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Pore-scale simulation of vortex characteristics in randomly packed beds using LES/RANS models

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HIGHLIGHTS

- A method is proposed to build real geometric structures of randomly packed beds.
- LES and RANS methods are employed to predict vortex shape and evolution features.
- Distribution characteristics of vorticity and velocity are analysed.
- The Q criterion is used to identify vortex structures and evolution of vortexes.
- The spatial scale of the maximum eddy and the time-scale of eddy merging are concluded.

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ABSTRACT

Turbulent flow characteristics and vortex behaviors in the pore space of real packed beds under different flow conditions is numerically investigated. Real geometric structure of randomly packed beds is modeled using the discrete element software LIGGGHTS. Both LES and RANS methods are employed to predict vortex shape and evolution features at pore scale in actual packed beds. The numerical model is validated corresponding to experimental data, a good agreement is achieved between predicted results and measurements. Based on the computational results, the distribution characteristics of vorticity and velocity in multiple representative special structures are analysed, such as the channel formed by two pellets, similar triangle area formed by compact spherical walls and channel. Besides the effects of special structures on vortex shape and turbulence intensity is studied, such as the guiding and friction effect by the side spherical wall on gas motion, and strong shear force on both sides of the main channel. The Q criterion is used to identify vortex structures and capture distribution and evolution of vortexes in the computational domain. Moreover, the effect of inlet velocity on the position and shape of eddies is investigated, and eddy morphological changes under unsteady inlet conditions are also discussed., At last, a comparison between LES and RANS methods shows that the LES method can capture more details of the distribution and shape of the vortexes in the pore space, and therefore it is more suitable to the complicated flow field in porous media.

1. Introduction

Packed beds are widely employed in energy engineering, e.g. in combustion reactor (Diglio et al., 2017; Deshpande et al., 2017; Guo and Zhu, 2015; Guo et al., 2014; Noorman et al., 2010), separator (Jansens et al., 1995) and adsorber (Chen et al., 2015). Combustion of premixed gases in packed beds has many advantages, such as the low emissions of NOx and CO, high power density, large range of modulation, etc. It can be widely applied in IC (internal combustion) engines, low calorific gas burners, VOC (volatile organic compound) oxidizers, and radiation heaters.

Analysis of the combustion in packed beds reveals that the complex flow field inside the bed plays an important role in affecting the combustion efficiency and NOx, CO emission. In recent years, the literature covering experimental research on the flow through packed beds is vast. Gräf and Rühl (2014) investigated the heat transport characteristics of catalytically coated sponge packings

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and of a packed bed of spherical shell-catalysts by performing the exothermal hydrogenation of benzene in a tubular reactor with cooled wall, and found that when sponge supports were compared among each other, the thermal conductivity coefficient of the solid material have the strongest impact on heat transfer. Koplik et al. (1984) showed how to calculate the electrical conductivity and the fluid flow permeability of a disordered random medium. Pereza and Laluezaa (2011) presented a new type of implantable drug eluting device, and placed particles inside the hollow interior of a porous medical grade stainless steel pin mimicking, the mechanical behavior of the porous was tested and found satisfactory. Alam et al. (2009) gave a calculation about the permeability of model paper coating structures with different particle sizes and shapes. Monazam and Spenik (2013) investigated the adsorption of carbon dioxide (CO_2) by immobilized polyethylenimine (PEI) on mesoporous silica in packed bed. To research the mixing hydrodynamics characteristics of the packed bed reactor Rehman and Dahman (2012) examined the effects of packing, gas redistributor, sparger configuration, gas flow rate, and liquid height on the mixing time and superficial liquid velocity by the tomography images.

Recently the interest in numerical methods and models in CFD (Computational Fluid Dynamics) has been continuously increasing. Such models are an important alternative to experiments, as their cost is much lower and they offer unlimited access to the bed and flow parameters. The modeling approaches can be divided in two main groups: (a) Construction, simplification and optimization of the packed bed structure, such as: Boccardo et al. (2015) developed a novel open-source and easily accessible work-flow based on Blender, and a rigid-body simulation tool developed for computer graphics applications has been presented. Ayeni and Wu (2016) presented DEM-CFD simulations of a gas–solid fluidized bed and compared to experimental results of the small scale challenge problem (SSCP) from the National Energy Technology Laboratory. It has been well recognized that the pressure drop and the solid velocity profile are over-predicted with the widely used constitutive relations for gas–solid flows in the Eulerian two-fluid frame work. Li and Park (1998) used packing permeability to give a prediction of mass transfer rate in granular media and fibrous. A novel process based on an impinging stream-rotating packed bed (IS-RPB) was proposed for preparing nanoscale zero-valent iron (NZVI) and degrading nitrobenzene (NB) simultaneously by Weizhou Jiao and Qin (2017). Vitaly Gitis and Rubinstein (2010) suggested a phenomenological model of deep-bed filtration, it combined an advection-dispersion equation with an equation of nonlinear multistage accumulation kinetics, including dispersion and accounts for temporal and spatial changes in media porosity. Tashman et al. (2003) used a non-staggered grid scheme to simulated the fluid flow in granular microstructure, and found that spherical glass beads have higher permeability coefficients than Silica and Ottawa sand. Petera and Nowicki (2013) proposed the full heterogeneous model of the fixed-bed reactor and developed a new algorithm for numerical solution of the mathematical model. Peters (2002) investigated a packed bed composed by a finite number of individual particles with different properties and sizes and gave a research on the processes such as heat-up, pyrolysis, drying, oxidation and gasification of each particles. (b) investigating characteristics of flow, heat transfer and combustion in packed bed, such as: Jafari and Zamankhan (2008) conducted a numerical study of flow behavior through random packing of non-overlapping spheres in a cylindrical geometry using a commercially available computational fluid dynamics package, and dimensionless pressure drop had been studied for a fluid through randomly packed bed at different Reynolds numbers based on pore permeability and interstitial fluid velocity. Alam et al.(2006) related the microstructural characteristics of porous media to their through-flow properties by researching the complex anisotropic particle packings. Yang and Luo (2014) presented a numerical modeling of the gas-solid motion in a 3-D lab-scale double slot-rectangular spouted bed with a partition plate in the parallel framework of CFD-DEM coupling approach, in this work solid motion was tracked with the discrete element method, and the gas motion was solved by the $k–\varepsilon$ turbulence model. Comparing numerical simulations and experiments with packings of glass bead, Moldrup et al. (2001) gave a study on the distribution of ions up to the formation of first crystals in a drying porous medium at the surface. Dong and Sosna (2017) obtained radial temperature profiles in a thin tube fixed-bed reactor packed with glass spheres and steatite rings at different packing heights and different flow rates. Matthews et al. (1996) identified subtle changes in void space dimensions by generating void space models of the correct porosity. Chalermsinsuwan and Gidaspow (2011) researched the system hydrodynamics of fluid catalytic cracking (FCC) particles in a thin bubbling fluidized bed with 2-D and three-dimensional (3-D) computational domains, and found that all the evaluated system hydrodynamic values in the thin radial system direction were lower in the 3-D computational domain than in the thick radial system direction. Henneke and Ellzeya (1999) investigated the low-velocity filtration combustion reaction of lean methane/air in packed bed, and carried out the one-dimensional model including gas-phase interphase heat exchange, transport, radiation, and solid conduction. Hannaoui and Horgue (2015) gave a simulation of gas–liquid trickle flows inside fixed beds of spherical particles with using the pore network model, while found that the pore network model only estimates liquid saturation value in the throats between pores, it caused the liquid saturation values overestimated, so the values should be corrected after calculation.

Bear (2013) pointed out that, when the Reynolds number based on the mean pore diameter (Re_d) was close to 10, turbulent vortexes appeared in the pores of porous media, and with the increasing of Re_d, the turbulent flow regime covered the whole flow region gradually. Recently, through experiment Patil and Liburdy (2013a, 2013b, 2015) discovered that turbulent flow had a gradual development in the packed beds, and when $Re_d > 2800$, the generation rate and dissipation rate of the turbulent kinetic energy approached their stable value gradually. Furthermore, they revealed that the anisotropy of turbulence was quite obvious in the pores, and the longitudinal integral length scale was about 0.1 times the hydraulic diameter of the packed bed, which was about 2 times of the transverse integral length scale.

At present, the numerical methods for solving the turbulence problems are mainly divided into three categories, namely, direct numerical simulation (DNS), Reynolds average Navier-stokes (RANS) and large eddy simulation (LES) (Pope, 2000) in the numerous researches of turbulent flows in the packed beds. DNS and RANS are the methods mainly used, for example, Bai et al. (2009) and Eppinger et al. (2011) presented a research on the flow field in structured and random packed beds by standard k-ε turbulent model; Dixon et al. (2012) researched the distribution of velocity, temperature and energy in random packed beds using Standard k-ε turbulent model in the Re_d range of 1600 to 27,000; Tabib et al. (2013) simulated the flow field and heat transfer in random packed beds with spheres, cylinders and fluted ring, using realizable k-ε turbulent model at low Re_d. The RANS models, however, can only provide average information of turbulent flow fields, and hardly satisfy the study of complex turbulent structure in the randomly packed bed.

On the other side, Ookawara et al. (2007) applied DNS to simulating both flow and energy transport in randomly packed beds at Re_d about 510; Atmakidis and Kenig (2009), Riefler et al. (2012) and Boccardo et al. (2015) investigated the hydrodynamics in randomly packed beds using DNS, and in their cases Re_d was relatively