REGULAR PACKING TYPES FOR CFD SIMULATION OF SCF EXTRACTION AND REACTION EQUIPMENT

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Fixed-bed structure study and its effects in heat and mass transfer has been widely reviewed by several authors. Determination of geometrical properties of randomly packed beds with computational simulation has conduced to the development of algorithms for simulating the construction of random packings in cylindrical containers. Regular packing of spheres has also been studied, developing uniform geometries; geometry-based models and computational algorithms have permitted to develop flow profile predictions in packed columns. Computational Fluid Dynamics (CFD) has proven to be a powerful tool to numerically solve fluid motion and transfer equations. There has been a fast growing in the study of applications in fluid flow and heat transfer, and have been used to analyse flow patterns in fixed-bed equipment and to predict heat transfer parameters in studied cases. In this work we review prior aproaches to geometrical sphere-based models for packed beds and propose three different geometrical arrangements for packed bed equipment computer simulation relevant to SCF extraction equipment design. These models are to be used in CFD simulation of supercritical extraction and reaction equipment. Fluid analyzed is taken to be CO_2 in supercritial conditions, with an uniform velocity at the bed inlet and a fixed velocity condition around the spheres and at the wall. Neither thermal nor mass transfer boundary conditions are considered.

INTRODUCTION

An understanding of the fluid transport within the void space of a porous medium is of fundamental importance to many chemical engineering systems such as fixed bed extraction or catalytic reaction equipment, with special relevance in heat and mass transfer studies. Experimental and theoretical studies of flow through such systems often treat the porous medium as an effectively homogeneous system and concentrate on the bulk properties of the flow. Such an approach neglects completely the complexities of the flow within the void space of the porous medium, reducing the description of the problem to macroscopic average or effective quantities. The details of this local flow process may, however, be the most important factor influencing the behaviour of a given physical process occurring within the system, and are crucial to understanding the detailed mechanisms of, for example, heat and mass dispersion and interface transport.

I – FIXED BED STRUCTURE

Packed beds structure study and its effects over heat and mass transfer have been extensively reviewed. Geometrical properties of randomly packed beds have been obtained using computational simulation [1], developing algorithms that allow to create computer applications that simulate the construction of a random packing in a cylindrical container. Fixed bed packing with homogeneous or non-homogeneous spheres has also been studied [2-4]. Differences in heat and mass dispersion behaviour of homogeneous and non-homogeneous packed beds have been proved to be slight, and dispersion in a bed with a mixture of particle sizes follows the prediction for bed of monosized particles, if an average particle size is used in calculations [5]. Geometry-based models and computational algorithms have permitted to predict flow profiles in packed columns [6].

II – GEOMETRICAL MODELS

Sphere packing is a mathematical problem by which is tried to determine how tightly equal spheres can be packed in a vessel of known volume (unit cell). Three different regular models from sphere packing theory have been selected for this study: simple cubic packing, face-centered cubic packing, and hexagonal close packing.

In simple cubic packing, spheres are stacked directly next to and on top of each other.

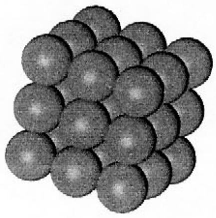

Figure 1: Simple cubic packing

In face-centered cubic packing, the bottom layer has spheres directly next to each other; spheres in the next layer are placed in the crevices of the underlying layer. In this packing scheme, every other layer directly overlies each other.

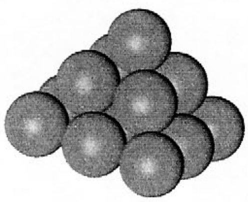

Figure 2: Face-centered cubic packing

In hexagonal close packing, each layer has spheres placed diagonally next to each other. The next layer of spheres is placed in the crevices between spheres on the bottom layer. Every third layer directly overlies each other.

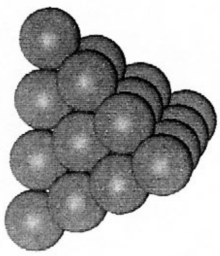

Figure 3: Hexagonal close packing

Packing density can be calculated determinating the fraction of a cube's volume occupied by the spheres. The packing densities and corresponding bed porosities are:

$$\rho_p = \frac{V_{spheres}}{V_{cube}} \tag{1}$$

$$\phi = 1 - \rho_p \tag{2}$$

GEOMETRICAL MODEL	PACKING DENSITY	BED POROSITY
Simple cubic	$\frac{\pi}{6}$	$1-\frac{\pi}{6}$
Face-centered cubic	$\frac{\pi}{3\sqrt{2}}$	$1-\frac{\pi}{3\sqrt{2}}$
Hexagonal close	$\frac{\pi}{3\sqrt{2}}$	$1-\frac{\pi}{3\sqrt{2}}$

Table 1: Packing densities and bed porosities of geometrical models

III – MESH GENERATION FOR CFD ANALYSIS

Computational Fluid Dynamics (CFD) has proven to be a powerful tool to numerically solve Navier-Stokes equations in complex 2D and 3D passages. There has been a rapid growth in the study of applications in fluid flow and heat transfer, and several authors have used it to analyse flow patterns in fixed-bed equipment and to predict heat transfer parameters in studied cases [7-8].

For mesh generation purposes, and in order to determinate the most important phenomena involved in this case, a dimensionless analysis of Navier-Stokes equations was done, obtaining the magnitude order of dimensionless groups shown in the study. Turbulence intensity has been calculated to 4 %.

According to this analysis, the most important term in the momentum balance will be the one that involves frictional pressure drop within the bed. Viscous forces will be of low apportation to calculations, and there's a boundary layer problem to be taken into account when defining mesh density. It also becomes clear that a transient analysis must be done.

Dimensionless group	Magnitude order
St	10^0
Re	$10^1 - 10^2$
Eu	$10^3 - 10^4$
Fr	$10^{-7} - 10^{-5}$
M	$10^{-7} - 10^{-6}$
Pr	10^1
Br	$10^{-12} - 10^{-11}$
Ec	$10^{-14} - 10^{-12}$

Table 2: Magnitude order of dimensionless groups

The mesh should be very fine near to the surface of the spheres, in order to properly define and capture the boundary layer problem involved. In order to simulate contact points between particles, a mesh manipulation strategy should be adopted; either the overlapping of particles or the creation of small elements with fluid properties and zero velocity condition imposed between the particles can be used for this purpose.

Boundary conditions applied to the model are as follows:

1. Constant velocity at the inlet, i.e., plug flow at $z = 0^-$
2. Constant pressure at the outlet
3. Constant velocity ($v = 0$ m/s) at elements simulating contact points between particles
4. Constant normal velocity ($v = 0$ m/s) at the particle surface

The mesh used in this model was an unstructured tetrahedral mesh, with special attention to flow-constricted areas near particle-to-particle contact points.

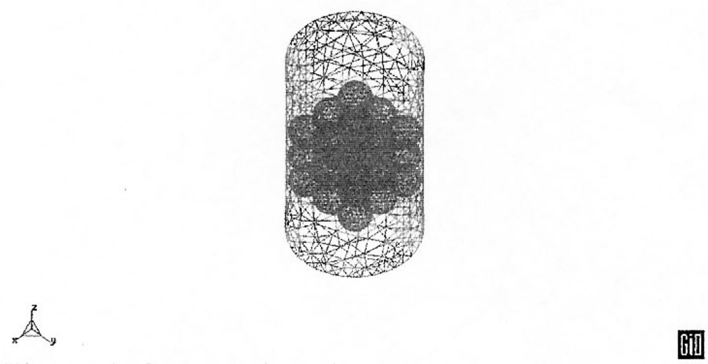

Figure 4: Generated mesh

IV - MODEL ANALYSIS

The Navier-Stokes equations for fluid flow, together with a turbulence model when necessary, were solved using a commercial available finite elements code, GiD® (Version 7.0 – Centro Internacional de Métodos Numéricos en Ingeniería CIMNE-UPC). The code includes modules for geometry creation, model generation, solution of equations and post-processing.

The fluid was taken to be CO_2 under supercritical conditions (165 bar, 310 K) in mostly laminar flow regime (Re< 500).

V - RESULTS: VELOCITY PROFILES

Velocity profiles for laminar model were obtained numerically solving the proposed model.

Laminar model was correctly solved up to *Re* = 500. For higher Reynolds' number, computational time was increased by 5 and numerical results were not stable. Velocity profiles shown strong radial flow components between crevices inside the bed.

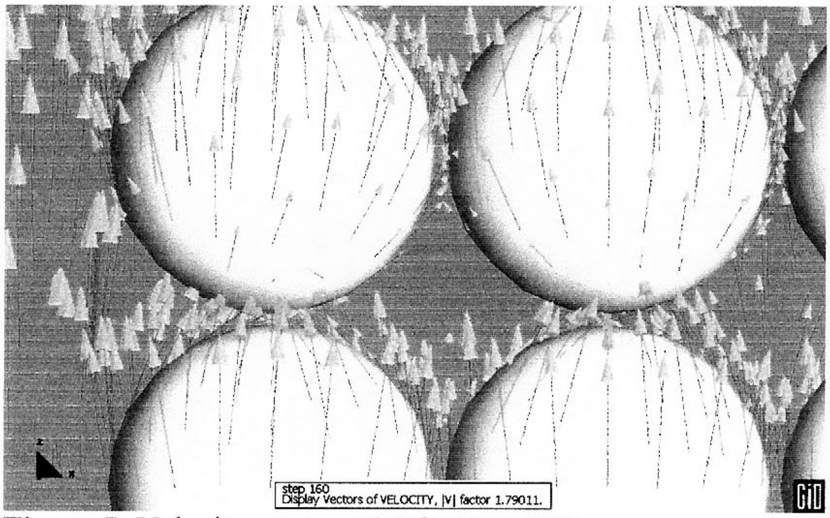

Figure 5: Velocity vectors plot for Re = 110

CONCLUSIONS

- Pressure drop calculation is the most relevant term in momentum balance equation for the conditions applied to the model
- Laminar model can be applied for *Re* below 500, if no eddy viscosity calculation is required. At higher Reynolds' number, numerical results are questionable, and care would be required in selecting an appropriated turbulence model.
- Velocity profiles show strong radial components within the bed of particles. This is directly related to heat and mass dispersion calculation, and should be taken into account in future models developing.

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