

TRANSPORT PROCESSES OF ACTIVE AGENTS INDUCING THE BI-FLUX PHENOMENON

Luiz Bevilacqua - COPPE/UFRJ

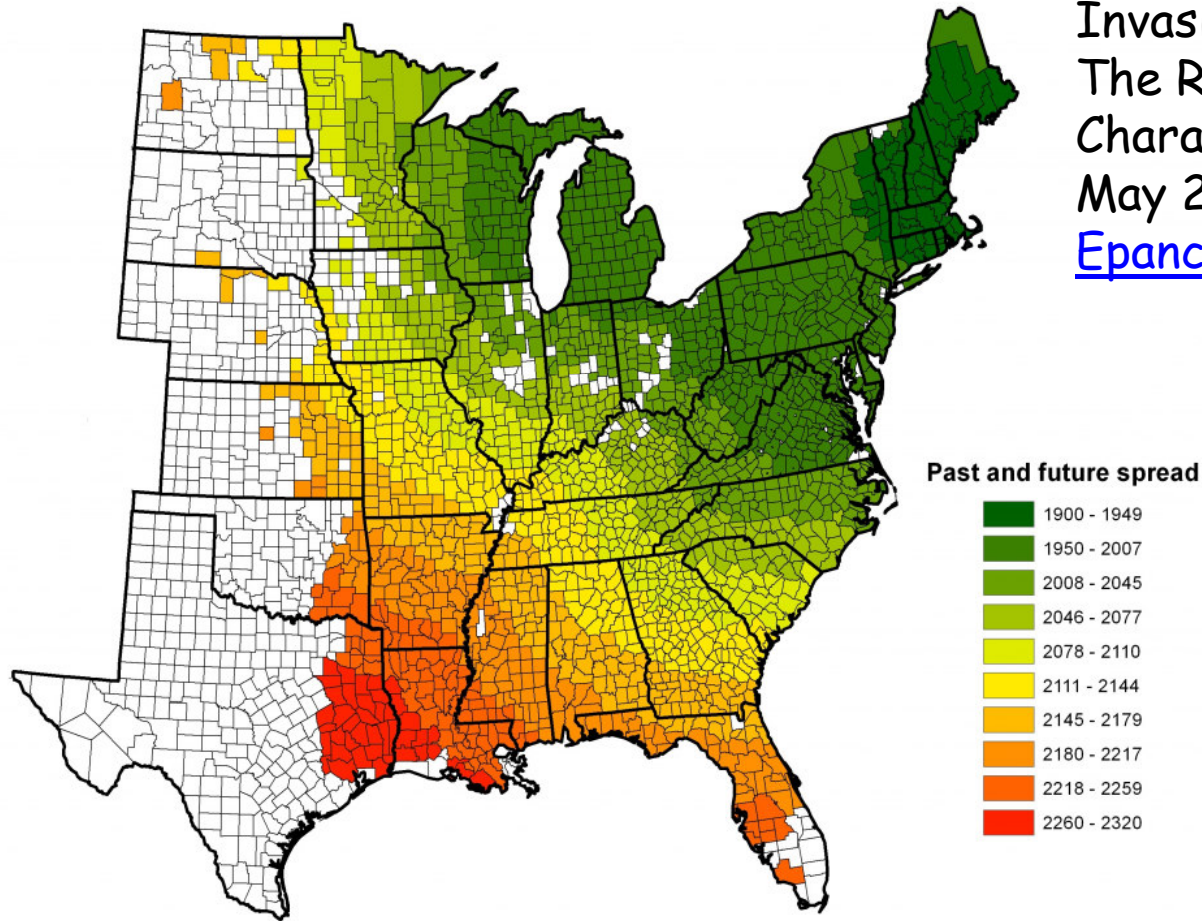
Maosheng Jiang - COPPE/UFRJ

INVADING SPECIES



INVADING SPECIES

Examining the Benefits of
Invasive Species Prevention:
The Role of Invader Temporal
Characteristics
May 20, 2015 | [Rebecca
Epanchin-Niell](#)



Past and predicted future spread of the gypsy moth.

SPREADING OF INFECTIOUS DISEASES

Malaria in the Asia-Pacific Region By [J. Kevin Baird](#) Global Research, November 13, 2015; [The Asia-Pacific Journal, Vol. 13, Issue. 44, No. 1](#) 9 November 2015

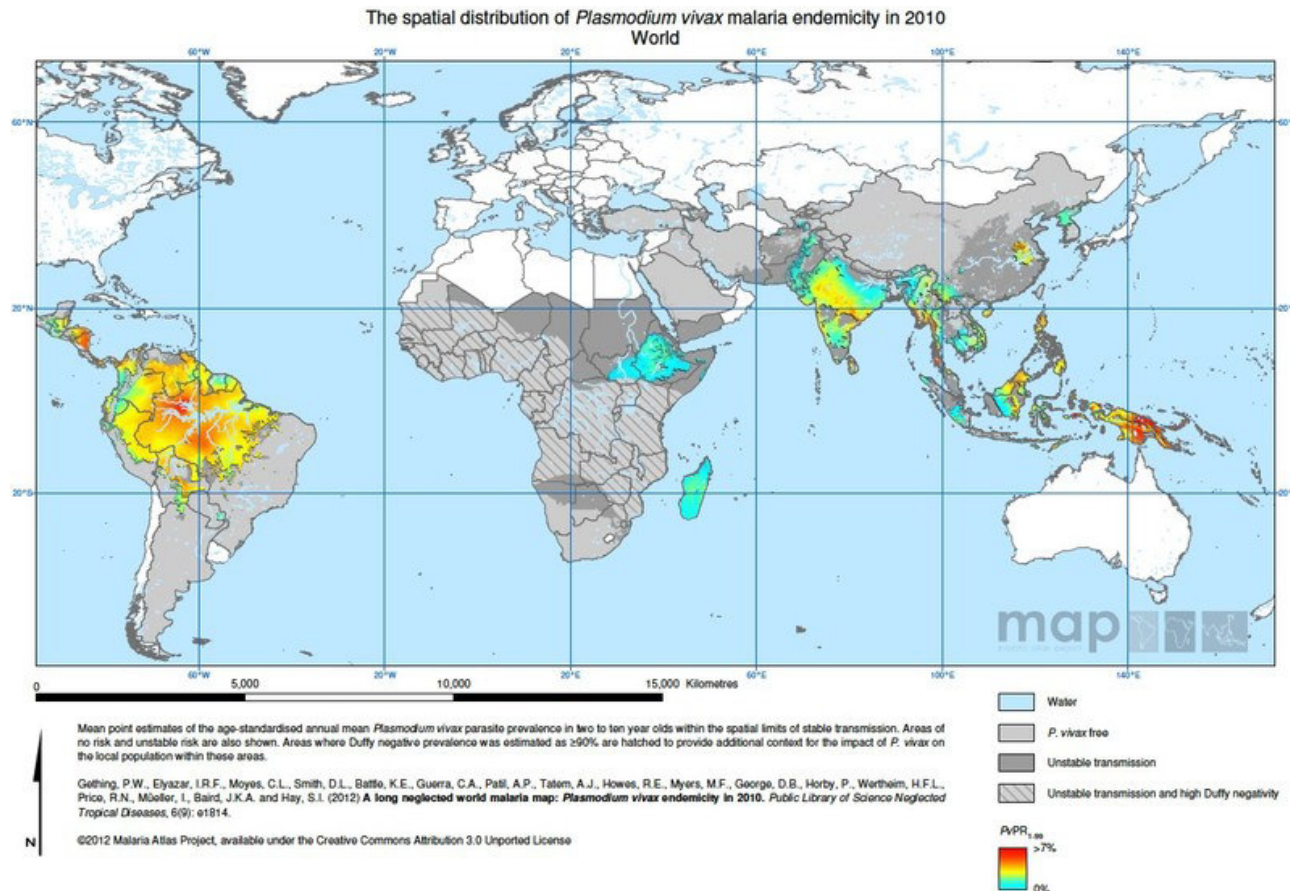


Figure 2. Maps showing the distribution of malaria risk globally for *Plasmodium falciparum* (top) and *Plasmodium vivax* (bottom). See color keys in Figure 3. Courtesy of the [Malaria Atlas Project](#), University of Oxford, United Kingdom

CLASSICAL APPROACH: REGULAR AND ANOMALOUS PROCESSES

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial p}{\partial x} \right) + \quad (\text{sources/sinks})$$

ARE THERE REFERENCES OR
EXPERIMENTAL EVIDENCE OF
RETENTION PHENOMENA IN ANY
PHYSIC-CHEMISTRY OR
BIOLOGICAL PROCESS?

THE ANSWER IS YES

SOME EXAMPLES OF DIFFUSION WITH RETENTION

1. Diffusion and Retention Processes in a Bentonite Near Field (WP2.5)
NF-PRO Annual Meeting, 2006, El Escorial, Spain (Euro-Comm)
2. Extracellular space structure revealed by diffusion analysis; C. Nicholson, E. Syková
3. Retention phenomena in non-Newtonian fluids flow, 2003, D'Angelo, Fontana, Chertco, Rosen
4. Hydrogen bulk retention in graphite and kinetics of diffusion, 2002, H. Atsumi
5. Effect of Liquid-Phase Diffusion Resistance on Retention Time in Gas-Liquid Chromatography, Jan-Chan Huang. Richard Madey
6. Laboratory determination of water retention and diffusion coefficient in unsaturated sand, 2004, K. Badv and M. R. Faridfard

Hydrogen bulk retention in graphite and kinetics of diffusion

H. Atsumi *

Department of Nuclear Engineering, Faculty of Science and Engineering, Kinki University, Kowakae 3-4-1, Higashi-Osaka, Osaka 577-8502, Japan

$$\frac{dN(r,t)}{dt} = D\nabla^2 N(r,t) + \Sigma_d N_t(r,t) - \Sigma_t N(r,t)C(r,t),$$

$$\frac{dN_t(r,t)}{dt} = -\Sigma_d N_t(r,t) + \Sigma_t N(r,t)C(r,t),$$

$$\frac{dC(r,t)}{dt} = \Sigma_d N_t(r,t) - \Sigma_t N(r,t)C(r,t),$$

where N is the local concentration of free hydrogen atom, N_t is that of trapped hydrogen atom, C is the concentration of vacant trap, D is the true diffusion coefficient of free hydrogen, Σ_d is the thermal detrapping rate constant for trapped hydrogen and Σ_t is the trapping rate constant for free hydrogen

Extracellular space structure revealed by diffusion analysis

Charles Nicholson and Eva Syková

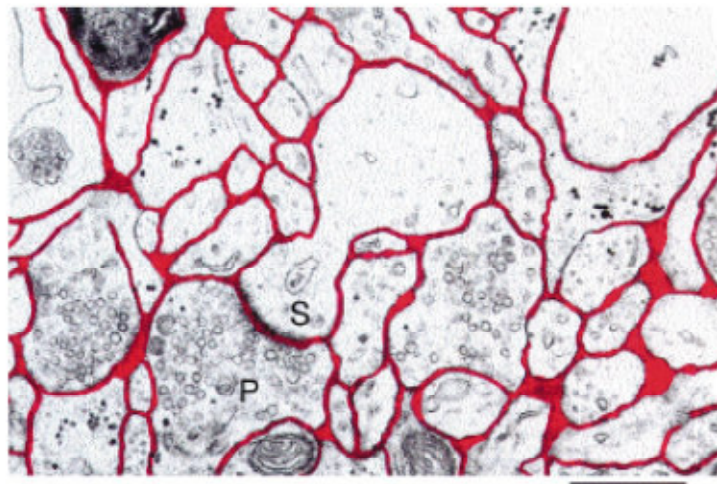


Fig. 1. Geometry of extracellular space. Electronmicrograph of small region of rat cortex with prominent dendritic spine (S) and presynaptic (P) terminal. The ECS is outlined in red. Note the foam-like structure, multiple connectivity, simple convex cell surfaces and presence of 'lakes' where the space widens. The ECS is probably reduced in width due to fixation procedure. Scale bar, 1 μ m. Figure kindly provided by Dr C.B. Jaeger.

proteoglycans and glycosaminoglycans^{6,7}. The matrix composition varies with the cytoarchitectonics⁸, but we know little about its density and we lack reliable evidence that it affects diffusion. The ECS allows glucose to reach brain cells from the blood vessels. It provides a low-resistance path that completes the circuit

$$\frac{\partial C}{\partial t} = \frac{D}{\lambda^2} \nabla^2 C + \frac{Q}{\alpha} - \mathbf{v} \cdot \nabla C - \frac{f(C)}{\alpha} \quad (1)$$

Hydraulic, Diffusion, and Retention Characteristics of Inorganic Chemicals in Bentonite (PhD Thesis)

Naim Muhammad

$$\frac{\partial C}{\partial t} = \frac{D^*}{R_d} \cdot n \cdot \frac{\partial^2 C}{\partial x^2} = D_a^* \left(\frac{\partial^2 C}{\partial x^2} \right) \quad (7.10)$$

The value of $(D^* n/R_d)$, replaced by D_a^* , is defined as the “apparent diffusion coefficient” by many researchers (Quigley *et al.* 1987; Li and Gregory, 1974).

LABORATORY DETERMINATION OF WATER RETENTION AND DIFFUSION COEFFICIENT IN UNSATURATED SAND

K. BADV* and M. R. FARIDFARD

Department of Civil Engineering, Urmia University, P.O. Box 165, Urmia, Iran
(*author for correspondence, e-mail: k.badv@mail.urmia.ac.ir, Tel: 0098-441-277-7040,
Fax: 0098-441-277-7022)

(Received 4 December 2003; accepted 3 August 2004)

It has been reported that, the transport of contaminants through soil by advection and diffusion can be described by the advection – diffusion equation (King *et al.*, 1993; Goodal and Quigley, 1977; Desaulniers *et al.*, 1981; Quigley and Rowe, 1986; Rowe *et al.*, 1988; Rowe and Sawiki, 1992; Schackelford and Daniel, 1991). In case of diffusion (and absorption, where appropriate) this equation is written for one-dimensional conditions as:

$$(\theta + \rho K_d) \frac{\partial c}{\partial t} = \theta D \frac{\partial^2 c}{\partial z^2} \quad (1)$$

Retention phenomena in non-Newtonian fluids flow

M.V. D'Angelo*, E. Fontana, R. Chertcoff, M. Rosen

*Grupo de Medios Porosos, Facultad Ingeniería, Universidad de Buenos Aires, Paseo Colón 850,
1063 Buenos Aires, Argentina*

PHYSICA A 327 (2003) 44-48

quently modify the concentration tracer profile. Various processes may be at the origin of the retention phenomena: for instance, the existence of adsorption processes, mechanical trapping or inaccessible or stagnant volume zones. In order to take them into account, a new term has to be added to the dispersion–convection equation which then expresses as [2]

$$\frac{\partial C}{\partial t} + \vec{U} \cdot \nabla C = D_{\parallel} \nabla_{\parallel}^2 C + D_{\perp} \nabla_{\perp}^2 C - \frac{\rho}{\phi} \frac{\partial \Gamma}{\partial t}, \quad (1)$$

where Γ is the term that represents the total phenomena that produce the retention effects (usually a non-linear isotherm); C is the average concentration; ρ is the medium density; ϕ is the medium porosity; U is the average velocity; D_{\parallel} and D_{\perp} are the dispersion coefficients in the parallel and normal flow direction, respectively (in general,

NEW BIOLOGICAL MODELS

ENZYME DIFFUSION

Joshua Wand , **Enzymes surf the heat wave , *Nature*, 517, 149-150 (2015)**

Molecular diffusion of some enzymes is enhanced when they catalyse reactions, but the reason for this was obscure. Dissipation of heat generated by catalysis through the protein is now thought to propel the molecules.

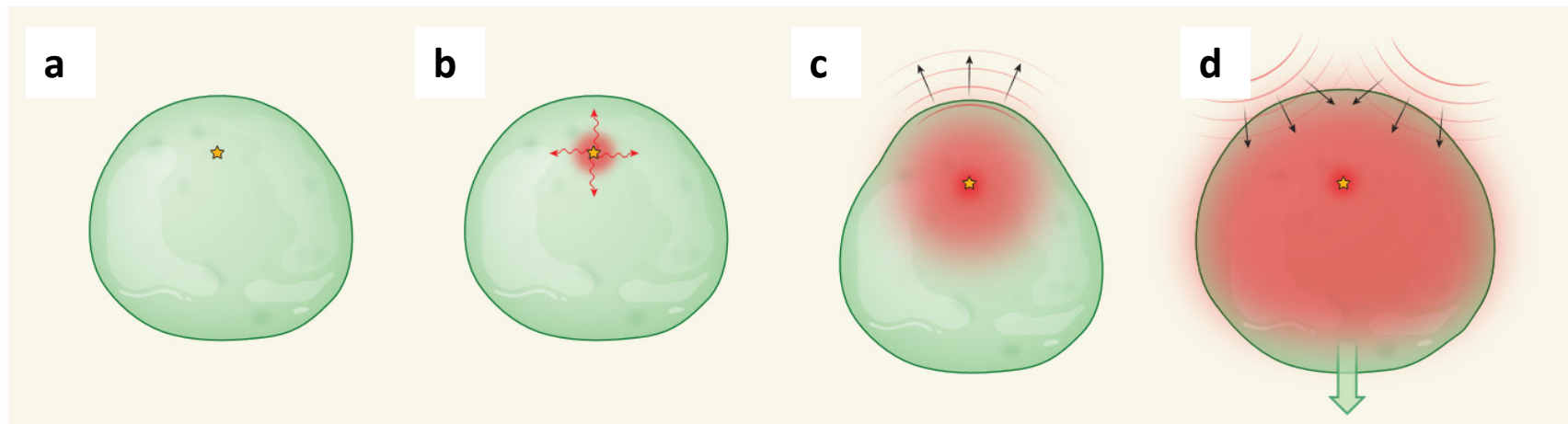


Figure 1 | The chemoacoustic model of anomalous enzyme diffusion.

Riedel *et al.*² report that dissipation of heat generated during enzymatic reactions increases the diffusion of certain enzyme molecules. **a–c**, They suggest that heat released at the active site (yellow star) during a catalytic event generates a radial deformation wave that causes the enzyme to rapidly expand; orange

areas indicate passage of the wave. This causes acoustic waves (black arrows) in the surrounding solvent. **d**, If reflected back on the protein, the waves cause the molecule to move (green arrow). Because enzyme molecules also undergo rotational Brownian motion (not shown), this mechanism of locomotion will not generate overall motion in a particular direction.

NEW BIOLOGICAL MODELS

ENZYME DIFFUSION

***Nature*, 517, 227-230 (2015)**

The heat released during catalytic turnover enhances the diffusion of an enzyme

*Clement Riedel¹, Ronen Gabizon, Christian A. M. Wilson, Kambiz Hamadani¹,
Konstantinos Tsekouras, Susan Marqusee, Steve Presse & Carlos Bustamante*

A stochastic model (detailed in the Supplementary Information and Extended Data Figs 6, 7 and 8) describes the enhanced diffusion upon catalysis in terms of the heat released by the chemical reaction. In this model, we assume that enzymes transiently diffuse more quickly—with diffusion coefficient D_1 —for some short period of time, dt , following a chemical reaction. Otherwise, the enzyme displays its diffusion coefficient in the absence of substrate, D_0 . The net diffusion coefficient in the presence of substrate, D , is therefore the ensemble average over both subpopulations with the probability of observing an enhanced diffusion proportional to V , the reaction rate. We then relate the enhanced diffusion coefficient, D_1 , to the amount of heat, Q , evolved by an enzymatic reaction. To do so, we assume that the kinetic energy of the enzyme's centre-of-mass immediately following a reaction is proportional to some fraction c of Q . From this simple model, we obtain the following expression

$$D = D_0 + \frac{2\gamma Q}{3\zeta^2} mV = D_0 + \alpha V$$

which shows a diffusion coefficient enhancement linear in V and Q , where m is the mass of the enzyme, ζ is the relaxation timescale associated with the enzyme displacement following an enzymatic turnover, and γ is an effective friction coefficient for the enzyme (see Supplementary Materials)

CONTINUUM FORMULATION OF DISTURBED (DELAYED) DIFFUSION PROCESSES

**A NEW ANALYTICAL FORMULATION
OF DISTURBING EFFECTS ON
PARTICLE DIFFUSION PROCESSES**

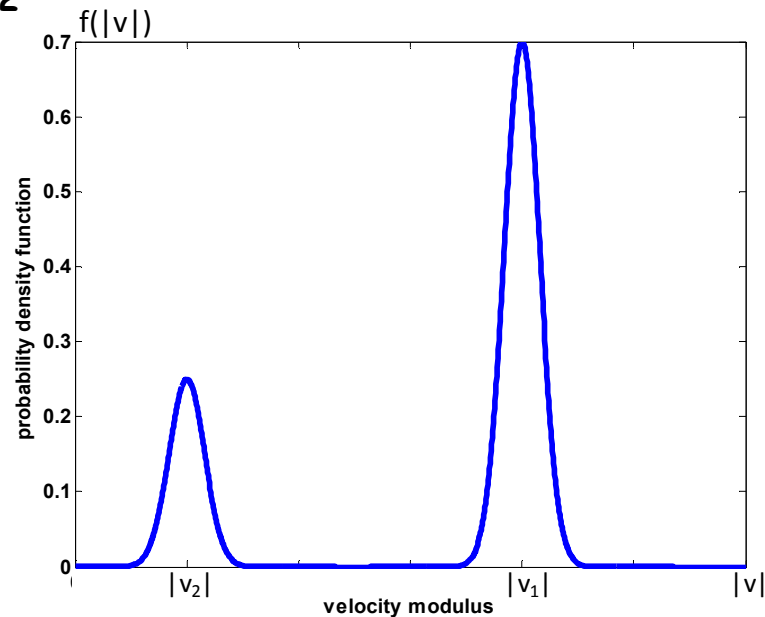
**INTRODUCTION OF A BIMODAL
SPEED DISTRIBUTION TO MASS
TRANSFER PROBLEMS**

FUNDAMENTAL HYPOTHESIS

- I. The system is self-contained in the sense that all possible internal reactions preserve the total mass in the diffusion process.
- II. There are neither sinks nor sources in the system. All particles are under a continuous state of excitation, that is, moving continuously.
- III. There are two distinct energy states $E_1(\mathbf{p}_1, L_1)$ and $E_2(\mathbf{p}_2, L_2)$, corresponding to the two subsets of particles, β and $(1 - \beta)$ respectively, where \mathbf{p} represents the linear momentum and L the angular momentum.
- IV. Particles in the system are either in the energy state I or in the energy state II

FUNDAMENTAL HYPOTHESIS

Under certain circumstances particles travelling in a continuum media may be divided into two distinct sets. The first set of particles $\beta p(x, t)$ is excited with a linear velocity $|v_1|$ - **energy state I** - corresponding to the flux Ψ_1 and the second set $(1-\beta)p(x, t)$ is composed by particles excited with linear velocity $|v_2|$ - **energy state II** - corresponding to the flux Ψ_2

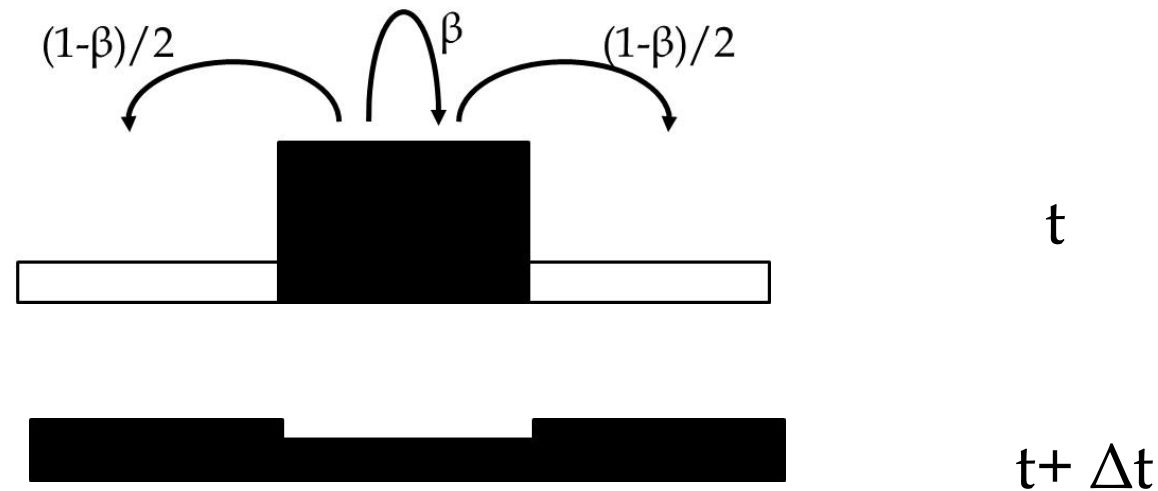


Bimodal velocity distribution

DERIVATION OF THE FUNDAMENTAL EQUATION

THE DISCRETE APPROACH

DISCRETE FORMULATION DIFFUSION WITH RETENTION



$$p_n^t = (1 - \beta)p_n^{t-1} + \frac{1}{2}\beta p_{n-1}^{t-1} + \frac{1}{2}\beta p_{n+1}^{t-1}$$

$$p_n^{t+1} = (1 - \beta)p_n^t + \frac{1}{2}\beta p_{n-1}^t + \frac{1}{2}\beta p_{n+1}^t$$

DISCRETE APPROACH TO DIFFUSION PHENOMENA

Reduce the right hand side terms to the reference time $t-1$

$$p_n^t = \alpha p_n^{t-1} + \frac{1}{2}(1-\alpha)p_{n-1}^{t-1} + \frac{1}{2}(1-\alpha)p_{n+1}^{t-1}$$

$$p_n^{t+1} = \alpha^2 p_n^{t-1} + \alpha(1-\alpha)(p_{n-1}^{t-1} + p_{n+1}^{t-1}) + \frac{1}{4}(1-\alpha)^2(p_{n-2}^{t-1} + p_n^{t-1} + p_{n+1}^{t-1} + p_{n+2}^{t-1})$$

Subtract to get

$$p_n^{t+1} - p_n^t = (1-\alpha) \left[-\frac{1}{2}(p_{n-1}^{t-1} + p_{n+1}^{t-1}) + \alpha(p_{n-1}^{t-1} + p_{n+1}^{t-1} - p_n^{t-1}) + \frac{1}{4}(1-\alpha)(p_{n-2}^{t-1} + 2p_n^{t-1} + p_{n+2}^{t-1}) \right]$$

DISCRETE APPROACH TO DIFFUSION PHENOMENA

$$\frac{\Delta p_n^{t+\Delta t}}{\Delta t} = \beta \left\{ \frac{1}{2} \frac{L_0^2}{T_0} \frac{\Delta^2 p_n}{\Delta x^2} - (1 - \beta) \frac{1}{4} \frac{L_1^4}{T_0} \frac{\Delta^4 p_n}{\Delta x^4} \right\}^{t-\Delta t}$$

Taking the limit when $\Delta x \rightarrow 0$ and $\Delta t \rightarrow 0$ and assuming $p(x,t)$ sufficiently smooth the continuum equivalent to the discrete formulation is obtained:

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

GENERALIZED BI-FLUX DIFFUSION EQUATION

From the discrete approach to the mass conservation principle Equation for the bi-flux diffusion

$$\frac{\partial p}{\partial t} = \beta \frac{\partial}{\partial x} - (1 - \beta) \frac{\partial}{\partial x}$$

Primary Flux (Fick's law)

$$\Psi_1 = -D \frac{\partial p(x, t)}{\partial x} \vec{e}_1$$

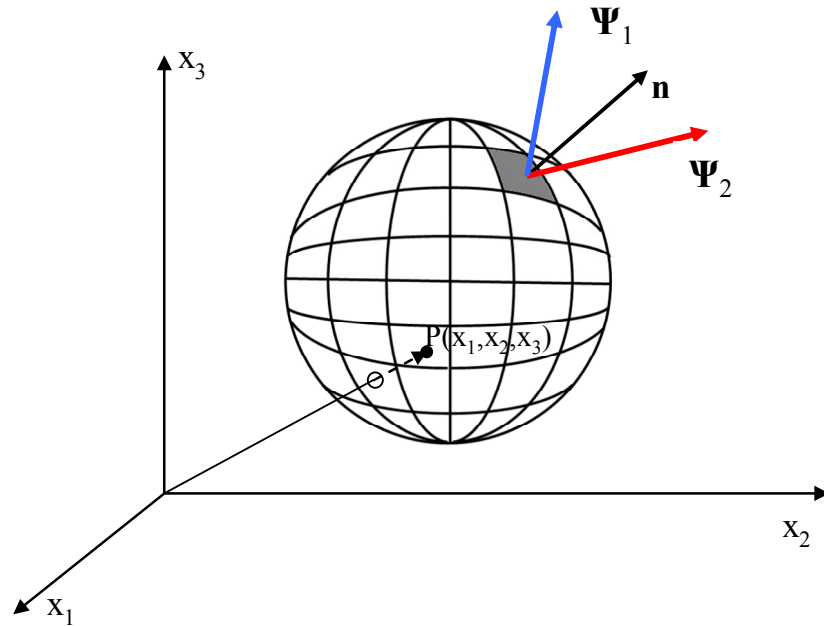
D: diffusion coefficient

Secondary Flux. Subsidiary to the principal flux

$$\Psi_2 = R\beta \left(\frac{\partial^3 p(x, t)}{\partial x^3} \right) \vec{e}_1$$

R: reactivity coefficient

MASS CONSERVATION



According to the previous hypothesis the net flux through the boundary element dS is:

$$\Psi \cdot \mathbf{n} dS = (\beta \Psi_I + (1 - \beta) \Psi_{II}) \cdot \mathbf{n} dS$$

$$0 < \beta < 1$$

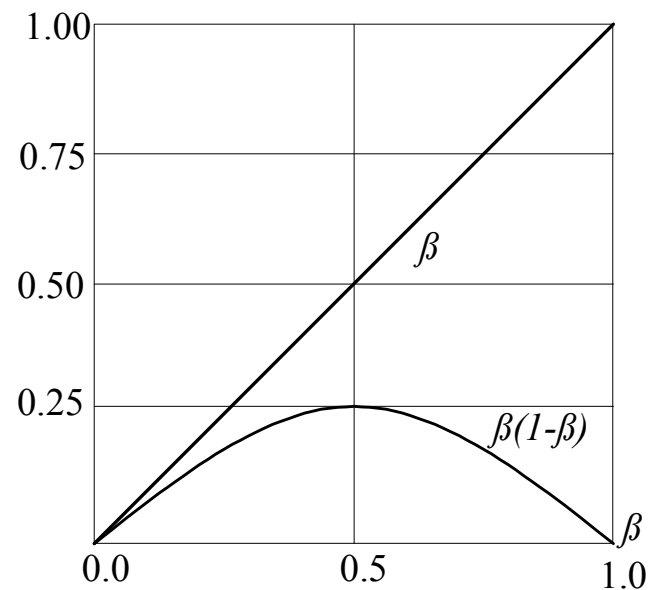
Introducing this expression in the mass conservation equation and since the specific mass ρ is constant we arrive at:

$$\frac{\partial}{\partial t} \int_V \rho(x, t) dV + \int_{\partial V} (\beta \Psi_I + (1 - \beta) \Psi_{II}) \cdot \mathbf{n} dS = 0$$

GOVERNING EQUATION OF TWO-SPEED DIFFUSION PROCESS

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \operatorname{div}(\beta \operatorname{grad}(Dp(\mathbf{x}, t))) - \operatorname{div}(R\beta(1-\beta)\nabla^2(\operatorname{grad}(p(\mathbf{x}, t))))$$

$$\frac{\partial p(x, t)}{\partial t} = \frac{\partial}{\partial x} \left[\beta D \frac{\partial p(x, t)}{\partial x} \right] - \frac{\partial}{\partial x} \left[\beta(1-\beta)R \frac{\partial^3 p(x, t)}{\partial x^3} \right]$$



PHYSICAL MEANING OF THE BOUNDARY CONDITIONS

THE BOUNDARY CONDITIONS ARE DETERMINED ONCE WE KNOW AT THE BOUNDARY:

The concentration : $p_0(t)$

The gradient of the concentration : $grad(p_0(t)) \quad \psi_1 \rightarrow$

The time variation of the concentration: $\partial^2 p_0(t)/\partial t^2$

The gradient of the time variation of the concentration : $\beta grad(\partial^2 p_0(t)/\partial t^2) \quad \psi_2 \rightarrow$

THE DIFFERENT TYPES OF SOLUTIONS FOR THE FOURTH ORDER EQUATION

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

Two cases of closed solutions will be considered

$$\phi(x, t) = \phi_0 g(t) \cos(\pi x/2)$$

$$\phi(x, t) = \phi_0 g(t) \cosh(x)$$

SIMPLE PROBLEMS-CLOSED SOLUTIONS

CASE I

$$\phi(x, t) = \phi_0 g(t) \cos(\pi x/2)$$

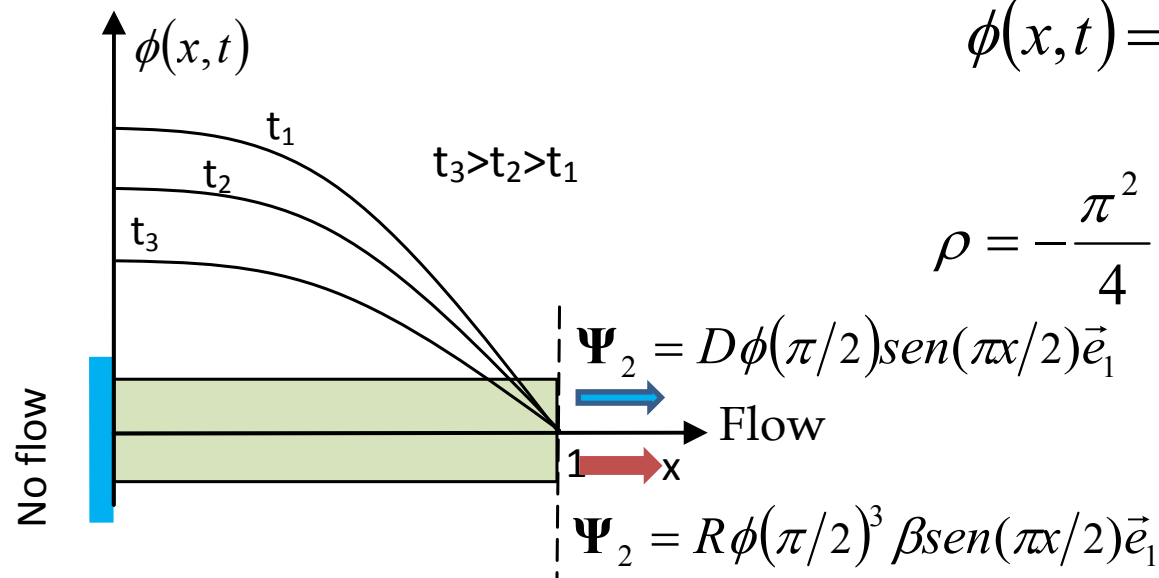
$$\left. \frac{\partial^3 \phi}{\partial x^3} \right|_{x=0} = 0; \quad \left. \frac{\partial \phi}{\partial x} \right|_{x=0} = 0; \quad \left. \frac{\partial^2 \phi}{\partial x^2} \right|_{x=1} = 0; \quad \phi|_{x=1} = 0$$

Solution

$$\phi(x, t) = \phi_0 e^{\rho t} \cos\left(\frac{\pi x}{2}\right)$$

$$\rho = -\frac{\pi^2}{4} D \beta \left(1 + \frac{\pi^2}{4} r (1 - \beta) \right)$$

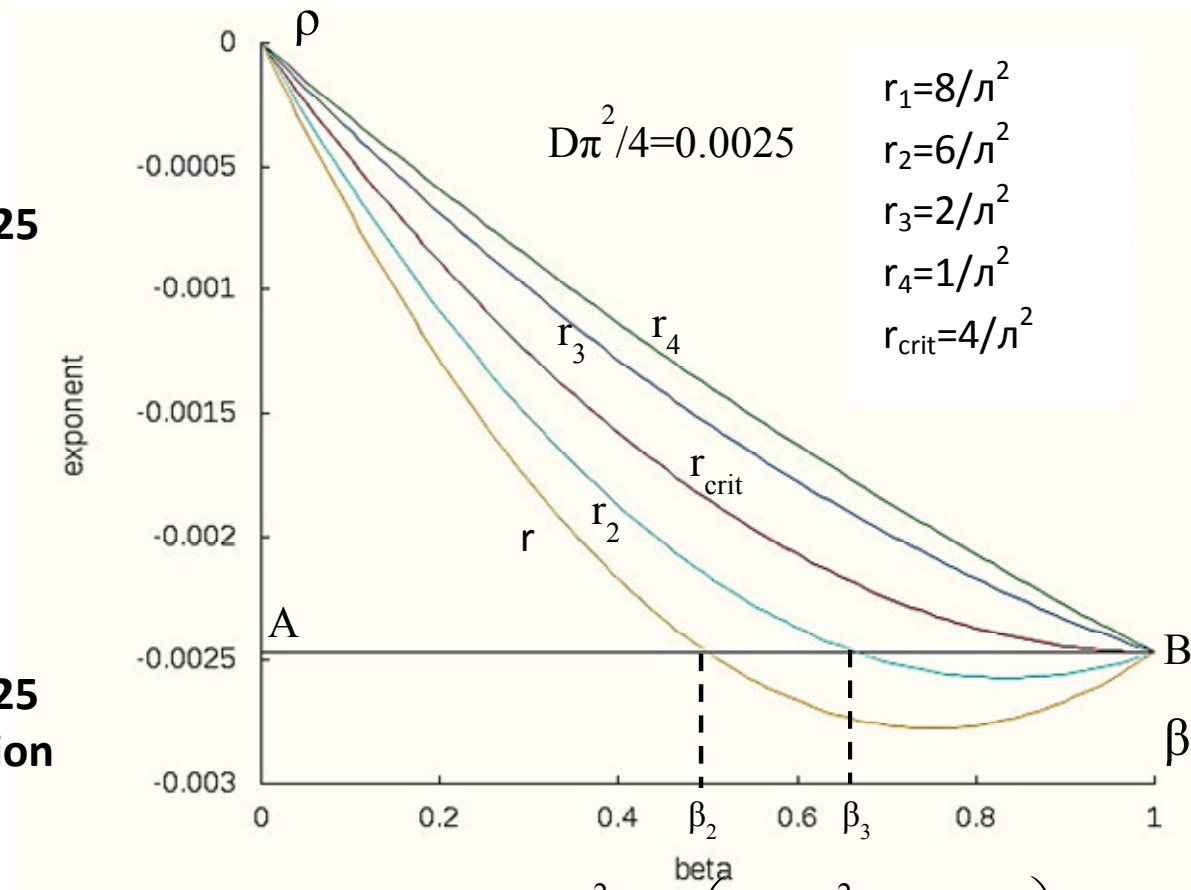
$$r = R/D$$



SIMPLE PROBLEMS-CLOSED SOLUTIONS CASE I

$\rho > -0.0025$
delay

$\rho < -0.0025$
acceleration

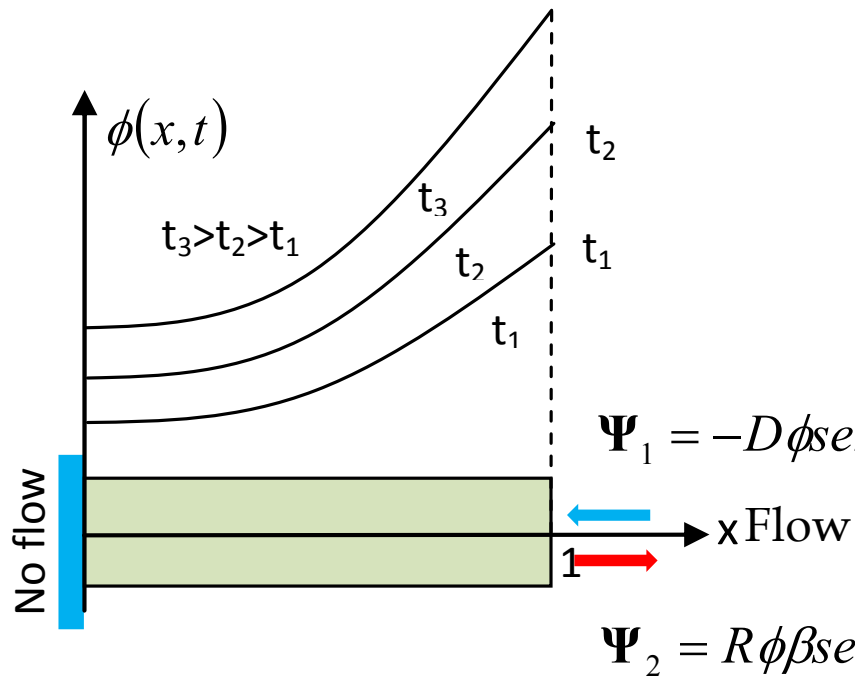


$$\rho = -\frac{\pi^2}{4} D\beta \left(1 + \frac{\pi^2}{4} r(1-\beta) \right)$$

SIMPLE PROBLEMS-CLOSED SOLUTIONS CASE II

$$\phi(x, t) = \phi_0 g(t) \cosh(x)$$

$$\left. \frac{\partial \phi}{\partial x} \right|_{x=0} = 0 \quad \left. \frac{\partial^3 \phi}{\partial x^3} \right|_{x=0} = 0 \quad \left. \frac{\partial^2 \phi}{\partial x^2} \right|_{x=1} = \phi \Big|_{x=1} \quad \left. \frac{\partial^3 \phi}{\partial x^3} \right|_{x=1} = \left. \frac{\partial \phi}{\partial x} \right|_{x=1}$$



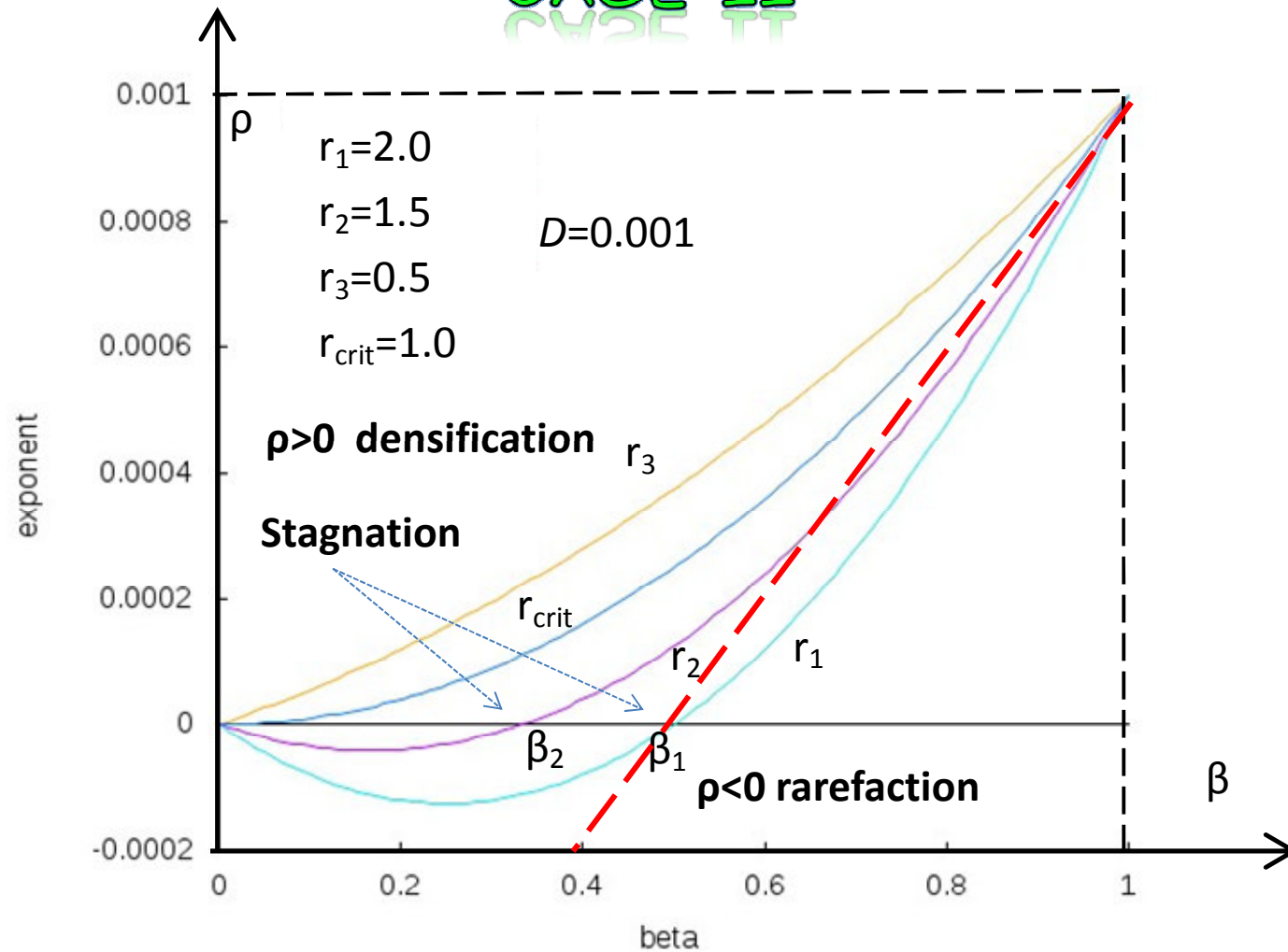
Solution

$$\phi(x, t) = \phi_0 e^{\rho t} \cosh(x)$$

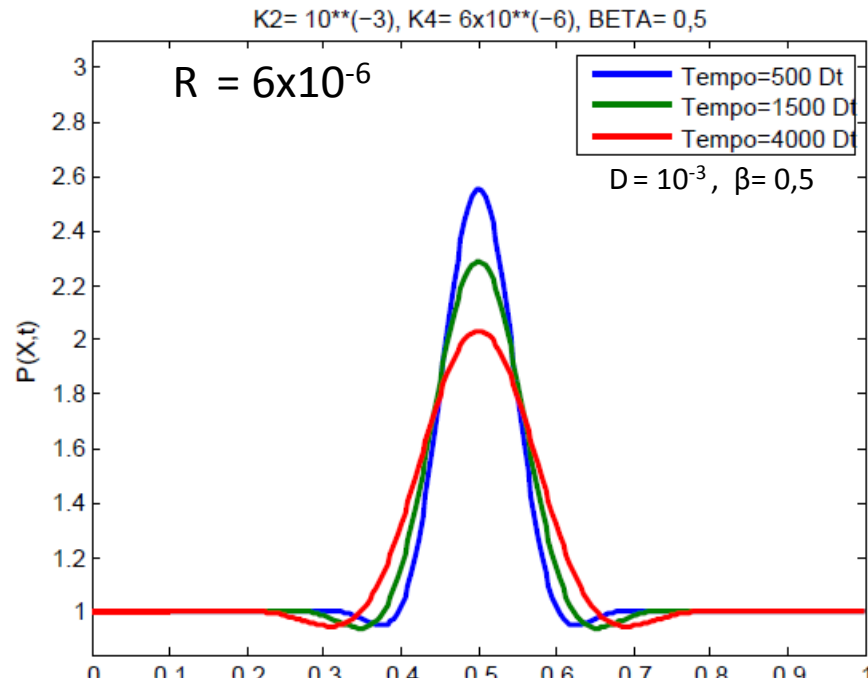
$$\rho = D \beta (1 - r(1 - \beta))$$

$$r = R/D$$

SIMPLE PROBLEMS-CLOSED SOLUTIONS CASE II



$$\rho = D\beta(1 - r(1 - \beta))$$



ANOMALY FOR A CONCENTRATED PULSE

$$p(x,0) = \frac{1}{\sqrt{\pi\theta}} \exp\left(-\frac{x^2}{\theta^2}\right)$$

Broadbridge P. (2008) *Entropy diagnosis for fourth order partial differential equations in conservative form*. Entropy 10:365-379

