Enhanced heat transfer in small diameter packed beds

C. T'Joen, J.R. van Ommen, M. Rohde



Introduction: packed beds

- Packed bed = "stacking of particles within a confinement"
- Stacking can be ordered (e.g. FCC, BCC) or random
- Different particle shape / size distribution possible
- Focus here: "small" random packed beds of spherical particles
- Applications:
 - Catalytic chemical (multi-tubular) reactors: e.g. Fischer-Tropsch process, the production of phthalic anhydride and terephthaldehyde and the epoxidation of ethylene oxide
 - Nuclear reactors: pebble bed reactor (VHTR)



Introduction: packed beds

Advantages:

- High specific surface area (+porous sphere)
- Easy to construct and maintain
- Option to refill 'online' (VHTR)
- Disadvantages:
 - Complex structure: heat/mass transfer?
 - Flow bypass near the wall: 'local ordening'
 - High pressure drop
 - Hot spots in the near wall zone





Packed bed thermo-hydraulics

Complex interaction between different heat transfer modes:

- Conduction: sphere-sphere, within the sphere
- Convection: complex geometry, wakes, flow bypass, hot spots
- Radiation: sphere to bed, bed to wall
- Mass transfer: chemical reactions
- Different scales:
 - Inside the spheres
 - Inside the bed



Packed bed thermo-hydraulics

Bed heat and mass transfer Catalyst pellet heat and mass transfer phenomena phenomena Intra-pellet heat Catalyst pellets/ inert conduction Intra-pore Multicomponent solid-Convective heat diffusion gas mass transfer transfer in coolant Intra-pore Heat transfer convection Tube wall between packed bed and wall Catalyst pellet Radial heat conduction in packed bed Diffusion across film Axial convective heat transfer in gas Heat conduction Radial Heat transfer diffusion/dissipation between solid and gas Catalytic reaction on pore surface Radial conduction in tube walls Energy carried by solid-gas Heat transfer between diffusive mass transfer tube and coolant

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- Different scales:
 - Inside the spheres
 - Inside the bed
- Difficult to model!
- Current approaches: porous media \leftrightarrow 3D CFD?



Porosity

- Measure for the local amount of 'void'
- Near the wall: 'local ordening'
 - More open structure
 - Results in flow bypass, 'channeling'
- Strong impact on bed thermo-hydraulics
- Effect increases as bed becomes smaller
 - $D_{bed} \sim 20-50 \text{ x } D_{sphere}$





Measuring porosity profiles?

- Various techniques exist: gamma beam attenuation used @ DUT
- Provide radially averaged porosity data
- Can be modified to provide axial data





Simulating random beds?

- Generating a true random bed?
- Numerical models:
 - Monte Carlo rejection method
 - Discrete Element Method
 - Overlap removal method (in-house code, G. Auwerda)



Simulating flow and heat transfer?

- Using both commercial and open-source CFD tools
- Fluidity (Imperial College London) and Openfoam
- Benchmark done for flow and heat transfer: CSP with N = 1



Benchmarking the codes

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- Fluidity (Imperial College London) and Openfoam
- Benchmark done for flow and heat transfer : CSP with N = 1



Benchmarking the codes

- Model inter-comparison (NRG:DNS, TUD:LES)
- Triple periodic domain with inter-pebble gaps
- Diagnostics: velocity field (domain mean and rms, plus probes)





Source: Shams et al. (NRG)



Benchmarking the codes

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A Structured Tube for Gas-Liquid Reactions D. Vervloet, F. Kapteijn, J. Nijenhuis, J.R. van Ommen **Tubular reactor Random packing** Structured packing (Dumped particles) (Channel network) G + L G + L<u>Length</u> ~10¹ m Radius G/L flow, ~10⁻² m ΔΡ, **Catalyst** Heat transport/transfer, dispersion, bypassing, G/L contact, **RTD** ~10⁻³ m G/L distribution **Reaction-diffusion.** film transport resistances

Different phenomena, at different length scales: complex interaction

Objective: decouple phenomena \rightarrow optimize performance



A Structured Tube for Gas-Liquid Reactions





A Structured Tube for Gas-Liquid Reactions

Experimental results (packed bed vs structured packing):

- Superior pressure drop
- Superior heat transfer
- Flatter temperature profiles
- Comparable mass transfer



Modelling of Fischer-Tropsch reactor (1-D) based on these parameters:

• Much higher selecitivity $P_{syngas} = 30$ bar, syngas ratio = 1.7, $d_p = 1.5$ mm, $d_t = 5.0$ cm for C5+! **Varying T**. **Optimum T and** α





Outlook: further improvements?

- New proposal to STW-OTP: looking for partners (input)!
- Goal: <u>further optimise small packed random beds with 'smarter'</u> walls and particles for single phase fluids
- Smart walls: reduce porosity variation but with good heat transfer →dimples, grooves, combinations?
- Smart particles: use varying particle sizes or non spherical shapes to dampen porosity oscillations
- Method: combined experimental and numerical (2 PhD): experiments will be used to validate 3D CFD (OpenFoam)



Proposed project outline

Experimental section

- Design experimental HT setup
- Validation experiments (tube flow)
- First heat transfer test cases (groove and a dimple case)

Numerical section

- Set up Openfoam code (RANS, LES)
- Code benchmarking
- Code validation: test case data
 (groove and dimple)
- Experimental parameter study: heat transfer and pressure drop, porosity profiles...
- Optimization (e.g. surrogate methods) using 'Design of Experiments'

Design guidelines for optimized systems



Project framework

Project team: 2 sections of Delft University of Technology

- 'Product and Process Engineering' (PPE): J. R. van Ommen
- 'Physics of Nuclear reactors' (PNR): C. T'Joen, M. Rohde
- Large expertise available:
 - Large experimental facilities + computational cluster
 - Expertise in heat transfer and fluid flow experiments
 - Measurement setup for local porosity profiles
 - CFD + experimental benchmark data for packed beds (PNR, PPE)
 - VHTR projects on neutronics (PNR, EU project)
 - Structured tube project for Fischer Tropsch (PPE)



Conclusions

- Packed bed thermo-hydraulics are very complex due to the interaction of different heat/mass transfer mechanisms, on different scales and the complex random geometry.
- An overview was presented of current activities at DUT related to packed bed thermo-hydraulics (experimental and computational)
- A new STW research proposal is being drafted by PNR/PPE (DUT), goal: to further optimise small packed random beds with 'smarter' walls and particles for single phase fluids, providing new design guidelines



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