DIFFUSION WITH RETENTION EFFECTS: APPLICATIONS IN BIOLOGY, SOCIAL SCIENCES AND ENGINEERING

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MOTIVATION

KNOWLEDGE TRANSFER IN A PRODUCTION CHAIN

INVADING SPECIES

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

Commonly Mechanisms to Simulate the Diffusion-Retention Effects

Using an “apparent diffusion coefficient”

Introducing a “time-delay process”

Using a succession of “equivalent sinks and sources”

$$\frac{\partial p}{\partial t} = \beta D \frac{\partial^2 p}{\partial x^2} + F\left(p, t; \beta\right)$$

$F(p,t;\beta)$

t

$$\int_0^\infty F\left(p, t; \beta\right) dt = 0$$

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

Naim Muhammad

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

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

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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:

$$(\theta + \rho K_{\mathrm{d}})\frac{\partial c}{\partial t} = \theta D \frac{\partial^2 c}{\partial z^2} \tag{1}$$

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Hydrogen bulk retention in graphite and kinetics of diffusion

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$$\frac{\mathrm{d}N(r,t)}{\mathrm{d}t} = D\nabla^2 N(r,t) + \Sigma_{\mathrm{d}} N_{\mathrm{t}}(r,t) - \Sigma_{\mathrm{t}} N(r,t) C(r,t),$$

$$\frac{\mathrm{d}N_{\mathrm{t}}(r,t)}{\mathrm{d}t} = -\Sigma_{\mathrm{d}} N_{\mathrm{t}}(r,t) + \Sigma_{\mathrm{t}} N(r,t) C(r,t),$$

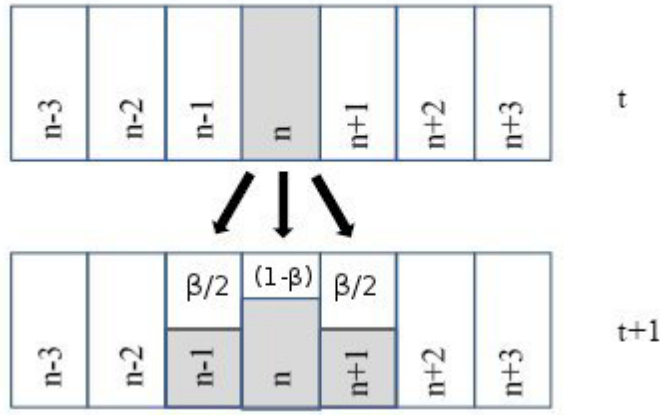
$$\frac{\mathrm{d}C(r,t)}{\mathrm{d}t} = \Sigma_{\mathrm{d}} N_{\mathrm{t}}(r,t) - \Sigma_{\mathrm{t}} N(r,t) C(r,t),$$

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, $\sum_d$ is the thermal detrapping rate constant for trapped hydrogen and $\sum_t$ is the trappingrate constant for free hydrogen

MEANINGFUL INSIGHT FROM A SIMPLE ANALYSIS

DISCRETE APPROACH TO DIFFUSION PHENOMENA

1. Symmetric Diffusion-Retention



Rule

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

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

$$0 \le \beta \le 1$$

$\beta = 0$ stationary regime

$\beta = 1$ symmetric diffusion with no retention

$0 < \beta < 1$ retention-diffusion phenomena

DISCRETE APPROACH TO DIFFUSION PHENOMENA

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

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

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

Subtract to get

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

DISCRETE APPROACH TO DIFFUSION PHENOMENA

After a careful separation of discrete variables

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

$$+ (1-\beta)\beta\frac{1}{4}\left[-p_{n-2}^{t-1} + 4p_{n-1}^{t-1} - 6p_n^{t-1} + 4p_{n+1}^{t-1} - p_{n+2}^{t-1}\right]$$

Limit $\beta \to 0$ stationary regime

Limit $\beta \to 1$ symmetric diffusion with no retention

Recall

$$\Delta^2 p_k = p_{k-1} - 2p_k + p_{k+1}$$

$$\Delta^4 p_k = -p_{k-2} + 4p_{k-1} - 6p_k + 4p_{k+1} - p_{k+2}$$

DISCRETE APPROACH TO DIFFUSION PHENOMENA

If p_n is the discrete representation of $p(x_n)$ and $p(x)$ is sufficiently smooth it is possible to write:

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

Where L_0, L_1 and T_0 are scale factors.

$$\Delta x = L_0/m = L_1/\sqrt{m} \qquad \Delta t = T_0/m^2$$

DISCRETE APPROACH TO DIFFUSION PHENOMENA

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

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

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

FUNDAMENTAL PROPOSITION FOR DISTURBED DIFFUSION PROCESSES

PROPOSITION. Suppose a one-dimensional diffusion process consisting of N particles moving in a homogeneous, isotropic supporting medium according to the Fick s law. If a fraction f(N) of the diffusing particles is temporarily disturbed along their trajectories due to some mechanical, physical, chemical or physicochemical interaction with the medium, the governing equation must include a fourth order differential term of the form:

$$-\Gamma\beta(1-\beta)\frac{\partial^4 p}{\partial x^4}$$

Where Γ *is a time-independent material constant;* $(1-\beta)$ *is the particle fraction temporarily trapped,* $0 < \beta \leq 1$, *and p(x,t) is the particle concentration.*

A Numerical Experiment for a Diffusion-Retention Problem

Semi-Discrete Finite Element Approximation

Hermite's Cubic Interpolation

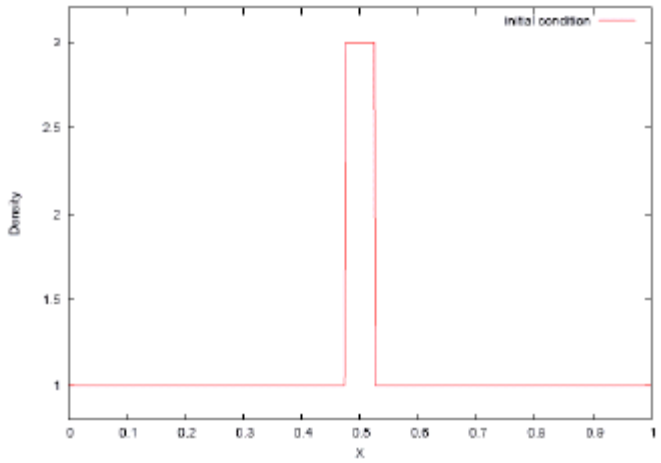
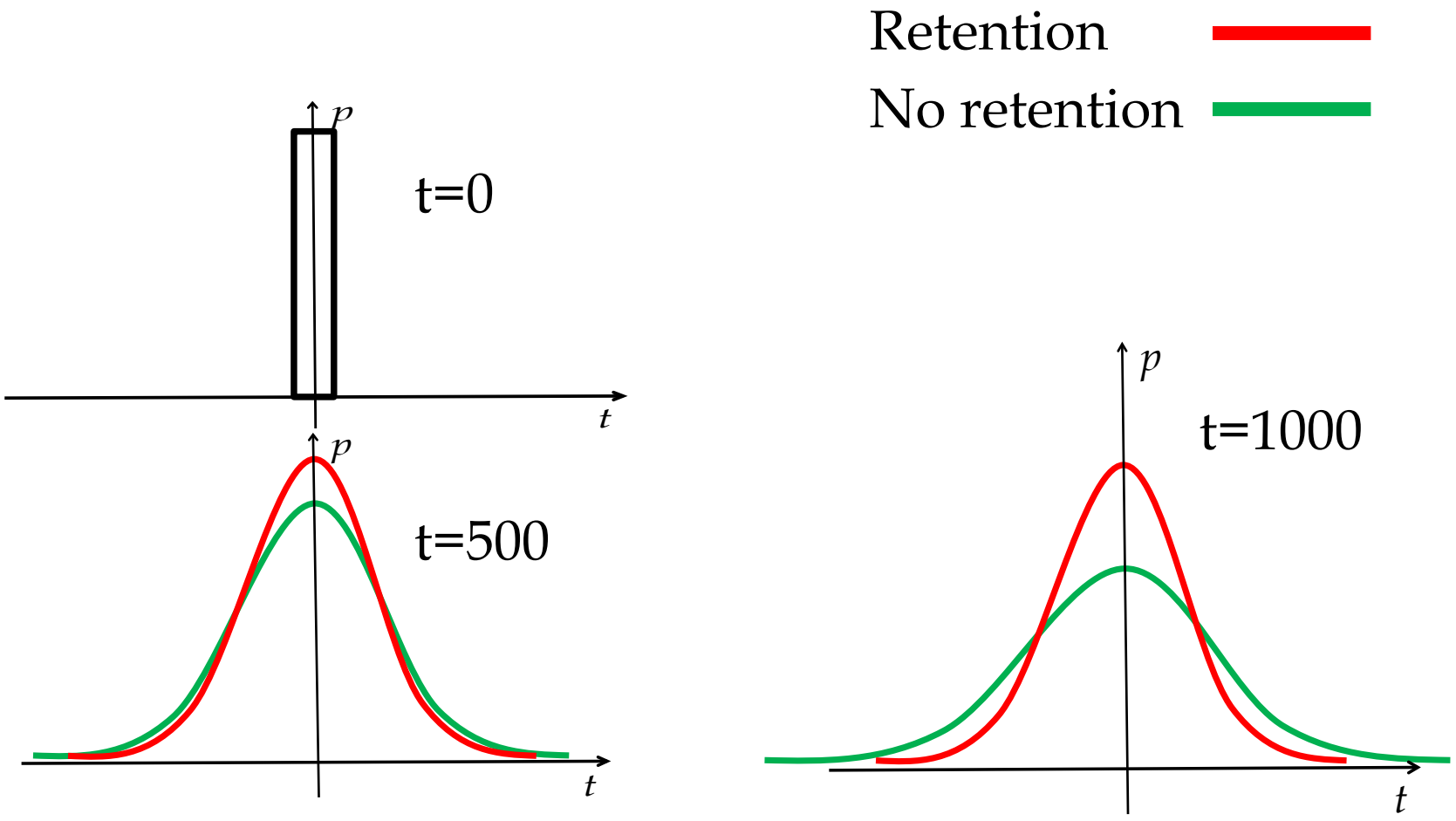


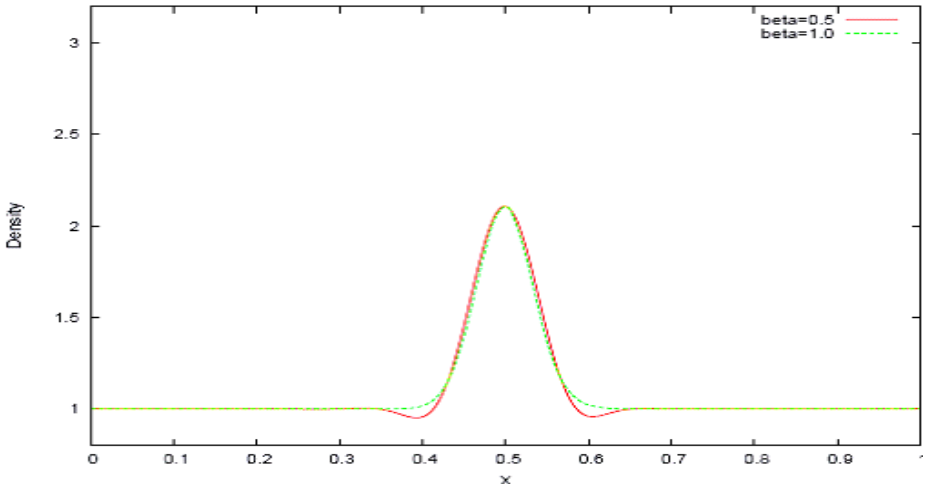
Fig.1 – Initial Condition

Boundary conditions

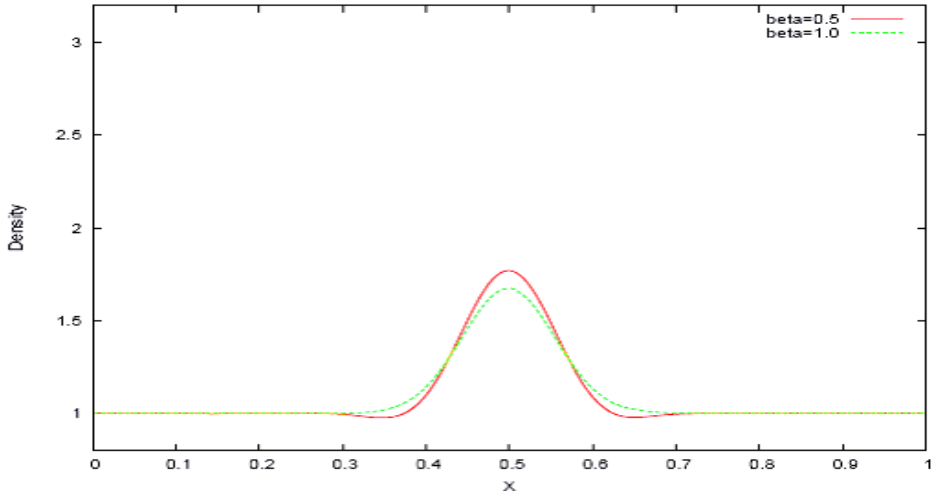
$$p(0) = p(1) = 1; \quad \frac{\partial p}{\partial x}(0) = \frac{\partial p}{\partial x}(1) = 0$$

CHECKING THE EXPECTED EFFECT OF RETENTION

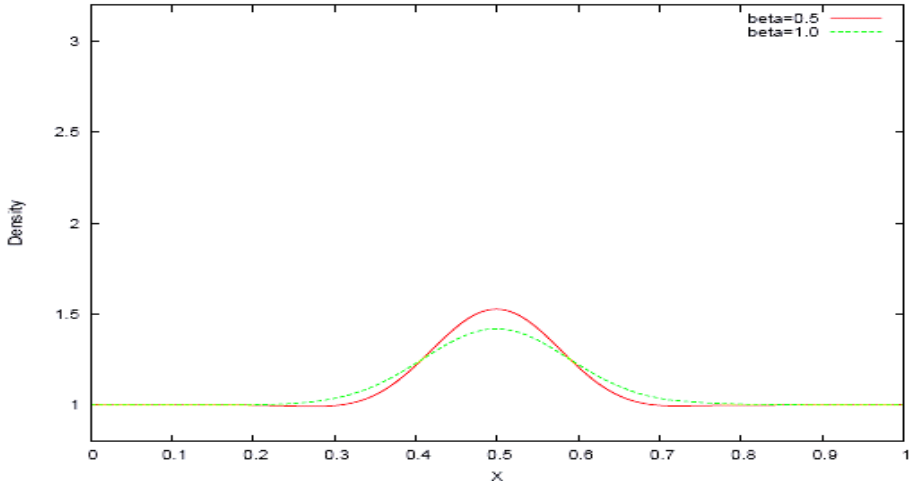




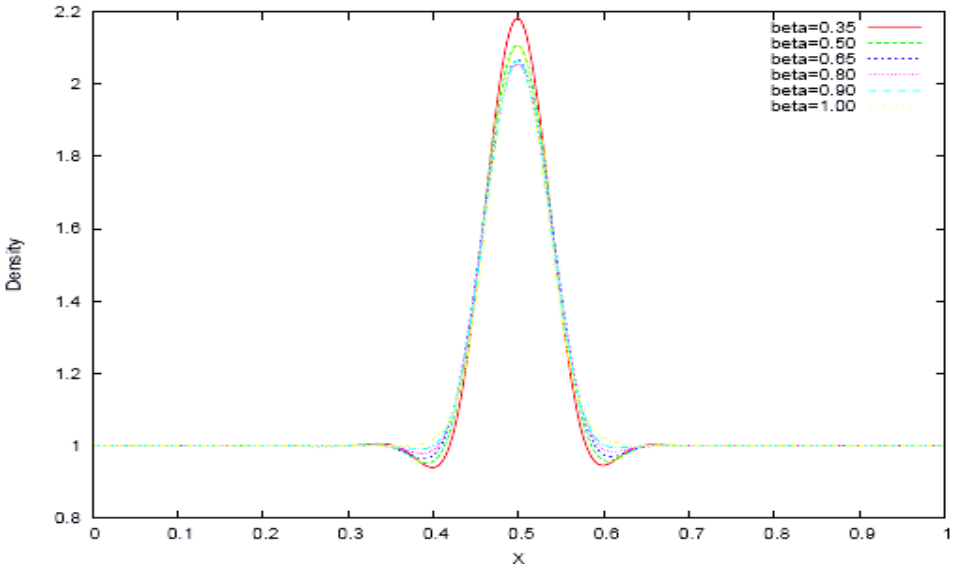
(a) Time 500Δt



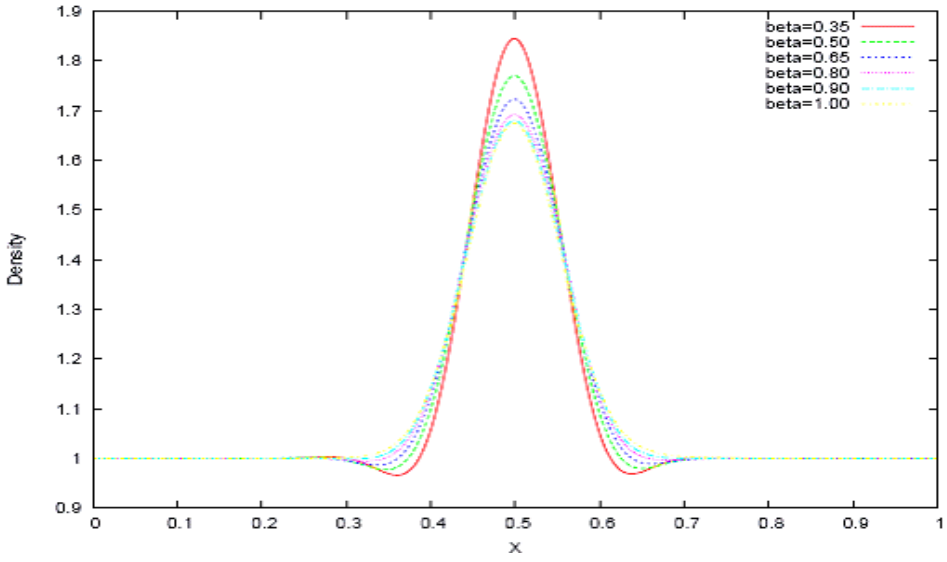
(b) Time 1500Δt



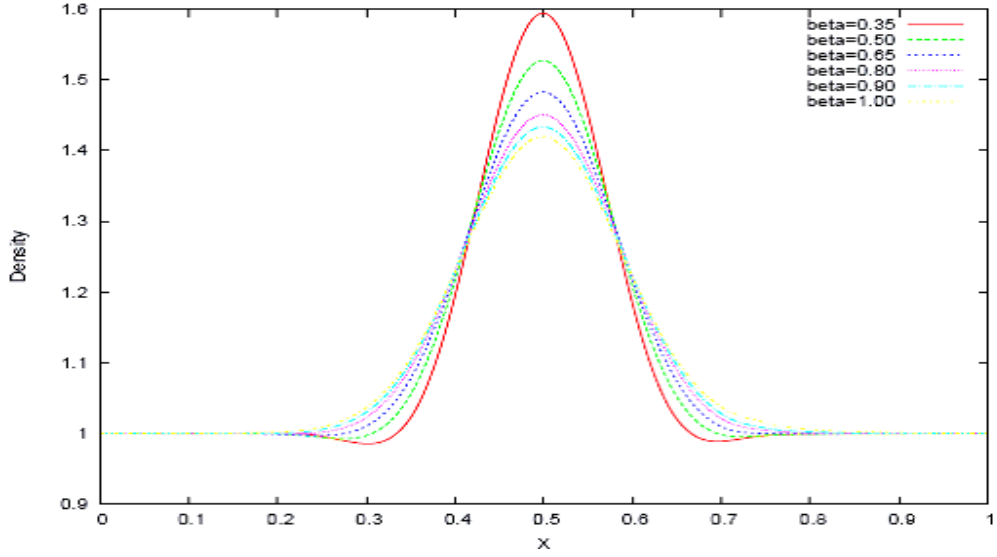
(c) Time 4000Δt



(a) Time 500Δt



(b) Time 1500Δt



(c) Time 4000Δt

CONTINUUM FORMULATION OF DISTURBED (DELAYED) DIFFUSION PROCESSES

CONTINUUM APPROACH OF DIFFUSION PHENOMENA

The equation derived with the discrete approach:

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

….may be used for the analysis in a continuous medium?
We have to face the following aspects:

1. The proposed fourth order equation doesn't contain any indication that a fraction of the mass retained, meaning zero velocity, still stand.
2. Therefore both particle sets β and (1−β) are flowing continuously.
3. Which are the laws controlling the respective fluxes?
4. How the hypothesis of retention in the discrete approach leads to a flow in the continuous model?
5. Is retention the only possible outcome? Is it possible to have acceleration?

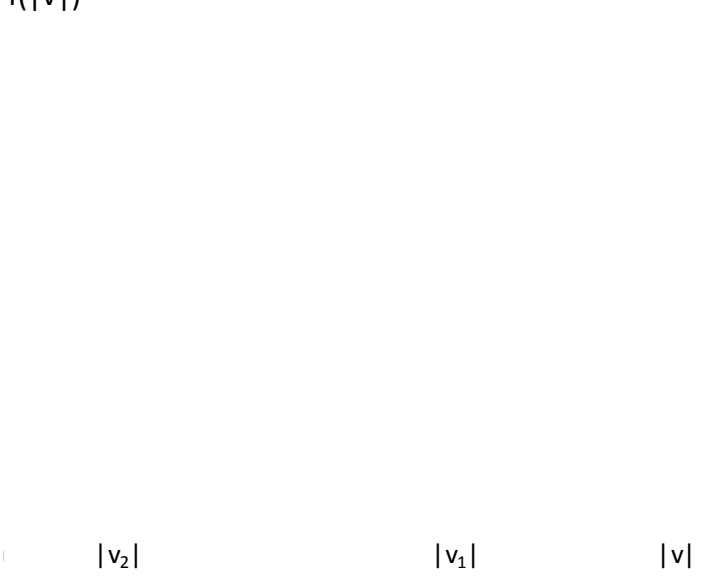
A NEW ANALYTICAL FORMULATION OF DISTURBING EFFECTS ON PARTICLE DIFFUSION PROCESSES

Introduction of a two-speed approach to mass transfer problems

A BY-VELOCITY MODEL PROPOSAL

FUNDAMENTAL HYPOTHESIS

Under certain circumstances particles travelling in a continuum media may be divided into two distinct sets. To the first set $\beta p(x,t)$ belong particles excited with a linear velocity $|\mathbf{v}_1|$ – **energy state I** – and to the second set $(1-\beta)p(x,t)$ belong particles excited with linear velocity $|\mathbf{v}_2|$ – **energy state II** –



FUNDAMENTAL HYPOTHESIS

- The mass conservation principle applies for any arbitrary volume contained in the system. That is, all possible internal reactions do not modify the total mass in the diffusion process.
- There are neither sinks nor sources in the system. All particles are under a continuous state of excitation, that is, moving continuously.
- The system is conservative and it is in thermodynamic equilibrium.
- There are two distinct energy states $E_1(\boldsymbol{p_1},\boldsymbol{L_1})$ and $E_2(\boldsymbol{p_2},\boldsymbol{L_2})$, corresponding to the two subsets of particles, β and $(1-\beta)$ respectively, where $\boldsymbol{p}$ represents the linear momentum and $\boldsymbol{L}$ the angular momentum.
- Particles in the system are either in the energy state I or in the energy state II

THE ONE-DIMENSIONAL CASE

Let $\boldsymbol{\Psi}_I$ and $\boldsymbol{\Psi}_{II}$ represent the fluxes corresponding to **state I** and **state II** respectively. The law governing $\boldsymbol{\Psi}_I$ is:

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

Which is the classical Fick s law. *D* is the primary diffusion coefficient.

Now let us introduce a second law for the energy state II.
The flux of particles belonging to the **energy state II** is given by:

$$\boldsymbol{\Psi}_{II} = \beta R\frac{\partial^2}{\partial x^2}\left(\frac{\partial p(x,t)}{\partial x}\right)\vec{e}_1$$

Note that the flux in **energy state II** depends on the mass fraction β moving according to the classical rule. *R* will be called as secondary diffusion coefficient.

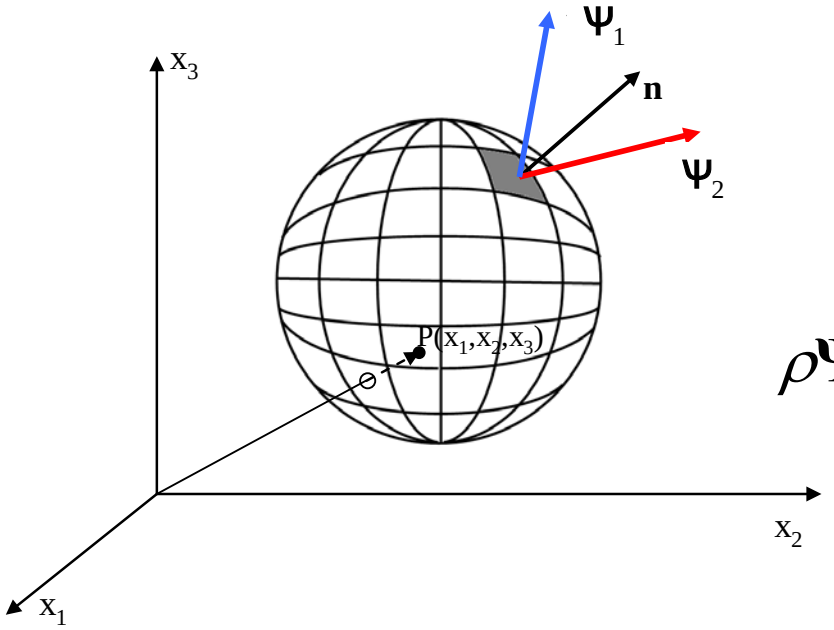
PRIMARY AND SECONDARY FLUXES

The set E_1 is essential, always exists and corresponds to the primary flux.

The flux Ψ_2 however depends on the fraction β of the particles associated to the flux Ψ_1. That is, the energy state E_2 is controlled by the energy state E_1 in such a way that E_2 cannot stand by itself, it only exists if the state E_1 exists. This correlation between both states justifies the origin of the state E_2 as an outcome of a disturbing effect on the state E_1, which is the principal phenomenon.

Initially it was thought that equation (1) would govern exclusively temporary retention or delaying effects. As it will be seen below this is not strictly true. More precisely the equation (1) in fact represents diffusion subjected to flux disturbances encompassing delay, acceleration or stagnation depending on the relative values of R, β and the boundary conditions.

MASS CONSERVATION



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

$$\rho\boldsymbol{\Psi}.\mathbf{n}dS = \rho\left(\beta\boldsymbol{\Psi}_{\mathbf{I}} + \left(1-\beta\right)\boldsymbol{\Psi}_{\mathbf{2}}\right).\mathbf{n}dS$$

$$0 < \beta < 1$$

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

$$\frac{\partial}{\partial t}\int_{V} p\left(x,t\right)dV + \int_{\partial V}\left(\beta\boldsymbol{\Psi}_{I} + \left(1-\beta\right)\boldsymbol{\Psi}_{II}\right).\mathbf{n}dS = 0$$

GOVERNING EQUATION OF TWO-SPEED DIFFUSION PROCESS

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

For uni-dimensional problems

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

For β, *D* and *R* independent of *x* we arrive at the original equation:

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

CHARACTERISTIC CASES OF BI-VELOCITY DIFFUSION IN A HOMOGENEOUS MEDIUM

DIFFUSION WITH RETENTION

Particular case of one dimensional diffusion with retention in a homogeneous medium that is *R*,*D* and β independent of *x*.

$$\frac{\partial p(x,t)}{\partial t} = \beta D\left(\frac{\partial^2 p(x,t)}{\partial x^2} - (1-\beta) r \frac{\partial^4 p(x,t)}{\partial x^4} \right)$$ With $r=R/D$

The solutions depend on the parameter β, *r* and *D* and we may write:

$$p = p(x,t;r,D,\beta)$$

Now from the fundamental hypothesis disturbances are controlled by the retention coefficient *R* and the fraction of diffusing particles β. So it is plausible to admit that β is a function of *R* or *r*, therefore:

$$p = p(x,t;\beta(r),D)$$

CONDITION FOR DIFFUSION WITH RETENTION

Suppose that we dealing with a retention process, then it is expected that increasing values of *R* or *r* (the diffusion coefficient *D* is supposed to be constant) the time delay of the diffusion process will also increase. So retention prevails provided that the following condition holds:

$$\frac{dp}{dr} = \frac{\partial p}{\partial r} + \frac{\partial p}{\partial \beta}\frac{d\beta}{dr} > 0$$

or

$$\boxed{\frac{d\beta}{dr} > -\frac{\partial p}{\partial r} \Big/ \frac{\partial p}{\partial \beta}}$$

THIS MEANS THAT r CAN NOT BE IMPOSED INDEPENDENTLY OF β IF RETENTION IS THE EXPECTED DISTURBANCE.

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

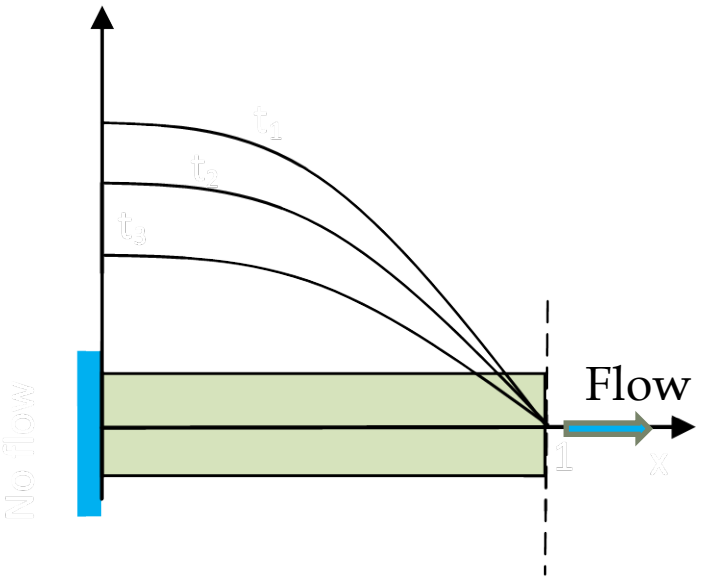
$$\phi(x,t) = \phi_0 g(t) \cos(\pi x/2)$$

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

SIMPLE PROBLEMS-CLOSED SOLUTIONS
CASE I

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

$$\partial^3\phi/\partial x^3\Big|_{x=0} = 0; \qquad \partial\phi/\partial x\Big|_{x=0} = 0; \qquad \partial^2\phi/\partial x^2\Big|_{x=1} = 0; \qquad \phi\Big|_{x=1} = 0$$



Solution

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

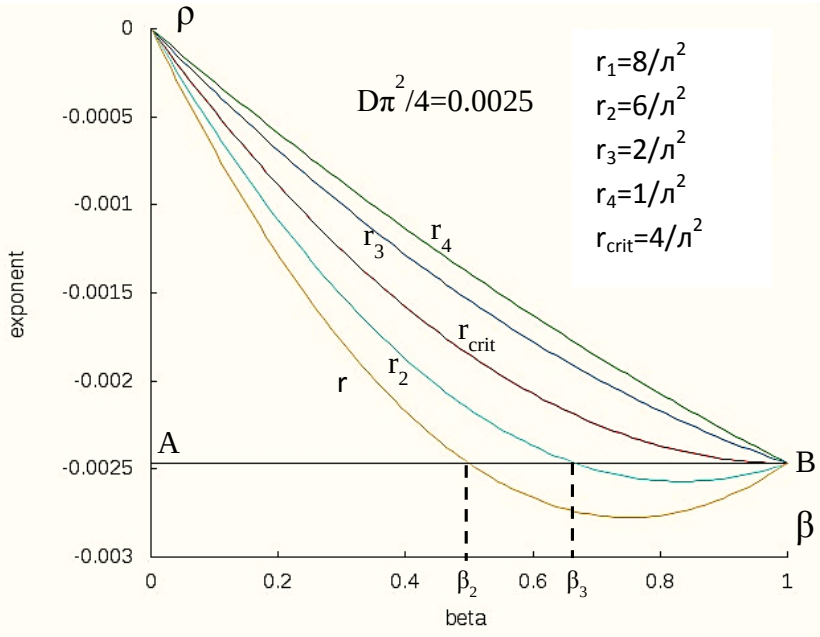
$$\rho = -\frac{\pi^2}{4} D\beta\left(1 + \frac{\pi^2}{4} r(1-\beta)\right)$$

r=R/D

SIMPLE PROBLEMS-CLOSED SOLUTIONS
CASE I

ρ>−0.0025
delay

ρ<−0.0025
aceleration

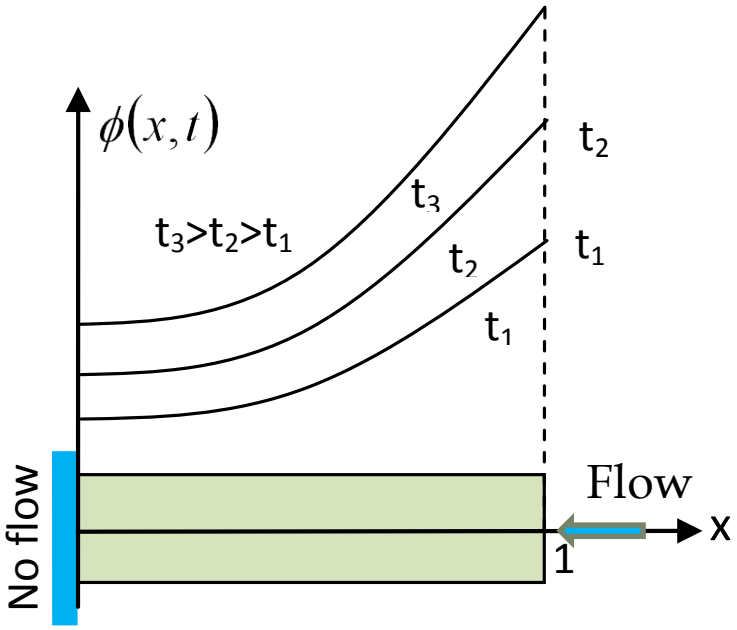


The figure shows the variation of ρ with β for different values of r. If r increases retention will be only possible for decreasing values of β that is for an increasing fraction of trapped particles. The retention effect is activated only for the pairs (r,β) above the line AB. The curve corresponding to $r_c = (R/D)_c$ divides the set of curves into two groups. For $r<r_c$ all curves represent delay. For $r> r_c$ only the branches above AB represent retention.

SIMPLE PROBLEMS-CLOSED SOLUTIONS
CASE II

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

$$\partial\phi/\partial x\big|_{x=0} = 0 \qquad \partial^3\phi/\partial x^3\big|_{x=0} = 0 \qquad \partial^2\phi/\partial x^2\big|_{x=1} = \phi\big|_{x=1} \qquad \partial^3\phi/\partial x^3\big|_{x=1} = \partial\phi/\partial x\big|_{x=1}$$



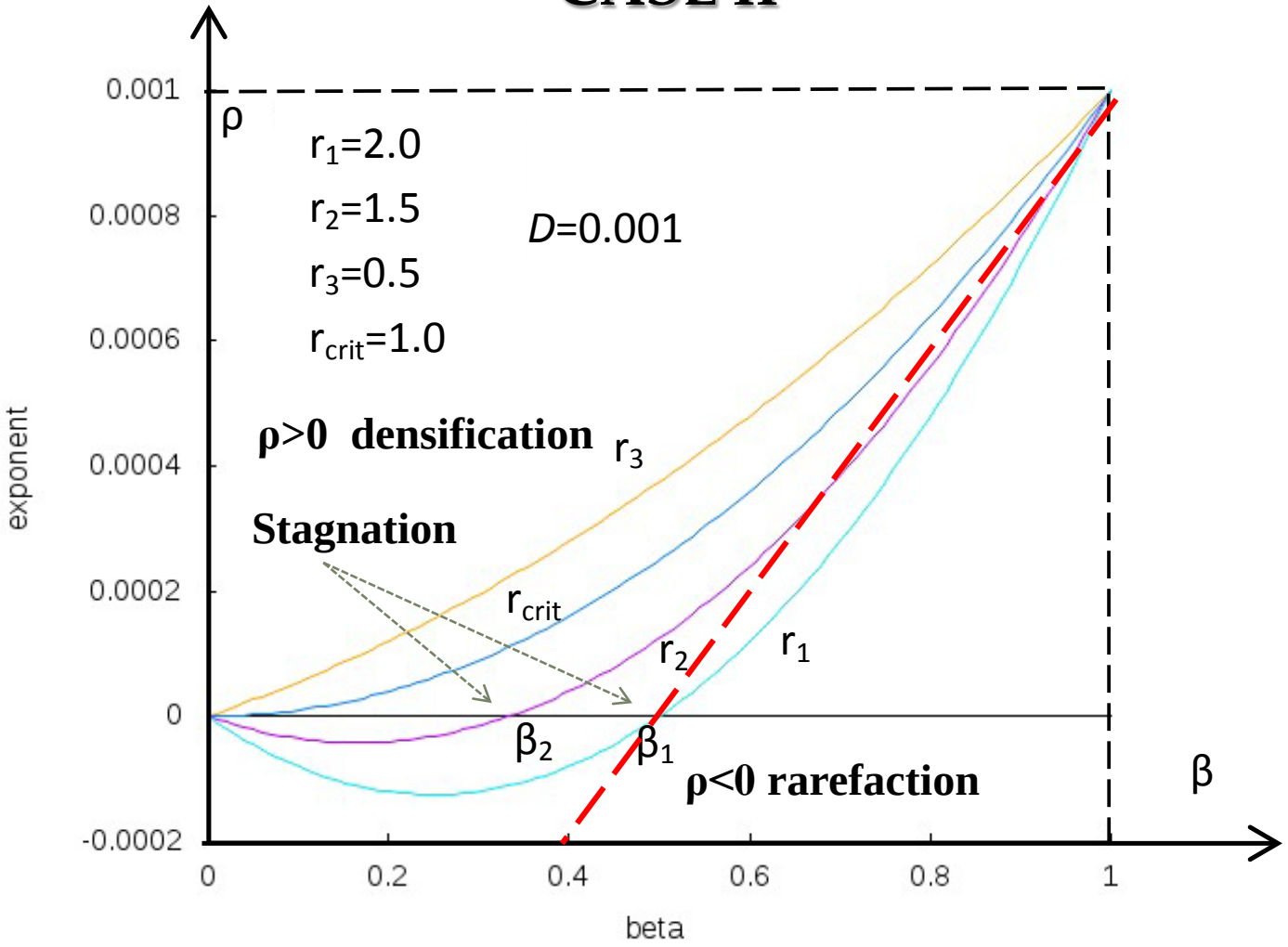
Solution

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

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

r=R/D

SIMPLE PROBLEMS-CLOSED SOLUTIONS
CASE II



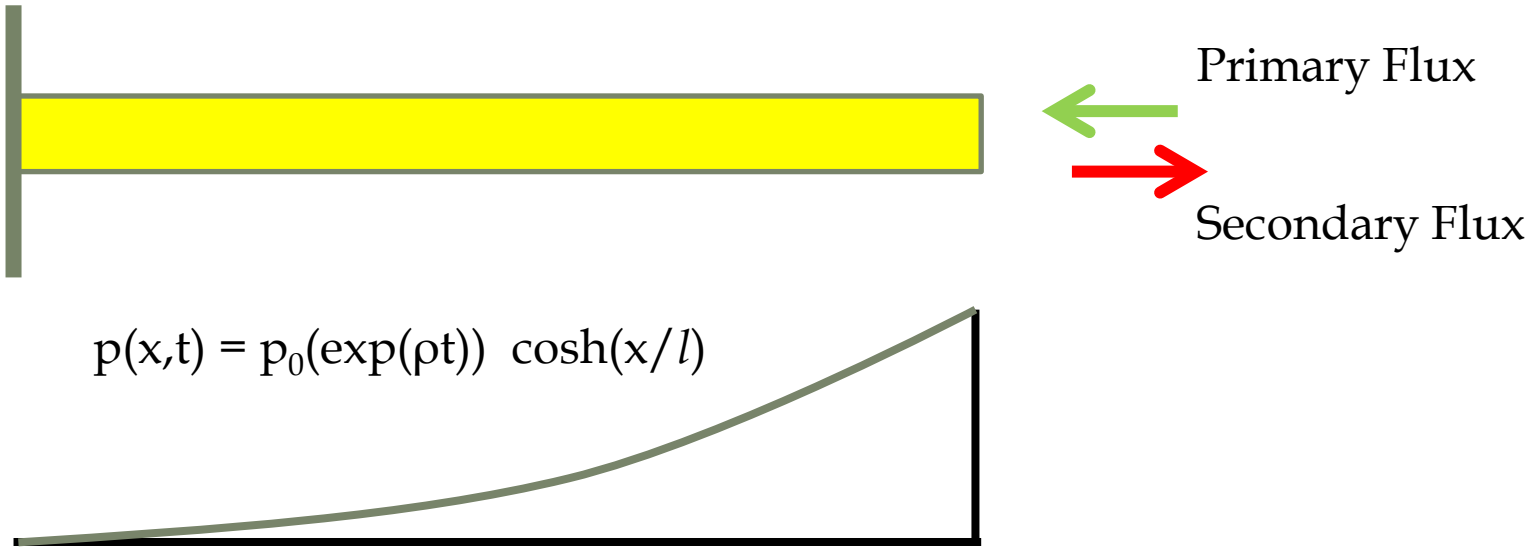
A Model for the Knowledge Transfer in a Production Chain

$$Cp_t = \beta D p_{xx} - \beta(1-\beta) R p_{xxxx} + Bp$$

C: Cognitive Impedance
D: Knowledge Permeability
B: Creativity
R: Knowledge Retention

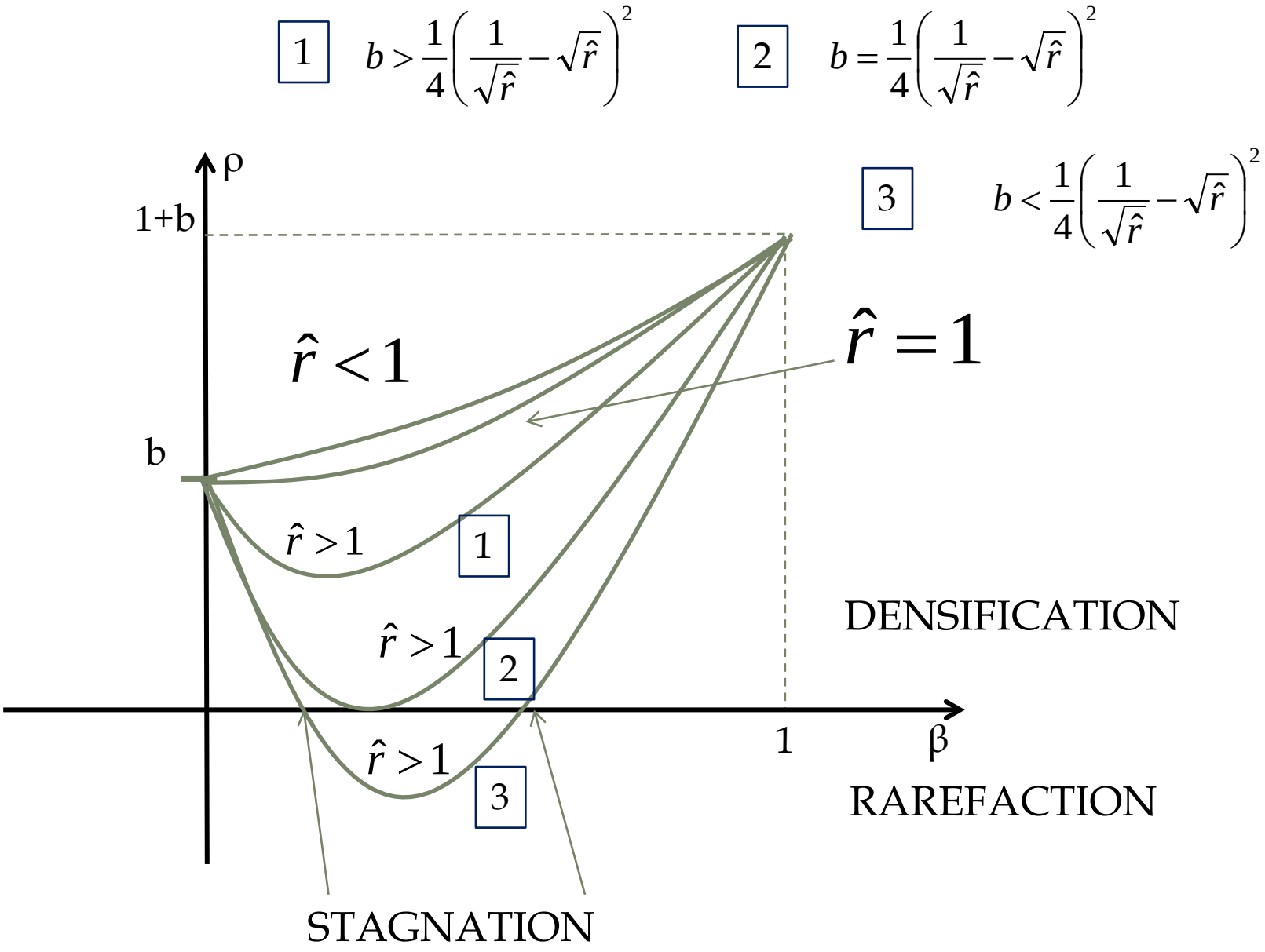
$$q_\tau = \beta q_{\xi\xi} - \hat{r}\beta(1-\beta) q_{\xi\xi\xi\xi} + bq$$

$$\tau = \frac{D}{Cl^2} t \qquad \hat{r} = \frac{R}{Dl^2} \qquad b = \frac{B}{D} l^2 \qquad \xi = \frac{x}{l} \qquad q = \frac{D}{l^2} p$$



Using the new variables: $q = q_0 e^{\rho t} \cosh(\xi)$

$$\rho = \beta - \hat{r}\beta(1-\beta) + b$$


1
$b > \frac{1}{4}\left(\frac{1}{\sqrt{\hat{r}}} - \sqrt{\hat{r}}\right)^2$
2
$b = \frac{1}{4}\left(\frac{1}{\sqrt{\hat{r}}} - \sqrt{\hat{r}}\right)^2$
3
$b < \frac{1}{4}\left(\frac{1}{\sqrt{\hat{r}}} - \sqrt{\hat{r}}\right)^2$
ρ
1+b
b
$\hat{r} < 1$
$\hat{r} = 1$
$\hat{r} > 1$
1
$\hat{r} > 1$
2
$\hat{r} > 1$
3
1
β
DENSIFICATION
RAREFACTION
STAGNATION

Results:

For a small retention, or very high diffusion, or for a long knowledge chain,
($\hat{r}<1$ or $\hat{r}=1$), densification will always occur.
Under these conditions, for any value of β, the secondary flux is smaller
than the primary flux.

For a very high retention, or a very small diffusion, or a very short knowledge chain,
rarefaction could occur in some situations (case 3).
To avoid rarefaction, (knowledge chain collapse possibility),
the creativity b must be high.

THE GENERALIZED MULTI-FLUX PROCESSES

The two sets of particles or bi-flux theory can be generalized to a large sequence of nested kinematical energy sets of particles or multi-flux diffusion phenomena. Indeed, let us assume the existence of m nested excitation states $\{\mathcal{E}_1,\mathcal{E}_2, \ldots \mathcal{E}_m\}$. Let β_i be the fraction of mass belonging to the excitation state $\mathcal{E}_i$ (i=1,2…m). Since all the particles in the system must be in some excitation state, clearly : $\beta_1 + \beta_2 + ... + \beta_m = 1$

Assume that the generalized rate of mass flow is given by:

$$\Psi_1 = -D_1 \frac{\partial p}{\partial x} \vec{e}_1$$

$$\Psi_n = (-1)^n \left(\prod_{i=1}^{n-1} (\beta_i) \right) \left(D_n \frac{\partial^{2n-1} p}{\partial x^{2n-1}} \vec{e}_1 \right) \qquad (\mathrm{n} = 2...\mathrm{m})$$

For homogeneous media the mass conservation principle leads to the generalized governing equation:

$$\frac{\partial p}{\partial t} + \sum_{n=1}^{m} (-1)^n \left(\prod_{i=1}^{n} (\beta_i) \right) \left(D_n \frac{\partial^{2n} p}{\partial x^{2n}} \right) = 0$$

Remark: for n>1, ε_n exists if and only if ε_{n-1} exists

For 3 different fluxes:

$$\frac{\partial p}{\partial t} - \beta_1 D_1 \frac{\partial^2 p}{\partial x^2} + \beta_1 \beta_2 D_2 \frac{\partial^4 p}{\partial x^4} - \beta_1 \beta_2 (1 - \beta_1 - \beta_2) D_3 \frac{\partial^6 p}{\partial x^6} = 0$$

This multi-flux approach may be useful to represent diffusion processes in a complex flow. Particularly, if the parameters D_n and β_n are taken as stochastic variables it would be possible to develop a kind of turbulent diffusion theory, although very much complex.

CONCLUSIONS

- The derivation of the governing equation for diffusion with retention obtained from the discrete approach has shown unequivocally that a fourth order partial differential term is required together with a control parameter β representing the fraction of diffuse particles following the classical Fick's law.
- The velocity of the particles belonging to the complementary fraction $(1-\beta)$ has to be governed by a new law that according to the analytical derivation is proportional to the third derivative of the concentration multiplied by β which is consistent with the physical meaning of a disturbance effect on the classical diffusion process.
- Retention is not a theoretical hypothesis, there are a considerable number of reports demonstrating that retention is an observable phenomenon. Several of these reports do not mention capture of particles, that is, the existence of sinks to explain the delay. Therefore it is expected that the retention phenomenon is due to some disturbance that delays the motion of a fraction of the particles.

CONCLUSIONS

- As shown above the solutions depend strongly on the parameters r and β. It is also presumably possible the existence of a functional relation $F(r,\beta) = 0$ characterizing physic-chemistry interactions. For these cases it is not possible to assign values of β independently of r. Physic-chemistry reaction may not allow for external control but may depend on random factors in which case the fraction β may well be a stochastic variable.
- On the other hand if we are dealing with a class of problems that allows for external control, like invading populations, spreading of contagious diseases, capital flow, knowledge transfer and other similar evolutionary processes, the combination of r and β may be adjusted to obtain a predetermined behavior.

CONCLUSIONS

- Experimental research
- Thermodynamic coupling – Energy conservation
- Energy transport – Heat conduction
- Population dynamics
- How β varies with r. Dependence on the entropy $\beta=\beta(s)$
- Mathematical analysis (PDE)
- How can disturbance effects be induced in the system
- Control of the diffusing (delayed) fraction
- Mpemba effect and other odd behaviors
- Coupling with vortex motion (3-d)
- Particle dynamics
- Application to other problems of mass –energy transfer

BASIC REFERENCES

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[2] Bevilacqua L, Galeão, A, Costa, F P, 2011, *A New Analytical Formulation Of Retention Effects On Particle Diffusion Processes***,** Proceedings of the Brazilian Academy of Sciences, 83(4), 1-22.

[3] Galeão, A.C., Bevilacqua, L., Delphin, S., Costa, F. P., *A Numerical Solution of the Diffusion-Retention Problem in Homogeneous Media,* Proceedings ENCIT, 2010.

[4] Bevilacqua, L. Galeão, A.C.N.R., *A Bi-Velocity Approach for Diffusion Processes Subjected to Retention Effects,* XXIII ICTAM, Beijing, China, 2012. (aceito para publicação).

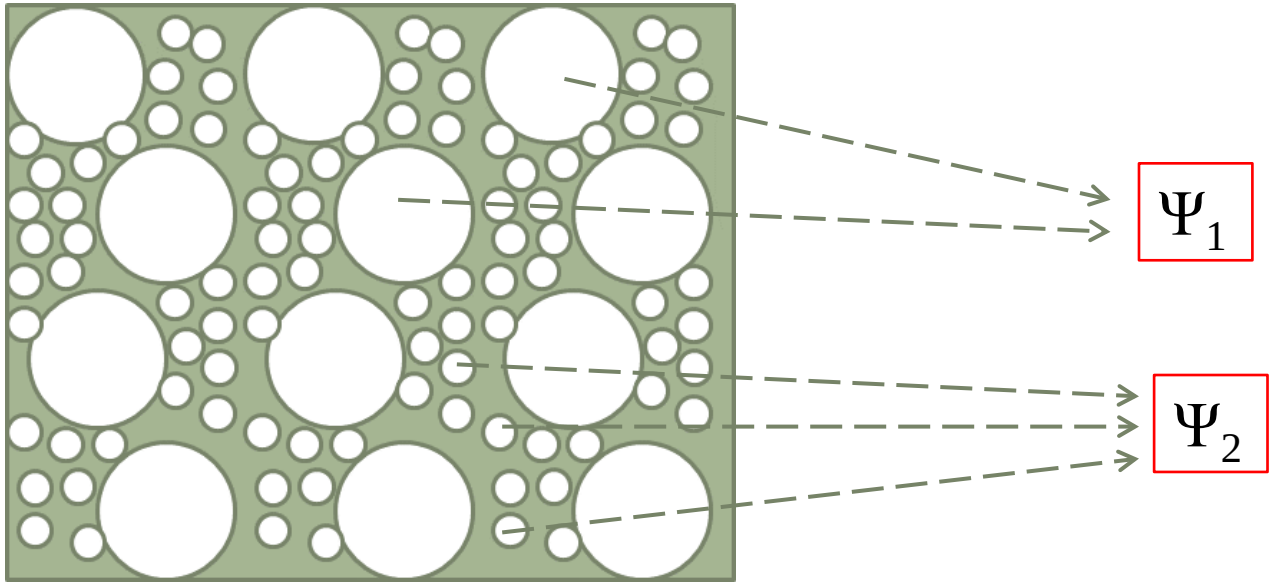
[5] Delphin, S., Galeão, A.C., Bevilacqua, L., *Modelling Establishment Processes of Biological Invasions.* Abstracts of MMA 2011, Sigulda, Latvia,2011.

[6] Bevilacqua, L. Galeão, A.C.N.R, *Derivation of the Equation of Mass Transfer with Retention and the Korteweg Devries Equation.*Proceedings COBEM 2011.

THANKS FOR THE ATTENTION

ILLUSTRATION OF A POSSIBLE BI-FLUX ADJUSTED MEDIUM

Particles may diffuse through the tubes with different diameters with two different flow speed. In any case the secondary flux only will be triggered if the primary flux is active.



STEADY STATE SOLUTION

For the steady condition the total flux must be constant:

$$\beta\Psi_1 + (1-\beta)\Psi_2 = C \rightarrow const.$$

With the primary and secondary flux laws we get

$$\beta\left(-D\frac{\partial p}{\partial x}\right) + (1-\beta)\left(\beta R\frac{\partial^3 p}{\partial x^3}\right) = C$$

For a homogeneous medium we have after integration

$$\frac{\partial^2 p}{\partial x^2} - \frac{D}{(1-\beta)R}\,p = C_1 x + C_2$$

With C_1 and C_2 equal zero:

$$p = A\exp\left(\sqrt{\alpha}\right) + B\exp\left(-\sqrt{\alpha}\right) \qquad \alpha = \frac{1}{r(1-\beta)} \qquad r = \frac{R}{D}$$

THE PHYSICAL COMPATIBILITY OF THE BI-FLUX DIFFUSION EQUATION

Some results seem to be unlikely. No clear physical support or not yet well established theory

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

Except if some external action is imputed on the system it is expected that the following relation holds:

$$R=0 \rightarrow \beta=1$$

The equation derived before requires a side condition.

R and β are independent parameters only if some external action is imposed. Otherwise there must be a functional relation:

$$F(R, \beta)=0$$

THE PHYSICAL COMPATIBILITY OF THE BI-FLUX DIFFUSION EQUATION

As a first approach let us take:

$$R = (1-\beta)R_0$$

$\beta = 1$ only primary flux is present $R = 0$
$\beta = 0$ no flux at all $R = R_0$

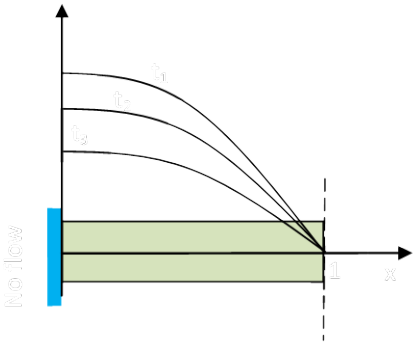
R_0 is a material constant. It is the maximum possible secondary flux coefficient. For $R = R_0$ no flux is possible, particles flow is completely blocked.

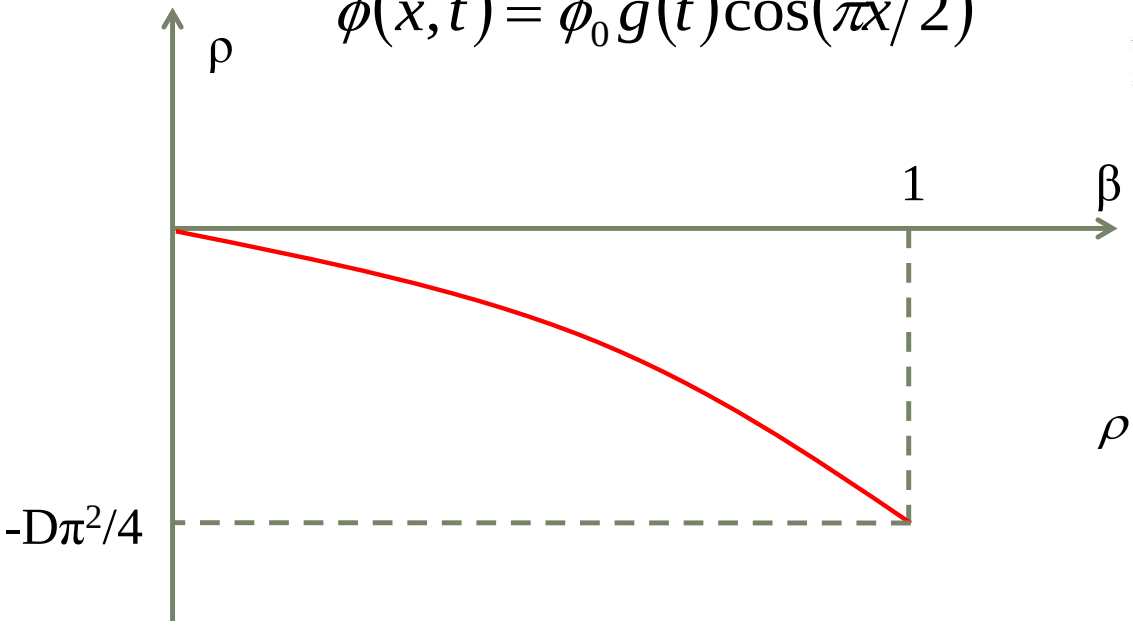
With the hypothesis of a linear dependence between R and β the fundamental equation reads:

$$\frac{\partial \phi}{\partial t} = D\beta \frac{\partial^2 \phi}{\partial x^2} - \beta(1-\beta)^2 R_0 \frac{\partial^4 \phi}{\partial x^4}$$

REVIEW OF PREVIOUS CASES

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





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

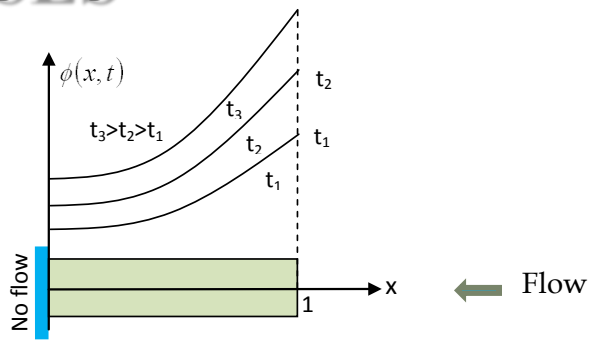
$$\rho = -\frac{\pi^2}{4} D\beta\left(1+\frac{\pi^2}{4} r_0(1-\beta)^2\right)$$

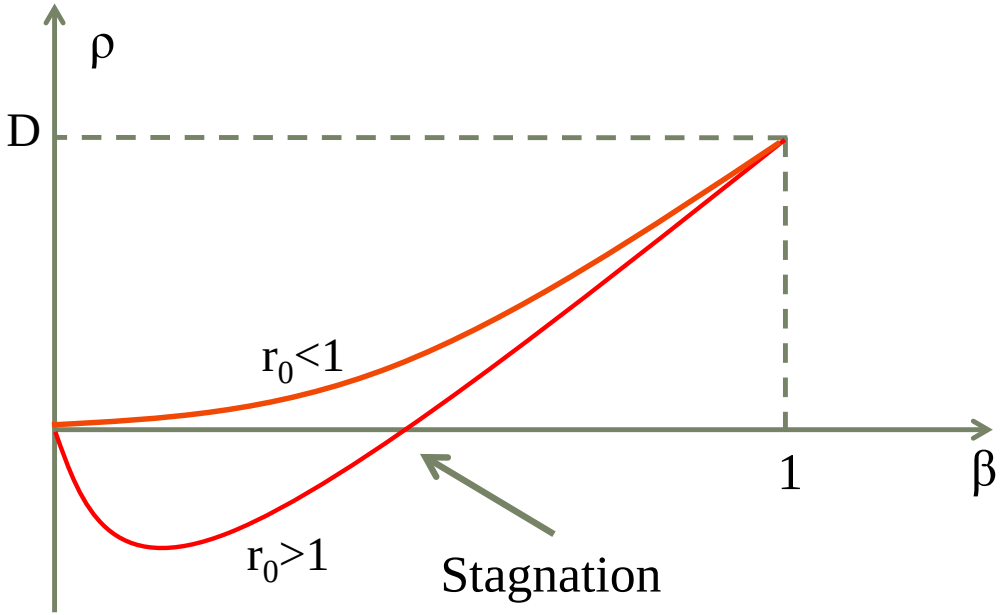
$$r_0 = R_0/D$$

System will be always delayed for $\beta < 1$ irrespectively of the value of r_0.

REVIEW OF PREVIOUS CASES

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



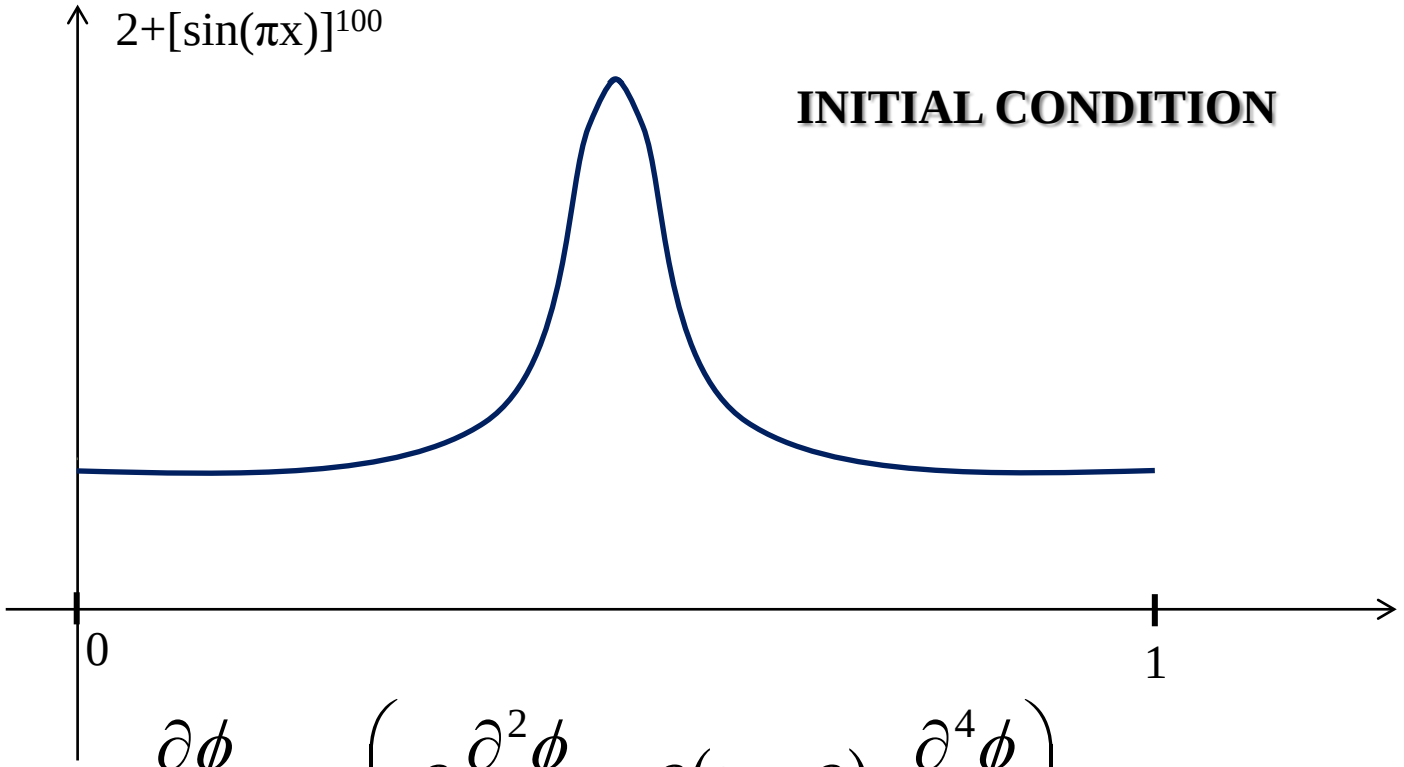


$$\phi(x,t) = \phi_0 e^{\rho t}\cosh(x)$$

$$\rho = D\beta\left(1 - r_0(1-\beta)^2\right)$$

$$r_0 = R_0/D$$

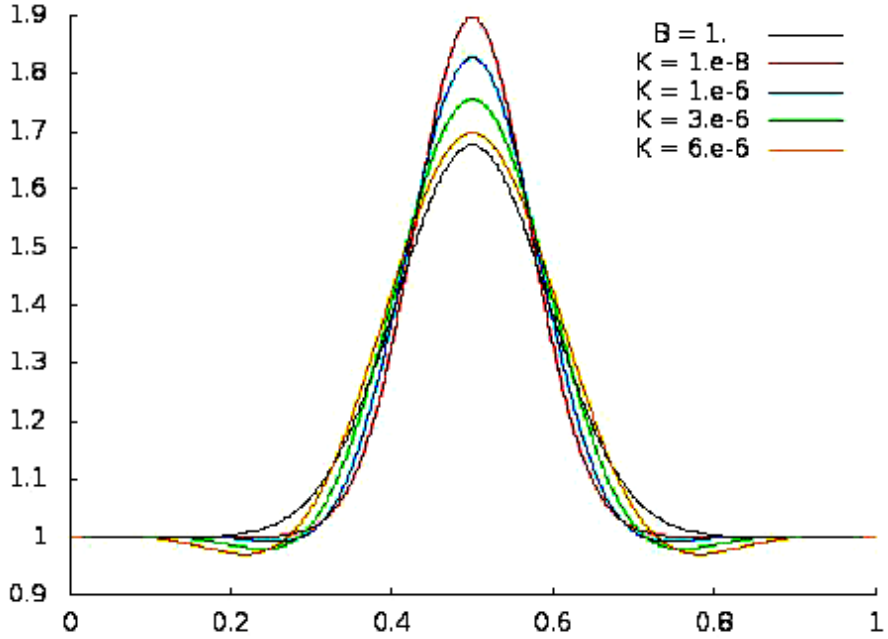
DEPENDENCE OF THE SOLUTION ON THE PARAMETERES β AND r = R/D

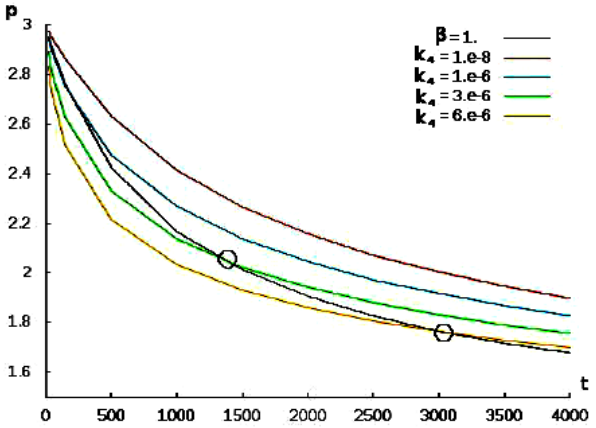


$$\frac{\partial \phi}{\partial t} = D\left(\beta \frac{\partial^2 \phi}{\partial x^2} - \beta(1-\beta) r \frac{\partial^4 \phi}{\partial x^4} \right)$$

K_4 =1x10^{-8}, 1x10^{-6}, 3x10^{-6}, 6x10^{-6}, $K_2 = 10^{-3}$ D ≡K_2 R ≡K_4

β= 1.0, β= 0,5





Time = 4000Δt

ELEMENTARY BOUNDARY CONDITIONS

The first two boundary conditions are classical.
The first boundary condition is the concentration level at the boundary that is:

$$p(\hat{x},t) = p_0(t)$$

The concentration gradient at the boundary gives the second boundary condition.

$$\Psi_I = -D\frac{\partial p(\hat{x},t)}{\partial x} = \phi_D(t) \quad \Rightarrow \quad \frac{\partial p(\hat{x},t)}{\partial x} = -\frac{\phi_D(t)}{D}$$

ELEMENTARY BOUNDARY CONDITIONS

Considering the fourth boundary condition and from the previous definitions we have:

$$\frac{\partial^3 p(\hat{x},t)}{\partial x^3} = \frac{\phi_R(t)}{\beta RD}$$

The governing equation reads:

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

Now for β small or close to one $\beta(1\text{-}\beta)RD \ll 1$ from which follows:

$$\frac{\partial^2 p(\bar{x},t)}{\partial x^2} \approx \frac{1}{\beta D}\frac{\partial p(\bar{x},t)}{\partial t}$$

ELEMENTARY BOUNDARY CONDITIONS

From the fourth boundary condition

$$\frac{\partial^3 p(\hat{x},t)}{\partial x^3} = \frac{\phi_R(t)}{\beta RD}$$

And with

$$\frac{\partial^2 p(\hat{x},t)}{\partial x^2} \approx \frac{1}{\beta D}\frac{\partial p(\hat{x},t)}{\partial t}$$

We have

$$\frac{\partial^3 p(\hat{x},t)}{\partial x^3} = \frac{\beta}{D}\frac{\partial}{\partial x}\left(\frac{\partial p(\hat{x},t)}{\partial t}\right)$$

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 : $grad(p_0(t))$

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

The gradient of the time variation of the concentration : $grad(\partial p_0(t)/\partial t)$