Biot Number Effects on the Local Heat and Mass Transfer Rate in Fixed and Fluidized Beds

Stefan Radl[1], Florian Krainer[1], Thomas Puffitsch[1] and Christoph Kloss[2]

[1]Graz University of Technology, Institute of Process und Particle Engineering, Graz, Austria. [2]DCS Computing GmbH, Linz, Austria

©Simulation Science Group, IPPT, TU Graz. Web: http://goo.gl/HXB5xm. Email: radl@tugraz.at.

parScale
A Compilation of Particle Scale Models

Introduction and Motivation

Heat and mass transport in fluid-particulate systems is of key importance to engineer, optimize, and understand processes such as

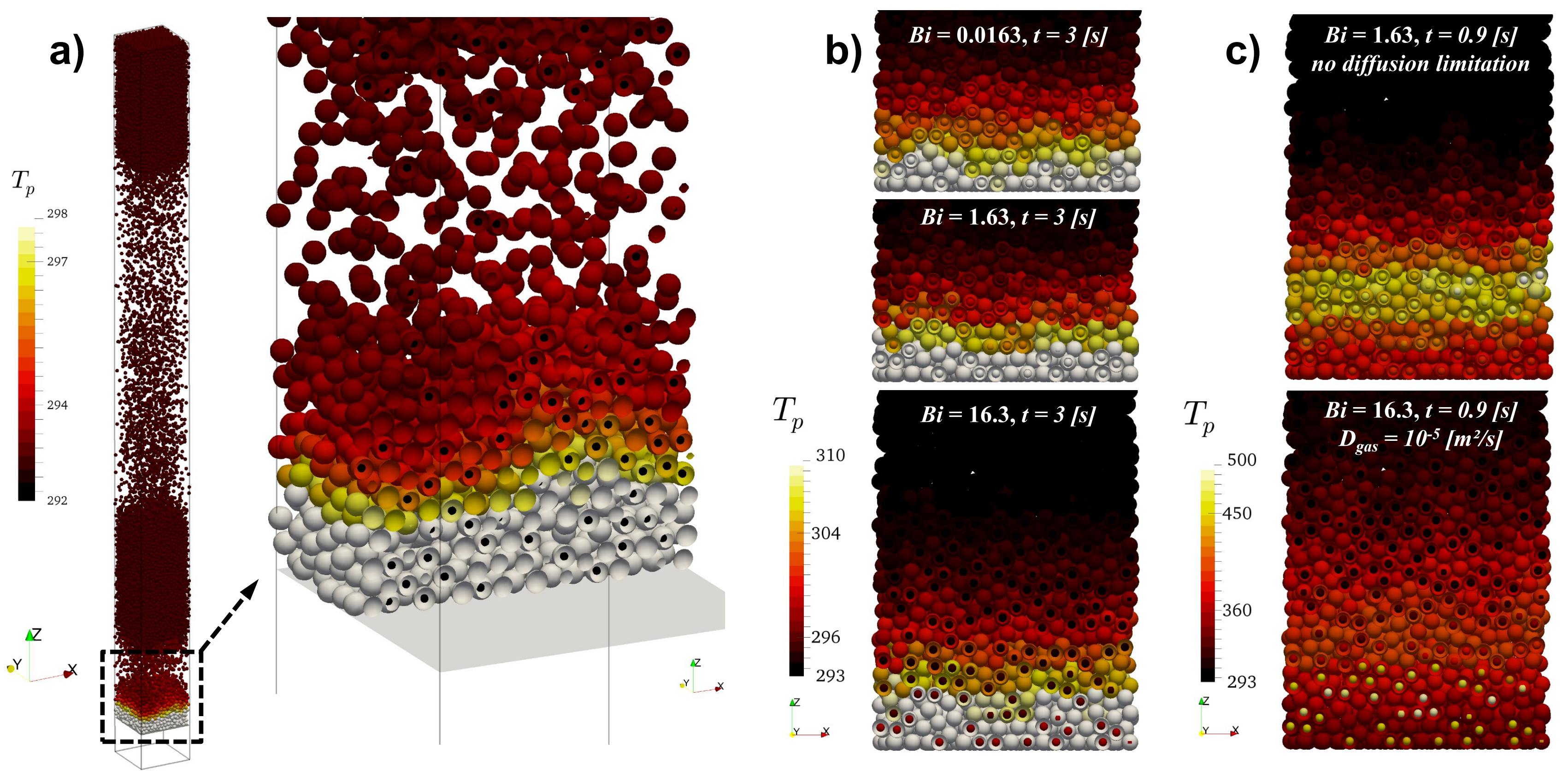
- **Chemical Loop Combustion (CLC) and CL-Reforming processes,**
- **catalytic reactions involving porous or non-porous particles, or**
- **biomass gasification & combustion.**

A key parameter to judge on the importance of intra-particle transport phenomena (i.e., heat and mass transport within the particle) is the Biot number defined as:

$$Bi \equiv \frac{\alpha_{fp}\, d_p}{\lambda_p} \qquad\qquad Nu \equiv \frac{\alpha_{fp}\, d_p}{\lambda_f}$$

The Biot number relates the convective transfer rate to the particle surface (i.e., α_{fp}) to the conductive heat transfer rate in the particle (i.e., λ_p/d_p), and is closely related to the Nusselt (or Sherwood) number *Nu*. A key challenge is to model particulate processes characterized by *Bi* >>1, since resolving intra-particle temperature and concentration gradients is key to predict transport phenomena and reactions within a particle. This is especially true in case particles are moving (see Figure 1), or change their morphology and composition.

Here we present the novel simulation tool *ParScale*, which is designed as a library that can be linked to any particle motion solver. The tool is publicly available via https://github.com/CFDEMproject, licensed under the LGPL v3 (http://www.gnu.org/licenses/lgpl-3.0.html), and is embedded into a multi-scale, open-source simulation platform centred around LIGGGHTS® and CFDEM®. A variety of verification cases, as well as documentation for *ParScale* is available online. *ParScale* relies on the *CVODE* integrator available in the *SUNDIALS* (https://computation.llnl.gov/casc/sundials) package, and hence is suitable to study stiffly-coupled systems (e.g., strongly exothermic reactions).



Base case simulation parameters: Bi = 16.3, W/D/H: $15 \cdot d_p$ / $15 \cdot d_p$ / $200 \cdot d_p$, x- and y-periodic, d_p = 2 mm, U_s = 2 m/s, T_{in} = 323 [K].

Figure 1. Temperature distribution in a fluidized, and a packed bed setup (25,000 particles, each particle is discretized using 10 radial points; a: fluidized bed with close-up view near the inlet, b: packed bed, c: reactive packed bed).

1D Model for Heat and Mass Balances

As a baseline model, we consider integral heat and mass balances for the fluid and particle phase. These balance equations are spatially discretized using a one-dimensional finite-difference approach, assuming a homogeneous particle temperature. Thus, we solve the following system of equations for the particle phase (a similar equation can be written for the fluid phase):

$$\partial_t T_p = \frac{6\alpha(z)}{d_p \rho_p c_{p,p}}\left(T_a - T_p\right) + D_p\, \partial_{zz} T_p$$

We use a second-order accurate, implicit formulation for temporal discretization, i.e. the Crank-Nicolson method, as well as a robust technique to treat the exchange terms for an efficient integration of the equations. Our model considers particle and gas-phase dispersion (with the dispersion coefficients D_p and D_f for the particle and fluid phase, respectively) to account for the effect of pseudo-turbulence and the agitation caused by bubbles in case of fluidized beds.

CFD-DEM Simulation Approach

CFD-DEM simulations of a monodisperse gas-particle fluidized bed, as well as a packed bed were performed. The integration of the governing equations for fluid and particle flow is done by the LIGGGHTS®/CFDEM® package. The newly established *ParScale* package is used to compute the intra-particle profiles. Particle-particle and particle-wall interactions are computed using the Hertz theory with a tangential history component. Rolling friction is taken into account using an elastic-plastic spring-dashpot model [1]. Heat conduction due to particle-particle contacts is accounted for using a model available in LIGGGHTS®. In this study the Nusselt correlation of Deen et. al [2], as well as the fluid-particle drag force correlation proposed by Beetstra et. al [3] was used.

To couple the gas and the particle phase we use a semi-implicit finite volume based PIMPLE algorithm. A smoothing model is used to smear-out the particle information, e.g. the particle concentration ϕ_p, over cells that contain, or are located next to particles [4].

Results

The simulations indicate that the gas temperature profiles (see Fig. 2a), as well as the total transferred heat are marginally affected by the Biot number. However, the particles' surface temperature is drastically affected by the Biot number: we observe higher surface temperatures at higher Biot numbers. This is true for packed beds (see Fig. 1b), as well as for fluidized beds (Fig. 2b). A more dramatic effect is observed for reactive systems (see Fig. 1c), where the temperature and conversion profiles change drastically with Bi.

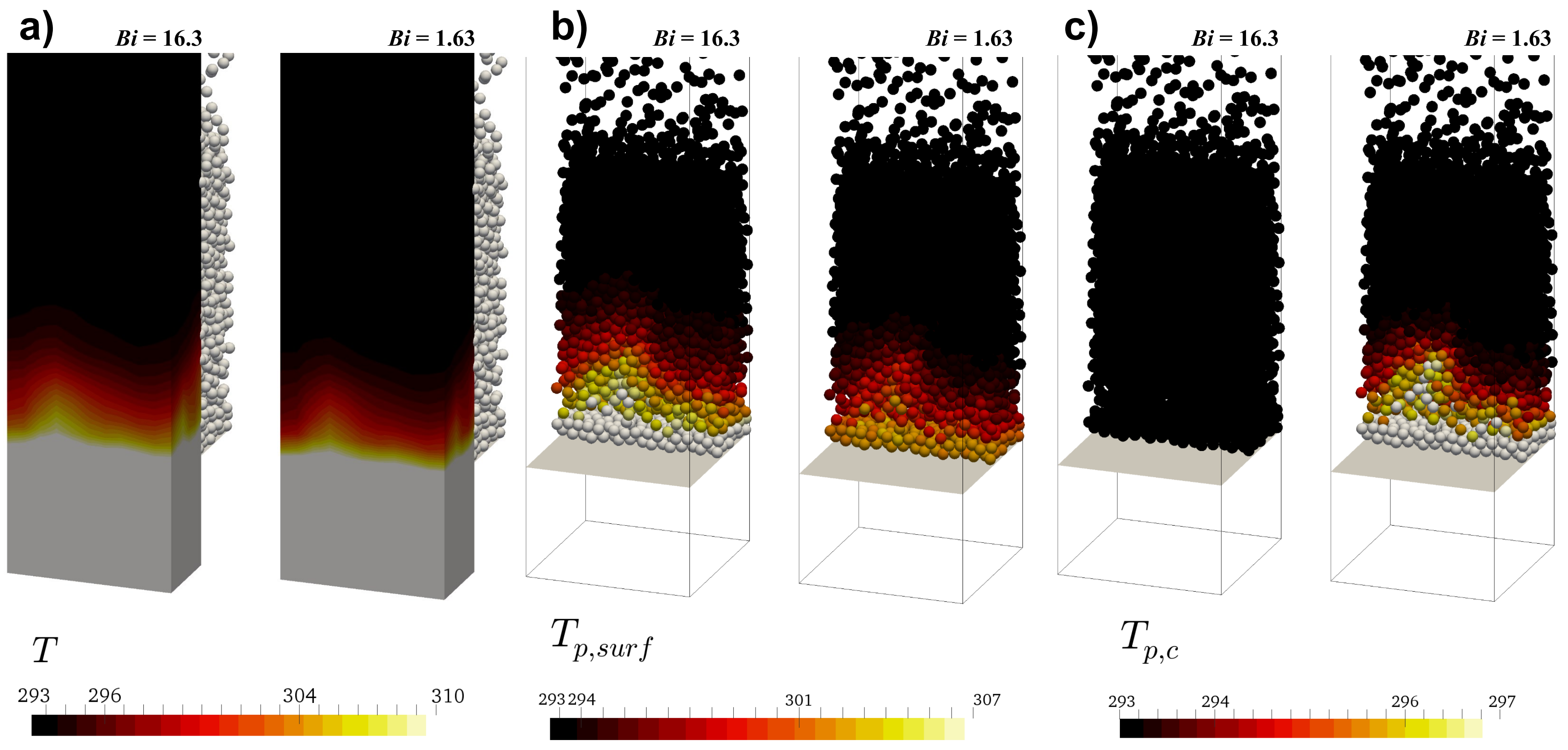


Figure 2. Temperature distribution in a fluidized bed (*t* = 1.1 [s]; a: fluid temperature, b: particle surface temperature, c: particle center temperature).

Results of a more quantitative analysis of the temperature distribution are shown in Fig. 3 (the temperature considered here is the particle's volume-averaged temperature). The effect of *Bi* appears to be smaller here, except for extreme Biot numbers of order 16 or larger. Thus, we expect a minimal effect on the local (particle-averaged) mean temperature. The 1D model captures the main trends for packed beds, however for fluidized beds D_p must be calibrated.

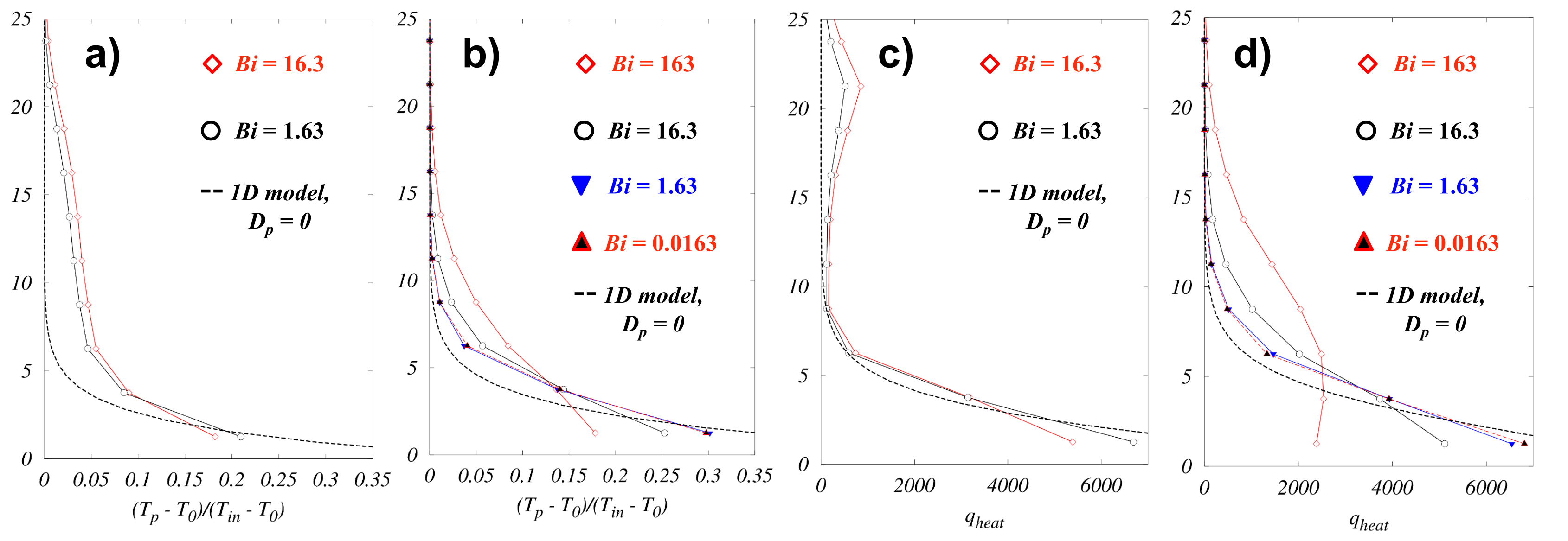


Figure 3. Mean particle temperature profiles (a: fluidized bed *t* = 0.8 [s], b: packed bed *t* = 1.2 [s]), as well as corresponding heat fluxes (c, d).

Acknowledgement
SR, TP, and CK acknowledge funding through the NanoSim project (http://www.sintef.no/projectweb/nanosim). SR and TP acknowledge support by "NAWI Graz" by providing access to dcluster.tugraz.at. LIGGGHTS® and CFDEM® are registered trade marks of DCS Computing GmbH, the producer of the LIGGGHTS® and CFDEM® software.

DCS LIGGGHTS CFDEM SEVENTH FRAMEWORK PROGRAMME NanoSim NAWI Graz

References

[1] C. Goniva, C. Kloss, N.G. Deen, J.A.M. Kuipers, S. Pirker, Influence of Rolling Friction Modelling on Single Spout Fluidized Bed Simulations, Particuology 10 (2012) 582–591.

[2] N.G. Deen, E.A.J.F. Peters, J.T. Padding, J.A.M. Kuipers, Review of direct numerical simulation of fluid–particle mass, momentum and heat transfer in dense gas–solid flows, Chem. Eng. Sci. 116 (2014) 710–724.

[3] R. Beetstra, M. van der Hoef, J.A.M. Kuipers, Drag force of intermediate Reynolds number flow past mono- and bidisperse arrays of spheres, AIChE J. 53 (2007) 489–501.

[4] S. Radl, B. Capa Gonzales, C. Goniva, S. Pirker, State of the Art in Mapping Schemes for Dilute and Dense Euler-Lagrange Simulations, Progress in Applied CFD (2015) 103–112.