Heat transfers in fixed beds made with wood chips

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Fixed bed reactors are widely used in the fields of energy or chemical engineering, with applications ranging from thermal energy storage to catalytic pellets fixed beds or to biomass transformation beds. Woody biomass is an important source for second generation bio-fuels production [1,2]. Through different thermochemical transformation processes, like gasification or pyrolysis, biomass can produce a large variety of compounds with a quality highly depending on the raw materials properties but also on the process specification, particularly the temperature or the heating rate. Wood biomass is generally converted in fixed bed reactors, under the form of pellets which can have undergone different kinds of pre-treatments, like drying, to increase the efficiency of the overall process. Thermal uniformity of the fixed bed is essential for the quality of generated products. However as wood is both a poor heat conductive material and an exothermic reactive material, uniform temperatures in the bed are difficult to achieve and to control. Being able to predict the heat transfer coefficient in the complex geometry of a fixed bed of wood chips would thus help in the comprehension of the thermal phenomena involved and would allow to better control biomass conversion processes.

The volumetric heat transfer coefficient is assessed through steady-state Direct Numerical Simulations (DNS). Laminar, incompressible and steady-state Navier-Stokes equations, i.e. continuity and momentum conservation, are solved in the fluid phase. An energy equation is added to the system, in both solid and fluid phases. Written in terms of a classical one-way coupling temperature equation, this energy equation includes heat convection (in the fluid phase only), heat conduction (in both fluid and solid phases), and a volumetric heat source term (in the solid phase only). This set of equations has been implemented in a dedicated multi-region solver using a segregated implementation, within the frame of OpenFOAM® version v1812, compatible with the latest releases. In the fluid phase region, Navier-Stokes equations and the fluid temperature equation are solved. In the solid region, only the solid temperature equation is solved. At the fluid-solid interface, which corresponds to the wood particles surfaces, a non-slip wall is imposed on fluid velocity and a zero gradient pressure condition is applied. Concerning the temperature variables at the fluid-solid interface, the coupling boundary condition between the fluid and solid regions ensures an equality of temperatures and an equality of heat fluxes between both sides:

$$T_{Fluid/wall} = T_{Solid/wall} \quad \text{and} \quad k_{Fluid} \nabla T_{Fluid/wall} = k_{Solid} \nabla T_{Solid/wall}$$

where k denotes the thermal conductivity.

Fixed beds geometries are generated using the in-house Discrete Element Method (DEM) code Grains3D or the opensource DEM solver LMGC90. The Grains3D DEM solver accounts for all the collisions between the particles and the reactor walls, in order to determine the contact points and the resulting contact forces [3,4]. The collision detections is based on the Gilbert-Johnson-Keerthi algorithm [5]. More details about Grains3D parallelization methods, contact force models and extension to non-convex particles of arbitrary shapes can be found in the article of Wachs et al. [3,4]. Grains3D was used for the generation of fixed beds of spheres, necessary for thorough validation of our computational chain, and LMGC90 was used for the generation of parallelepiped wood chip packings.

Meshing is performed using the utility `snappyHexMesh`. The wood chips parallelepipeds are input as STL objects in the geometry section of the `snappyHexMeshDict`. A surface based refinement level increment (typically 2 or 3) is used on all the surfaces of the parallelepipeds. A global `gapLevelIncrement` (typically value 1) was used to ensure a correct capture of the thin gaps in regions where the chips can be tangent.

Validation of the workflow was performed on a single sphere case and then on a 60 spheres fixed bed larger case. Predictions of Nusselt number versus Reynolds number were compared with literature correlations, in particular Whitaker's correlation [6]. The workflow is then applied to a packed bed of torrefied wood particles, taken from the article of Bouzarour [7]. The heat transfer coefficient, with a constant heat source term inside the solids taken from Bouzarour [7], is computed for different Reynolds numbers. Table 1 summarizes the results. A sample flow structure and temperature variation inside the fixed bed are presented on

Figure 1.

As a conclusion, we present in this article an OpenFOAM® workflow for the computation of heat transfer coefficient computation in fixed beds, showing an application to wood biomass transformation and a better understanding of the risks of thermal run-aways.

Table 1 : Heat transfer coefficient versus Reynolds number

Velocity (mm/s)	Particle Reynolds	h ($W/m^2/K$)	Nusselt
2.5	1	4.88	0.87
5	2	4.72	0.85
12.5	5	11.36	1.04
25	10	22.73	1.37

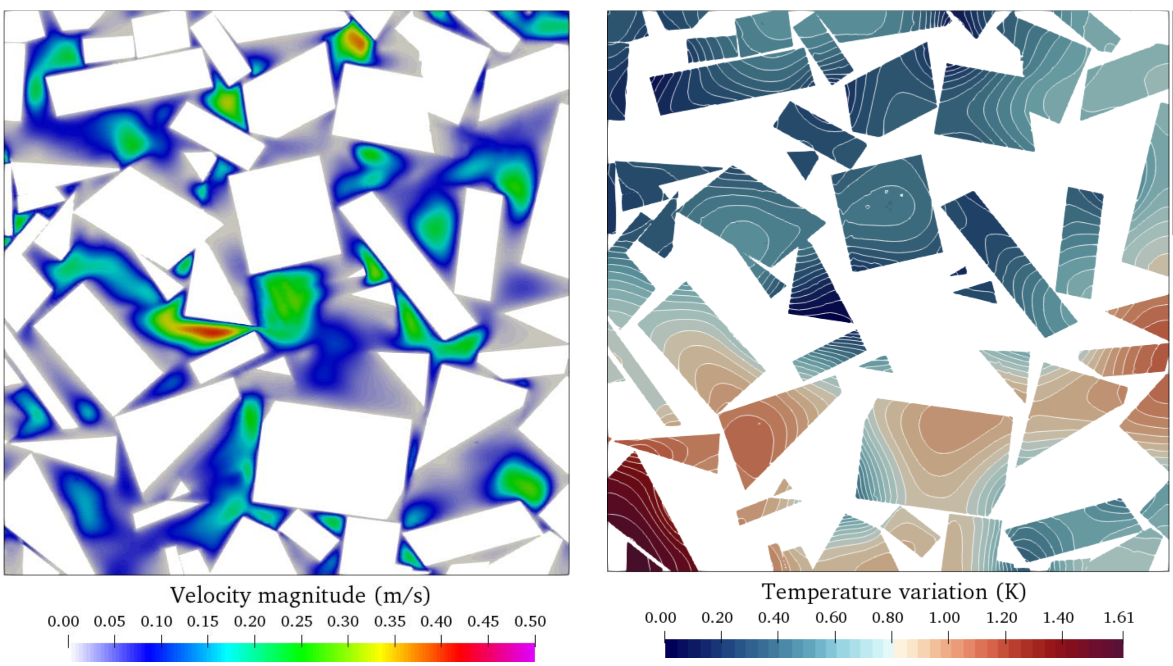

Figure 1 : Velocity (left) and temperature variation (right, T(z) - min(T(z)) at z = 27 Dp, Re = 10 across a wood chip bed under constant heat source of 5.32 kW/m^3

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