

Application of the Extended Discrete Element Method (XDEM) in Computer-Aided Process Engineering

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1 Abstract

A novel technique referred to as Extended Discrete Element Method (XDEM) is developed, that offers a significant advancement for coupled discrete and continuous numerical simulation concepts. The Extended Discrete Element Method extends the dynamics of particles as described by the classical discrete element method (DEM) by additional properties such as the thermodynamic state or stress/strain in conjunction with a continuous phase. Thus, it treats the solid phase representing the particles and the fluidised phase generally a fluid or a gas as two distinguished phases that are coupled through heat, mass and momentum transfer. An outstanding feature of the numerical concept is that each particle is treated as an individual entity that is described by its thermodynamic state e.g. temperature and reaction progress and its position and orientation in time and space. The thermodynamic state includes one-dimensional and transient distributions of temperature and species within the particle and therefore, allows a detailed and accurate characterisation of the reaction progress in each particle. Computational fluid dynamics (CFD) describes the continuous phase with its temperature and velocity distribution in conjunction with the composition of the fluid phase. Thus, the proposed methodology provides a high degree of resolution ranging from scales within a particle to the gas phase as global dimensions of the reactor.

2 Keywords

reaction engineering, modelling, continuous/discrete approach

3 Bakground

Numerical approaches to model multi-phase flow phenomena including a solid e.g. particulate phase may basically be classified into two categories: All phases are treated as a continuum on a macroscopic level of which the two fluid model is the most well-known representative [1]. It is well suited to process modelling due to its computational convenience and efficiency. However, all the data concerning size distribution, shape or material properties of individual particles is lost to a large extent due to the averaging concept. Therefore, this loss of information on small scales has to be compensated for by additional constitutive or closure relations.

An alternative approach considers the solid phase as discrete, while the flow of liquids or gases is treated as a continuum phase in the void space between the particles, and therefore, is labelled the Combined Continuum and Discrete Model (CCDM) [2, 3, 4, 5]. Due to a discrete description of the solid phase, constitutive relations are omitted, and therefore, leads to a better understanding of the fundamentals. This was also concluded by Zhu et al. [6] and Zhu et al. [7] during a review on particulate flows modelled with the CCDM approach. It has seen a mayor development in last two decades and describes motion of the solid phase by the Discrete Element Method (DEM) on an individual particle scale and the remaining phases are treated

by the Navier-Stokes equations. Thus, the method is recognized as an effective tool to investigate into the interaction between a particulate and fluid phase as reviewed by Yu and Xu [8], Feng and Yu [9] and Deen et al. [10].

Initially, such studies are limited to simple flow configurations [3, 2], however, Chu and Yu [11] demonstrated that the method could be applied to a complex flow configuration consisting of a fluidized bed, conveyor belt and a cyclone. Similarly, Zhou et al. [12] applied the CCDM approach to the complex geometry of fuel-rich/lean burner for pulverised coal combustion in a plant and Chu et al. [13] modelled the complex flow of air, water, coal and magnetite particles of different sizes in a dense medium cyclone (DMC). For both cases re-markedly good agreement between experimental data and predictions was achieved.

The CCDM approach has also been applied to fluidised beds as reviewed by Rowe and Nienow [14] and Feng and Yu [9] and applied by Feng and Yu [15] to the chaotic motion of particles of different sizes in a gas fluidized bed. Kafuia et al. [16] describe discrete particle-continuum fluid modelling of gas-solid fluidised beds.

However, current CCDM approaches should be extended to a truly multi-phase flow behaviour as opposed to the Volume-of-Fluid method and the multi-phase mixture model [17]. Furthermore, particle shapes other than spherical geometries have to be taken into account to meet engineering needs according to Zhu et al. [6] and Zhu et al. [7]. This efforts should ideally be complemented by poly-disperse particle systems since all derivations have done for mono-sized particles as stated by Feng and Yu [9]. All these efforts should contribute to a general link between continuum and discrete approaches so that results are quantified for process modelling.

4 eXtended Discrete Element Method (XDEM)

The Extended Discrete Element Method (XDEM) is a numerical technique that extends the dynamics of granular material or particles described by the classic Discrete Element Method (DEM). This extension is achieved through additional properties such as thermodynamic state, stress/strain, or electro-magnetic field for each particle. Contrary to a continuum mechanics concept, XDEM aims at resolving the particulate phase with its various processes attached to the particles. While the Discrete Element Method predicts position and orientation in space and time for each particle, the Extended Discrete Element Method additionally estimates properties such as internal temperature and/or particle distribution, or mechanical impact with structures.

The Discrete Particle Method (DPM) considers each particle of an ensemble as an individual entity with motion and thermodynamics attached to it. The motion module of the Discrete Particle Method handles a sufficient number of geometric shapes that are believed to cover a large range of engineering applications. The thermodynamics module incorporates a physical-chemical approach that describes temperature and arbitrary reaction processes for each particle in an ensemble. Relevant areas of application include furnaces for wood combustion, blast furnaces for steel production, fluidized beds, cement industry, or predictions of emissions from combustion of coal or biomass. The exchange of data between continuous and discrete solutions requires careful coordination and a complex feed- back loop so that the coupled analysis converges to an accurate solution. This is performed by coupling algorithms between the Discrete Particle Method to the Finite Volume e.g. Computational Fluid Dynamics and to structural engineering e.g. Finite Element Method (FEM).

4.1 Computational Fluid Dynamics (CFD) Module

Packed beds can be characterised as a type of porous media in which fluid flow behaves more like an external flow. The flow may be accurately described for a continuum approach by averaging relevant variables and parameters on a coarser level. This leads to a formulation where the actual multiphase medium consisting of

solid matrix and fluid is treated as one homogeneous continuum. The continuity equation of the fluid phase f writes as:

$$\frac{\partial}{\partial t} \left(\varepsilon_f \langle \rho_f \rangle^f \right) + \vec{\nabla} \cdot \left(\varepsilon_f \langle \rho_f \rangle^f \langle \vec{v}_f \rangle^f \right) = \dot{m}_{s,f}''' \quad (1)$$

Gas flow within a porous media like a packed bed of particles exhibits higher Reynolds numbers and thus drag shifts from linear to nonlinear behavior. Thus, phase interaction terms in averaged momentum equation need to be accounted for and appropriately model the non-linearity. This can be achieved by using the Brinkmann or Forchheimer relations [28, 29]. Faghri et al. [29] state that these "empirical momentum relationships are heuristically related to the volume-averaged momentum equation through reasonable observation" This leads to the following equation for conservation of momentum for a porous bed:

$$\frac{\partial}{\partial t} \left(\varepsilon_f \langle \rho_f \rangle^k \langle \vec{v}_f \rangle^f \right) + \vec{\nabla} \cdot \left(\varepsilon_f \langle \rho_f \rangle^f \langle \vec{v}_f \vec{v}_f \rangle^f \right) \quad (2)$$

$$= \vec{\nabla} \cdot \left(\varepsilon_f \langle \vec{v}_f' \rangle^f \right) - \frac{\mu_f}{k} \varepsilon_f \langle \vec{v}_f \rangle^f - \frac{C_f \langle \rho_f \rangle^f}{k^2} \varepsilon_f^2 \langle \vec{v}_f \rangle^f \langle \vec{v}_f \rangle^f \quad (3)$$

where K is the permeability of the bed and C_f the dimensionless drag coefficient. Both parameters can be obtained from empirical relations which are tabulated for various types of porous media [29]. For example for a packed bed with voidage ε_f consisting of spherical particles having diameter D_P the following relations hold [29, 30]:

$$K = \frac{D_P^2 \varepsilon_f}{150(1-\varepsilon_f)^2} \quad (4)$$

$$C_f = \frac{1.75(1-\varepsilon_f)}{D_P \varepsilon_f^3} \quad (5)$$

Conservation of energy in a porous medium consisting of a gas and a solid phase is accounted for by volume-averaging the corresponding energy equation of multiphase systems and writes as follows:

$$\begin{aligned} & \frac{\partial}{\partial t} \left(\varepsilon_f \langle \rho_f \rangle^f \langle h_f \rangle^f \right) + \left(\varepsilon_f \langle \rho_f \rangle^f \langle \vec{v}_f h_f \rangle^f \right) \\ &= -\vec{\nabla} \cdot \langle \vec{q}_f'' \rangle + \frac{\partial p_f}{\partial t} + \langle \vec{v}_f \rangle \cdot \vec{\nabla} \langle p_f \rangle + \sum_{i=1}^M \left\langle \frac{S_p}{V_{REV}} h_{p,f} (\Delta T_i) \right\rangle \end{aligned} \quad (6)$$

where the last term of the right hand equation 6 reflects the coupling between DPM and CFD for heat transfer simulations.

4.2 Motion Module

The Discrete Element Method (DEM), also called a Distinct Element Method, is probably the most often applied numerical approach to describe the trajectories of all particles in a system. Thus, DEM is a widely accepted and effective method to address engineering problems in granular and discontinuous materials, especially in granular flows, rock mechanics, and powder mechanics. Pioneering work in this domain has been carried out by Cundall [31], Haff [32], Herrmann [33] and Walton [34]. The volume of Allen and Tildesley [35] is perceived as a standard reference for this field. For a more detailed review the reader is referred to Peters [36].

4.3 Thermodynamic Module

An individual particle is considered to consist of a gas, liquid, solid and inert phase whereby the inert, solid and liquid species are considered as immobile. The gas phase represents the porous structure e.g. porosity of a particle and is assumed to behave as an ideal gas. Each of the phases may undergo various conversions by homogeneous, heterogeneous or intrinsic reactions whereby the products may experience a phase change such as encountered during drying i.e. evaporation. The need for heterogeneous reactions was pointed out by Chapman [37], while intrinsic rate modelling was emphasised by Rogers et al. [38] and Hellwig [39] to capture accurately the nature of various reaction processes. Furthermore, local thermal equilibrium between

the phases is assumed. It is based on the assessment of the ratio of heat transfer by conduction to the rate of heat transfer by convection expressed by the Peclet number as described by Peters [40] and Kansa et al. [41]. According to Man and Byeong [42] one-dimensional differential conservation equations for mass, momentum and energy are sufficiently accurate. The importance of a transient behaviour is stressed by Lee et al. [43] and Yetter et al. [44]. Transport through diffusion has to be augmented by convection as stated by Rattea et al. [45] and Chan et al. [46]. In general, the inertial term of the momentum equation is negligible due to a small pore diameter and a low Reynolds number as pointed out by Kansa et al. [41]. The conversion module already contains relevant and validated kinetic data that allows predicting both temperature distribution and chemical reactions for an individual particle. This concept is applied to each particle within the packed bed of which spatial and temporal distributions are resolved accurately.

5 Results and Discussion

The following results present predictions of the flow behaviour, temperature distribution and reaction processes in a packed bed including relevant validation.

5.1 Flow characteristics of randomly packed beds

In a classical continuous representation of particulate matter either experimental data or empirical correlations are employed to determine both total surface of the particles and the distribution of void space between them. Of particular interest and investigations is the distribution of porosity in near wall regions and its effect on flow, heat and mass transfer. These disadvantages are omitted by the current approach. XDEM evaluates the available surface for heat transfer and void space influencing the flow distribution. A reactor was randomly filled with particles and the final arrangement allowed assessing local heat and mass transfer conditions. In particular the the distribution of velocity and porosity are shown in fig. 1.

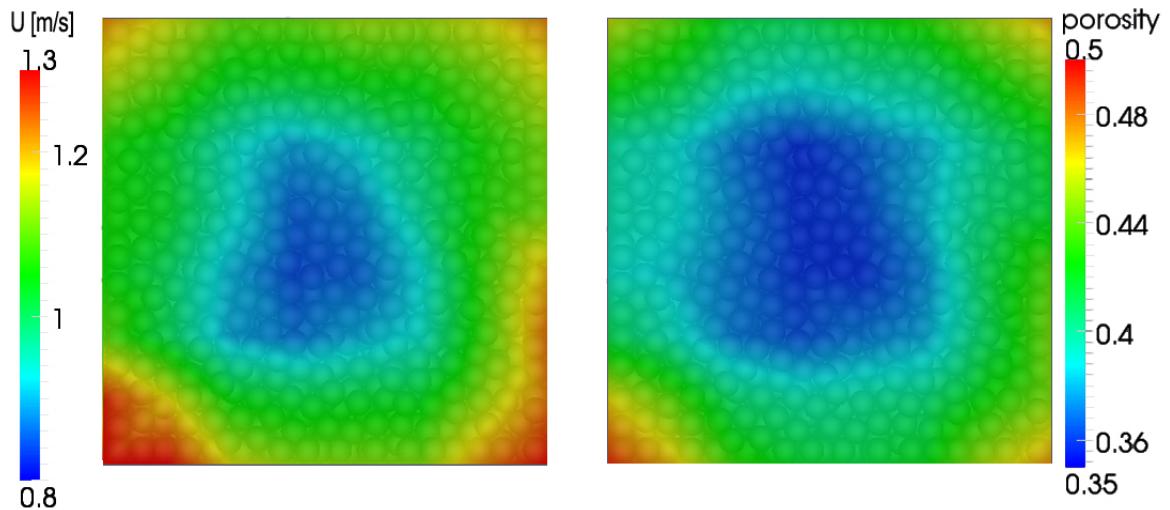


Figure 1: Distribution of flow and porosity in a randomly packed bed

An important characteristic of packed beds is the wall effect, this is manifested by an increased porosity around the inner walls. In these regions, the fluid flow experiences less drag resulting in an increased mass flow rate along the walls as depicted in fig. 1. It contributes to an increased heat transfer to the walls, and thus may causes increased thermal losses of the entire reactor.

5.2 Temperature distribution in a randomly packed bed

Heat-up of a randomly packed bed reactor was experimentally investigated by Peters et al. [47, 48] and therefore, was used to validate the current approach. Among the experiments carried out, heat-up of slate particles was chosen, for which the evolution of temperatures at different positions along the centre line of the packed bed was measured. A cylindrical reactor was randomly packed with particles of spherical shape and equal diameter that amounts to a bed height of 10 cm and represents experimental conditions. In order to avoid a fluidised bed at higher air velocities, the hot gas to heat the packed bed streamed downward through the bed. This arrangement causes the packed bed to heat from top to bottom as depicted in fig. 2 as a comparison between measured and predicted temperatures versus time at different axial positions in the packed bed.

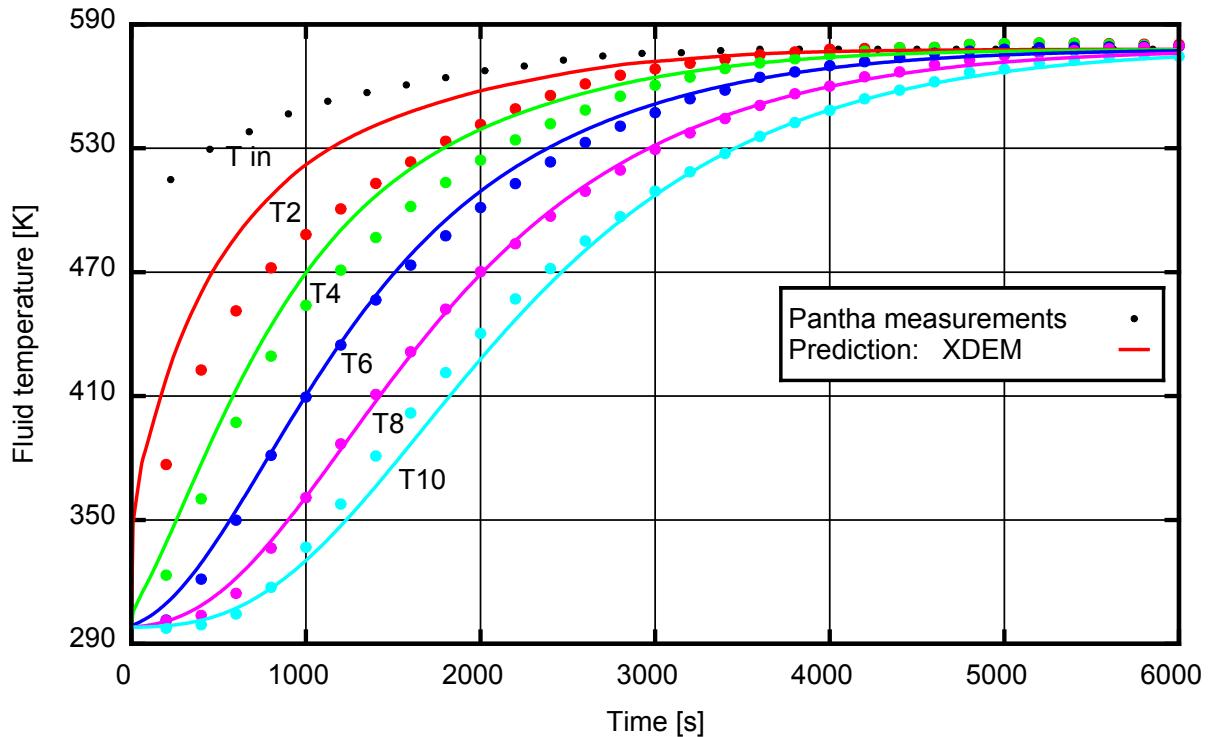


Figure 2: Comparison of temperatures between measurements and predictions at different axial positions in the packed bed

The temperatures at different axial position increase exponentially from top to bottom until steady-state conditions are reached and predictions agree well with measurements. A more detailed view of the temperature fields of both particles and gas is shown in fig. 3 for different times during the heat-up process.

The temperature distributions at different times shows that the temperature is distributed heterogeneously among the particles and that no plain temperature front propagates through the packed bed. In particular the wall effect manifests itself during the heat-up by a rather uneven spatial distribution of particle temperatures. There exists a region near the inner wall of the reactor where air has less access and therefore, a retarded rise of particle temperatures occurs.

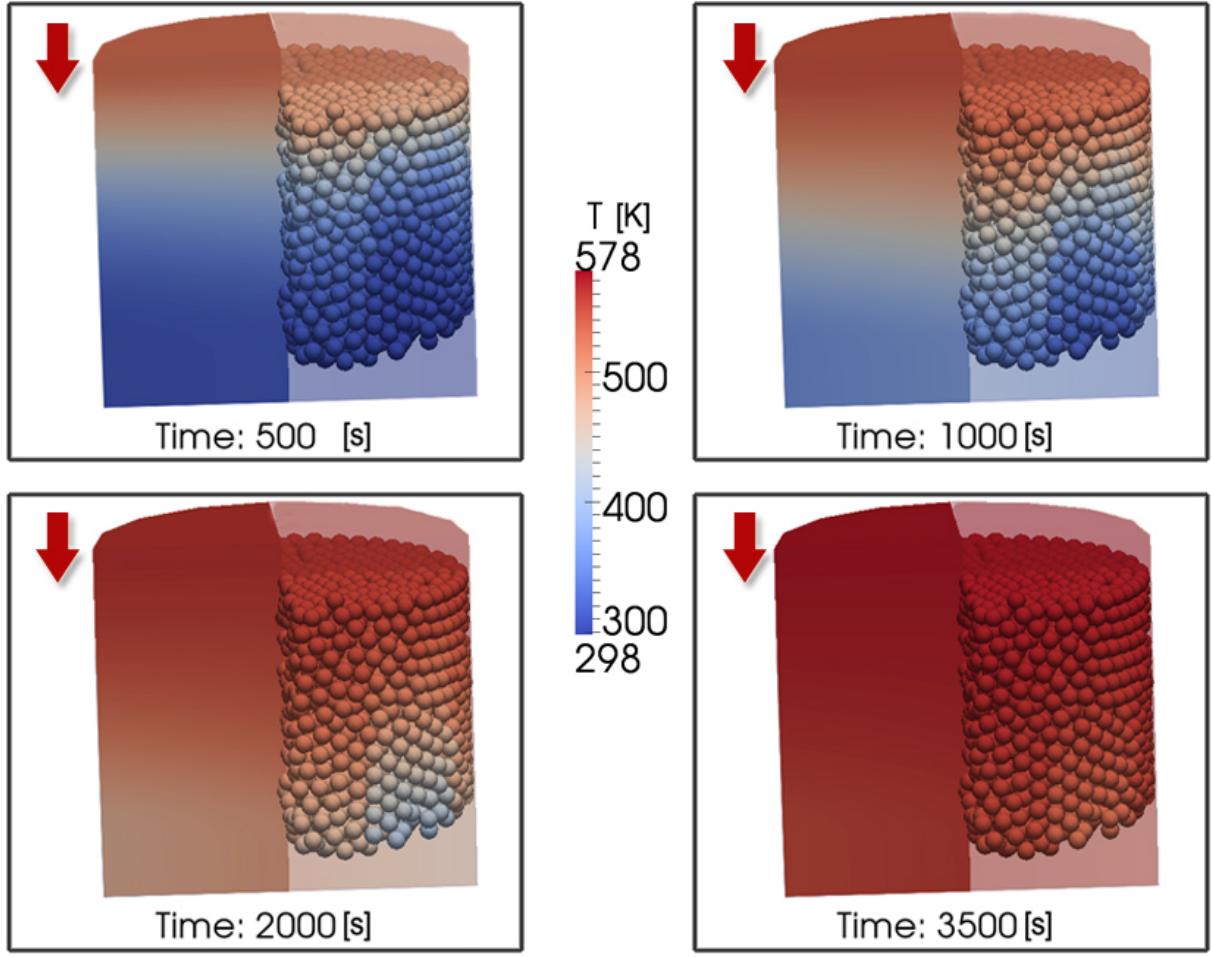


Figure 3: Distribution of gas and particle temperatures in a randomly packed bed

5.3 Drying of a randomly packed bed

Similar to the set-up presented in the previous section, drying of wood particles was predicted and compared to experimental results. Fig. 4 shows the drying process in form of an integral loss of moisture versus the drying period of 100 minutes for two temperatures of the incoming gas of $T = 408\text{ K}$ and $T = 423\text{ K}$. After an initial period for heat-up of the packed bed, during which heat is transferred from the gas to the particles, evaporation conditions are met. Hence, some particles have reached the evaporation temperature so that water vapour inside the particle is generated and successively transported into the gas phase. This process is affecting more and more particles that reduces the total weight of the packed bed. The latter was also measured and very good agreement between measurements and predictions was achieved as depicted in fig. 4.

Since the XDEM methodology resolves individual particles in conjunction with the gas phase, details of the underlying physics are revealed. These detailed results are depicted in fig. 5 at different instances of time for which both water content of the particles and gas temperature is shown.

During the initial period of 1000 s as shown in fig. 5a no drying takes place because the incoming hot gas is heating up the particles to the evaporation temperature. After 2000 s first particles have reached the evaporation temperature and consequently reduce their water content. As seen by the distribution of the water content of individual particles in fig. 5b, the drying process proceeds rather heterogeneously within a cross-sectional viewed from the top of the packed bed. This is due to the in-homogeneously distributed particles that affect both flow distribution heat transfer to the gas phase and between particles in contact. This rather heterogeneous drying pattern progresses through the packed bed as shown in the following sub-figures of fig. 5 and is not comparable to a drying front propagating through a bed as often assumed by many authors.

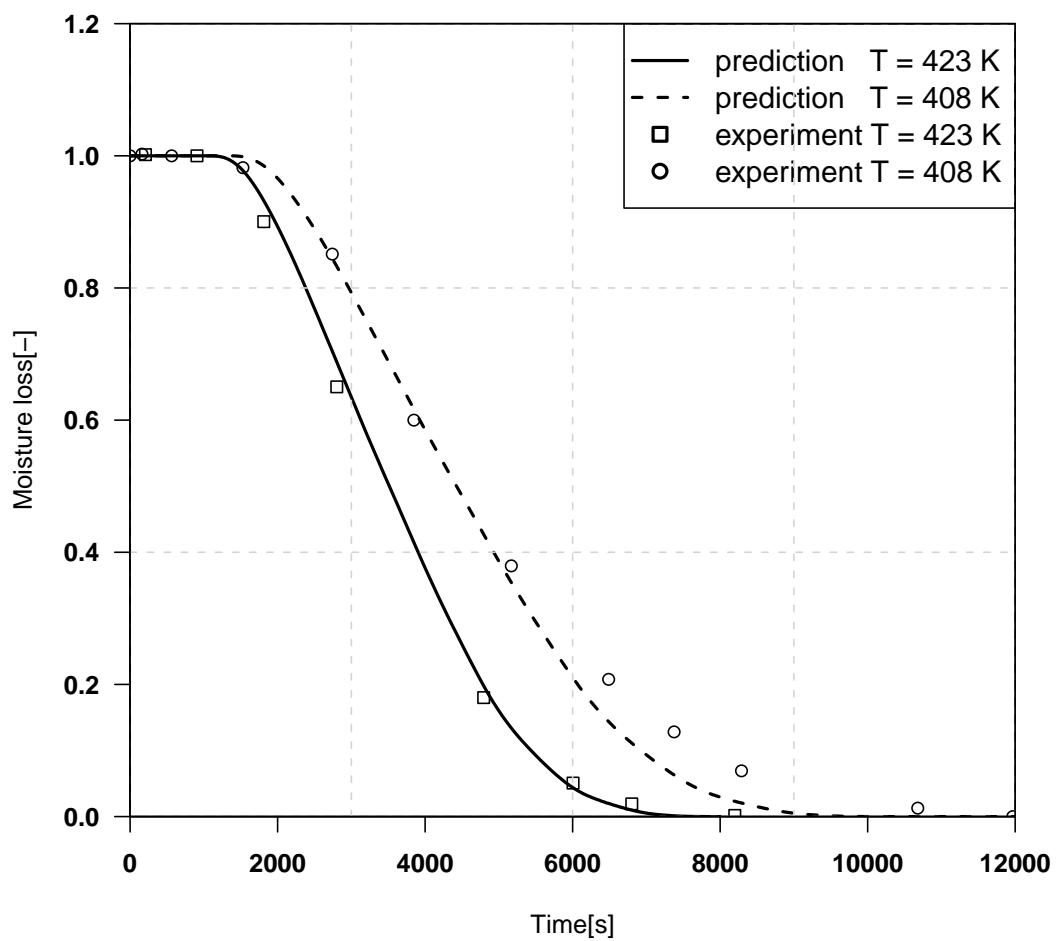


Figure 4: Comparison between measurements and predictions for drying of a randomly packed bed

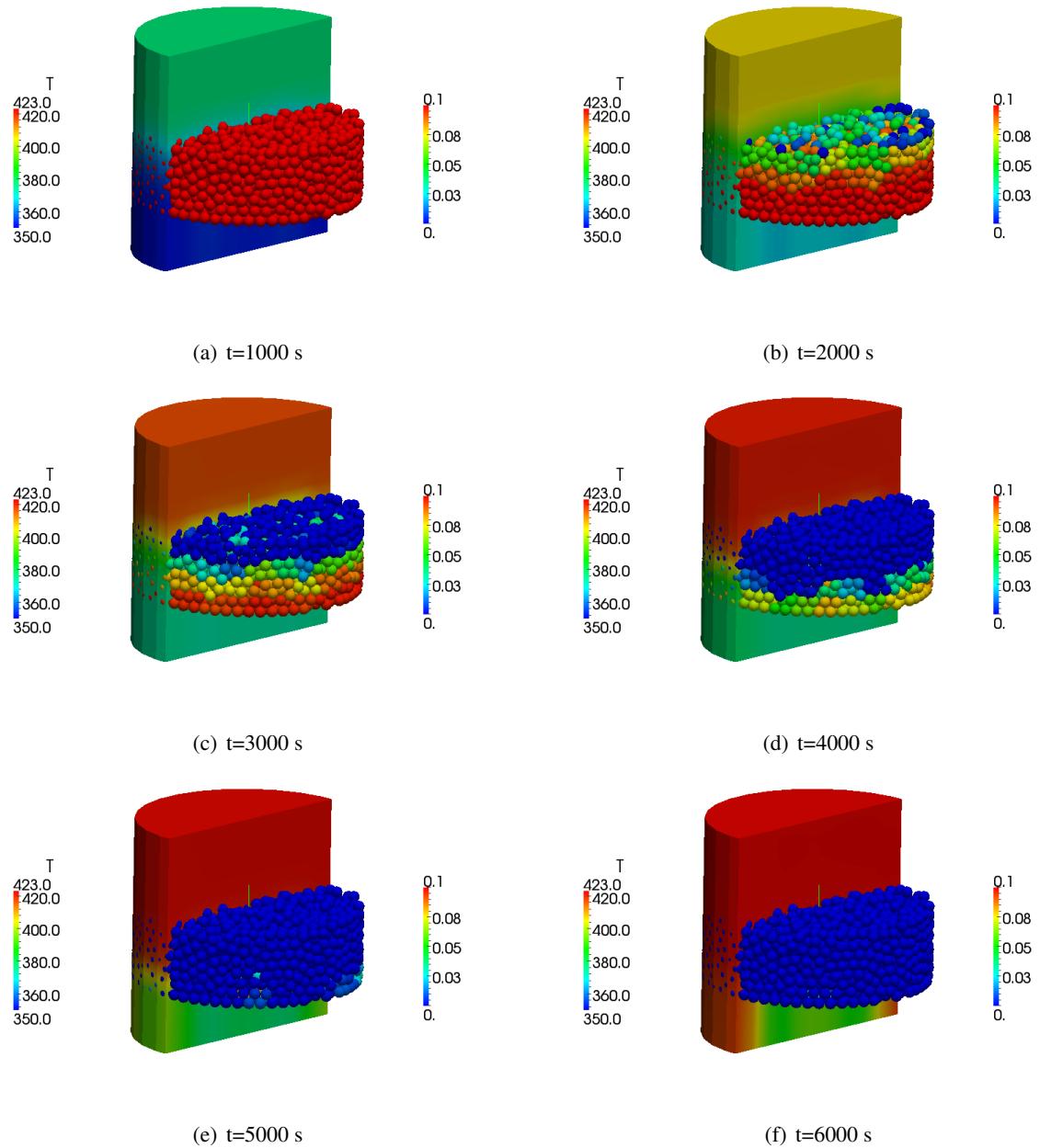


Figure 5: comparison with experiment data a) inlet temperature equal to 408 K b) inlet temperature equal to 423 K

6 Conclusions

Within this study a comprehensive numerical model for heat and mass transfer of granular material in contact with a gas phase is presented to predict drying of particulate materials in a packed bed. The current approach of the Extended Discrete Element Method (XDEM) resolves the particles as a discrete phase of individual particles so that the packed bed consists of a finite number of particles. The thermodynamic state of each particle is described by one-dimensional and transient differential conservation equations that are solved by fast and efficient algorithms.

The flow of a gaseous fluid is through a packed bed is perceived as flow through a porous media of which the distribution is estimated from the geometrical arrangement of particles. Temperature, velocity, pressure and composition of the gas phase is predicted by well developed and state-of-the-art computational fluid dynamics approaches. The particles interact with the flow in their vicinity by heat and mass transfer. Thus, detailed properties of both individual particles and the gas phase are obtained that allow a more accurate and complete interpretation of the underlying physics. The predicted results were compared to experimental data that yielded very good agreement.

7 Authors' Contributions

BP developed the theoretical and numerical frame work of the XDEM. XB is responsible for software development and implementation. AE validated heat transfer for a packed bed, while FH and AM concentrated on mass transfer between particles and gas phase in a packed bed. MM takes the responsibility for the motion of particles in a chemical reactor.

8 Author's Information

A graduate in Mechanical Engineering (Dipl.-Ing.) and PhD from Technical University of Aachen, he is currently head of the Thermo-/Fluidynamics section at the University of Luxembourg and an academic visitor to the Lithuanian Energy Institute (LEI). After a post-doctoral research associate at Imperial College of Science, Technology and Medicine, University of London, UK, he established a research team dedicated to thermal conversion of solid fuels at the Karlsruhe Institute of Technology (KIT) and worked hereafter in industry at AVL List GmbH, Austria. His research activities at the University of Luxembourg include thermo-/fluid dynamics in particular multi-phase flow, reaction engineering, numerical modelling, High Performance Computing (HPC) and all aspects of particulate materials such as motion and conversion from which he derived the Extended Discrete Element Method (XDEM).

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