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ESTIMATION OF INTRINSIC VISCOSITY OF APPLE CELLS BY NUMERICAL SIMULATION

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extensional flow, Einstein equation, COMSOL Multiphysics

ABSTRACT

A numerical simulation approach was proposed to estimate the intrinsic viscosity of particles with complex geometry. The approach is based upon the solution of the mass and the momentum conservation equations for an incompressible Newtonian fluid under steady-state creeping flow around the particle. The reliability of the approach is demonstrated after solving the problem for fluid flow around a small sphere, whose effect is known after theoretical work. The approach is then applied in solving the same problem for different apple cells. The intrinsic viscosity varies with the particle shape and its orientation, between 2.6 and 4.6.

INTRODUCTION

Understanding the rheology of food materials is essential for the standardized characterization of raw materials and innovative products, as well as for optimized industrial processing (Fischer and Windhab 2011). In the case of apple purees, bulk measurements have allowed to evaluate the influence of particles size and insoluble solids content on the suspension rheological properties (Espinosa-Muñoz et al. 2013); further, direct observation has demonstrated the ability of apple cells to compress and decrease their volume when the concentration of the suspension increases (Leverrier et al. 2017). As a complement to experimental work, numerical simulation can provide useful information linking these two scales (bulk and cell). Indeed, the rheology of particle-fluid suspensions through numerical simulation has been studied since the 1990's, for instance by solving the dynamics of the solid particles combined with a Lattice Boltzmann approach for the fluid phase in the case of spheres, cylinders, or disks (Ladd and Verberg 2001).

It is clear that many of the complex phenomena associated with a flowing suspension cannot be explained by using a classical Newtonian description of a fluid with an ef-

fective viscosity. The volume fraction of the particles in a suspension (volume occupied by particles per unit volume of suspension) has often been assumed to be the only variable that influences the observed rheological properties of the suspension. Experimental evidence has shown that this is incorrect and that other factors, such as the shape and size distribution of the particles, the presence of electrical charges, and the type of flow being experienced must be considered (Jeffrey and Acrivos 1976). The study of the hydro-dynamical contributions of non-Brownian particles to the rheology of suspensions usually starts with diluted systems, i.e., those in which there are so few particles that occasional collisions between particles can be ignored. In such case everything one needs to know can be obtained from studying the flow around a single particle (Mewis and Wagner 2012, p.41).

Einstein (1906) has shown that the viscosity η of a diluted suspension of rigid spheres, treated as an incompressible homogeneous liquid, divided by the viscosity η_ℓ of the pure liquid, can be expressed as a linear function of the volume fraction of particles, ϕ :

$$\eta / \eta_\ell = 1 + \alpha \phi . \quad (1)$$

The parameter α is called intrinsic viscosity, being equal to 2.5 for very diluted spherical particles. Since then, much work has been devoted in describing the relative viscosity of disperse systems as a function of the concentration of the dispersed phase: equations have been developed on a theoretical foundation; theoretical equations have been adapted to empirical results; and empirical expressions have been reformulated in such a way that the Einstein equation (1) is obtained at very low concentration. Fifty years ago, dozens of formulas were already available (Rutgers 1962).

Theoretical computation of the relative viscosity due to very diluted ellipsoidal particles has demonstrated that the parameter α in the Einstein equation (1) can assume values from 2 up to 10 depending on the particle shape and orientation (Jeffery 1922). These findings have provided a physical, micro-structural explanation of observations, including changes of rheological regime as the volume fraction increases (Mueller et al. 2010).

Looking for a method to investigate the role played by the particle shape on the intrinsic viscosity, we propose a numerical simulation approach for studying the effect on the flow of a liquid around a particle suspended in it. In this contribution two kinds of particles are considered: spheres, as a way to assess the reliability of the approach; and some apple cells, in order to explore the potential of our approach in the case of irregularly-shaped particles.

METHODS

Particles in the liquid constitute obstacles to fluid flow; hence their presence distorts the flow field. Further, there is friction at the surface of particles. Both effects are expected to increase the energy dissipation during flow, and hence the apparent viscosity, above that of the pure suspending medium (Mewis and Wagner 2012, p.46).

Our rationale is based on the thought experiment of Einstein (1906) in his theoretical analysis dealing with the viscosity of diluted suspensions. In a first step, we solve an extensional stationary fluid flow problem associated with the presence of a very small particle placed in the center of a volume of incompressible Newtonian liquid. The viscous dissipation W is calculated by integrating $\eta_\ell(\dot{\gamma})^2$ over the liquid volume under consideration, where η_ℓ is the viscosity of the liquid phase, and $\dot{\gamma}$ is the shear rate field. The second step involves the solution of the problem but without the particle in the liquid volume. This second problem is associated with a smaller viscous dissipation W_ℓ , due to a shear rate field $\dot{\gamma}_\ell$ which does not exhibit the features characterizing the flow disturbances occurring in the first problem. The relative viscosity η/η_ℓ due to the presence of the particle in the liquid volume is finally obtained by computing the ratio W/W_ℓ .

The mass and momentum conservation equations for an incompressible Newtonian fluid under stationary conditions can be written as:

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

$$\rho(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot (-p\mathbf{I} + \eta_\ell(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)), \quad (3)$$

where \mathbf{u} is the velocity (magnitude in $\text{m}\cdot\text{s}^{-1}$) and p the pressure (Pa); ρ is the liquid density ($\text{kg}\cdot\text{m}^{-3}$) and η_ℓ its viscosity (Pa.s).

Following Einstein, here we consider extensional flow around the particle. The computational domain is a cube; two opposite faces are associated with outflow, while the four remaining ones correspond to inflow. At the particle surface, the velocity field is assumed to vanish. At the two outlet boundaries, the pressure p is assumed to vanish under no viscous stress. At the four inlet boundaries, the velocity components u, v, w are prescribed as:

$$u = A(x - x_0), \quad v = B(y - y_0), \quad w = C(z - z_0), \quad (4)$$

where the coordinates (x_0, y_0, z_0) indicates the barycenter of the particle. On account of the incompressibility of the liq-

uid, the constants $A, B,$ and C must fulfill the condition $A + B + C = 0$. Three scenarios are here considered:

- $A = 1, B = C = -1/2$; outflow through the cube faces which are parallel to the plane YZ;
- $B = 1, A = C = -1/2$; outflow through the cube faces which are parallel to the plane XZ; and
- $C = 1, A = B = -1/2$; outflow through the cube faces which are parallel to the plane XY.

Only one scenario is required in assessing the relative viscosity due to spheres. In the case of apple cells, the application of these scenarios is equivalent to consider three arbitrary orientations for the particle in respect to the fluid flow. The liquid is characterized by the density $\rho = 1000 \text{ kg}\cdot\text{m}^{-3}$ and the dynamic viscosity $\eta_\ell = 0.001 \text{ Pa}\cdot\text{s}$ (similar to pure water at 20°C). This problem is solved under creeping regime: Reynolds number is smaller than 1.5 for all the cases.

Equations (2) and (3) need to be solved firstly with the particle at the center of the computational domain, and later in its absence. These equations are solved through the finite-element method as implemented in the simulation package COMSOL Multiphysics software (version 5.2.0.220; COMSOL, Inc., Burlington, Massachusetts) (Zimmerman 2006). Three-dimensional domains are commonly approximated by a mesh of polyhedrons in the process of setting up the equations for finite-element analysis. In this study the domains are subdivided into large numbers of small, non-overlapping tetrahedrons, which allow suitable geometrical approximations of virtually any three-dimensional shape. Discretization of equations (2) and (3) considers first-order Lagrange finite elements for the velocity components and the pressure. The solution of the linear system obtained after discretization of governing equations is reached through the direct solver PARDISO (Schenk and Gartner 2004). Satisfactory convergence of the numerical model is reached in looking for a relative tolerance smaller than 10^{-6} .

SPHERES

Figure 1A illustrates the computational domain, built around a sphere corresponding to the volume fraction of 0.4%. Figure 1B displays model predictions of the velocity field, after solving the fluid flow problem in the presence of that sphere. Velocities vanish in the vicinity of the sphere, as a consequence of friction (no slip condition at the particle surface). This leads to distortion of the flow field, which is put in evidence in Figures 1C and 1D.

Model predictions of the relative viscosity were obtained at different mesh resolutions. Solving the problem with the coarser mesh required less than 2 Gb-RAM and few seconds; the application of the finer mesh required above 190 Gb-RAM, and results were available after some days of work on a Windows-7 64-bit SP1, Intel Xeon CPU ES-2630 v3 @ 2.40 GHz, 192 Gb-RAM computer.

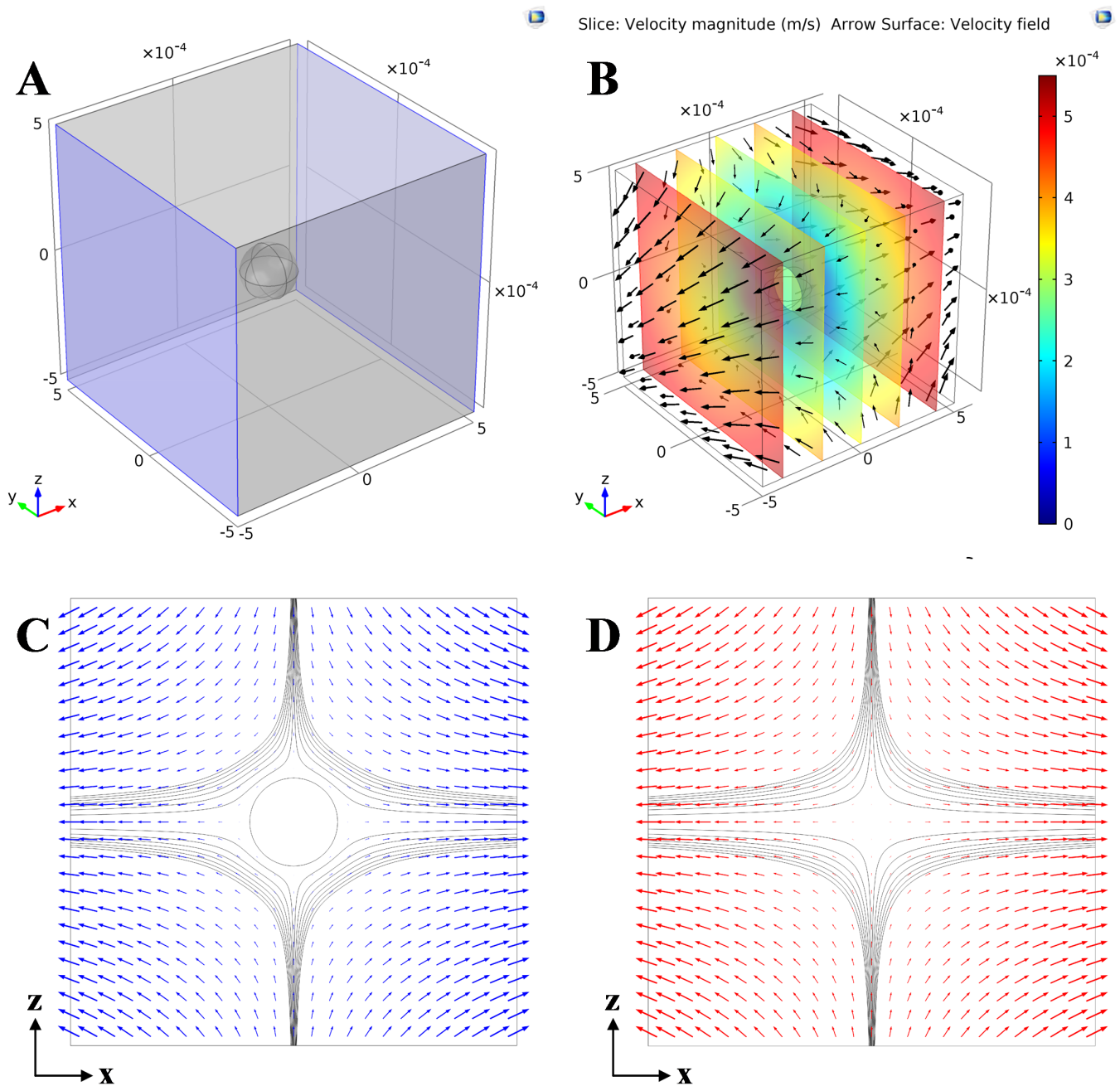


Figure 1: Display **A** shows the computational domain for a sphere corresponding to the volume fraction of 0.4 %, where the blue faces indicate domain outlets when outflow boundary conditions correspond to $A = 1$. Display **B** presents model predictions of the velocity field around such a sphere, in 3D representation; the same model predictions are presented in display **C** with the help of streamlines and velocity vectors in the plane $Y = 0$. Display **D** presents model predictions of the velocity field in the absence of the sphere. Dimensions are expressed in meters.

Figure 2 summarizes results obtained for spheres corresponding to the volume fractions of 0.1 % and 0.4 %. Model results converged with the mesh resolution, and the values predicted for the relative viscosity due to such spheres became quite stable above 5×10^5 mesh elements. Even applying the highest mesh resolution, there is a difference between values predicted for the relative viscosity from the model and those from the Einstein equation (1); further, such a difference increases with the volume fraction. In fact, the intrinsic viscosity is defined for infinitely small volume fraction as $\alpha = \lim_{\phi \rightarrow 0} (\eta - \eta_\ell) / (\eta_\ell \phi)$. Assuming a volume fraction of 0.4 % in numerical simulation leads to slightly overestimate the intrinsic viscosity, $\alpha_{0.4\%} \sim 2.54$, whereas using 0.1 % gives $\alpha_{0.1\%} \sim 2.50$.

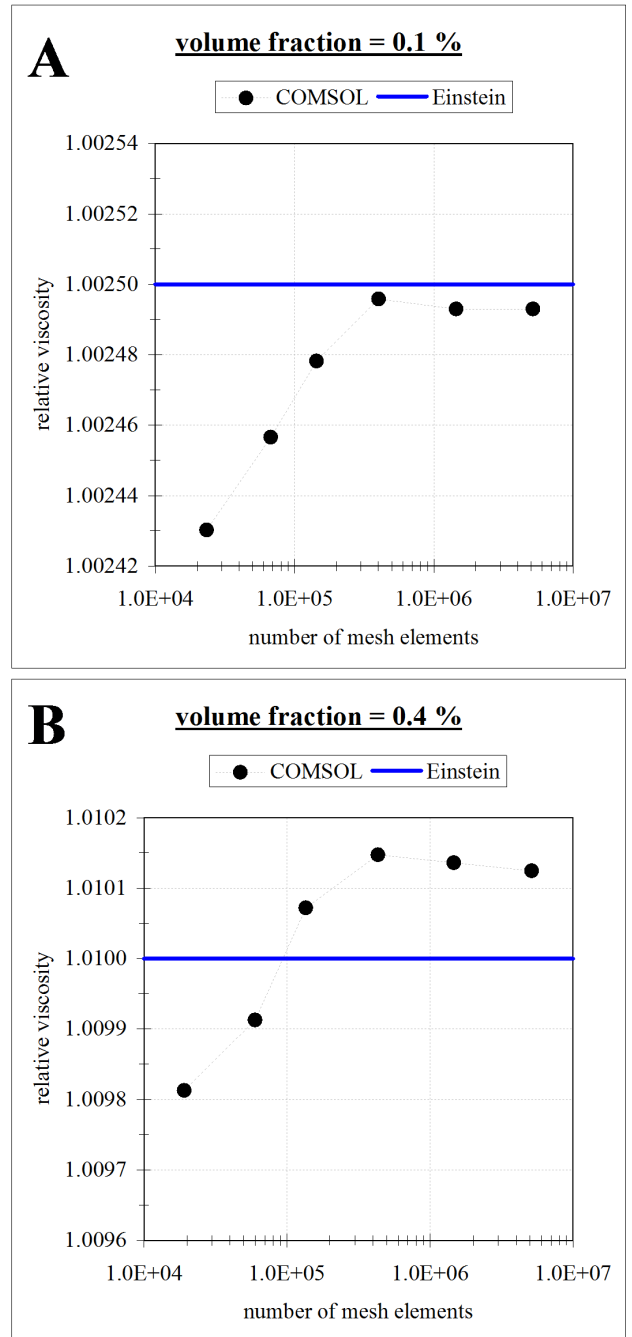


Figure 2: Model predictions of the relative viscosity due to spheres, after assuming a volume fraction of 0.1 % (A) and 0.4 % (B), as function of the number of mesh elements. Blue lines indicate the value as estimated from the Einstein equation (1) for $\alpha = 2.5$.

APPLE CELLS

The application of numerical modeling to problems involving real food particles constitutes a challenging task. On one hand, the irregularly-shaped particles that we found in real-world problems can exhibit very complex geometrical features. Under such conditions, the construction of the computational domain needs to include a realistic representation of the particles of interest as provided by image acquisition and post-processing. On the other hand, meshing algorithms can forbid the construction of relatively coarse meshes for detailed geometries. As noted above, higher is the resolution in meshing the computational domain, larger is the computer memory required and longer is the simulation time needed for reaching a satisfactory solution.

Our numerical modeling approach was applied to three apple cells (Leverrier et al., 2017). The volume occupied by each apple cell was about 1.36, 3.40 and $1.27 \times 10^6 \mu\text{m}^3$, respectively; the geometry of each cell was obtained using confocal microscopy and three-dimensional reconstruction. These apple cells were sampled from a moderately diluted apple puree (0.47 g of insoluble solids per 100 ml of suspension; volume fraction of 0.43); the cells are expected do not change their shape under fluid flow.

Three steps were conducted in order to consider those apple cells in our numerical approach.

- Firstly, the volume associated with each cell was subdivided into a large number of tetrahedrons. This was performed through the Simpleware software environment and its +FE Mesh Generation Module (version 2016.09-SP1; Synopsis, Inc., Mountain View, California). Looking for a detailed representation of the cells, a relatively high meshing resolution was considered; the resulting volume meshes are constituted by about 1.8 , 3.7 , and 2.3×10^6 tetrahedrons.
- Secondly, the file containing the volume mesh generated by Simpleware was imported into the COMSOL environment, in which we created a 3D representation of the apple cell considered. The results obtained can be appreciated in Figure 3.
- Lastly, a cubic computational domain was built, whose center coincides with the cell barycenter. The volume fraction corresponding to the cell is assigned, hence the cube volume becomes a multiple value of the cell volume (say, 250 times higher for a volume fraction of 0.4 %).

The standard options of the COMSOL Multiphysics mesh generator gave origin to great heterogeneity in the size of elements. Hence, the subdivision of the computational domain was customized in order to generate a large number of tetrahedrons with similar size. The shortest edge of mesh elements was set to be a sub-multiple of the side L of the liquid

cube representing the computational domain; and the ratio of their longest edge to the shortest edge was set to be 4.

Figure 4 shows results reached for the apple cells after assuming the volume fraction $\phi = 0.1 \%$ and 0.4% , taking into account the three sets of flow boundary conditions. Sensitivity tests were performed on the mesh resolution in solving the flow problem for the three apple cells in the case of boundary conditions associated with $A = 1$. Quite stable results were obtained above 10^6 mesh elements; hereafter only the results obtained with the finest mesh are discussed.

Table 1 translates model predictions of relative viscosity into estimates of intrinsic viscosity. All the values are higher than 2.5, associated with the Einstein equation (1). This was expected as a consequence of the irregular, non-spherical shape of particles under consideration. Essentially the same estimates of intrinsic viscosity are obtained from model simulations performed for $\phi = 0.1 \%$ and 0.4% . Table 1 indicates that, for a given particle, the intrinsic viscosity depends on the particle orientation with respect to the flow boundary conditions. The relative standard deviation (or coefficient of variation) of α is smaller for one cell (#1) than for the other two, without any apparent reason from the visual inspection of their 3D appearance. As shown in Figure 3, each apple cell exhibits a variety of geometrical features, including convex and concave regions, as well as rugged and smooth areas. It seems difficult to anticipate the influence of the geometrical features exhibited by an apple cell on its intrinsic viscosity.

SUMMARY AND FUTURE WORK

- Results obtained for spheres demonstrated the reliability of our approach for volume fractions below 0.4%. Differences between model results and estimates from the Einstein equation (1) remained below 2 % of the intrinsic viscosity value (2.54 instead 2.5 for $\phi = 0.4\%$).
- Model predictions of the intrinsic viscosity due to an isolated apple cell are higher than for a sphere. Such an increase depends on the cell shape as well as on its orientation with respect to the extensional flow.

Results presented above were obtained after placing the cube center at the particle barycenter. In fact, we should consider the position at which the forces exerted by the fluid on the particle exhibit null resultant. Such a steady-state position of the particle could differ slightly from its barycenter. Further, only three different orientations were considered in obtaining the results shown above. Two conditions deserve attention regarding the estimation of the intrinsic viscosity. At low shear (Peclet number < 1), thermal agitation dominates, and the particle orientation is random. Therefore the intrinsic viscosity at low shear should be based on the averaged value obtained from numerous orientations. Inversely, at high shear (Peclet number > 100), thermal agitation becomes negligible; the particle orientation is expected to be in

the direction corresponding to the lowest viscous dissipation, say to the lowest intrinsic viscosity. The latter could also be obtained by turning the particle until the torque vanishes. Finally, a larger set of apple cells should be considered in order to obtain statistically significant values.

The determination of the intrinsic viscosity of apple cells can be useful to estimate the volume fraction which is occupied by solid particles in apple juices or apple purees. Indeed, one could progressively dilute the apple-based food product, searching conditions where the suspension viscosity becomes a linear function of the concentration; then, knowing the viscosity of the continuous phase (e.g. the supernatant after centrifugation), the volume fraction could be estimated from the measurement of the suspension viscosity.

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AUTHOR BIOGRAPHY

ARTEMIO PLANA-FATTORI studied Atmospheric Sciences in the Universidade de Sao Paulo and later in the Université de Lille. After 20 years teaching and conducting research in Brazil, he joined AgroParisTech in 2010, where he has working with numerical modeling applied to food engineering.

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CHRISTOPHE DOURSAT and GIANA ALMEIDA are Professors, CASSANDRE LEVERRIER is Assistant Professor, and GABRIELLE MOULIN is Assistant Engineer, all at AgroParisTech.

EVEN OU contributed to this study in the scope of his research internship at AgroParisTech.

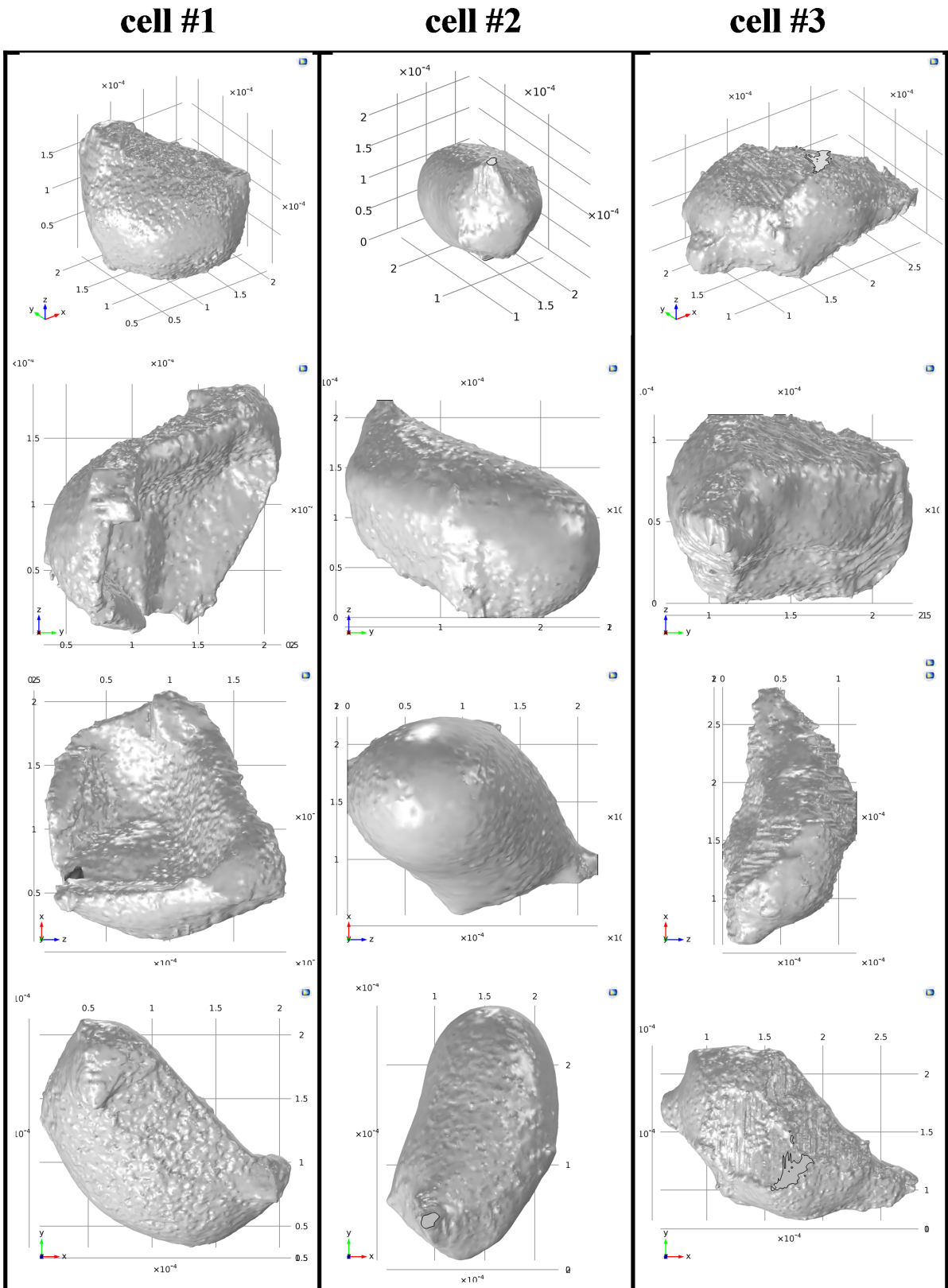


Figure 3: The apple cells here considered, after 3D reconstruction by the COMSOL Multiphysics geometry builder. The second, third, and fourth rows from the top exhibit the apple cells facing one of the cube outlets, when applying the flow boundary conditions associated with $A = 1$, $B = 1$, and $C = 1$, respectively (see METHODS). Dimensions are expressed in meters.

$\phi = 0.1 \%$					
cell	$A = 1$	$B = 1$	$C = 1$	average	RSD
#1	4.47	4.25	4.53	4.42	0.03
#2	2.67	3.42	2.92	3.00	0.13
#3	3.75	3.24	2.92	3.31	0.13

$\phi = 0.4 \%$					
cell	$A = 1$	$B = 1$	$C = 1$	average	RSD
#1	4.55	4.33	4.62	4.50	0.03
#2	2.70	3.46	2.95	3.04	0.13
#3	3.81	3.30	2.97	3.36	0.13

Table 1: Estimates of the intrinsic viscosity α , from the results displayed in Figure 4. RSD stands for relative standard deviation (i.e. coefficient of variation).

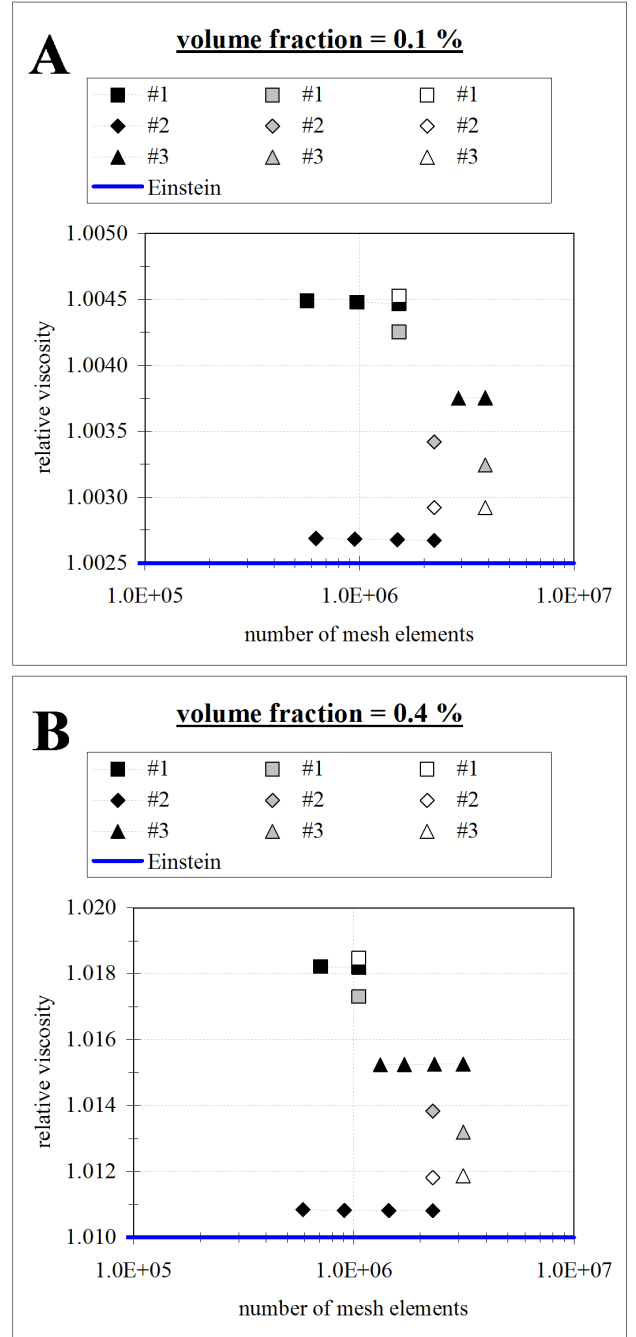


Figure 4: Model predictions of the relative viscosity due to the three apple cells as a function of the number of mesh elements, by assuming a volume fraction of 0.1 % (A) and 0.4 % (B). Blue lines indicate values associated with the Einstein equation (1) for $\alpha = 2.5$. Black, gray, and open symbols indicate results obtained after assuming the flow boundary conditions associated with $A = 1$, $B = 1$, and $C = 1$, respectively.