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Validation method for the systematization of results based on a similarity concept

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The development of a functional methodological approach is presented here, to clarify a globally valid way of evaluating the precision of mathematical modeling of physical and/or chemical processes. Starting from the description of the system, a phenomenon accompanied by a disclaiming hypothesis is investigated, against which the knowledge is accumulated with time. Moreover, the possibility of the evolution of any phenomenon being interrupted when a parameter overpasses a critical threshold, after which the hypothesis is not any more valid, is introduced. This possibility should be obtained through the dependence of a selected macroscopic quantity (marker) on a specific parameter. To apply this methodology, the problem of Stokes flow through a granular medium of spheroidal grains has been selected as an indicative case study. The prolate spheroidal configuration is considered, since the results for the oblate spheroid can be recovered via a simple transformation. Therein, the three-dimensional flow fields are initially constructed analytically via the Papkovich-Neuber differential representation, which provides the velocity and pressure fields in terms of harmonic spheroidal eigenfunctions. Next, under the Kuwabara-type spheroidal 2D unit cell concept, the above expressions degenerate to the axisymmetric case, and the full solution is then obtained, keeping the leading terms of the series, which are adequate for most engineering applications for specific aspect ratio of the spheroids. In the sequel, the aforementioned problem is solved numerically for a 3D extension of the same model, where this numerical solution has been achieved by using the finite volumes method, while the resulting linear systems were approximated by applying the well-known successful over-relaxation concept. Finally, outcomes by both models have been compared via the above methodology, resulting to objective and reliable accuracy criteria.

1 | INTRODUCTION

Simulations is a powerful tool, mainly used when the experimentation regarding a specific problem is either infeasible or costly ineffective to be implemented. Nevertheless, it is always necessary to evaluate simulations' outcomes in a globally valid way, for their results to be widely accepted by scientific community. Usually, this validation process is fragmented by the point of view of the researcher, the available techniques/materials, the knowledge accumulated etc..[1,2] Although it is widely accepted that a theory is usually criticized by falsification, mathematical models are often tested by validation; thus, a set of validations checks for all the main results should be undeniably performed.[3]

The study of physical phenomena is mainly based on the concept of physical similarity. Two physical phenomena are similar if the numerical values for the characteristics of one phenomenon enable one to derive the numerical values for the characteristics of the other by a simple conversion, which is analogous to transferring from one system of units of measurement to another. For any set of similar phenomena, all the corresponding dimensionless characteristics must have the same numerical values.[4] To apply similarity theory in a physical system, it is first necessary to define a relevant class of phenomena that, in general, are not similar to one another; therefore, a subclass of similar phenomena must be identified within this class after applying a set of similarity criteria and particular conditions.[5]

This work presents a step-by-step methodology for evaluating the results of simulations in a globally valid manner. This evaluation inevitably results to a specific macroscopic quantity that adequately describes the phenomenon along with the hypothesis against which the system is investigated. In general, scientists do not investigate phenomena but perceptions of phenomena that have been derived in the context of a hypothesis via the logical combination of empirical observations, as well as conclusive theoretical and practical interpretations.[6] As a case study, the above methodology has been applied on the problem of flow through granular porous media, where the analytical solution for spheroidal-in-cell model and the numerical results are compared with predictions produced by applying the Darcy's law to evaluate its validity in the present case.

We derive the solution of the problem of creeping flow through a swarm of stationary spheroidal particles, immersed in a Newtonian fluid that moves with a uniform and constant mean interstitial velocity in the axial direction. Under the assumption of very small Reynolds number, an axisymmetric Stokes flow in a spheroidal envelope of appropriate shape and dimensions is adopted as a fair approximation to the flow around a typical particle of the swarm, in accordance with the concept introduced by Kuwabara.[7] In general, Kuwabara's approach becomes very popular due to the advantages of the easily obtained analytical form of the velocity field, being therefore applicable to coupled and/or uncoupled mass and heat transfer problems. The inner spheroid, which represents one of the particles in the assemblage, is solid, whereas the outer spheroid represents a fictitious fluid envelope identifying the surface of a unit cell (spheroid-in-cell). This idea provides a useful and effective way to model flow through a swarm of spheroidal particles. The volume of the fluid cell is chosen so that the solid volume fraction in the cell coincides with the volume fraction of the swarm. The appropriate boundary conditions, resulting from these assumptions, can be used to determine the flow fields as full series expansion via the Papkovich-Neuber representation, which represents the velocity and the total pressure fields in terms of harmonic functions and is proved to be widely applicable to spherical[8-10] and spheroidal[11,12] geometry. The same problem is solved numerically for the corresponding 3D case, where the numerical implementation has been incorporated via the finite volumes method, whereas the obtained linear systems were approximated by applying the well-known successful over-relaxation concept. Finally, outcomes by both models have been compared using the introduced technique, resulting to objective and reliable accuracy criteria.

Section 2 provides the relative theoretical principles of the proposed method, and the main Section 3 includes the analytical and numerical application to the wide spectrum of physical phenomena involving porous media, followed by their connection through the applicability of the applied theoretical approach. The final Section 4 is devoted to a discussion of the results drawn in this work.

2 | THEORY DEVELOPMENT

Scientists may investigate a phenomenon in order to support a theory, since theories may have gaps and inconsistencies that need to be completed. The major tool for obtaining experience in the physical world is based on reproducing the physical phenomena in a controlled environment, ie, within a lab or field experimentation procedure, is actually based on similarities between phenomena or classes of physical phenomena, whose identification lies among the fundamental considerations of a physical scientist in charge. This reproduction should be in a standard and repeatable manner. In fact, the perception of a phenomenon is deriving in the context of a hypothesis via the logical combination of empirical observations, as well as conclusive theoretical and practical interpretations. Therefore, there is an infinite number of phenomena, which claim to represent an objective reality with a higher or a lower precision level.

The ability to correctly infer the values of quantities in one physical system from knowledge of the values of the quantities in a system that is physically similar to it rests on the ability to correctly establish that the two systems are similar. Towards this aim, the necessity of an existent classified knowledge has already been accepted. A powerful tool assisting this classification is the similarity that assures and requires a mapping between the various phenomena. Once two systems have been identified as similar, one may be able to draw a similarity mapping to keep certain relationships about quantities in one system the same as in the other. Precisely, the concept of similarity assures and pre-requisites that a mapping between elements of the system exists, having also the property to preserve the structure of the situation that is relevant to the phenomenon of interest. In other words, when two systems/states are similar, a similarity mapping must be able to be drawn based on keeping certain relationships, quantities, or elements in one system the same as in the other.

Observations of events expressed in the laboratory are considered informative about things and events that go beyond the specifics of the observed case, in support of a broader theoretical approach. This is possible due to the assumption that there is a class of events or situations that are similar to a given event, and that a given event is informative of other events in that class. A question now arises: what determines the class of other events to which an observation is made on a specific setup, is deemed similar? The answer, apparently, refers to a comparison of various considerations of the same object or to a comparison among various objects on a common hypothesis. Specific well-posed criteria are necessary to identify similarity. For that, it is widely accepted that a classification of the existing knowledge is necessary. However, a major difficulty to that is the definition of the specific similarity criteria, in order to assure that similarity indeed exists. Evidently, a researcher applying improper similarity criteria might obtain erroneous or meaningless results, yet, still spending significant amounts of resources. Accordingly, poor similarity criteria could lead to a research duplication (and, therefore, to an effort's and resources' waste), due to the lack of a deeper insight on the existing experience and knowledge regarding the phenomenon under current consideration.[13]

It is rather clear that the description of a system must take in account both the physical principles of the system along with a physical description of the system. To provide an integrated "cycle-of-understanding" for such a system, this description has always to be transformed accordingly to human cognition, in order to obtain a description that is consistent with the way that intelligence translates the phenomena. This stage produces the necessary categories, ie, the expression of the system behavior and the definition of the boundary conditions, both classified in terms of logic. Any system of physical interest can be described through a typical "in-process-out" context. The above concept can be picturized through the scheme described in Table 1.

The necessity and success of a classification scheme are originated from the need and aim at the applied capability to correctly describe the system, based on the eventual reflections of the way our mind composes the phenomena. The overall classification scheme has to cover the hypothesis' context possibilities for the system in question and regulate the system boundaries (classification frame) via impacting on each and every systemic participant, in-principal. Conclusively, the classification will also reflect the theoretical solidness of the mathematical concept, independent of the empirical experience, in which case the resultant model must be capable of assessing the shaped categorical imperative of the hypothesis.

It is essential to primarily consider the conceptual description of the system, in the basis of an "in-process-out" context was converted into the necessary justification methodological approach by incorporating the optimum and minimal, yet straightforward systemic participants. In simple terms, the basic context turned into the following principal description: "matter" along with "energy" produce "outcome" via specific "relationships."[14,15] These four entities constitute the categorical descriptors for such a system. All categories have to satisfy the hypothesis' context possibilities for the system in question. Having adequately considered and investigated all levels and categories, it is necessary to regulate the boundaries of the model via impacting on each and every systemic participant, in-principal. Conclusively, the classification will also reflect the theoretical solidness of the model, independent of the empiric experience, in which case the model shall be capable of assessing the shaped categorical imperative of the hypothesis.

TABLE 1 The methodology for describing a state and understand a phenomenon

Step	Action
1	Define the system under investigation, where a physical phenomenon takes place.
2	Identify the disclaiming hypothesis, against which the system is under investigation.
3	Define the relative state through steps 1 and 2.
4	Describe mathematically the state through fundamental principles and balances.
5	Calculate the macroscopic quantity, against which the tool should be assessed.
6	Outcome: The understanding of the phenomenon in a specific level.

Following the above, the categorical description of the system was developed. We concluded an adequate classification frame of at least a 12 cells scheme, consisted of four main structural categories extended up to three empirically defined levels.[15] These levels denote the degrees of freedom for a set of conditions within a critical judgment. In practice, all levels of a given category condense the impact of this systemic participant where it is the cohesion among the systemic orders that are also considered. It is worth-mentioning that the amount of the cells is very well defined in terms of mathematics: the rows are four due to the four entities involved. Overall, it is all four categories at all three levels that should contain all universal hypotheses' possibilities for a food system during its shelf-life. Each individual “category-level” cell represents the particular conditions for a systemic activity. In a sense, each cell is a “hypothesis disclaiming class,” a structural contributor to the possibility of the overall hypothesis disclaim. Furthermore, summary of the classes embraces the cohesion within the system context, rather than the independent interpretational risks due to the theoretical impregnation of the observations. Cross sections of the classification cells actually provide the much-needed space for intersubjectivity, or, ie, they allow for the maximum objectivity in validating the hypothesis. The common ground among all classes' interactions shall eventually deliver the basic principles behind the phenomena, the cohesions in the food system, the only physically meaningful and responsible, potential conditions of knowledge.[16]

The sequence of steps about the methodology for describing a state and understanding a phenomenon, presented in Table 1, is readily applied in order to address the problem of flow through a granular medium of spheroidal grains, where the complexity of the porous structures allows for assuming very complex phenomena in local scale, which should be integrated to normal macroscopic ones.

3 | ENGINEERING APPLICATION

In this work, the above methodology is applied in a problem of physical and engineering interest, in order to show how the above methodology could be applied for engineering purposes. Flow through granular media has been selected as a main promotive case study, assuming the spheroidal geometry to fit the particles' shape, as it is readily depicted in Figure 1. This application is of high importance, since flow problems in porous media have attracted the attention of industrialists, engineers, and scientists from varying disciplines, such as chemical, environmental, and mechanical engineering, geothermal physics, and food science. It is widely acceptable that dense materials do not actually exist: even the most compact artificially developed material is of a small porosity and must be treated as porous itself. Consequently, the study of flow and transport in porous media is applicable in a very wide range of fields, with practical applications in modern industry and environmental areas. In all these disciplines, transport phenomena and transformation occur in porous media domains at a wide range of scales, from the microscopic to the field scale.

Besides the wide spectrum of applications that porous media have attain during last centuries, they are not transparent; thus, it is necessary from scientific point of view to describe a process without any local observation, based only on macroscopic data regarding the inlet and the outlet of the domain.[17] In this context, Darcy's law[18] is considered as a widely accepted tool for the successful estimation of the velocity field developed within a given porous medium. It is

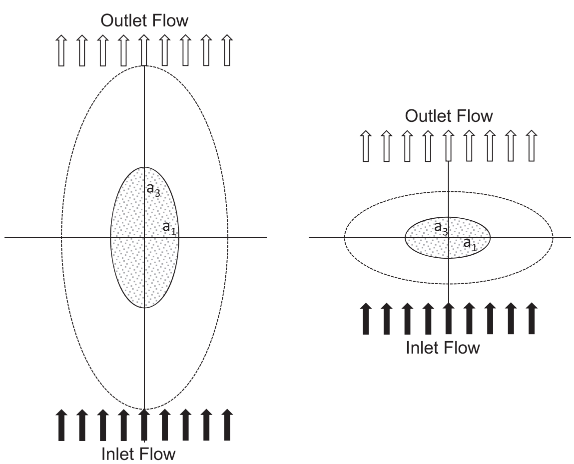

FIGURE 1 Formulation of the problem for both the prolate and the oblate spheroidal geometry

important to note here that Darcy's law is a macroscopic expression, while the complexity of porous structures allows for assuming very complex phenomena in local scale, which should be integrated to normal macroscopic ones.

Mathematical modeling of transport processes in porous media is a powerful tool employed whenever experimentation is either expensive or difficult due to the nature of the process under consideration. Presenting the advantage of analytical solutions for the flow and transport equations, cell models establish an authoritative tool for engineering applications regarding porous media.[14] The conceptual idea behind them is that the medium is considered as an assemblage of similar unit cells gathered in a regular manner; therefore, the unit cell is the adequate representative of the whole medium (see Figure 1). In other words, the processes occurring through the porous structure are described sufficiently by those occurring in the unit cell. The shape of the core could be spherical, cylindrical, and spheroidal or in the most general case ellipsoidal, while the outer liquid envelope is of the same shape. For many interior and exterior flow problems involving small particles, spheroidal geometry provides a very good approximation, since impurities agglomerate in the direction of the flow, establishing the particular prolate spheroidal shape. The thickness of the surrounding fluid layer is adjusted so the ratio of the solid volume to the volume of the liquid envelope to represent exactly the solid volume fraction of the porous medium. Finally, the boundary conditions imposed on the outer surface of the envelope are supposed to adequately represent the interactions between the grains. Precisely, the definition of the problem is presented in the following Table 2, where the general methodology introduced in Table 1 is now limited to the particular application for the Stokes flow through a swarm of particles in granular porous media.

For the sake of simplicity, the laminar flow of a Newtonian fluid through a porous medium of spheroidal grains has been considered, adopting the Kuwabara's approach for spheroidal cells.[11,12]

3.1 | Analytical approach

Given the semifocal distance $c > 0$ of the prolate spheroidal geometry for $1 \leq \tau < +\infty$, $-1 \leq \zeta \leq 1$, and $\varphi \in [0, 2\pi)$,

$$x_1 = c\sqrt{\tau^2 - 1}\sqrt{1-\zeta^2}\cos\varphi, \quad x_2 = c\sqrt{\tau^2 - 1}\sqrt{1-\zeta^2}\sin\varphi \text{ and } x_3 = c\tau\zeta, \tag{1}$$

in terms of the Cartesian coordinates, then to every fixed value of $\tau_0 \in (1, +\infty)$, there corresponds a unique prolate spheroid with major semiaxes $a_3(\tau_0) = c\tau_0$, minor semiaxes $a_1(\tau_0) = c\sqrt{\tau_0^2 - 1}$, and eccentricity $\varepsilon(\tau_0) = 1/\tau_0$, that is

$$S_{\tau_0}: \frac{x_1^2 + x_2^2}{c^2(\tau_0^2 - 1)} + \frac{x_3^2}{c^2\tau_0^2} = 1 \text{ with aspect ratio } a = \frac{a_3(\tau_0)}{a_1(\tau_0)}, \tag{2}$$

which degenerates to a sphere of radius $c\tau_0 \to r_0$ as $c \to 0^+$.

The governing equations of the steady, non-axisymmetric, creeping flow (Reynolds number $\mathrm{Re} \ll 1$) of an incompressible (constant mass density ρ), viscous (constant dynamic viscosity μ) fluid, around particles embedded within a

TABLE 2 Application for Stokes flow through granular media

Theory	Application
Phenomenon	Flow through granular porous media.
Hypothesis	Darcy's law.
State	The flow through granular media is adequately described by Darcy's law.
Mathematical description	Geometry: Spheroidal (prolate and oblate). Flow: Laminar. Model: Kuwabara's unit cell. Solution: Either analytical or numerical. Microscopic result: Velocity field.
Macroscopic quantity	Volumetric flow rate, Q.
Outcome	$\lambda = \frac{Q_{A/N}}{Q_D}$, where $Q_{A/N}$ refers to analytical (A) and numerical (N) results, while Q_D is the volumetric flow rate from Darcy's law.

smooth, bounded domain $\Omega(\mathbb{R}^3)$, resembling the granular medium, connect the biharmonic velocity field $\mathbf{v}$ with the harmonic total pressure field P via the partial differential equations

$$\mu\Delta\mathbf{v}(\mathbf{r}) = \nabla \mathrm{P}(\mathbf{r}) \text{ and } \nabla\cdot\mathbf{v}(\mathbf{r}) = 0 \text{ with vorticity } \boldsymbol{\omega}(\mathbf{r}) = \nabla\times\mathbf{v}(\mathbf{r}) \text{ for every } \mathbf{r}\in\Omega\left(\mathbb{R}^3\right). \tag{3}$$

Papkovich-Neuber proposed a 3D differential representation of the solution for Stokes flow (3), in terms of the vector $\boldsymbol{\Phi}$ and scalar Ψ harmonic potentials, ie,

$$\mathbf{v}(\mathbf{r}) = \boldsymbol{\Phi}(\mathbf{r}) - \frac{1}{2}\nabla(\mathbf{r}\cdot\boldsymbol{\Phi}(\mathbf{r}) + \Psi(\mathbf{r})) \text{ and } \mathrm{P}(\mathbf{r}) = -\mu\nabla\cdot\boldsymbol{\Phi}(\mathbf{r}), \text{ where } \Delta\boldsymbol{\Phi}(\mathbf{r}) = \mathbf{0},\ \Delta\Psi(\mathbf{r}) = 0 \text{ with } \mathbf{r}\in\Omega\left(\mathbb{R}^3\right). \tag{4}$$

The gradient differential operator ∇ (note that $\Delta = \nabla\cdot\nabla$), in prolate spheroidal coordinates, assumes the form

$$\nabla = \frac{1}{c\sqrt{\tau^2-\zeta^2}}\left[\sqrt{\tau^2-1}\,\hat{\boldsymbol{\tau}}\frac{\partial}{\partial\tau} - \sqrt{1-\zeta^2}\,\hat{\boldsymbol{\zeta}}\frac{\partial}{\partial\zeta}\right] + \frac{1}{c\sqrt{\tau^2-1}\sqrt{1-\zeta^2}}\hat{\boldsymbol{\varphi}}\frac{\partial}{\partial\varphi} \text{ for } \tau\in[1,+\infty),\ \zeta\in[-1,1] \text{ and } \varphi\in[0,2\pi), \tag{5}$$

while $\hat{\boldsymbol{\tau}}$, $\hat{\boldsymbol{\zeta}}$, and $\hat{\boldsymbol{\varphi}}$ denote the coordinate vectors of the system. The Papkovich-Neuber general solution covers three-dimensional flow fields. For 2-D flows, as in our case, a considerable reduction is possible, where relationships

$$\partial\mathbf{v}(\mathbf{r})/\partial\varphi = \mathbf{0} \text{ and } \hat{\boldsymbol{\varphi}}\cdot\mathbf{v}(\mathbf{r}) = 0 \text{ for } \mathbf{r}\in\Omega\left(\mathbb{R}^3\right) \tag{6}$$

secure the rotational symmetry of the prolate spheroidal system, implying that the velocity is independent of the azimuthal angle φ and that its vector lives on a meridian plane.

The Kuwabara-type spheroid-in-cell model considers two confocal prolate spheroids. The inner one, indicated by S_α, at $\tau = \tau_\alpha = a_3/c$, is solid and stationary. It lives within a fictitious fluid spheroidal layer, which is confined by the outer spheroid indicated by S_β, at $\tau = \tau_\beta = b_3/c$, where a_3 and b_3 are the corresponding major semiaxes of the two spheroids. A uniformly approaching velocity $\mathbf{U} = U\hat{\boldsymbol{x}}_3$, in the positive direction of x_3-axis, generates the axisymmetric flow in the fluid layer between the two spheroids. The two double sets of boundary conditions are given by

$$\hat{\boldsymbol{\tau}}\cdot\mathbf{v}(\mathbf{r}) = 0,\ \hat{\boldsymbol{\zeta}}\cdot\mathbf{v}(\mathbf{r}) = 0 \ \text{ on } \tau = \tau_\alpha \ \text{ and } \hat{\boldsymbol{\tau}}\cdot\mathbf{v}(\mathbf{r}) = -U\hat{\boldsymbol{x}}_3\cdot\hat{\boldsymbol{\tau}},\ \hat{\boldsymbol{\varphi}}\cdot\boldsymbol{\omega}(\mathbf{r}) = 0 \text{ on } \tau = \tau_\beta, \tag{7}$$

where $\zeta\in[-1,1]$ and $\varphi\in[0,2\pi)$. The first two equations of Equation 7 express the non-slip flow conditions. The third relation within Equation 7 implies that there is a flow across the boundary of the fluid envelope S_β, while, according to Kuwabara's argument, the vorticity is assumed to vanish on the external spheroid, as shown by the last condition in Equation 7. This completes the statement of a well-posed boundary value problem.

The complete representation of the Papkovich-Neuber harmonic potentials in Equation 4, which are regular on the axis of symmetry, is given in terms of the associated Legendre functions of the first P_n^m and of the second Q_n^m kind of degree n = 0, 1, 2, ... and of order m = 0, 1, 2, ..., n via the formulae

$$\left\{\begin{matrix}\boldsymbol{\Phi}(\mathbf{r})\\ \Psi(\mathbf{r})\end{matrix}\right\} = \sum_{n=0}^{\infty}\sum_{m=0}^{n}\sum_{s=e,\,o}\left[\left\{\begin{matrix}\boldsymbol{e}_{n,in}^{m,s}\\ d_{n,in}^{m,s}\end{matrix}\right\}P_n^m(\tau) + \left\{\begin{matrix}\boldsymbol{e}_{n,ex}^{m,s}\\ d_{n,ex}^{m,s}\end{matrix}\right\}Q_n^m(\tau)\right]P_n^m(\zeta)f^{m,s}(\varphi) \text{ with } f^{m,s}(\varphi) = \left\{\begin{matrix}\cos m\varphi, & s=e\\ \sin m\varphi, & s=o\end{matrix}\right.,\ \mathbf{r}\in\Omega\left(\mathbb{R}^3\right), \tag{8}$$

where s denotes either the even (e) or the odd (o) part of the potentials, while we attain both interior (in) and exterior (ex) solutions. The unknown vector and scalar constant coefficients $\boldsymbol{e}_{n,in/ex}^{m,s} = a_{n,in/ex}^{m,s}\hat{\boldsymbol{x}}_1 + b_{n,in/ex}^{m,s}\hat{\boldsymbol{x}}_2 + c_{n,in/ex}^{m,s}\hat{\boldsymbol{x}}_3$ and $d_{n,in/ex}^{m,s}$, respectively, must be evaluated through the proper boundary conditions. Inserting, now, the potentials (8) within the general solution (4), we perform some tedious calculations in view of Equation 5 to obtain the general 3D set of the flow fields, which under the action of the axial symmetry conditions (6), reduces to a simpler 2D form for our purposes. Therein, reinforcing boundary conditions (7) and applying standard orthogonality relations for the special functions $P_n^m(\zeta)$ for $-1\le\zeta\le 1$, we calculate the aforementioned constants in a closed-type form in the sense of solving easy-to-handle linear algebraic equations with the aid of cut-off techniques.

However, the leading terms (LT) of these series solutions turn out to be satisfactory for engineering applications so long as the aspect ratio of the spheroids remains within moderate bounds, say ~1/5 < a < ~5 (incorporating both prolate and oblate spheroids). Thus, the leading term of the expansion of the velocity is denoted by

$$\mathbf{v}^{(LT)}(\tau,\zeta)=\upsilon_{\tau^{(LT)}}(\tau,\zeta)\hat{\boldsymbol{\tau}}+\upsilon_{\zeta^{(LT)}}(\tau,\zeta)\hat{\boldsymbol{\zeta}} \text{ for any } \tau_\alpha\le\tau\le\tau_\beta \text{ and } |\zeta|\le 1, \tag{9}$$

whereas the components of $\mathbf{v}^{(LT)}$ read as

$$\upsilon_{\tau^{(LT)}}(\tau,\zeta)=\frac{U}{D\sqrt{\tau^2-\zeta^2}\sqrt{\tau^2-1}}\left[-\frac{L_2}{3}-\frac{5G_4(\tau_\beta)}{2G_1(\tau_\beta)}P_1(\tau)+\left(\frac{L_2}{3}+\frac{1}{14}\right)P_2(\tau)-\frac{1}{14}P_4(\tau)-\frac{L_1}{3}Q_0(\tau)+\frac{L_1}{3}Q_2(\tau)\right]P_1(\zeta) \tag{10}$$

and

$$\upsilon_{\zeta^{(LT)}}(\tau,\zeta)=\frac{U}{D\sqrt{\tau^2-\zeta^2}}\left[\frac{5G_4(\tau_\beta)}{4G_1(\tau_\beta)}-\frac{L_2}{2}P_1(\tau)+\frac{1}{4}P_3(\tau)-\frac{L_1}{2}Q_1(\tau)\right]P_1^1(\zeta) \tag{11}$$

for every $\tau_\alpha\le\tau\le\tau_\beta$ and $|\zeta|\le 1$. On the other hand, the leading term of the total pressure field series implies

$$\mathrm{P}^{(LT)}(\tau,\zeta)=\mathrm{P}_0+\frac{U\mu}{Dc(\tau^2-\zeta^2)}\left[-\frac{5G_4(\tau_\beta)}{2G_1(\tau_\beta)}-\frac{15}{2}P_3(\tau)\right]P_1(\zeta) \text{ for every } \tau_\alpha\le\tau\le\tau_\beta \text{ and } |\zeta|\le 1, \tag{12}$$

whereas P_0 is an arbitrarily chosen constant reference pressure, whose value depends on the physical problem. Finally, the corresponding leading expression for the vorticity is

$$\boldsymbol{\omega}^{(LT)}(\tau,\zeta)=\frac{U\hat{\boldsymbol{\varphi}}}{Dc(\tau^2-\zeta^2)\sqrt{\tau^2-1}}\left[\frac{5}{14}(P_2(\tau)-P_4(\tau))+\frac{5G_4(\tau_\beta)}{2G_1(\tau_\beta)}P_1(\tau)\right]P_1^1(\zeta) \text{ with } \tau_\alpha\le\tau\le\tau_\beta \text{ and } |\zeta|\le 1. \tag{13}$$

The implicated constants yield

$$L_1=G_4(\tau_\alpha)P_1(\tau_\alpha)-G_2(\tau_\alpha)P_3(\tau_\alpha)+M\left[\frac{G_2(\tau_\alpha)}{P_1(\tau_\alpha)}+P_1(\tau_\alpha)\right] \text{ and}$$
$$L_2=H_2(\tau_\alpha)P_3(\tau_\alpha)-G_4(\tau_\alpha)Q_1(\tau_\alpha)-M\left[\frac{H_2(\tau_\alpha)}{P_1(\tau_\alpha)}+Q_1(\tau_\alpha)\right] \tag{14}$$

with

$$M=\frac{5P_1(\tau_\alpha)}{P_1(\tau_\beta)}G_4(\tau_\beta) \text{ and } D=\frac{1}{2G_2(\tau_\beta)}\left[L_2G_2(\tau_\beta)-3G_4(\tau_\beta)+L_1H_2(\tau_\beta)\right]. \tag{15}$$

The relative special functions within expressions (9) to (13) are given for convenience reasons as

$$G_1(x)=-P_1(x)=-x,\ 2G_2(x)=1-x^2,\ 8G_4(x)=(5x^2-1)(1-x^2),\ 4H_2(x)=(1-x^2)\ln\frac{x+1}{x-1}+2x \tag{16}$$

and

$$2P_2(x)=3x^2-1,\ 2P_3(x)=x(5x^2-3),\ 8P_4(x)=35x^4-30x^2+3,\ Q_1(x)=P_1(x)Q_0(x)-1,\ 2Q_2(x)=2P_2(x)Q_0(x)-3x, \tag{17}$$

where either $x\equiv\tau\in[\tau_\alpha,\tau_\beta]$ or $x\equiv\zeta\in[-1,1]$, while

$$P_1^1(x)=\sqrt{1-x^2},\ 2Q_0(x)=\ln\frac{1+x}{1-x} \text{ for } x\equiv\zeta\in[-1,1] \text{ and } P_1^1(x)=\sqrt{x^2-1},\ 2Q_0(x)=\ln\frac{x+1}{x-1} \text{ for } x\equiv\tau\in[\tau_\alpha,\tau_\beta]. \tag{18}$$

The above results (9) to (13) with (14) to (19) correspond to the leading term of a stream function $\psi^{(LT)}$, which admits

$$\psi^{(LT)}(\tau,\zeta)=\frac{Uc^2}{D}\left[-\frac{5G_4(\tau_\beta)}{2G_1(\tau_\beta)}G_1(\tau)+L_2G_2(\tau)-\frac{1}{2}G_4(\tau)+L_1H_2(\tau)\right]G_2(\zeta)\text{ for any }\tau_\alpha\le\tau\le\tau_\beta\text{ and }|\zeta|\le 1, \tag{19}$$

as a fair approximation of the flow behavior.

The corresponding results for the oblate spheroid can be readily obtained through the simple transformation

$$\tau\to i\lambda\text{ and }c\to -i\bar{c}\text{ with }i\equiv\sqrt{-1}, \tag{20}$$

being the imaginary unit, while $0\le\lambda<+\infty$ and $\bar{c}>0$ are the characteristic variables of the oblate spheroidal geometry.

3.2 | Numerical simulation

For the simulation of the flow through the spheroidal structure, the flow module of the CFD–ACE+ has been used. Both, inlet and outlet flows, in and out of the porous medium volume, with the velocity magnitude set by the user as normal velocity, can be simulated to obtain velocity and pressure fields. The flow of the gas phase has been set as laminar flow due to the low to medium Reynolds number occurring by the velocity magnitude used. The governing equations are produced through the fundamental principles of mass conservation (there is no loss or gain of mass in the system) and the Newton's second law. In particular, conservation laws of the form of the generic transport equation constitute the Navier-Stokes equations, in which the conserved variables are the mass, momentum, and total energy. The simplest component of this system of partial differential equations is always the continuity equation, where it is rather straightforward to arrive at the Navier-Stokes equations by simple mathematical manipulations.[18] By discretizing in space, the Navier-Stokes equations have been integrated numerically by using the finite volume method, which in particular corresponds to a generalized discrete algebraic equation,[19] which can be handled accordingly.

When such a system is formulated for each computational cell, it results in a set of coupled nonlinear algebraic equations, where no direct matrix inversion method is available to solve it. Therefore, an iterative procedure is employed in CFD–ACE+ at every time step, where an equivalent linear equation is formed by evaluating the link coefficients with the values of available at the end of the previous iteration. The linear system was solved by using successful over-relaxation scheme, which is adequate for successfully solving linear systems of big amount of equations and unknowns.

For the simulations, a number of HP Compaq 6000 Pro MT PCs were used with Intel Core ™2 Duo CPU E7500 at 2.93GHz and 2GB RAM memory. The solver was installed on a Windows 7—32Bit operating system. By discretizing the geometry in 109 792 cells, approximately 300 iterations were needed to achieve convergence within 10 to 26 minutes, depending on the parameters' values. In accordance to the stream function (19), which is the main analytical result, typical microscopic results are presented in Figure 2.

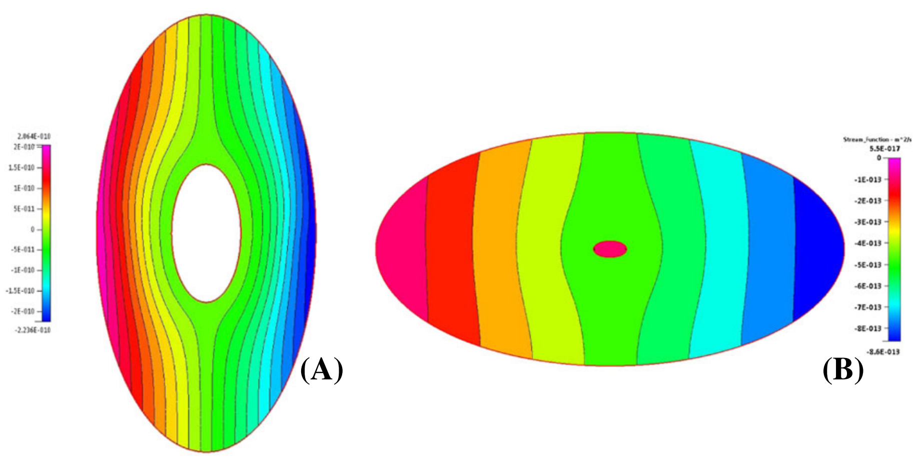

FIGURE 2 Stream function for prolate (A) and oblate (B) spheroidal geometry [Colour figure can be viewed at wileyonlinelibrary.com]

The parameters used were as follows: the spheroids were of aspect ratios $0.2 < a < 5$, in order to model both prolate and oblate cases, while for this range, the first terms of the series are sufficient for most engineering applications. If V, V_s, and V_l are the volumes of our system, the solid and the liquid phase, respectively, then $V = V_s + V_l$, while in terms of the fraction $\gamma = V_s/V$ of the solid phase, the porosity is $\varepsilon = 1 - \gamma$. To be compatible with the use of the leading terms, we are obliged to use $\gamma < 0.3$, while Reynolds number $10^{-4} < \text{Re} \equiv \rho U[2a_1(\tau_0)]/\mu < 10^{-2}$ with $\tau_0 \in [\tau_\alpha, \tau_\beta]$ to secure the laminar flow assumption. In Table 3, we summarize the values used in the simulations.

3.3 | Results and discussion

To quantify the agreement between the obtained analytical and the performed numerical results with Darcy's law predictions, the ratio λ is used (see the outcome in Table 2). It is important to note here that this law could be applicable under the prerequisite of known permeability. To obtain this value, the reverse problem is considered: by solving the micro-scale problem, the velocity and the pressure fields could be obtained; therefore, it is easy to apply pressure gradient and flowrate to Darcy's formula in order to calculate the permeability value. The preceding set of diagrams represent λ as a function of the solid volume fraction in the prolate (see Figure 3) and the oblate (see Figure 4) spheroidal coordinate system.

It is clearly depicted that the Darcy's law is of high accuracy when Kuwabara's spheroidal-in-cell model is applied to describe flow through spheroidal grains. This good agreement can be attributed to the identical velocity values of U used both in Darcy's law calculations and in simulations. Furthermore, the numerical simulations present better accuracy than the analytical one, due to the simplifications applied in the analytical treatment, where only the first term of the series was utilized, approximating the solution through polynomials. The comparison between numerical and analytical results shows that the optimal agreement is achieved for low solid volume fraction values (high porosities) and high axis ratios, as expected, where the above simplifications become insignificant.

TABLE 3 Parameters used in the simulations

Parameter	Value
Density	997 kg/m^3
Dynamic viscosity	0.000855 kg/ms
Porosity	0.995, 0.9, 0.8, 0.7
Reynolds	0.0001, 0.001, 0.01
Aspect ratio	2/1, 0.5/1
Permeability (for aspect ratio 2/1)	0.409, 0.00789, 0.00251, 0.00127 m^2
Permeability (for aspect ratio 0.5/1)	0.15600525, 0.02581777, 0.000779, 0.000345 m^2

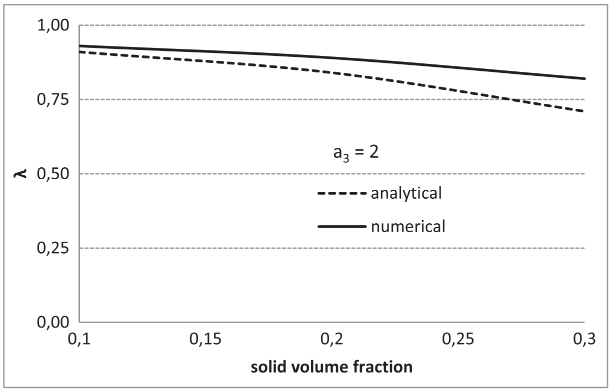

FIGURE 3 Validation of Darcy's law against solid volume fraction in prolate spheroidal geometry

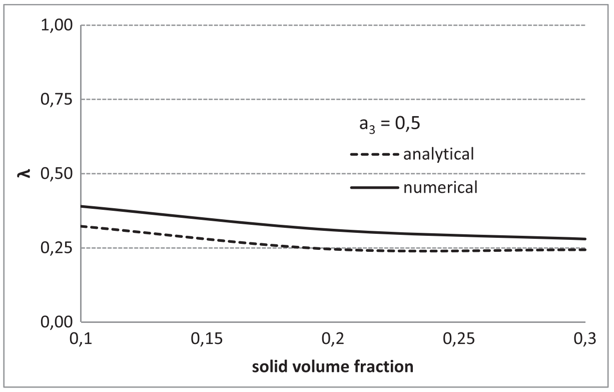

FIGURE 4 Validation of Darcy's law against solid volume fraction in oblate spheroidal geometry

4 | CONCLUSIONS

In the present work, a well-defined methodology has been established in order to validate simulations' results in a globally valid manner. This methodology initially identifies the system and the phenomena occurring there and describes mathematically the processes using fundamental principles and balances.

The solution of the mathematical problem leads to one macroscopic quantity that has been accepted as indicator of the validity of the disclaiming hypothesis. The above methodology has been successfully applied to the problem of flow through a swarm of spheroidal solid grains, where simulation results have been evaluated against Darcy's law predictions. The quality of this agreement further strengthens the power of the presented methodology as a unique engineering tool.

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