ON SIMULATION OF SOFT MATTER AND FLOW INTERACTIONS IN BIOMASS PROCESSING APPLICATIONS

Uldis Strautins, Maksims Marinaki
Institute of Mathematics and Computer Science, University of Latvia, Latvia
uldis.strautins@lu.lv, maksims.marinaki@lu.lv

Abstract. In this research, we extend our studies of the extraction process from diverse plant materials, introducing advancements to our previous models. Our framework considers dynamic elements by taking into account the motion of the particles, departing from the statical particle assumption in prior articles. Several methods such as moving geometries or modified equations for a system with moving particles in Lagrangian coordinates are introduced to boost the precision of our simulations, taking into account the complex dynamics of the solvent and its interaction with the plant material. Expanding beyond our focus on supercritical carbon dioxide (scCO2), our research is addressing some different applications. Besides the traditional solvent-based extractions, we consider potential applications in filtration, wood industry processes, etc. This allows our model to adapt to diverse industrial contexts with varied extraction mediums. Our coupled system of equations contains fluid dynamics equations for solvent flow, reaction-advection-diffusion equations for solute, and equations governing remaining solute concentration in biomass. The exchange of active material between solid and fluid is modelled by the Langmuir law. Applying finite volume techniques and implemented in the Octave/Matlab environment, our model captures the temporal evolution of two and three dimensional solute distribution and solvent velocity field. This modular framework facilitates the integration of tailor-made laws to represent diverse plant materials, ensuring versatility across applications. Through our simulations, we present the analysis of our modified model's performance and discuss its advantages and limitations. This research is a slight step forward in understanding and optimising extraction processes, offering valuable insights for industries involved in functional foods, nutraceuticals, pharmaceuticals, cosmetics, filtration, and wood processing.

Keywords: biomass, virtual design, PDEs, hydrodynamics.

Introduction

There are many applications that require flow simulations that take into account the detailed particle motion in the flow. One of them is supercritical carbon dioxide extraction (scCO2) – a process that has gained vast popularity nowadays, and we also recognize some broader applications. Industries ranging from pharmaceuticals to cosmetics, functional foods to the wood sector – all deal with the potential usage of natural resources. Bearing in mind such a variety of applications a rather detailed description of the underlying processes is required. In this paper we extend our investigations of the extraction process from various plant sources, implementing enhancements of our previous models. We use our prior simulation results and develop our model to the extent where we can thoroughly describe the process to the point when tracking the motion of each single particle in the flow is possible.

Various approaches for simulating low to moderate Reynolds number flow of particle laden fluid through complex geometry have been proposed in articles and literature, starting from simulations resolving the boundary of the particles to mesh free methods to mixed eulerian-lagrangian methods such as the fictitious domain method, which requires no re-meshing of the computational domain.

In [1] various numerical simulation methods for studying the motion of rigid particles suspended in fluid are considered. The choice of the method should account for the fluid to solid density ratio, more about that in [2]. Regarding the comparison between the solutions obtained using the continuous model and simulations evaluating the forces on each particle individually, article in [3]. More on modern numerical methods that play a significant role in the analysis of complex particulate flows in [4]. Recent progress using particle-resolved direct numerical simulations to discover new multiphase flow physics and develop models are reviewed in [5]. Also, the present paper is a logical continuation of recently published [6], where the extraction process was considered for random and stationary particle distribution. The paper [7] provides a basic mathematical model founded on the Broken-and-Intact Cell (BIC) approaches with the applications in simulating the extraction of bioactive compounds from plants using supercritical fluid. The article [8] gives a review of mathematical modelling methods used in the extraction process, along with a thorough analysis of the mathematics behind the different stages in the procedure. In [9; 10] there is an explanation of the finite volume method and its application in numerical simulation, covering surface and volume integral approximations, cell interpolation methods, and treatment of the resultant systems of algebraic equations.

In the present article, we address a more general mathematical model of similar processes. Similar as in [6], we propose a coupled system of equations consisting of fluid dynamics equations describing the flow of the solvent and reaction-advection-diffusion equations for the solute, as well as equations describing the remaining concentration of the solute in biomass. By applying the Langmuir law, our model describes the exchange of active materials between the solid and the fluid phases. Notably, we do not presume homogeneity in the initial solute distribution or extraction parameters, allowing our model to describe the non-homogeneous plant material mixtures. We introduce advancements in modelling particle dynamics, which are characterised by the dynamics of their centre of gravity (COG) under the influence of hydrodynamic and gravitational forces. Our approach incorporates drag coefficients, accounting for surface area considerations, such as employing the Stokes drag coefficient. Moreover, we model the force exerted by particles on the fluid using a three-dimensional Gaussian kernel. Notably, the movement of particles serves as sources of solute within the system. By executing our simulations, we obtain the temporal evolution of the solute three-dimensional distribution and the velocity field of the solvent. We track the patterns of the particle depositions and thus step-by-step make our models more realistic. This approach enables a rather detailed description of extraction processes within virtual designs. Furthermore, our model's modular nature facilitates the incorporation of laws tailored to specific plant materials. The obtained framework potentially could be applied for a spectrum of plant materials. Practical examples show its utility in real-world applications and advancements in different technologies.

Materials and methods

In [6] a model was presented where the biomass particles were fixed, and the exchange of the active compound between the biomass particles and the solvent was simulated by advection-diffusion-reaction equations. Here we extend this model by adding particle dynamics in two stages: first the particles are injected in the extraction chamber, and then they form a "biomass cake" where the particles are essentially immobile. Every particle carries a time dependent amount of the active compound and releases it during the extraction process, allowing for simulating inhomogeneous batches.

We propose a system of partial differential equations consisting of fluid dynamics equations (1)-(2) describing the flow of the solvent and reaction-advection-diffusion equations for the solute (3), plus equations describing the remaining concentration of the active compound in the biomass (4):

$$\frac{\partial v}{\partial t} + \nabla \cdot (v \otimes v) = -\nabla p + \frac{1}{Re} \triangle v + f, \tag{1}$$

$$\nabla \cdot v = 0, \tag{2}$$

$$\frac{\partial \varphi}{\partial t} + \nabla \cdot (v\varphi) = \alpha \triangle \varphi + R(\varphi, \psi), \tag{3}$$

where v – solute velocity;
p – pressure;
f – density of external forces acting on the solute;
$\varphi(r, t)$ – the concentration of the active compound in the solvent;
$R(\varphi, \psi)$ – rate of release of the solute from the biomass particles;
α – diffusivity of the solute in the solvent.

The concentration of the active compound ψ is the sum over individual particles:

$$\psi = \sum_i c_i(t) W(x - x_i(t)). \tag{4}$$

Here $c_i(t)$ is the time dependent concentration of the active compound in i-th particle and the function W is the Gauss kernel (defined below) representing the distribution of the active compound in the finite sized particle. The summation is over all the particles in the computational domain at the time. The rate of exchange of the active compound in i-th particle is

$$\frac{dc_i(t)}{dt} = k \left(\frac{Kc_i(t)}{Kc_i(t) + 1} - \varphi(x_i(t), t) \right). \tag{5}$$

Also function $\psi(r,t)$ represents the concentration of the active compound bounded in the particles interpreted as "intact" cells in BIC models [7]. The exchange rate into the solvent is

$$R(\varphi,\psi) = k\left(\varphi_{eq} - \varphi\right), \tag{6}$$

$$\varphi_{eq} = \frac{K\psi}{K\psi + 1}. \tag{7}$$

We utilize the Langmuir adsorption isotherm in our study, although it is worth mentioning that our software framework allows for the straightforward incorporation of alternative laws. In the simulations outlined in this paper, we approximate this law under conditions where the parameter k equals one dimensionless unit and K is five times greater. As for the Reynolds number in our standard simulations, it falls within a specific range between 0.6 and 8 in numerical values. The inlet boundary condition is:

$$\alpha\frac{\partial\varphi}{\partial n} + v_n\varphi|_{inlet} = 0, \tag{8}$$

provided that the inflowing solvent has $\varphi = 0$. The diffusion coefficient α was taken to be one unit. The remaining boundary conditions are $\varphi_n = 0$ at the walls. We additionally apply suitable boundary conditions for velocity and pressure, including homogeneous Neumann conditions for pressure at the rigid walls, either pressure or velocity conditions at the inflow, and Dirichlet pressure at the outlet.

Particle dynamics are described by their COG dynamics, influenced by hydrodynamic forces and gravity forces:

$$m_i\dot{x}_i = F_H + \frac{\rho_s - \rho_f}{\rho_s}m_i g. \tag{9}$$

Here dots over variables denote the time derivative, ρ_s and ρ_f denote density of the biomass particles and solvent respectively, and the hydrodynamic force acting on the i-th particle is

$$F_H = C_D(v(x_i,t) - \dot{x}_i) \tag{10}$$

and C_D is the total drag coefficient. For computations in the present article, we use the Stokes drag for a sphere with the radius a:

$$C_D = 6\pi\mu a. \tag{11}$$

The force the particles exert on the fluid is modelled by the 3d Gauss kernel:

$$W = (2\pi\sigma^2)^{-\frac{3}{2}}exp(-x^2/2\sigma^2), \tag{12}$$

where σ – related to the particle radius a.

By the third Newton's law, the back-coupling force exerted by the particles on the fluid is

$$f(x,t) = -\sum_i F_H \cdot W\left(x - x_i(t)\right). \tag{13}$$

In the presence of buoyancy or sedimentation of the particles we need to consider particle collisions with walls. We treat them as inelastic collisions: normal velocity component to the wall is set to zero in case of contact (particle sticks to the wall). The equations are discretized by using finite volume techniques and currently implemented in Octave/Matlab environment. We use the voxel geometry and it facilitates particle-wall collision detection. In the section below we present some graphical results produced by our code and discuss several features thereof.

Results and discussion

In the following figures we present the results of our simulations for different geometry settings. Similarly, as in [6], we will use the randomly allocated obstacles. In order to show how the process works, we will also use simpler (channel-type) domains. The determined obstacle geometry is the first test example for behaviour of particles. We start off with the setting containing one cylindrical obstacle and track the motion of the particles. The velocity field obtained by solving (1)-(2) has been used in order to solve the discrete version of (9)-(10). In Fig. 1 we can see sample trajectories of particles in domain with an obstacle (left). Particles deposit at the obstacle, chamber floor and at outflow (green dots represent particle contact with obstacles, right).

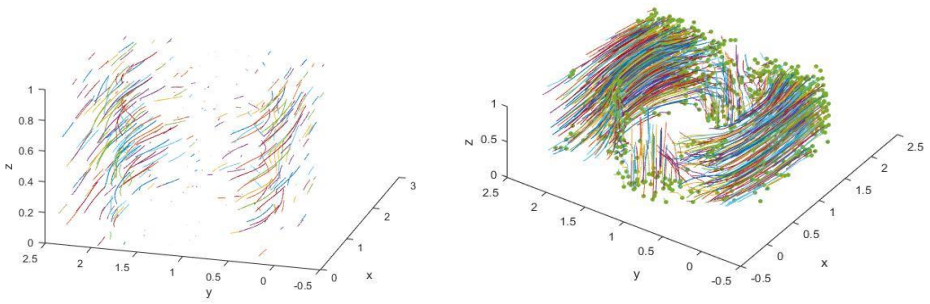

Fig. 1. **Trajectories of particles in domain with cylindrical obstacle**

Moreover, we consider the same process, but for different types of obstacle allocation. We randomize the obstacle positions and track the particles in the domain corresponding to more real-life settings for extraction and other applications. In Fig. 2, the extraction process in an inhomogeneous porous domain, characterised by predefined obstacles, is graphically represented. New particles are deposited at the outlet and near the obstacles. The solute concentration graph is on the left panel. Particle trajectories and deposition sites are on the right panel.

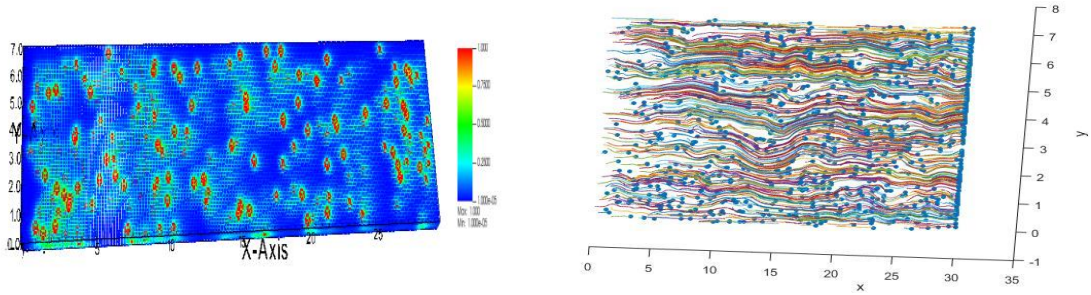

Fig. 2. **Extraction process in inhomogeneous porous domain**

In order to observe the behaviour of different portions of particles, forming a sort of a biomass "cake" – something of a wide interest in the application in terms of the appearance of certain layer-type patterns, we consider a channel type domain as well. In Fig. 3 we graphically represent the results of the filling simulation of a rectangular channel domain. We can observe the sample particle trajectories and deposition sites (blue dots, left panel). Also, one can see the formation of the biomass "cake" with 12000 particles. Deposition sites of the first 3000 particles are represented with yellow dots, next 3000 particles - with green dots, then blue, then red (right panel).

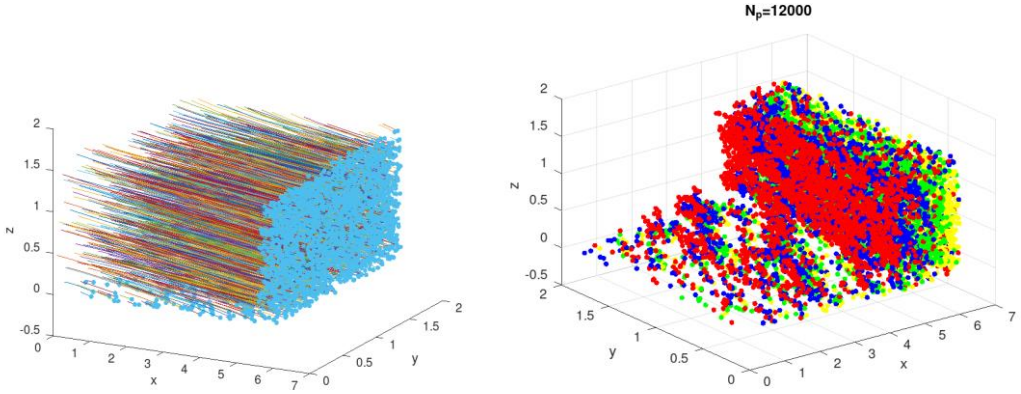

Fig. 3. **Filling simulation of rectangular channel domain**

Afterwards, once the modified setting has been obtained, several possibilities such as updating of the problem geometries or forces in the system have been examined experimentally. The modification of forces has shown more promising and experimentally stable results. The back-coupling of the system

has been performed by incorporating the back-coupling force exerted by the particles on the fluid (13) into the velocity equations (1)-(2). This led to certain changes in the velocity fields. In Fig. 4 we graphically represent the velocity fields for both settings as in Fig. 3 above. We can observe the decrease of the total flow for the same pressure gradient and also flattening of the velocity profile.

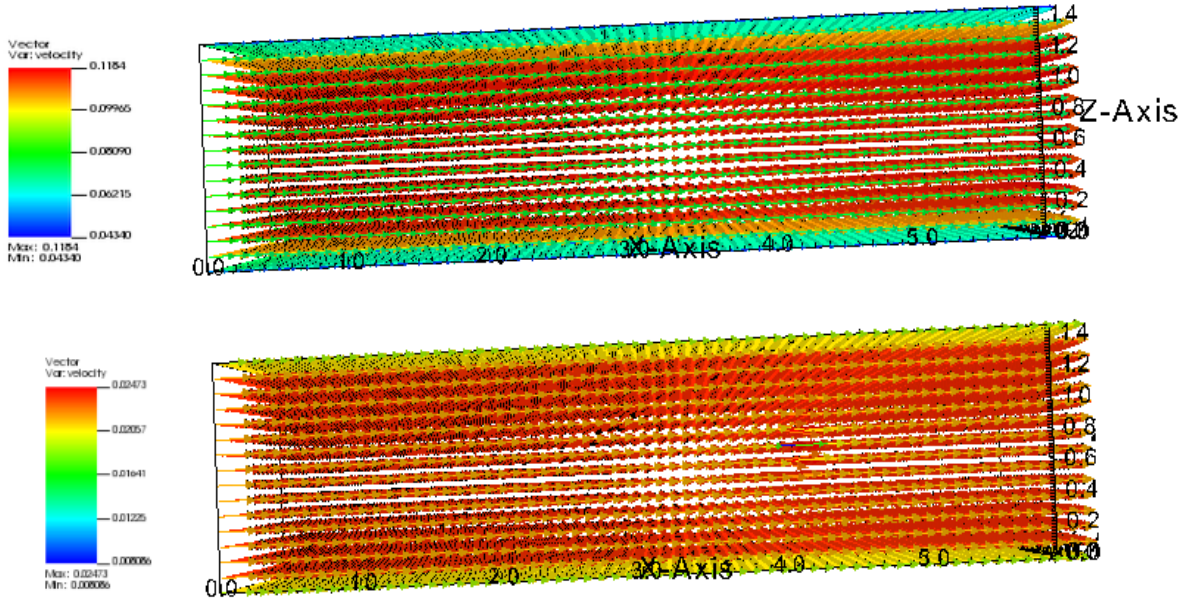

Fig. 4. **Velocity fields for the filling simulation in the (x, z) plane, same geometry as in Fig. 3:** upper panel – no flow interaction with particles; lower panel – interaction with particles; note the decrease of flow rate (at the same pressure drop) and flattening of velocity profile in the right panel

Conclusions

Biomass extraction process with continuous biomass feed can lead to rich and complex fluid-structure interaction. We have proposed a model describing in detail the dynamics and deposition of particles on the extractor walls and the back-coupling of the particle induced flow resistance in the Navier-Stokes framework. The simulation examples show particle trajectories travelling to the deposition site and deposition patterns, the back-coupling to solvent flow, as well as the dynamics of solute transfer from the biomass particles to the solvent.

The parameters in the model need more accurate estimations for practical applications, depending on the specific type of biomass and active compound in question. This would require more thorough analysis of problem parametrization and the experimental data together at once. The present study is of potential interest for multidisciplinary research and in case of presence of such data, future works should consider developing of methods for parameter estimation.

Our future endeavours will also include a creation of a coupled Navier-Stokes - Darcy solver, where the biomass “cake” is to be considered as a porous medium.

Author contributions

Conceptualization, U.S. and M.M.; methodology, U.S. and M.M.; software, U.S. and M.M.; validation, U.S. and M.M.; formal analysis, U.S. and M.M.; investigation, U.S. and M.M.; data curation, U.S. and M.M..; writing – original draft preparation, U.S. and M.M.; writing – review and editing, U.S. and M.M.; visualization, U.S. and M.M. All authors have read and agreed to the published version of the manuscript.

References

[1] Maxey M. Simulation Methods for Particulate Flows and Concentrated Suspensions. Annual Review of Fluid Mechanics, 49(1), 2017, pp. 171-193, doi:10.1146/annurev-fluid-122414-034408

[2] Xia Y., Yu Z., Deng J. A fictitious domain method for particulate flows of arbitrary density ratio. Computers & Fluids, 193, 2019. DOI: 10.1016/j.compfluid.2019.104293.
[3] Idelsohn S. R., Gimenez J. M., Löhner R., Oñate E. A multiscale approach for the study of particle-laden flows using a continuous model. Computer Methods in Applied Mechanics and Engineering, 401(a), 2022. DOI: 10.1016/j.cma.2022.115174.
[4] Zohdi T. I. An Introduction to Modeling and Simulation of Particulate Flows. SIAM, 2007.
[5] Shankar S. Multiphase flows: Rich physics, challenging theory, and big simulations. Phys. Rev. Fluids, 5(11), 2020.
[6] Strautiņš U., Marinaki M. On modelling on three dimensional flow in extraction of biologically active substances from plants. Engineering for Rural Development, 22, 2023, pp. 204–209.
[7] Sovová H. Broken-and-intact cell model for supercritical fluid extraction: Its origin and limits. The Journal of Supercritical Fluids, vol. 129, 2017, pp. 3-8.
[8] Sneps-Sneppe M., Kalis H. On Diffusion Processes and Medical Plants Processing. Modern Information Technologies and IT Education, vol. 16(1), 2020, pp. 132-138.
[9] Ferziger J.H., Peric M. Computational Methods for Fluid Dynamics. Springer, 2002. 423 p.
[10] Versteeg H., Malalasekera W. An Introduction to Computational Fluid Dynamics. The Finite Volume Method. Prentice Hall, 2007. 257 p.