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Transient Diffusion in Nuclear Fuels Processes

Kal Renganathan Sharma

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TRANSIENT DIFFUSION IN NUCLEAR FUELS PROCESSES

KAL RENGANATHAN SHARMA

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PREFACE

Sir Isaac Newton wrote his *Philosphiae Naturalis Principia Mathematica* in 1687. Although Albert Einstein improved upon Newton's laws of motion in the early 20^{th} century the work of Newton has not been fully applied to explain fundamental phenomena in engineering. The Fourier's law of heat conduction, Fick's law of mass diffusion, Newton's law of viscosity and Ohm's law of electricity are not sufficient to describe transient events in heat condution, molecular diffusion, momentum transfer and electrical conduction. The 4 laws were developed from empirical experimental observations. They violate the Onsager principle of microscopic reversibility and as pointed out by Lifshitz imply a infinite propagation of disturbance. As Einstein showed light is the speediest of velocities. The "blow-up" and singularities found in the surface flux expression during transient diffusion subjected to constant wall concentration at the boundary developed using Fick's second law of diffusion can be removed and bounded surface flux expressions obtained when the analogous Cattaneo & Vernotte heat condution equation in molecular diffusion is used. Thus in one dimension;

$$J_A = -D_{AB}\frac{\partial C_A}{\partial x} - \tau_{mr}\frac{\partial J_A}{\partial t} \qquad \text{(i)}$$

Where, τ_{mr} is the mass relaxation time (secs) and D_{AB} the binary diffusivity (m^2/s), J_A is the mass flux (mole/m^2/sec). The *damped wave diffusion and relaxation equation* can be derived from: (i) Stokes-Einstein chemical potential formulation when the acceleration of molecules are accounted for; (ii) free electron theory when the acceleration of electrons are accounted for; (iii) kinetic theory of gases when the surface flux expression includes the accumulation of molecules at the surface in addition to the difference between the molecules leaving the surface less than the molecules arriving at the surface at a considered increment in time. Viscoelastic combination of Hooke's elastic element and the Newtonian viscous element (his second book was in Fluid Mechanics!) leads to a damped wave momentum transfer and relaxation that is analogous to Eq. (i).

Newton observed the apple fall from the tree. The net acceleration decreases to zero at the terminal settling velocity of objects under free fall. This is because of the changing drag force as a function of velocity. As the velocity of the falling object increases from zero at rest, the resultant force changes from the initial gravity force less the Archimedes buoyancy force to gravity force less the Archimeded buoyancy force less the fluid drag force. So the rate of acceleration which can be obtained by dividing the resultant force by the mass of the object is a pronounced phenomena during transient events. Similar to the velocity of the falling object in transient motion, the heat conduction in transient conduction, mass diffusion in transient diffusion can be better described by theory when acceleration is accounted for.

The primary goal of this work is to evaluate the use of the damped wave diffusion and relaxation equation to nuclear fuels processes. Simultaneous diffusion and autocatalytic reactions and the wave diffusion phenomena may have a combined effect of subcritical damped oscillations in concentration under certain conditions. Closed form analytical solutions are developed from the hyperbolic partial differential equations that govern the phenomena. The governing equations are obtained from mass balance under transient conditions. About 1000 equations and 35 illustrations are used to describe the manifestation of damped wave diffusion in nuclear fuels processes.

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About the Author

Dr. Kal Renganathan Sharma PE received all his three degrees in chemical engineering: i) B.Tech. from Indian Institute of Technology, Chennai, India, 1985; ii) M.S and ; iii) Ph.D. from West Virginia University, Morgantown, WV in 1987 and 1990 respectively. He serves currently as *Adjunct Professor, Chemical Engineering* at the Roy G. Perry College of Engineering at Prairie View A & M University, Prairie View, TX. He is the author of 9 books, 19 journal articles, 488 conference papers and 108 other presentations. He has instructed over 2450 students in 75 semesterwise courses. He has held a number of high level positions in engineering academia in India and USA. He is listed in Who's Who in America, Marquis Who's Who, New Providence, NJ. He has been commended by the International Biographical Center at Cambridge, UK. At the time of this writing (09-09-09) his earlier book *Bioinformatics: Sequence Alignment and Markov Models*, McGraw Hill Professional, New York, NY (2009) has been cataloged in over 436 libraries including the Library of Congress, British Library, Cambridge University, MIT, UC Berkeley, Stanford, etc. He has been inducted as fellow of Indian Chemical Society, Kolkata, India, member of New York Academy of Sciences, Phi Kappa Phi and Sigma Xi. He was won cash awards and papers are cited widely. His Professional Engineer registration is with the state of New Hampshire in 1995.

NOMENCLATURE

A	area across path of diffusion (m^2)
a	half-width of the finite slab (m)
C_A	concentration of species A (mol/lit)
C_p	heat capacity (J/mole/K)
D	binary diffusion coefficient (m^2/s)
F	frictional coefficient
$I_0(x)$	modified Bessel function of the zeroth order and first kind
$I_1(x)$	modified Bessel function of the first order and first kind
$I_{1/2}(x)$	modified Bessel function of the halfth order and first kind
J	molar flux (mole/sec)
$J_0(x)$	Bessel function of the zeroth order first kind
$J_1(x)$	Bessel function of the first order and first kind
$J_{1/2}(x)$	Bessel function of the halfth order and first kind
k'''	first order rate constant (s^{-1})
$K_0(x)$	modified Bessel function of the zeroth order and second kind
$K_1(x)$	modified Bessel function of the first order and second kind
$K_{1/2}(x)$	modified Bessel function of the halfth order and second kind
k	thermal conductivity (w/m/K)
l	length of the cubical box containing gas molecules (m)
m	mass of molecule (kg)
M	molecular weight (kg/mole)
N_m	number of molecules in the system
n	number of molecules per unit volume (#/lit)
q	heat flux (w/m^2)
k_B	Boltzmann constant (J/molecule/K)
k*	dimensionless rate constant ($k'''\tau_r$)

P_{tot}	total pressure (N/m^2)
R	universal molar gas constant (J/mole/K)
R_o	radius of solute molecule (m)
R_{crit}	critical radius of nuclear fuel rod (m)
S	storage coefficient $\frac{\rho C_p}{\tau_r}$ ($w/m^3/K$)
T	temperature (K)
T_s	surface temperature of fuel rod (K)
t	time (s)
u	dimensionless concentration
U	heat source ($w/m^3/K$)
U*	dimensionless heart source $\frac{U}{S}$
v_m	velocity of molecule (m/s)
V	function of time only
w	wave concentration (dimensionless)
x	space coordinate (m)
X	dimensionless distance $\frac{x}{\sqrt{D\tau_r}}$
X_{pen}	penetration distance (dimensionless)
$Y_0(x)$	Bessel function of the zeroth order and second kind
$Y_1(x)$	Bessel function of the first order and second kind
$Y_{1/2}(x)$	Bessel function of the halfth order and second kind

Greek

α	thermal diffusivity (m^2/s)
	relativistic transformation variable, $\eta=\tau^2-X^2$
ξ	wave coordinate
λ_n	Eigen values in Fourier infinite series solution
μ	viscosity (kg/m/s)
ϕ	function of space only
ρ	density (kg/m^3)
τ_r	relaxation time (s), mass
τ_{lag}	inertial lag time