CHAOS AND SELF-STRUCTURING BEHAVIORS IN LUNG AIRWAYS

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In the framework of the Scale Relativity Theory with fractal arbitrary constant, a numerical simulations of aerosol dynamics in the lung is obtained. As a result, chaoticity and self-structuring can be observed in the aerosol dynamics. Moreover, a Kelvin-Taylor type effect appears at the aerosol colony periphery.

Keywords: aerosol dynamics**,** aerosol colonies, Scale Relativity Theory, chaoticity, self-structuring, respiratory diseases, aerosolotherapy

1. Introduction

Although aerosol depositions in the lungs are often looked upon in the context of industrial hygiene, aerosols also play an important clinical role. Three principal mechanisms (inertial impaction, gravitational sedimentation and Brownian diffusion) account for the majority of aerosols deposition in the lungs. Deposition depends upon the mode of inhalation, the nature of the particles and the physical characteristics of the subject inhaling these particles. Radioaerosols are widely employed in measurements of total and regional deposition, and topographical distribution may also be determined. Aerosols play an important role in the treatment of various forms of respiratory diseases, those with the bronchodilators, anti-inflammatories and antibiotics for the therapy of bronchial asthma, COPD, bronchiectasis etc. being particularly important. On average only 10% of the therapeutic aerosols dose actually reaches the lungs. The rate of removal of insoluble radioaerosols deposited in the lungs may be used as an index of mucociliary transport. Aerosols are also used in a variety of other diagnostic and research procedures, particularly for ventilation scanning, alveolar clearance, measurement of alveolar permeability, and for measuring the size of pulmonary air spaces [1][2].

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The size, mode and flow rate of the particles of drugs administered by aerosols way are very important in the treatment of the acute respiratory diseases and, especially, of the chronic inflammatory diseases, which are found worldwide among the people of all ages. The aerosol administration of drugs for respiratory diseases is one of the basic methods of pulmonary rehabilitation. The inhalator way of the drugs administration in the treatment of respiratory diseases is more advantageous than oral or parenteral administration because it allows selective treatment of the respiratory tract by pulmonary local action and by acquiring higher drug concentration in the lung, and simultaneously by decreasing the risk of occurrence of side effects due to the low level of drug in the blood [1][2].

Molecular biology is driving scientists to the innermost reaches of the aerosol's ultimate mechanisms, complexity, and capacity to evolve. Moreover, advances in Mathematics, Physics, Chemistry, and Biology are showing how far–reaching the powers of self–organization can be. These advances hold implications for the origin of life itself and for the origins of order in the ontogeny of every organism. Rather than the consequence of natural selection alone, the order inherent in the great complexity within the aerosols may be largely self–organized and spontaneous [3]. As a consequence, the lung morphology (structure) and functionality by means of aerosol dynamics can be assymilated to a complex system.

A fundamental property of complex systems is that of emergence, which can be thought of as a new property or behavior, which appears due to non–linear interactions within the system; emergence may be considered the 'product' or by–product of the system. Until now, the concept of emergence has been mainly used as an explanatory framework [4], to inform the logic of action research or as a means of exploring the range of emergent potential of simulation of real complex systems [5][6][7][8][9].

In order to underline the connection between emergence and self–organization, one can discuss the features of the four meta–classes–first introduced in McDonald and Weir [10]. Features were considered potential meta–classes if (i) they were generated by non–linear interactions (ii) they were independent with respect to a domain (iii) they were a central building block for system interactions and (iv) their existence causes the open up of a new system potential. Self–organization, which implies detailed organizational structure and new system interactions emergence as a result of the behavior rules of the system entities, is a well known feature of real complex systems. The term self–organization is often used to describe the dynamics of complex systems, emergence or the specific organizational changes brought about through the autonomous entity behavior. Thus, self–organization can be defined as the structural change in a complex system due to nonlinear, possibly noise-generating interaction.

In the present paper we propose a new model for analyzing lung aerosol dynamics, taking into account that the aerosols movement trajectories are continue but non-differentiable curves (fractal curves).

2. Mathematical Model

Let us consider the dissipative approximation of motions on fractal paths. In such context, for irrotational motions of the aerosols that take place in a lung airways matrix,

$$\nabla \times \hat{\boldsymbol{V}} = 0, \quad \nabla \times \boldsymbol{V}_D = 0, \quad \nabla \times \boldsymbol{V}_F = 0\,, \tag{1a-c}$$

we can choose the aerosol's complex velocity $\hat{\boldsymbol{V}}$ of the form [11]

$$\hat{\boldsymbol{V}} = -2i\frac{\lambda^2}{\tau}\left(\frac{dt}{\tau}\right)^{(2/D_F)-1} \nabla \ln\psi = \boldsymbol{V}_D - \boldsymbol{V}_F\,, \tag{2}$$

where $\phi \equiv \ln\psi$ is the complex aerosol's velocity scalar potential. In relation (1) and (2), $\boldsymbol{V}_D$ is the differentiable and scale resolution independent velocity, $\boldsymbol{V}_F$ is the non-differentiable and scale resolution dependent velocity, λ is the spatial resolution scale, τ is the temporal resolution scale, dt is the scale resolution, D_F is the arbitrary constant fractal dimension, and ψ is the wave function. For details on the physical meaning of these quantities, see refs. [12][13][14].

By using the fractal operator of motion from [11] and using the method described in [12][13][14] it results:

$$\frac{\hat{d}\hat{\boldsymbol{V}}}{dt} = \frac{\partial \hat{\boldsymbol{V}}}{\partial t} + \hat{\boldsymbol{V}} \cdot \nabla \hat{\boldsymbol{V}} - i\frac{\lambda^2}{\tau}\left(\frac{dt}{\tau}\right)^{(2/D_F)-1} \Delta \hat{\boldsymbol{V}} = -\nabla U, \tag{3a}$$

or, furthermore

$$\frac{\hat{d}\hat{\boldsymbol{V}}}{dt} = -\frac{\lambda^2}{\tau}\left(\frac{dt}{\tau}\right)^{(2/D_F)-1} \nabla\left[i\frac{\partial \ln\psi}{\partial t} + \frac{\lambda^2}{\tau}\left(\frac{dt}{\tau}\right)^{(2/D_F)-1} \frac{\Delta\psi}{\psi}\right] = -\nabla U \tag{3b}$$

where U is the external scalar potential. The equation (3b) can be integrated, yielding:

$$\frac{\lambda^4}{\tau^2}\left(\frac{dt}{\tau}\right)^{(4/D_F)-2} \Delta\psi + i\frac{\lambda^4}{\tau^2}\left(\frac{dt}{\tau}\right)^{(4/D_F)-2} \frac{\partial\psi}{\partial t} - \frac{U}{2}\psi = 0\,. \tag{4}$$

up to an arbitrary phase factor which may be set to zero by a suitable choice of the phase of ψ. Relation (4) is a Schrödinger type equation.

For $\psi = \sqrt{\rho}e^{iS}$, with $\sqrt{\rho}$ the amplitude and S the phase of ψ, the complex velocity field (2) takes the explicit form:

$$\hat{\boldsymbol{V}} = 2\frac{\lambda^2}{\tau}\left(\frac{dt}{\tau}\right)^{(2/D_F)-1}\nabla S - i\frac{\lambda^2}{\tau}\left(\frac{dt}{\tau}\right)^{(2/D_F)-1}\nabla \ln\rho\,,$$

$$\boldsymbol{V}_D = 2\frac{\lambda^2}{\tau}\left(\frac{dt}{\tau}\right)^{(2/D_F)-1}\nabla S\,, \boldsymbol{V}_F = \frac{\lambda^2}{\tau}\left(\frac{dt}{\tau}\right)^{(2/D_F)-1}\nabla \ln\rho\,. \tag{5}$$

By substituting (5) in (3a), and separating the real and the imaginary parts, up to an arbitrary phase factor which may be set at zero by a suitable choice of the phase of ψ , we obtain:

$$\frac{\partial \boldsymbol{V}_D}{\partial t} + \left(\boldsymbol{V}_D\cdot\nabla\right)\boldsymbol{V}_D = -\nabla\left(Q+U\right),$$

$$\frac{\partial \rho}{\partial t} + \nabla\cdot\left(\rho\boldsymbol{V}_D\right) = 0\,, \tag{6}$$

with Q the specific aerosol's fractal potential

$$Q = -2\frac{\lambda^4}{\tau^2}\left(\frac{dt}{\tau}\right)^{(4/D_F)-2}\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}} = -\frac{\boldsymbol{V}_F^2}{2} - \frac{\lambda^2}{\tau}\left(\frac{dt}{\tau}\right)^{(2/D_F)-1}\nabla\cdot\boldsymbol{V}_F \tag{7}$$

The first equation (6) represents the conservation law of aerosol momentum, while the second equation (6) represents the conservation law of aerosol probability density. Through the aerosol fractal velocity field, $\boldsymbol{V}_F$, the specific aerosol fractal potential Q is a measure of non-differentiability of the aerosols trajectories, *i.e.* of their chaoticity. Therefore the equations (6) with (7) define the aerosol fractal hydrodynamic model (CFHM).

Since the position vector of the aerosol is assimilated with a stochastic process of Wiener type (for details see [15][16], ψ is not only the aerosol scalar potential of a aerosol complex velocity (through $\ln\psi$) in the frame of aerosol fractal hydrodynamics, but also aerosol density of probability (through $|\psi|^2$) in the frame of a aerosol Schrödinger type theory. It results the complementarity of these two formalisms (the formalism of the aerosol fractal hydrodynamics and the one of the aerosol Schrödinger type equation). Moreover, the chaoticity, either through turbulence in the aerosol fractal hydrodynamics approach, either through stochasticization in the aerosol Schrödinger type approach, is generated only by the non – differentiability of the aerosol's movement trajectories in a fractal space.

3. Numerical simulation of the aerosol dynamics process

In the following, using (6) in an axial symmetry we analyze the dynamics of the aerosol, assuming that the aerosol – extraaerosolular medium interaction mimes the dynamics of a barotropic type fluid [17]. Thus, we can choose

$\sigma_{il} = \rho c^2 \delta_{il}$, where ρ is the aerosol density, c is a characteristic grow velocity of the aerosol and δ_{il} is the Kronecker symbol. The presence of an external perturbation in the form of extraaerosolular medium is specified only by adequate initial and boundary conditions (e.g. spatio-temporal Gaussian). In this situation, let us introduce the normalized coordinates

$$\omega t = \tau, kr = \xi, kz = \eta, \frac{V_{Dr} k}{\omega} = V_\xi, \frac{V_{Dz} k}{\omega} = V_\eta, \frac{\rho}{\rho_0} = N, \tag{8}$$

and by admitting the adiabatic expansion, equations (6) and (7) become:

$$\begin{gathered} \frac{\partial N}{\partial \tau} + \frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi N V_\xi\right) + \frac{\partial}{\partial \eta}\left(N V_\eta\right) = 0, \\ \frac{\partial}{\partial \tau}\left(N V_\xi\right) + \frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi N V_\xi^2\right) + \frac{\partial}{\partial \eta}\left(N V_\xi V_\eta\right) = -N^{\gamma-1}\frac{\partial N}{\partial \xi}, \\ \frac{\partial}{\partial \tau}\left(N V_\eta\right) + \frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi N V_\xi V_\eta\right) + \frac{\partial}{\partial \eta}\left(N V_\eta^2\right) = -N^{\gamma-1}\frac{\partial N}{\partial \eta}. \end{gathered} \tag{9}$$

For numerical integration we shall impose the initial conditions:

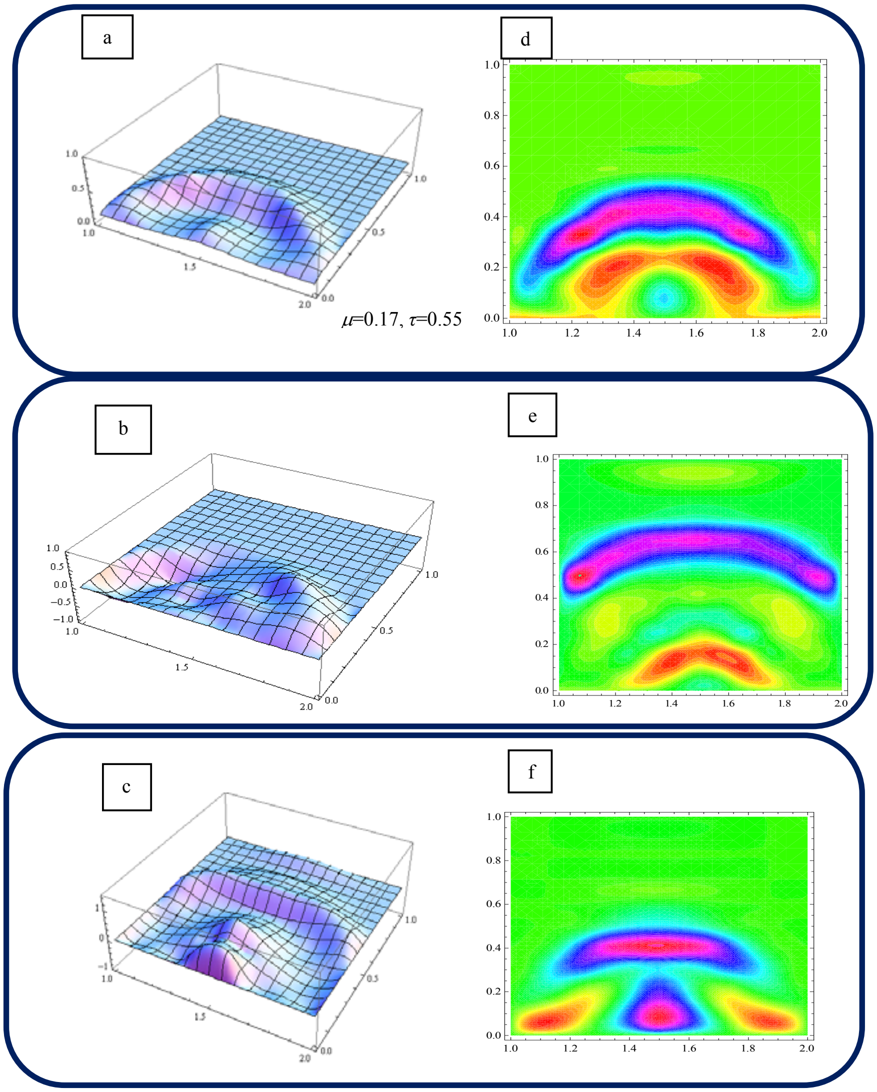
$$V_\xi\left(0,\xi,\eta\right) = 0, V_\eta\left(0,\xi,\eta\right) = 0, N\left(0,\xi,\eta\right) = \frac{1}{5}, 1 \le \xi \le 2, 0 \le \eta \le 1, \tag{10}$$

and the boundary ones:

$$\begin{gathered} V_\xi\left(\tau,1,\eta\right) = 0,\ V_\xi\left(\tau,2,\eta\right) = 0,\ V_\eta\left(\tau,1,\eta\right) = 0,\ V_\eta\left(\tau,2,\eta\right) = 0, \\ N\left(\tau,1,\eta\right) = \frac{1}{5},\ N\left(\tau,2,\eta\right) = \frac{1}{5},\ V_\xi\left(\tau,\xi,0\right) = 0,\ V_\xi\left(\tau,\xi,1\right) = 0, \\ V_\eta\left(\tau,\xi,0\right) = 0,\ V_\eta\left(\tau,\xi,1\right) = 0, \\ N\left(\tau,\xi,0\right) = \frac{1}{10\mu}\exp\left[-\left(\frac{\tau - \frac{1}{5}}{\frac{1}{5}}\right)^2\right]\cdot\exp\left[-\left(\frac{\xi - \frac{3}{2}}{\mu}\right)^2\right], N\left(\tau,\xi,1\right) = \frac{1}{5} \end{gathered} \tag{11}$$

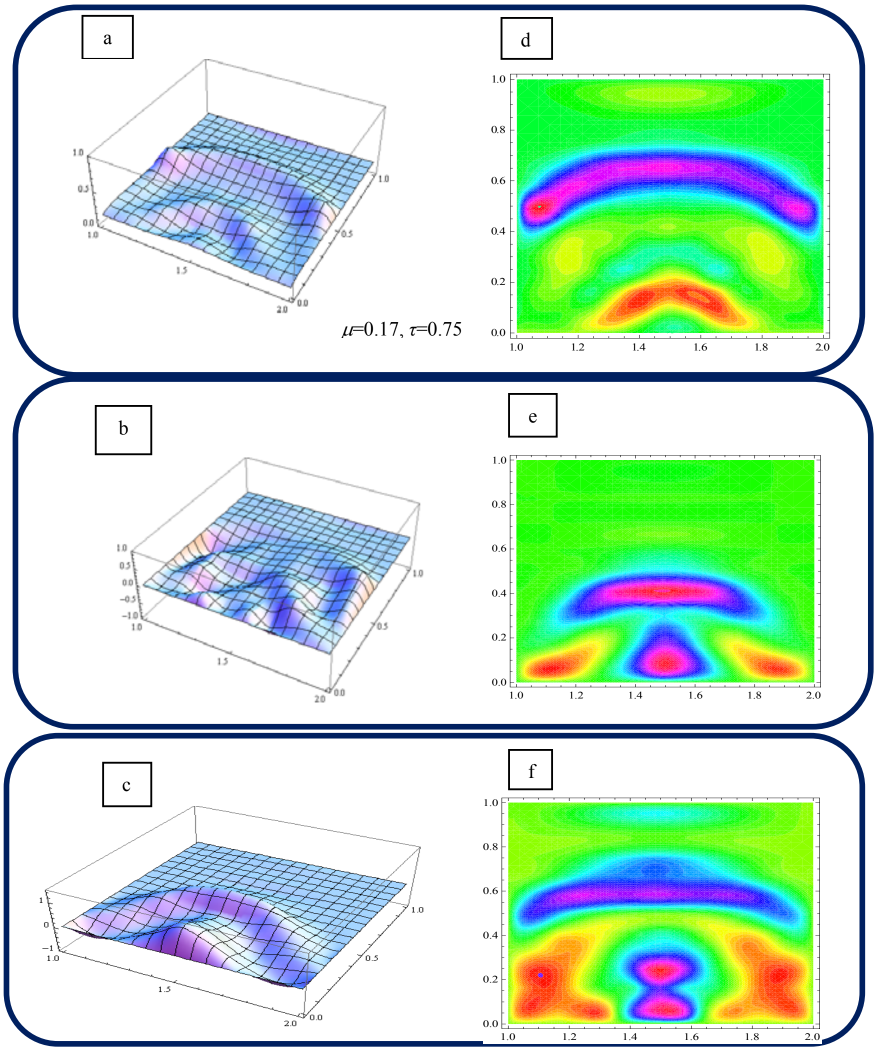
where ω is aerosol specific pulsation, k is the inverse of a aerosol specific length and ρ_0 is the aerosol equilibrium density.

The system (9) with the initial conditions (10) and the boundary ones (11) was numerically integrated using finite differences [18].



Figs. 1a-f. Three dimensional dependences of the normalized aerosol density field N, normalized aerosol velocities fields, V_ξ and V_η, on the normalized coordinates, ξ and η for the normalized time $\tau = 0.55$ and $\mu = 0.17$ (a, b, c); two dimensional contour of the normalized aerosol density field N, normalized aerosol velocities fields, V_ξ and V_η, for the same τ and μ (d, e, f).

In Figures 1a-f and 2a-f the dynamics of the normalized aerosol density field N and normalized aerosol velocities fields V_ξ and V_η , respectively, are plotted for the normalized time $\tau = 0.55$, respectively $\tau = 0.75$ for $\mu = 0.17$ (three dimensional and contour plot evolutions). The followings features of the aerosol expansion process result: i) the generation of two aerosol structures (see the dynamics from Figures 1a,d and 2a,d); ii) the symmetry of the aerosol normalized velocity field V_ξ with respect to the symmetry axis of the spatial-temporal Gaussian (see the dynamics from Figures 1b,e and 2b,e); iii) aerosol shock waves and aerosol vortices at the aerosol colony periphery for the aerosol normalized speed field V_η (see the dynamics from Figures 1c,f and 2c,f).



Figs. 2a-f. Three dimensional dependences of the normalized aerosol density field N, normalized aerosol velocities fields, V_ξ and V_η, on the normalized coordinates, ξ and η for the normalized time τ = 0.75 and μ = 0.17 (a, b, c); two dimensional contour of the normalized aerosol density field N, normalized aerosol velocities fields, V_ξ and V_η, for the same τ and μ (d, e, f).

4. Conclusions

In the fractal hydrodynamic frame of the Scale Relativity Theory with arbitrary constant fractal dimension, the lung aerosol dynamics are analyzed. Thus, using a numerical simulation of the aerosol dynamics process, both their chaoticity and self-structuring result. Moreover, a Taylor type effect can appear at the lung airways periphery, thus affecting the endothelium.

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