensional domain given by $x \in [-1,1]$, $y \in [-1,1]$. The diffusion coefficient $D = 0.1$ is constant but the reactivity coefficient is given by the following distribution law $R = 5\exp\left(-20x^2 - 20y^2\right)$. The secondary flux is assumed to follow the relation $\mathbf{\Psi}_2^{**}$ corresponding to the anisotropic effect in the concentration spreading. The relation between β and R is given by $\beta = \exp\left(-R^2/5\right)$. The initial condition is given by $q(x,y,0) = \exp\left(-10x^2 - 10y^2\right)$ and the boundary conditions correspond to no flux, both primary and secondary. The solution is presented in the

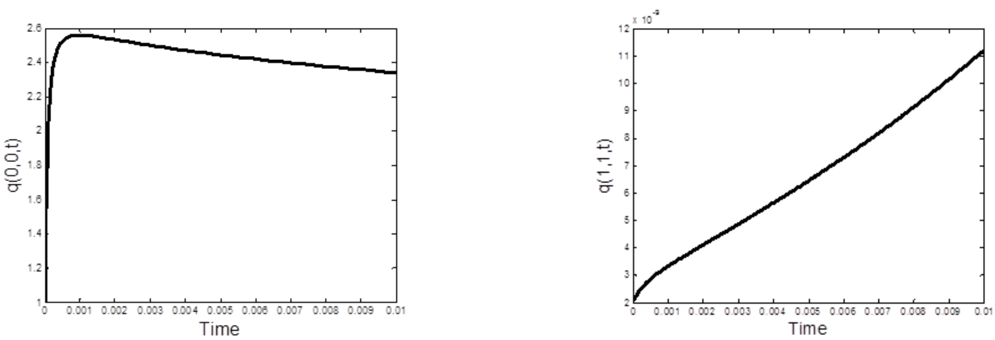

Fig.2. Time variation of the concentration at (0,0) and (1,1). Secondary flux defined with $\left|\mathbf{\Psi}_2^{**}\right| = \Delta\left(\beta\nabla q\right)$ equation 2-b

Fig.2. Clearly as t increases the concentration at $x = 0$, $y = 0$ increases growing in the opposite direction as compared with the classical solution. The effect of $R(x,y)$ concentrated around the center of the domain exerts an attraction effect pulling the particles towards the center. It is as if the

reactivity coefficient would be able to create an attraction field pulling the particles towards the center. Fig.2 shows the concentration at (0,0) and (1,1). The concentration at (0,0) grows very quickly and reaches its maximum q(0,0,001)= 2.55 for t=0.001. After reaching the maximum value the concentration decreases very slowly. It is expected that after a sufficiently long time the concentration distribution will approach a uniform configuration $q(x, y) =$ constant. The solution with the secondary flux defined as $\mathbf{\Psi}_2^*$ presents the same qualitative behavior except that the initial jump of the concentration at (x=0,y=0) is smaller. This type of behavior may well represent the scattering process of heat sensitive particles or the initial motion of cells with the reactivity coefficient associated to heat or nutrient sources respectively.

CONCLUSIONS

The bi-flux diffusion theory is new and despite the lack of a consistent experimental comprobation several challenges emerging from concrete problems as diffusion of living organism and particles sensitive to some energy source might better dealt with the proposed approach. Several points remain to be better clarified particularly the proper relationship between the particle fraction β and the reactivity coefficient R and the analysis of the influence of the secondary flux on the solution. The physical significance of the choice of the expression of the secondary flux should also be further investigated. It is also expected the reactivity coefficient R to be a function of the concentration which will lead to complex non-linear equations. Also the term $\beta(1-\beta)$ in the governing equation might lead to chaotic behavior . It is also interesting to note that complex capital flow might take advantage of a bi-flux process which is well appropriate to simulate real situations. Being a new approach it is necessary to join people interested in diffusion models to advance the analytical treatment and perform adequate experimental work.

ACKNOWLEDGEMENTS

This research was supported by the National Research Council CNPq, research grant 480865/2009-4, by CAPES/INMETRO Research Contract 076/2014 and the agreement CNPq-TWAS.

REFERENCES

Bevilacqua, L., Galeão, A.C.N.R., Simas, J.G., Doce, A.P.R.[2013], A new theory for anomalousdiffusionwith a bimodal flux distribution *J Braz. Soc. Mech. Sci. Eng.,* 35, pp: 431–440.

Silva, L. G., Knupp, D. C., Bevilacqua, L., Galeão, A. C. N. R. e Silva Neto, A. J., 2014, Inverse Problem in Anomalous Diffusion with Uncertainty Propagation, *Proc. 8th International Conference on Inverse Problems in Engineering: Theory and Practice*, 2014,Cracow, Poland.