SIGNIFICANCE OF THE MICROFLUIDIC CONCEPTS FOR THE IMPROVEMENT OF MACROSCOPIC MODELS OF TRANSPORT PHENOMENA

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Abstract Complexity of transport phenomena - ranging from macroscopic motion of matter, heat transfer, over to the molecular motions determining the overall flow properties of fluids, or generally aggregation states of matter – inhibited development of a single mathematical model describing simultaneously transport processes at all relevant scales. In classical engineering sciences at each scale level we have different equations, different fundamental variables and different methods of solution [4]. The established basis of the classical fluid dynamics – the Navier-Stokes equations [1, 3] - have apparently nothing in common with molecular physics. At the macroscopic scale of motion the molecular structure of matter and the microscopic molecular motions are ignored (even though they determine the local macroscopic behaviour) [1, 3, 4]. To describe multiphase flows, still other methods must be used – increasing further the number of equations, methods of solution etc. The serious disadvantage of this approach is, that equations describing macroscopic models (Navier-Stokes and there from derived equations), introduce multiple theoretical problems:

- higher order continuity requirements [3],

- numerous paradoxes in simple macroscopic flows (Bernoulli eq.),

- different equations with different fundamental variables and different methods of solution, build a set of disciplines devoted in principle to a single problem – dynamics of disperse systems.

Keywords: dynamics of disperse systems, single- and multiphase flows, interdisciplinary education

1. Introduction

Purpose of this work is mathematical model aiming at the broadest possible range of micro- and macroscopic transport phenomena with help of a minimum of basic concepts of corpuscular physics [2, 3]. This paper presents the created transparent and simple model of transport related phenomena designed to facilitate interdisciplinary education. It may be used to derive practically all basic equations describing phenomena caused by motion of matter understood as disperse system built of particles characterized by mass and velocity (momentum). The possible range of engineering applications starts with motion of elementary particles [2, 3], heat flow and generation, classical single and multiphase flows over to applications in non-relativistic astrophysics [7 - 12]. The difference between

the proposed method and classical methods of fluid mechanics [4] - is the applicability of a single, very limited set of basic concepts and equations to the possibly broadest range of phenomena. Thereby, elements of Statistical Physics [2], respectively of Microscopic Fluidics are applied to motion of particle systems under influence of forces defined by observed changes of the state of motion [7 - 13]. Model used in this work applies directly Newton 's second law [7 - 13]and conservation laws [1] to motion of matter understood as a disperse system [2, 3, 5 - 12]. Newton's law and relevant conservation laws define forces and bulk physical quantities of flowing systems as result of particle properties and interactions at considered micro scales and originate all resulting equations for practical application. Results show, that: the differential - integral formulation of Newton's second law and conservation laws provides a transparent common physical background of motion related phenomena across all technically relevant application scales.

2. Theoretical foundations

Newton's law used to define individually the possible interaction forces reads [11, 12]:

$$\underline{\mathbf{F}} = \frac{\mathrm{d}}{\mathrm{d}\,\mathrm{t}} \int_{\mathbf{V}} \rho \,\underline{\mathbf{v}} \,\mathrm{d}\mathbf{V} \tag{1}$$

The right side of the above equation represents the total time rate of change of momentum in Volume V (i.e. mass times acceleration = m <u>a</u>) in terms of the velocities <u>v</u> of volumes dV with density ρ within the time (t) interval dt. Vectors are marked by underlining. Thereby, critical for all derivations is, that: **time rate of momentum change defining the relevant forces** <u>F</u> **may be expressed in terms of momentum conservation [7-12]:**

$$\underline{F} = \frac{d}{dt} \int_{V} \rho \underline{v} dV = \frac{\partial}{\partial t} \int_{V} \rho \underline{v} dV + \int_{A} (\rho \underline{v}) \underline{v} \bullet \underline{dA}$$
(2)

Thereby A denotes the considered control surfaces, or their oriented (vector) elements dA. The above two equations define the particle-particle interaction forces (Applications of (1) below, [11, 12]). Result of application of eqs. (1) and (2) written in a form suitable to describe the macroscopic flow phenomena in process engineering applications reads [7 - 12]:

$$\frac{d}{dt} \int_{V} \rho \underline{v} dV = \int_{V} \rho \underline{g} dV - \int_{A} p \underline{dA} + \int_{A} \underline{t}(\eta) \bullet \underline{dA}$$
(3)

The forces <u>F</u> on the right side of (3) are identified as [11, 12]: gravity **g**, pressure p, friction <u>t</u> etc. acting in V and, respectively, on its limiting surfaces A. The double underlining denotes the considered term (here <u>t</u>) as tensor of second order. Thereby the so called "fluid quantities" are understood as result of averaged application of Newton's law eq. (1) and momentum conservation law eq. (2) to micro scale particle systems (fluid). Thus the statistical "fluid quantities" like density ρ , pressure p and friction \underline{t} (represented as function of the dynamical viscosity η), are all defined at the micro scale by molecular numbers, masses, volumes, average collision free paths etc. [2, 3, 7 - 13]. In compliance with this understanding "fluid quantities" like pressures p (similarly also the viscosity η) and such macroscopic equivalents as "body forces" are specialized representations of the averaged molecule impact forces. Mass conservation law used together with eqs. (1, 2, 3) reads [1, 13]:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbf{V}} \rho \, \mathrm{d}\mathbf{V} = \frac{\partial}{\partial t} \int_{\mathbf{V}} \rho \, \mathrm{d}\mathbf{V} + \int_{\mathbf{A}} \rho \, \underline{\mathbf{v}} \bullet \underline{\mathrm{d}\mathbf{A}} \tag{4}$$

Beside eqs. (1-4)the model uses conservation laws of other characteristic physical quantities transported with matter. Thus, e.g. for explanation of heat transfer in a particle system useful is representation of the stochastic, thermal molecule momentum in terms of the quadratic mean value of the thermal molecule velocity \underline{v}_{λ} in volume V along the mean free travelling path λ of the molecules. Using the general structure of the conservation laws as given e.g. in [1] we may write [8 - 13]:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbf{V}} \rho \, \mathbf{v}_{\lambda}^{2} \, \mathrm{d}\mathbf{V} = \frac{\partial}{\partial t} \int_{\mathbf{V}} \rho \, \mathbf{v}_{\lambda}^{2} \, \mathrm{d}\mathbf{V} + \int_{\mathbf{A}} \left(\rho \, \mathbf{v}_{\lambda}^{2} \right) \underline{\mathbf{v}} \bullet \underline{\mathrm{d}\mathbf{A}}$$
(5)

Where v_{λ} represents the thermal molecule velocity along its collision free path λ .

Besides advantages mentioned till now [7, 13] i.e.:

- simplicity combining the elementary school physics with e.g. process engineering (1), (3) [11, 12],
- conciseness and transparency of all above equations (1-5),
- simple application to the analysis of complex disperse (discontinuous) systems [7 13],
- applicability to arbitrary technical or natural material systems [12],
- simple derivation of the practically used parameters and dimensionless numbers [11, 12],

- physically coherent interpretation of the basic measured properties of matter [11, 12],
- analysis of experimental results [13].

The most important advantage of the model is its **ability to avoid paradoxes in practically relevant flows**.

3. Application examples: important advantage of the above model [7 - 13] is its simple applicability to the analysis of disperse systems at multiple scales of resolution. Newton's equation of motion applied to an arbitrary material disperse system defines its physical properties and the involved forces in terms of momentum exchange at particle level [7 - 13] (Fig. 1 below):



Fig. 1: Fluid modelled as a molecular disperse system [7 - 13]. Schematically shown are gas molecules in stochastic thermal motion. Arrows symbolize the thermal molecule velocities.

3.1 Derivations of the involved statistical physical quantities and e.g. of basic equations of continuum mechanics. Definitions of the statistical quantities like pressure, viscosity etc., used in descriptions of macroscopic flows, follow from the analysis of molecular motions in respect to chosen control surfaces A.

Basic examples are:

Thermal gas pressure: eq. (2) with

assumption: $v_{\lambda}(z \pm \lambda) = v_{\lambda}(z)$ results in [11, 12]:

$$p = \rho_{\rm G} v_{\lambda Z}^2 \tag{6}$$

Thermal pressure defines together with the molecular binding forces [12] the melting point of solids and the boiling point of liquids [12]. Result (6) shows in particular, that:

Temperature T is just an indicator of the stochastic thermal molecule velocities:

$$T = k v_{\lambda Z}^2$$
(7)

Gas laws: expressing density ρ_G in (6) by molecule numbers and masses in volume V we obtain [11, 12]:

$$\frac{p V}{T} = n_m R = \text{const}$$
(8)

with R representing the universal gas constant [1, 2]: $R\approx 8.314$ J/mol K.

Heat conductivity: from eq. (5), assuming [11, 12] that:

$$v_{\lambda}^{2}(x \pm \lambda) = v_{\lambda}^{2}(x) \pm \lambda \frac{\partial v_{\lambda}^{2}}{\partial x}$$
 (9)

We obtain:
$$\frac{\partial \Theta_{\rm C}}{\partial t}\Big|_{V_{\rm R}} = \frac{\partial}{\partial t} \int_{V_{\rm R}} \rho_{\rm G} v_{\lambda}^2 \, dV =$$

= $-\rho_{\rm G} v_{(\lambda x)} \lambda \frac{\partial v_{\lambda}^2}{\partial x} A_{\rm x}$ (10)

Where Θ_C is the content of heat momentum in the considered volume V_R of a substance. Thereby, the product: $\rho_G v_{(\lambda x)} \lambda$ defines the coefficient of thermal conductivity [11, 12]:

$$\kappa = \rho_{\mathbf{G}} \, \mathbf{v}_{(\lambda \mathbf{X})} \, \lambda \tag{11}$$

in:

Fourier 's law of heat conductivity [8-12]:

$$\frac{\partial \Theta_C}{\partial t} = -\kappa A_X \frac{\partial T}{\partial x}$$
(12)

(Extension to 3-D space by induction method [7 - 12]). The content of the thermal momentum Θ reads as [11, 12]: $\Delta \Theta = C_S \text{ m } \Delta T$ with C_s – heat capacity and $m = \rho V$ mass of the substance. It follows:

$$C_{s} \rho V \frac{\partial T}{\partial t} = -\kappa A_{x} \frac{\partial T}{\partial x}$$
 (13)

Bernoulli equation [1] requires implementation of simplifying assumptions in eq. (3) to reduce vector quantities to scalars, the derivation will here be omitted. The derived form reads [11, 12]:

$$\rho \frac{v_n^2}{2} + \rho g z_n + p_n =$$

$$= \rho \frac{v_1^2}{2} + \rho g z_1 + p_1 - \Delta P_T - \rho \int_{S_1}^{S_n} \frac{\partial v}{\partial t} ds$$
(14)

Thereby index n denotes the values of the marked quantities as belonging to the n-th point of the streamline containing the 1- st point (index 1), z represents the height in the potential field. Δp_T represents the influence of friction and the last term the influence of accelerations/decelerations along the streamline path s. In practical purposes most frequently used is the reduced form of eq. (14):

$$\rho \frac{v_n^2}{2} + \rho g z_n + p_n = \rho \frac{v_1^2}{2} + \rho g z_1 + p_1 \qquad (15)$$

The consequences of reducing vector quantities in eq. (3) to scalars and use of the form (15) are easily recognizable on example 2.a and 2.b below.

Dynamic viscosity follows accordingly [7 - 13] from eq. (2) for the macroscopic relative shearing motion of fluids at temperatures above absolute zero with assumption (Fig. 2:2 above) that e.g.:

$$v_{x}(z \pm \lambda) = v_{x}(z) \pm \lambda \frac{\partial v_{x}}{\partial z}$$
 (15)

Eq. (2) with inserted assumption (15) defines the statistical average of the friction force as:

$$F_{T,X} = \rho_G v_{\lambda Z} \lambda A_Z \frac{\partial v_X}{\partial Z}$$
(16)

Dynamic viscosity results accordingly as:

$$\eta = \rho_G \, v_{\lambda Z} \, \lambda \tag{17}$$

Navier – Stokes equations follow from eqs. (1), (2), (3) with approximations (15) and other [11, 12], introducing together the higher order continuity requirements of the continuum model [3, 5 -13]. As partial differential equations of second order they

require **double** integration and determination of integration constants [7-13]. Examples of technical calculations point to advantages of the system (1), (2), (3) in comparison with corresponding applications of the Navier – Stokes equations:

3.2 Examples of technical calculations. The following summarizes basic advantages of the model for technical calculations on simplest examples of educational and practical relevance:

Example 1: integral notation of equations based on micro fluidic concepts saves integration steps and makes calculations direct, short and simple [7 - 13] We consider Hagen - Poiseuille flow [1, 8 - 13] i.e. real, macroscopic, steady, laminar, fully developed flow in a pipe of circular cross-section:

Starting point here is the equation of macroscopic motion (3):

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V} \rho \, \underline{v} \, \mathrm{d}V = \int_{V} \rho \, \underline{g} \, \mathrm{d}V - \int_{A} p \, \underline{\mathrm{d}A} + \int_{A} \underline{\underline{t}} \, \bullet \underline{\mathrm{d}A} \, (18)$$

With the involved simplifying assumptions (circular, steady, horizontal, fully developed laminar flow) and the mean value theorem, for components along the flow direction follows:

$$0 = p_1 A_1 - p_2 A_2 + \eta A_W \frac{dv(r)}{dr}$$
(19)

Eq. (19) applied to a cylindrical volume V with radius 0 < r < R and length L and surfaces $A_1 = A_2$ and Aw defined by the proper geometrical relations results in:

$$0 = p_1 \pi r^2 - p_2 \pi r^2 + \eta 2\pi r L \frac{dv(r)}{dr}$$
(20)

Transformation of (20), simplifying, indefinite integration on both sides and determination of the constant C from the boundary condition v(r = R) = 0 results in:

$$v(r) = \frac{p_1 - p_2}{4 \eta L} \left(R^2 - r^2 \right)$$
(21)

The same analysis with help of the Navier-Stokes equations requires many more steps and is much more complex [12].

Example 2: use of the micro fluidic force concept improves at least the plausibility of the theoretically derived macroscopic results in engineering practice: Applying eq. (2):

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to:

a) change of flow direction in a steady, horizontal, frictionless flow from 1 to 2 by an arbitrary angle α shows, that change of direction of flow requires a corresponding force respectively, in terms of macroscopic terminology, the corresponding pressure difference:

$$\Delta p = \rho \, v_1 \, v_1 - \rho \, v_2 \, \cos \, (\alpha) \, v_2 \qquad (22)$$

With p_0 representing the reference pressure of the environment we may define the pressures at the entrance (1) and exit (2) as:

$$p_1 = p_0 + \Delta p$$
 and: $p_2 = p_0 - \Delta p$ (23)

Result (23) follows directly from eq. (3). It does not introduce any paradox and complies with the basic knowledge about the structure of matter. Analysis of the same problem with help of Bernoulli equation (15) is equally simple, but it predicts the pressure difference $\Delta p=0$ implying, that change of direction of motion requires neither force nor energy. From the point of view of school physics this is a paradox.

b) contraction of frictionless, steady flow of volumetric intensity Q through a horizontal element of cross-section area from A_1 to A_2 defines a single force F, which may, however, depending on the cross-section in which the force is applied (e.g. using a piston), generate two different pressures:

$$p_{l} = \frac{F}{A_{l}} = \rho Q^{2} \left\lfloor \frac{A_{l} - A_{2}}{A_{l}^{2} A_{2}} \right\rfloor$$

or:
$$p_2 = \frac{F}{A_2} = \rho Q^2 \left[\frac{A_1 - A_2}{A_1 A_2^2} \right]$$
 (24)

Analysis of the same problem with help of the Bernoulli equation (14 or 15) is equally simple, but it predicts a single pressure difference, equal exactly to the mean value of the both results (24), which do not include so many simplifying assumptions as Bernoulli eq. (14). The list of the above examples, elementary to the point of triviality, may be further extended. Important here is, that: it points to interpretation problems in complex technically relevant macroscopic flows as well.

c) complex flows e.g. in fluidized beds, and numerical calculations [12] provide further arguments in favour of use of the observed change of momentum (force) as a primary reference quantity for analysis of derived, statistical quantities like pressure.

Thereby, purpose of here qualitative discussion of an idealized fluidized bed is:

- to show the applicability of the method to the analysis of complex systems concerning simultaneously single- and multiphase flows,
- to show that, the observed changes of momentum (forces) are better suited to serve as primary reference quantities in system analysis, than the derived, statistical quantities like pressure,
- to imply the basic similarity of the behaviour of the considered system of disperse particles with the behaviour of an ideal gas (Fig. 1) or (Figs. 1 and 2) a melting solid,
- to introduce definitions of parameters resulting directly from eqs. (1-5).

Comparison with measurement results is not aimed at, because instrumental fulfillment of all theoretical assumptions of e.g. uniform velocity distribution, uniformity of particle properties etc. in a real fluidized bed is not possible.

To start with, we consider the schematic representation of a fixed bed shown in **Fig. 2** below.



Fig. 2. Schematic representation of particle bed at rest. Particles rest on the sieve and are supported with total force \underline{F}_S equal to total particle weight less weight of the displaced fluid.



Fig. Schematic representation 3 of fluidized particle bed. Particles are separated from each other by the flow and move freely above the supporting sieve. The average sedimentation velocity of the particles (e.g. black arrow \underline{w}_{g}) is approximately equal to the average upward interstitial fluid velocity (blue arrow). Flow intensity through the fluidized bed Q_{FB} is larger than flow intensity through the particle bed at rest Q_{FB} > Q_{PB} . The resulting length L_{FB} of the fluidized bed in steady state results from equilibrium of particle weight and drag exerted by the flow and exceeds the length of the particle bed at rest $L_{FB} > L_{PB}$.

The estimative analysis of the idealized fluidized bed starts with determination of forces F acting on particle. These result from equation (3) applied to particles. It reads:

$$\frac{d}{dt} \int_{V_{p}} \rho \underline{v} dV =$$

$$= \int_{V_{p}} \rho_{p} \underline{g} dV - \int_{A_{p}} p \underline{dA} + \int_{A_{p}} \underline{t}(\eta) \bullet \underline{dA} + \underline{F}_{s}$$
(25)

Thereby V_p is the volume filled by the particles; ρ_p is the density of the particles; A_p is respectively the particle surface regarded here as total wetted surface; <u>Fs</u> denotes the support forces acting on particles resting on the supporting sieve. For the upward direction follows [7, 11, 12]:

$$F_{\rm S} = (\rho_p - \rho_F) g V_p - k_{FB}(\text{Re}) \eta A_{\rm W} \frac{v_{rel}}{R_{\rm HP}}$$
(26)

Thereby ρ_F is the fluid density. The last term on the right side of eq. (26) represents direct extension of the micro fluidic derivation of the viscous friction force (eqs. (16, 17)) to technically relevant geometries. Thereby $k_{FB}(Re)$ is the drag coefficient characteristic for a given flow geometry, here for the particle bed.[8, 11, 12]; A_W is the wetted area of the particles, here is A_W = Ap; further <u>v</u>_{rel} the relative particle–fluid velocity i.e. the difference between the average interstitial fluid v and particle velocity w [7, 11, 12]:

 $\underline{\mathbf{v}}_{rel} = \underline{\mathbf{v}} - \underline{\mathbf{w}}$; \mathbf{R}_{HP} is the hydraulic radius estimating the boundary layer thickness in the pores between the particles [8, 11, 12]: $\mathbf{R}_{HP} = \mathbf{V}\boldsymbol{\epsilon} / \mathbf{A}_{W}$. The quotient of the interstitial velocity v and of the hydraulic radius \mathbf{R}_{HP} estimates the velocity gradient in the boundary layers of the interstitial spaces. This in conformance with the micro fluidic definition of the viscous force given by eq. (16). The above simplified form of eq. (25) is valid for particle phase for situations represented in Figs. 2 and 3 during all periods of time in which the average absolute velocity of the particles w_g along the gravity vector vanishes i.e. : $w_g = 0$ and $v_{rel} = v$.

The first term on the right side of the above eq. (26) represents weight of the particles reduced by weight of the displaced fluid (Archimedes law). The second term describes the viscous drag force. The only variable term on the right side of eq. (26) is the interstitial flow velocity v in spaces between the particles. Controlled by the flow intensity Q and by the geometry of the interstitial flow:

$$Q = v A \varepsilon$$
 (27)

A is the total cross-section of the column and ε represents the porosity of the considered particle ensemble.

Flow intensity Q defines several operation modes of the system:

I) Particle bed at rest is characterized by the condition of total particle weight less weight of the displaced fluid being larger than the drag exerted by the flow i.e., in respect to eq. (26) when: $F_S \ge 0$ (28)II) Unstable state of the bed beginning when the flow drag approaches the total weight of the particle bed diminished by the weight of the displaced fluid, so that the supporting force F_S (eq. (26)) vanishes (s. Fig. 4). The interstitial fluid velocity in spaces between the particles v is still smaller than the average absolute sedimentation velocity of the particles w_g . The porosity of the particles ε varies locally between porosity of fixed bed ε_{FB} and 1. Then following conditions prevail:

 $F_S = 0 \ ; \quad v < w_g \ ; \quad \epsilon_{FB} \le \epsilon \le 1$ (29)III) Steady state begins when the interstitial fluid velocity v reaches the sedimentation velocity of single particles wg throughout the whole particle bed at porosities ε just starting to exceed the porosity of a fixed bed ε_{FB} . This operation mode is approximated by equilibrium of drag and weight of single particles ($F_{s}=0$). Individual particles start moving freely in the flow as shown in Fig. 3 building together a macroscopic model of a liquid (compare Figs. 1 and 3). Porosity of the particles ε is estimated by an approximately continuous function of the flow intensity Q and of characteristic dimensions and velocities in the column as:

$$\varepsilon = \frac{Q}{W_g A} = \frac{v_F}{W_g}$$
(30)

Porosity of the fluidized particle layer increases continuously with increasing flow

intensity Q from porosity of the fixed bed ϵ_{FB} till the value of 1.

In respect to the calculation of pressures in the column it is to be remarked:

a) forces relevant for the behavior of the particles remain constant under steady operation conditions and allow simple analysis and fairly definite representation of results (s. Fig. 4 below)



Fig. 4: $F_S(i)$: force exerted by the particles on the supporting sieve (weight of the particles less weight of the displaced fluid and less viscous drag of flow in the fixed bed s. eq. 26). $F_G(i)$: Drag force on the particles in the fixed bed and in steady state of the fluidized bed (green line in and after the grey block of unstable operation mode), $F_L(i)$: viscous drag force exerted by the flow on the particles. $F_L(i)$ rises till unstable mode (grey block region) is reached. In the unstable region "anything" may occur. Red interrupted line shows viscous drag in the unstable bed increasing till bed breakup occurs (abrupt fall of the interrupted $F_L(i)$ line to $F_G(i)$ level).

b) calculation of pressures relates forces to the magnitudes of the cross-sections available to the flow. Free cross sections depend on the porosity. Thus pressure is a function of porosity and flow intensity: $p = f(\varepsilon(Q))$. It may also be calculated by relating forces to the column cross section A. This introduces the possibility of multiple interpretation of principally identical results (s. Fig. 5 below).



Fig. 5 Calculated pressures. It is recognizable that two different pressure values $(\Delta p_L(i) \text{ and } \Delta p_{L\epsilon}(i) \text{ may be derived from a single force value } F_L(i)$ (s. **Fig. 4**). The same is valid for the drag force $F_G(i)$, in fixed particle bed and in steady state of the fluidized bed (green line in and after the grey block of unstable operation mode).

Further increase of the flow intensity Q blows particles out of the column and begins the:

IV) Single phase flow mode. Interesting is here, that the analysis of the single phase flow does not require theoretical tools other than those used for the analysis of disperse particle systems (s. examples 1 and 2a, b above) and vice versa.

4. Conclusions: Explicit application of Newton's second law (eqs. (1), (2), (3)) and conservation laws in the differential-integral notation [1, 7 - 13] to fluids modelled basically as molecular disperse systems [7 -13], provides а self consistent. physically coherent, concise and simple description of non - relativistic transport phenomena. Set of equations to remember is very small and provides a transparent common physical background for multiple applications in process engineering.

In view of the experimental evidence gathered in the fields of corpuscular physics, also in the kinetic gas theory [2, 3], as well as in classical astrophysics [6], Newton's law represents the experimentally best confirmed law describing the non relativistic motion of matter generally. The purpose of the paper is to promote its use as an explicit reference standard and starting point of analysis of all phenomena in material systems, which may be discussed in terms of dynamics of disperse systems.

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