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On hyperbolicity and solution properties of the continual models of micro/nanoparticle aggregation and sedimentation in concentrated suspensions

Про гіперболічність і властивості розв'язків континуальних моделей агрегації та седиментації мікро/наночастинок у концентрованих суспензіях

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In continual mechanics sedimentation of aggregating particles in concentrated suspensions are determined by the mass and momentum conservation laws for each component of the suspension. The resulting quasilinear system of differential equations governing the flow could be hyperbolic, strongly strictly or weakly hyperbolic depending on the model accepted. The type and Eigenvalues of the matrix influence the characteristics of the pattern formation during the sedimentation that is essential for the model application in modern medical, microbiological and nanofluidic technologies. In this paper the hyperbolicity of the three-phase model of aggregation and sedimentation of micro/nanoparticles is studied.

Key Words: Aggregation, Sedimentation, Multiphase Continuous Media, Hyperbolic Systems, Eigenvalues, Characteristics.

В механіці суцільних середовищ седиментація частинок, що агрегують, у концентрованих суспензіях визначається законами збереження маси та імпульсу для кожного компонента суспензії. Отримана квазілінійна система диференціальних рівнянь, які керують течією, може бути гіперболічною, суворо або слабко гіперболічною залежно від прийнятої моделі. Тип та власні значення матриці задачі впливають на характеристики формування паттерну частинок під час їх седиментації, що є важливим для застосування моделі в сучасних медичних, мікробіологічних та нанофлюїдних технологіях. В даній роботі вивчається гіперболічність трифазної моделі агрегації та седиментації мікро і наночастинок.

Ключові слова: агрегація, седиментація, багатофазні суцільні середовища, гіперболічні системи, власні значення, характеристики.

Статтю представив д.ф.-м.н., проф. Жук Я. О.

1. Introduction

Sedimentation of aggregating particles in suspensions is widely studied in connection with direct engineering applications like testing the suspension stability and ageing, formation of the layered materials and coatings composed of solid nanoparticles of different size and shape, biological tests of red blood cells or platelet sedimentation of patients [1-4]. The pattern formation in the sediment, its continuity and mechanical properties depend on the solution of

the governing system of equations [2-5]. In this paper the Eigenvalues (EV), characteristics (Ch) and different types of solutions are studied on the model of three-phase suspension of solid aggregating particles developed in [3].

2. Mathematical background

Let us consider a concentrated suspension composed of solid particles and basic fluid (BF) some part of which could be captured inside the aggregations as a captures fluid (CF). The mass and

momentum conservation laws in the case of 1D sedimentation in a tube in the external non-uniform flow field can be finally formulated as a system of quasilinear differential equations

$$\frac{\partial \Phi_i}{\partial t} + \sum_{j=1}^n A_{ij} \frac{\partial \Phi_j}{\partial x} = B_i, \quad i = 1-3, \quad (1)$$

where $\bar{\Phi} = (H, C, V)^T$, H and C are volumetric concentrations of the aggregates and particles in them, V is the mean volume of the aggregates per unite volume, $A_{ij}(t, x, \Phi_j) \in C^1(\mathcal{R}^n, \mathcal{R}^n)$ and $B_i(t, x, \Phi_j) \in C^1(\mathcal{R}^n)$ are matrix and force vector.

As it is known from general theory [1], if the Jacobian $J_A(\bar{\Phi}) = |\partial A_{ij}(\bar{\Phi}) / \partial x_j|_{i,j=1,\dots,n}$ has real EV and diagonalizable, (1) is hyperbolic. When the EV are distinct, (1) is strongly hyperbolic, and when J_A is not diagonalizable, (1) is weakly hyperbolic and singular shocks can occur [1].

Hyperbolic systems can have discontinuous solutions even when the boundary conditions (BC) are smooth. Such discontinuities are called kinematic shocks, which must satisfy jump conditions and an entropy condition (admissibility condition) [1,4,6]. Depending on the hyperbolicity kind of (1), different types of sedimentation (ToS) may be observed [1] (Fig.1 a,b).

Fig.1. Sketch of ToS I (a) and ToS II, III (b); explanations are in the text.

ToS I corresponds to a sharp interface $l_1(t)$ separating the basic fluid zone ($z1$) from the particle sedimentation zone ($z2$) (Fig.1a), while ToS II and ToS III (Fig.1b) also have a transition zone (tz) between the aggregate sedimentation zone ($z3$) and the sediment zone ($z4$). In tz the concentration increases downwards continuously. ToS II shows a jump between the $z3$ and the tz , whereas in ToS III the jump is absent. The interfaces propagate as kinematic waves and the suspension dynamics is split into two regimes (Fig.1a,b): in one only hydrodynamic interactions

between the particles are dominant ($z2, z3$) and another in which the solid interactions between the particles are dominant ($z3, z4$) [1,2,4,6].

3. Mathematical problem formulation

The resulting system of equations for the 3-phase suspensions has the form [3]

$$\begin{aligned} \frac{\partial H}{\partial t} + A_{11} \frac{\partial H}{\partial x} + A_{12} \frac{\partial C}{\partial x} + A_{13} \frac{\partial V}{\partial x} &= \theta - B_1, \\ \frac{\partial C}{\partial t} + A_{21} \frac{\partial H}{\partial x} + A_{22} \frac{\partial C}{\partial x} + A_{23} \frac{\partial V}{\partial x} &= -B_2, \\ \frac{\partial V}{\partial t} + A_{33} \frac{\partial V}{\partial x} &= \frac{V^2}{C} (\Gamma^+ - \Gamma^-) - B_3, \end{aligned} \quad (3)$$

where θ is the rate of the CF accumulation, $\Gamma^\pm$ are rates of aggregation and disaggregation, A_{ik} , B_j , $\Gamma^\pm$ are known nonlinear functions of H, C, V ; the corresponding complex expressions are presented in [3]; the functions $B_{1-3} \neq 0$ here due to the presence of the non-uniform vertical field $G(x)$ instead of gravitation (for instance, centrifugal, magnetic or other force field). The BC for (3) are

$$t = 0, x \in [0, L]: H = H_0, \quad C = C_0, \quad V = V_0, \quad (4)$$

where C_0 and V_0 are the initial concentration and volume of a single particle; in the case of the perfectly uniform suspension $C_0 = H_0$.

The system (1) determines nonlinear flux function $F(\Phi)$, which needs special consideration in solving the initial value problem (3),(4). Any potential jump between $z1, z2, z3, tz$ and $z4$ must satisfy the Rankine-Hugoniot condition [1]

$$F(\Phi_{j+}) - F(\Phi_{j-}) = c_j(\Phi_{j+}, \Phi_{j-})(\Phi_{j+} - \Phi_{j-}), \quad (5)$$

where c_j is the jump propagation speed.

The Liu entropy condition requires that

$$c_j(\Phi_{j+}, \Phi_{j-}) \leq c_j(\Phi_{j+}, \Phi_j), \quad (6)$$

for all Φ in the Hugoniot locus inside $[\Phi_{j-}, \Phi_{j+}]$.

Here the existence of a complete set of EV for (3) and different ToS determined by (3), (4) for different model parameters taken from [3] for the suspension of human red blood cells are studied. As it was shown in [3], for such sets of parameters the discontinuity between $z1$ and $z2$ always exist while two more EV are solutions of the square equations and one of them could be negative. Theoretical sedimentation curves $l_1(t)$ can easily be checked in experimental measurements using the optical techniques, while the curves $l_2(t)$, $l_3(t)$, $l_4(t)$ are much more difficult for experimental studies.

4. Results and discussion

Solutions of the problem (3), (4) have been found by the method of characteristics [3,7]. The method had been validated by the particle dynamics method [8] and experiments [9]. The characteristic ch1 of the 1-st family separates z1 and z2 and moves with the speed $c_1 > 0$ at any set of material parameters. For the microparticles with high aggregation rate Γ^+ and $\Gamma^- \sim 0$ the length $l_2 - l_1$ of z2 is very short, while in the nanofluids it could be long enough due to high buoyancy of the nanoparticles [1]. At the low concentrations $C_0 < C^*$, C^* is a critical value, the cross-section of the ch1 and ch2 with negative speed $c_3 < 0$ (Fig.2a). The ch1 curves correspond to the experimentally observed sedimentation curves $l_1(t)$ and in Fig.2a $C^* \sim 0.25-0.3$ depending on the suspension parameters.

The nonlinear flux (5) can generate a centered rarefaction wave originating from the bottom (Fig.2b). This wave may be interpreted as a 'supersediment' consisted of the tz built above the sediment during sedimentation [1,5]. At some mode parameters and low external forces the tz layer built from $t=0$ and is formed by a series of thin layers with gradually increased (from $x=l_4(t)$ to $x=l_3(t)$) concentrations from $C=C^{**}$ in z3 to $C=1$ in z4 (Fig.1b). Existence or absence of the discontinuity at $x=l_4$ is determined by an additional condition that can be satisfied by different sets of suspension parameters and $G(x)$.

When the aggregation is high enough and the external force $G(x)$ grows monotonously, the z4 zone is formed quickly and another picture of zone distributions appear (Fig.2c). The rarefaction wave is represented by a fan of piecewise constant values split by the propagating fronts [1]. This solution strategy has been used for sedimentation modeling in bidisperse suspensions in [5]. At some combinations of the model parameters the discontinuity at $x=l_1+l_2+l_3$ (ToS III) is also presented as a fan-type structure proper to the rarefaction wave (Fig.2c). In the highly non-uniform fields $G(x)$ an additional jump at $x=x=l_1+l_2+l_4$ (ToS II) is formed (Fig.2d). Despite our case, in the uniform gravity field this structure is also uniform with the sublayers of gradually decreasing concentrations and, therefore, density.

Contrary to the 2-phase suspensions [1,4,5], in the 3-phase suspensions with the ability of rapid capture of the BF and its temporary absorption inside the sedimented aggregates in z3, release of the CF inside the zt will produce more

complex structures of the fan-type structures (ToS III) with a possibility with complex discontinuities with additional fan-type structures (ToS II) in each sublayer (Fig.3) depending on the relationships between the model parameters. This double structures are formed by the intersections of three family of characteristics of the system (3).

The corresponding bulky expressions for the conditions on the model parameters needed for development of each case (Fig.2a-d, Fig.3) are not presented here for brevity.

Fig.2. Characteristics of the 1-st and 2-nd families for (a) low $C_0=0.1; 0.15; 0.2$ and (b) high $C_0=0.35; 0.5$ values, in low- (c) and high- (d) intensity fields $G(x)$ at $C_0=0.4$.

Fig.3. Distribution of 3 families of characteristics for 3-phase suspensions with high BF capture ($\theta = 0.5$).

5. Conclusions

The complete sets of EV for the 3-phase suspension of aggregating particles sedimented in an external non-uniform field are computed for different sets of material parameters. It was shown, besides well-known ToS I,II,III, a more complex sets of characteristics can appear. That may be used in manufacture of complex layered nanomaterials with non-uniform physical properties as well as in medical diagnostics on blood sedimentation tests.

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