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DIRECT NUMERICAL SIMULATION OF REACTIVE FLOW THROUGH A FIXED BED OF CATALYST PARTICLES

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ABSTRACT
Many catalytic refining and petrochemical processes involve two-phase reactive systems in which the continuous phase is a fluid and the porous phase consists of rigid particles randomly stacked. Improving both the design and the operating conditions of these processes represents a major scientific and industrial challenge in a context of sustainable development. Thus, it is above all important to better understand all the intricate couplings at stake in these flows: hydrodynamic, chemical and thermal contributions. The objective of our work is to build up a multi-scale modeling approach of reactive particulate flows and at first to focus on the development of a microscopic-scale including heat and mass transfers and chemical reactions for the prediction of reactive flows through a dense or dilute fixed bed of catalyst particles. A first step is the upgrading and the validation of our numerical tools via analytical solutions or empirical correlations when it is feasible. Then we illustrate the assets of our simulation method on a reactive flow through a pack of different shapes of particles. Our method is implemented in our massively parallel numerical platform PeliGRIFF (Parallel Efficient LIbrary for GRains In Fluid Flow) that already enable us to improve the accuracy of predictions in scales which interest engineers in process engineering. In fine, this process will enable to take a step towards the enhanced design of semi-industrial processes.

INTRODUCTION
Since few years, the study of multiphase transport processes in porous media have acquired considerable attention. These applications include areas such as chemical catalytic reactors, petroleum reservoirs, coal combustors, production of chemicals bulk, petroleum refining, fine chemical pharmaceutics, biomass conversion, etc. Most catalytic refining and petrochemical reactions are operated with fixed bed reactors. In these reactors, catalyst particles are randomly stacked in a large cylindrical vessel and the reactants, usually gas and liquid, are streaming through the packed bed to react inside the catalyst pellets.
The efficiency of a catalyst reactor is quite difficult to estimate a priori because it depends on many factors including the micro-structure of the random packing of particles, the hydrodynamics of the flow through the fixed bed and the intrinsic chemical properties of the catalyst material. From a chemical engineering perspective, designing and optimizing the packed bed arrangement (such by modifying the catalyst shape, polydispersity ...) means finding the mechanism to minimize pressure drop while maximizing the effectiveness and the performance of the catalyst reactor.
A better understanding of the physics ruling reactor performances allows to design more efficient processes in term of chemical but also thermal and mechanical responses. Thus, catalyst development has been more and more concerned with the acquisition of accurate knowledge that can be up-scaled to industrial design, thus requiring better reactors and better analytical techniques.
The improvements of the numerical resolution of Navier-Stokes equations in the modeling of multiphase flows allow to study the main transport processes in the porous media and mostly account for non-Darcian effects such as the inertial, boundary, and variable porosity effects. Thus, fully-resolved simulations of the flow through a fixed bed of pellets are performed to better understand the effect of the local microstructure on the energy loss, i.e., pressure drop through the bed. However computing the detailed kinematics of the reactive flow through a porous media is not an easy task for the three following primary reasons:

1. The creation of the porous media geometry, i.e., the assembly of pellets (solid particles), itself, is not straightforward.
2. The interstitial domain geometry is quite complex which leads to issues in generating the mesh of the computational fluid domain.

3. The limitations related to the size of the studied physical phenomena inherent in non-Darcian effects.

For the first point, one common option in the literature is to perform a dynamic granular simulation of the filling stage, i.e., as all particles are poured into the container, where all collisions between particles are calculated. This type of method is not only efficient because it supplies a realistic assembly of particles but also imitates the filling process and hence allows one to investigate the influence of the type of filling process on the final microstructure of the assembly of particles (porosity, tortuosity, ...). Among the various computational methods available to simulate granular dynamics (Event-Driven method, Non-Smooth Contact Dynamics, Discrete Element ...), the Discrete Element Method (DEM) [2] is likely to be the most commonly used, with hundreds of publications in the international literature every year.

About the issues of the mesh generation, using a conforming mesh is an obvious choice especially when this latter is fixed. However, in the aim to have a code which can treat both fixed and moving solid particles, an interesting alternative is to use a fixed Cartesian structured mesh. This strategy often implies technical implementation efforts to compute fluid/solid interfacial transfers. In this spirit, Distributed Lagrange Multiplier/Fictitious Domain method (DLM/FDM) [8] which belongs to the class of non-boundary fitted methods like Immersed Boundary (IBM) [13], lattice-Bolztmann (LBM) [11] or Force Coupling (FCM) [1], has been applied with reasonable success to a variety of flow configurations including both fixed and moving solid particles [17,20].

Regarding the third point listed previously, the study of convective heat and mass transfers in laminar, transitional and turbulent flows is quite intricate especially when the effects of boundary layers predominate. Thus the determination of the Nusselt and Sherwood numbers is a fundamental result in the study in convective heat (resp. mass) transfer in porous media, as well as the determination of the drag coefficient. In order to accomplish this objective, a significant amount of research has been carried out and empirical correlations for the Nusselt and Sherwood numbers for a variety of configurations and boundary conditions have been established, with certain limitation, for a wide variety of current technological applications.

Numerically, the study of these multi-physics couplings has been poorly studied in the literature. Recently the most of DNS of particulate systems have been extended to include mass transfer and/or heat transfer [3,4,16,21]. These extensions were made possible thanks to the improvements and modifications of existing methods which provide satisfactory results to predict gas-solid particle mass and heat transfer coefficients for stationary arrays of spheres [3,4]. And regarding the consideration of non-spherically-shaped particles, our preliminary results using DNS, have proved that orientation and position of catalyst pellets could change significantly the apparent reactor performance [5,6,15].

PeliGRIFF [12] is a combination of an efficient DEM for particle/particle and particle/wall collisions and a DLM/FDM for the two-way fluid/particle momentum, energy and mass transfers. This model can treat both fixed and moving solid particles, convex and non-convex particles and flows with or without heat transfer in a range of particulate Reynolds numbers from 0 to 10^3 and Prandtl numbers from 0 to 10. The corresponding computations are highly demanding in terms of resources and time. However our code is fully parallel and can run on supercomputers of up to a few thousands of cores with reasonable scaling properties. And the goal is now to extend our preliminary study to more complex configurations of particles bed, especially for reactive fluid/solid flows.

The rest of the paper is organized as follows. We, first, give an overview of our numerical tools by describing the general framework of our DNS models: from the layout of particles to generate a porous media to the study of the reactive/thermal flows through a loosely packed bed of particles. Subsequently, recent results generated from DNS are presented. We will conclude with a perspective on future developments.

NOMENCLATURE

c_A	=	concentration of specie A
D_A	=	diffusion coefficient of specie A
K	=	friction coefficient
Lc	=	characteristic length
Nu	=	Nusselt number
P	=	region occupied by the particles
p	=	pressure field
Pe	=	Peclet number
Pr	=	Prandtl number
Re	=	Reynolds number
t	=	time
T	=	fluid temperature field
$\mathbf{u}$	=	fluid velocity field
Uc	=	characteristic velocity

Greek Symbols

α	=	thermal diffusivity
δ	=	boundary layer thickness
ε	=	volume fraction
ρ	=	density
μ	=	viscosity
λ	=	lagrangian multipliers
ψ	=	pseudo-pressure field
Ω	=	flow domain
$\partial\Omega$	=	flow domain boundary

Subscripts

f	=	fluid phase
p	=	solid phase
th	=	thermal

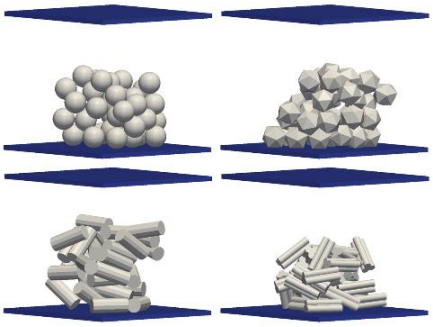

Figure 1: Examples of stacked particles. On the top: spheres (left) and icosahedrons (right); on the bottom: cylinders (left) and trilobe particles (right)

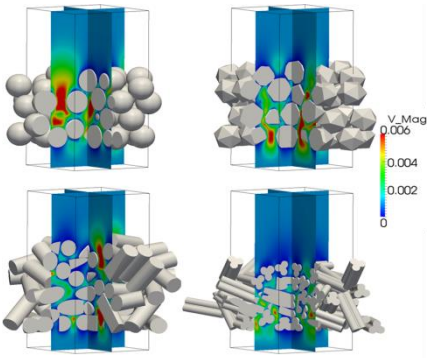

Figure 2: Flow through different particles layout : cross-section views of the velocity magnitude (Re~1)

1 Framework of DNS Models

The goal of our numerical work is to develop an innovative multi-physics modeling of reactive flows, and to make it available in the context of high-end CFD codes able to exploit the full potential offered by massively parallel super-computers for a medium to long term application to full-scale industrial configurations and their optimization. To achieve this objective, considerable efforts were and still are directed towards the numerical validations of the following steps that we detail in this section:

(a) loading procedure, micro-structure of the pack,
(b) hydrodynamics,
(c) and thermal/reaction couplings.

The transport phenomena in the fluid phase are governed by the conservation equations for momentum, mass, thermal energy and/or chemical species respectively given by

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\nabla\cdot\mathbf{uu}\right)=-\nabla p^n+\mu\nabla^2\mathbf{u} \tag{1}$$

$$\nabla\cdot\mathbf{u}=0 \tag{2}$$

$$\frac{\partial T}{\partial t}+\nabla\cdot\left(T\,\mathbf{u}\right)=\alpha\,\nabla^2 T \tag{3}$$

$$\frac{\partial c_A}{\partial t}+\nabla\cdot\left(c_A\,\mathbf{u}\right)=D_A\,\nabla^2 c_A \tag{4}$$

1.1 Grains3D : A Porous Media Maker

In order to generate a catalyst porous media, catalyst particles are randomly stacked (cf. Figure 1). The layout of particles is obtained as the result of a dynamic simulation of a granular media where particles are released at the top of the domain and settle under gravity. This simulation has been performed using a DEM solver Grains3D [19].

DEM is conceptually simple and easy to implement for spherical particles. However its extension to non-spherical and angular particles is more complicated in relation to the determination of the network of contacts. A way to handle this geometric problem is to use a collision detection techniques such as Gilbert-Johnson-Keerthi (GJK) algorithm for the geometric detection of the contact points.

Our numerical code has been validated in assorted granular flow configurations and in particular enables one to fill a container with any kind of shapes [6,19]. Catalyst shape is chosen in order to optimize the reactor performance. A new contribution relies on extending the modeling capabilities of Grains3D to non-convex particles. A strategy based on decomposing a non-convex shape into a set of convex ones appears to be the most obvious, though powerful, option [14].

1.2 DLM/FDM for the Hydrodynamics Coupling

The DLM/FD method used in our code PeliGRIFF implies to use a cartesian structured mesh of constant grid size, to solve the fluid conservation equations everywhere in the domain and to force the rigid body motion (motionless here) in the regions (filled of fictitious fluid) occupied by the particles [8]. Assorted variants at the discrete level have been suggested in the literature. Here, we combine the DLM/FDM with a Finite Volume/Staggered Grid discretization scheme for the fluid equations, a collocation-point method to discretize the particles on the fluid mesh and a second-order interpolation on the fluid velocity at the particle boundary (further details in [20]).

1. A classical L2-projection scheme for the solution of the Navier & Stokes problem: find $\boldsymbol{u}^{n+1/2}$ and p^{n+1} such that

$$\frac{\tilde{\boldsymbol{u}}-\boldsymbol{u}^n}{\Delta t}-\frac{1}{2\,\mathrm{Re}}\nabla^2\tilde{\boldsymbol{u}}=-\nabla p^n+\frac{1}{2\,\mathrm{Re}}\nabla^2\tilde{\boldsymbol{u}} -\frac{1}{2}\left(3\boldsymbol{u}^n\cdot\nabla\boldsymbol{u}^n-\boldsymbol{u}^{n-1}\cdot\nabla\boldsymbol{u}^{n-1}\right) \tag{5}$$

$$\nabla^2\psi=\frac{1}{\Delta t}\nabla\cdot\tilde{\boldsymbol{u}},\ \frac{\partial\psi}{\partial n}=0\ on\ \partial\Omega \tag{6}$$

$$\boldsymbol{u}^{n+1/2}=\tilde{\boldsymbol{u}}-\Delta t\nabla\psi \tag{7}$$

$$p^{n+1}=p^n+\psi-\frac{\Delta t}{2\,\mathrm{Re}}\nabla^2\psi \tag{8}$$

2. A fictitious domain problem: find $\boldsymbol{u}^{n+1}$ and λ_u^{n+1} such that

$$\frac{\boldsymbol{u}^{n+1}-\boldsymbol{u}^{n+1/2}}{\Delta t}-\lambda_u^{n+1}=0 \tag{9}$$

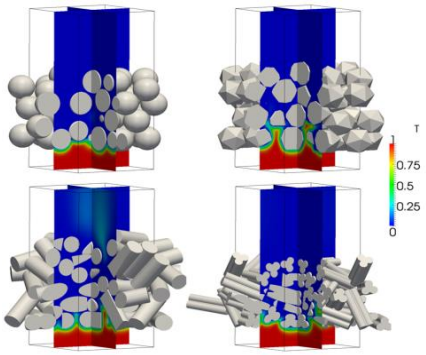

Figure 3: Flow with heat transfer (Pr~1) through different particles layout (Tp is fixed at 0).

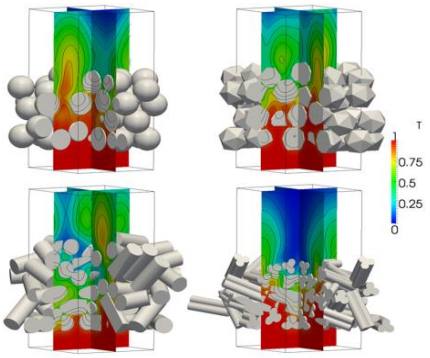

Figure 4: Flow with heat transfer through different non-isothermal particles layout.

$$\boldsymbol{u}^{n+1} = 0 \ \ in\ P \tag{10}$$

Finally, Reynolds number reads:

$$\mathrm{Re} = \frac{\rho L_c U_c}{\mu} \tag{11}$$

In the case of the flow through a fixed bed of particles, obvious choices for U_c and L_c are the fluid inlet velocity and the equivalent particle diameter, but other choices are also conceivable.

PeliGRIFF is an appropriate computational strategy to compute the flow and the pressure drop in a packed bed of particles. Main results have led to several publications, especially concerning the flows around polygonal isometric particles [17,20], cylinders [6] and shortly non-convex particles. As an illustration of our hydrodynamic simulations, we present, in figure 2, visualizations of flows through different particles layouts in a bi-periodic box. An upwards oriented velocity is imposed at the bottom-section (inlet) and an outflow boundary condition is set at the top-section (outlet).

1.3 DLM/FDM for the Heat/Mass Transfer Coupling

At each time, once the velocity field $\boldsymbol{u}^{n+1}$ is computed, it can be used to solve the convection-diffusion equation for a scalar field such as the fluid temperature for heat transfer or species concentration for mass transfer. For brevity, in this paper, only the heat transfer equations with fixed temperature on particles boundary and results will be presented. Hence, in the case where the temperature field is considered as homogeneous and isotropic on particles, we can use the same numerical toolbox as for velocity field:

3. In determining first the $T^{n+1/2}$ such that:

$$\frac{T^{n+1/2}-T^{n}}{\Delta t} - \frac{1}{Pe}\nabla^2 T^{n+1/2} = \frac{1}{Pe}\nabla^2 T^{n} - \frac{1}{2}\left(3\boldsymbol{u}^{n}\cdot\nabla T^{n} - \boldsymbol{u}^{n-1}\cdot\nabla T^{n-1}\right) \tag{12}$$

4. And a fictitious domain problem: find T^{n+1} and λ_T^{n+1} such that

$$\frac{T^{n+1}-T^{n+1/2}}{\Delta t} - \lambda_T^{n+1} = 0 \tag{13}$$

$$T^{n+1} = T_p \ \ in\ P \tag{14}$$

Finally, the Peclet number reads:

$$Pe = \frac{L_c U_c}{\alpha} = \mathrm{Re}\,\mathrm{Pr} \tag{15}$$

As for the rigid-body motion constraint, the temperature field of the porous media is constrained in the regions occupied by particles (further details in [18,21]).

To illustrate the coupling with heat transfer, we present in figure 3, some cross-section views of temperature field through an isothermal fixed bed of particles at fixed temperature of zero and the inlet temperature is imposed on the bottom-section at 1.

1.4 Advantages & Limitations of DLM/FD Couplings

The DLM/FD method is particularly efficient to solve fluid/solid interaction problems when the solid phase is homogeneous and isotropic. Firstly, in cases of flow coupled with mass or heat transfer, diffusive intra-particle processes require no artificial flow inside the solid body (due to rigid body constraint). Besides, a second advantageous property, the method of Lagrange multipliers is a powerful tool for solving this class of problems without the need to explicitly know gradients of velocity, concentration and temperature fields on fluid/solid interfaces. Thus, to extract fluid/solid forces, torques, mass or heat transfer flux, it is sufficient to compute volume integral of Lagrange multipliers.

However, by construction, the original DLM/FD formulation cannot take into account the heterogeneous and anisotropic phenomena inside particles. And from a chemical engineering perspective, catalyst particles are designed to be porous so that the reacting fluid can penetrate the particle to reach the reactive phase coated onto them. Main interest of heterogeneous catalysis is that the surface area available for reaction is very large. To investigate in this direction, in the spirit of [9], we recently added a new module to model the assorted chemical reactions that take place in the reactor [5]. We present in figure 4, in the same conditions that simulations illustrated in figure 3, except here, the intra particle diffusion is taken into account.

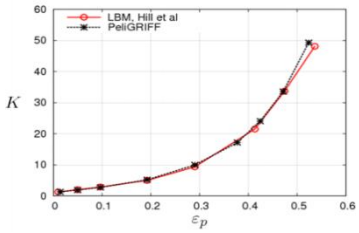

Figure 5: Comparison of our results with [11] in case of flow through random arrays of spheres at Re<<1

2 Results

At this stage, we have undertaken to validate our results with correlations of literature. And the cases of convective heat transfer through a fixed bed made of spherical particles, at a fixed temperature, are particularly well studied. In this section, recent results generated from DNS are presented.

2.1 Flow Through a Porous Media

In the case of Stokes flow through periodic ordered arrays of spheres, Zick & Homsy [23] proposed an analytical solution which links the imposed pressure drop, the mean velocity and the friction coefficient K. This case is convenient to investigate the space convergence of the computed solution with mesh refinement. And in order to validate our numerical solutions, when the Reynolds number Re > 1 and/or the arrays of spheres become random, we compare with other numerical methods such as IBM, LBM, etc.

Recently in [20], we proved using our numerical code [12] that a first-order convergence rate is obtained (around 1.3) in the case of Stokes regime, with a very satisfactory agreement with the analytical solution of [23]. Moreover, this trend is confirmed by the results obtained in the case of random arrays of spheres at Re<<1 that we compare with [11] in Figure 5. In [20], we present, in further details, both the results in the case of Stokes regime where 16 points per particle diameter is enough to have less than 4% of discrepancy from the reference solution, and the results in the case of moderate-Reynolds-numbers regime (Re < 100), in which at least 32 points are required to capture the hydrodynamic boundary layer effects.

2.2 Convective Heat Transfer Through Porous Media

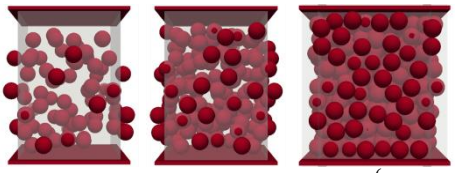

Figure 6: Particles configuration for $\varepsilon_f \in \{0.5,0.7,0.9\}$

We illustrate the assets of our numerical coupling method on flows with heat transfer through fixed beds of spheres. As proposed by [16], 3 particle configurations are studied, defined by a set of three fluid volume fractions $\varepsilon_f \in \{0.5,0.7,0.9\}$ (cf. figure 6).

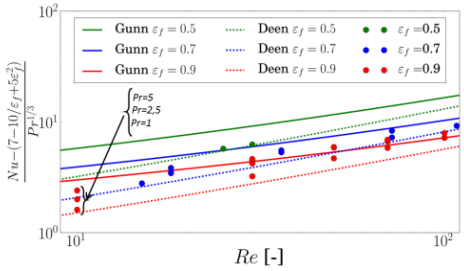

Figure 7: Comparison our numerical results (o-symbols) with Deen et al. [3] and Gunn et al. [10] correlations

The spheres are distributed in a random fashion over a bi-periodic computational domain. And concerning the fluid boundary conditions, an upwards oriented velocity is imposed at the bottom wall (inlet) and an outflow boundary condition is set at the top wall (outlet). The temperature is set to 0 everywhere at the initial time t = 0 except at the inlet where it is imposed to 1. And at the outlet a zero normal derivative is imposed for temperature. Finally, we set a zero velocity and a zero temperature in all particles. The thermal boundary layer being finer than hydrodynamic one, DNS with heat transfer require a spatial resolution much finer, for instance, in the case of a flat plate, the relation evolve as:

$$\frac{\delta_f}{\delta_{th}} = \mathrm{Pr}^{1/3} \tag{16}$$

To compare our numerical results, detailed in [7], we use two different Nusselt correlations of the literature: an empirical correlation established by Gunn [10] and a numerical correlation established by Deen et al. [3]. The Nusselt number is written as the following form:

$$\mathrm{Nu} = \left(7 - 10\varepsilon_f + 5\varepsilon_f^{\,2}\right)\left(1 + \mathrm{A}\,\mathrm{Re}^{0.2}\,\mathrm{Pr}^{1/3}\right) + \left(1.33 - \mathrm{B}\varepsilon_f + \mathrm{C}\varepsilon_f^2\right)\mathrm{Re}^{0.7}\,\mathrm{Pr}^{1/3} \tag{17}$$

Where the coefficients (A, B, C) are defined in Table 1.

Authors	A	B	C
Gunn [10]	0.7	2.4	1.2
Deen et al.[3]	0.17	2.31	1.16

Table 1: Coefficients for [3] and [10] correlations

Computed results obtained for three Prandtl numbers {1;2.5;5} and a range of Reynolds numbers from 10 to 100 are plotted in Figure 7. Overall, our results show the same trend as [3] and [10]. With some differences, in the case of Pr = 1, our results are closer to Deen's correlation for ε_f = 0.9 and when Pr > 1 our results are in an agreement with Gunn's predictions.

CONCLUSIONS

We have presented a multi-physics framework to examine the reactive flow through a fixed bed of catalyst particles. In this paper, we described how to build up this workflow, from the layout of particles to generate a porous media until the study of the hydrodynamic and thermal coupling. Then we focused on the analysis of

flows with heat transfer through a loosely packed bed of spheres at a fixed temperature, as a preliminary validation of our numerical methods.

An additional attention was given on the study of spatial resolution in order to capture the thickness of the hydrodynamic and thermal boundary layers in the cases of inertial regime.

Concerning the next steps of the just presented work, there are four levels of on-going validation:

1. To take into account of poly-dispersity of solid particles
2. To investigate local effects on random arrays of non-spherical pellets, namely the interaction at scale particle position and orientation with flow and reactant transport.
3. To enhance our numerical model to study with sufficient accuracy and stability the case of heterogeneous and anisotropic catalyst pellets.
4. To extend our approach to a two-way coupling i.e. to consider feedback of the chemical species conversion on the fluid properties.

More complete simulations and results on these ongoing works will be presented during the meeting.

Other forthcoming developments require a larger understanding of physical and numerical modeling before being implemented. Thus, two studied cases may be mentioned: the biomass gasification processes, in which the consideration of the (partial or complete) combustion of particles is primary, and the case of phase-change particles.

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