Enhanced Thermal Process Engineering by the Extended Discrete Element Method (XDEM)

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Abstract A vast number of engineering applications include a continuous and discrete phase simultaneously, and therefore, cannot be solved accurately by continuous or discrete approaches only. Problems that involve both a continuous and a discrete phase are important in applications as diverse as pharmaceutical industry e.g. drug production, agriculture food and processing industry, mining, construction and agricultural machinery, metals manufacturing, energy production and systems biology. 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 granular materials or particles as described through the classical discrete element method (DEM) to additional properties such as the thermodynamic state or stress/strain for each particle coupled to a continuum phase such as fluid flow or solid structures. Contrary to a continuum mechanics concept, XDEM aims at resolving the particulate phase through the various processes attached to particles. While DEM predicts the spacial-temporal position and orientation for each particle, XDEM additionally estimates properties such as the internal temperature and/or species distribution. These predictive capabilities are further extended by an interaction to fluid flow by heat, mass and momentum transfer and impact of particles on structures.

Keywords Extended Discrete Element Method, process engineering, multi-physics, modelling

1 Introduction

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 (TFM) 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 as compared to DNS- or LB-DEM and its capability to capture the particle physics better than the two fluid model. 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].

Within a mayor review on particulate flows modelled with the CCDM approach Zhu et al. [6] and Zhu et al. [7] concluded that the methodology is well suited to understand the fundamental physics of these flows. However, current models including software should be extended to multi-phase flow behaviour and to particle shapes other than spherical geometries to meet engineering needs. This efforts should lead to a general link between continuum and discrete approaches so that results are quantified for process modelling.

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 remarkedly good agreement between experimental data and predictions was achieved. The difficulty for particlefluid flow modelling arises usually for the solid phase within these applications, rather than the fluid phase as stressed by Yu and Xu [8]

The CCDM approach has also been applied to fluidised beds as reviewed by Rowe and Nienow [14] (get article) and Feng and Yu [9] (get article) 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 multiphase 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.

Although the CCDM methodology has been established over the past decade [2, 4], prediction of heat transfer is still in its infancy. Kaneko et al. [18] predicted heat transfer for polymerisation reactions in gasfluidised beds by the Ranz-Marshall correlation [19], however, excluding conduction. Swasdisevi et al. [20] predicted heat transfer in a two-dimensional spouted bed by convective transfer solely. Conduction between particles as a mode of heat transfer was considered by Li and Mason [21, 22, 23] for gas-solid transport in horizontal pipes. Zhou et al. [24, 25] modelled coal combustion in a gas-fluidised bed including both convective and conductive heat transfer. Although, Wang et al. [26] used the two fluid model to predict the gas-solid flow in a high-density circulating fluidized bed, Malone and Xu [27] predicted heat transfer in liquid-fluidised beds by the CCDM method and stressed the fact that deeper investigations into heat transfer is required.

Although Xiang [28] investigated into the effect of air on the packing structure of fine particles, it is not feasible for large structures due to limited computational resources. A recent review of Zhou et al. [6] shows that a lot of approaches concetrate on flow solely without heat or mass transfer. They stated that

- Microscale: To develop a more comprehensive theory and experimental techniques to study and quantify the interaction forces between particles, and between particle and fluid under various conditions, generating a more concrete basis for particle scale simulation.

- Macroscale: To develop a general theory to link the discrete and continuum approaches, so that particle scale information, generated from DEM or DEM-based simulation, can be quantified in terms of (macroscopic) governing equations, constitutive relations and boundary conditions that can be implemented in continuum-based process modelling.

- Application: To develop more robust models and efficient computer codes so that the capability of particle scale simulation can be extended, say, from two-phase to multiphase and/or from simple spherical to complicated non-spherical particle system, which is important to transfer the present phenomenon simulation to process simulation and hence meet real engineering needs.

Zhu et al. [29] reviewd extensively the theoretical background of CFD-DEM coupling, while Zhu et al. [7], Deen et al. [10] and Yu and Xu [8] gave a review focused on the applications of combined CFD and DEM simultions. review Zhu et al. [7] and Zhu et al. [6] concluded from their review that the coupled approach is well suited to understand the fundamnetal phhysics of particulate flows.

2 Extended Discrete Element Method (XDEM)

Contrary to a continuum mechanics concept, the Extended Discrete Element Method (XDEM) as developed by Peters [30, 31] aims at resolving the particulate phase with its various processes attached to the particles. 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 and stress/strain for each particle. 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. 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 Extended Discrete Element Method 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 (DPM) 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. 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 (CFD). For a more detailed review the reader is referred to Peters [31].

2.1 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 [32], Haff [33], Herrmann [34] and Walton [35]. The volume of Allen and Tildesley [36] is perceived as a standard reference for this field.

An ensemble of discrete and moving particles offers the highest potential to describe transport processes. Each of the particles is assumed to have different shapes, sizes and mechanical properties. Shapes such as barrel, block, cone, cube, cylinder, disc, double-cone, ellipsoid, hyperboloid , parallel-epiped, sphere, tetrahedron and torus are available and are shown in fig. 1.
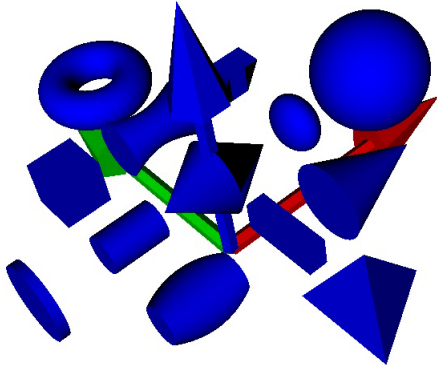

Figure 1. Different shapes for moving particles

Thus, the motion of particles is characterised by the motion of a rigid body through six degrees of freedom for translation along the three directions in space and rotation about the centre-of-mass.

By describing these degrees of freedom for each particle its motion is entirely determined. Newton's Second Law for conservation of linear and angular momentum describe position and orientation of a particle i as follows:

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \sum_{i=1}^{N} \vec{F}_{ij}(\vec{r}_j, \vec{v}_j, \vec{\phi}_j, \vec{\omega}_j) + \vec{F}_{extern} \qquad (1)$$

$$\bar{I}_i \frac{d^2 \vec{\phi}_i}{dt^2} = \sum_{i=1}^{N} \vec{M}_{ij}(\vec{r}_j, \vec{v}_j, \vec{\phi}_j, \vec{\omega}_j) + \vec{M}_{extern} \qquad (2)$$

where $\vec{F}_{ij}(\vec{r}_j, \vec{v}_j, \vec{\phi}_j, \vec{\omega}_j)$ and $\vec{M}_{ij}(\vec{r}_j, \vec{v}_j, \vec{\phi}_j, \vec{\omega}_j)$ are the forces and torquues acting on a particle i of mass m_i and tensor moment of inertia $\bar{I}_i$. Both forces and torques depend on position $\vec{r}_j$, velocity $\vec{v}_j$, orientation $\vec{\phi}_j$, and angular velocity $\vec{\omega}_j$ of neighbour particles j that undergo impact with particle i. The contact forces comprise all forces as a result from material contacts between a particle and its neighbours. Forces may include external forces due to moving grate bars, fluid forces and contact forces between the particles in contact with a bounding wall. This results in a system of coupled non-linear differential equations which usually cannot be solved analytically.

2.2 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. 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 [16] and Kansa et al. [17]. Conservation of mass, momentum and energy is described by transient and one-dimensional differential conservation equations. In general, the inertial term of the momentum equation is negligible due to a small pore diameter and a low Reynolds number, so that the flow may be approximated by Darcy's law as follows:

$$v = \frac{\mu}{k} \nabla p \qquad (3)$$

where v, μ, k and p denote gas velocity, viscosity, permeability and pressure, respectively.

However, conversion of mass for a specie Y_i and energy are described by appropriate differential equations as follows:

$$\frac{\partial Y_i}{\partial t} + \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n \vec{v} Y_i\right) = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n D_i \frac{\partial Y_i}{\partial r}\right)$$
$$+ \sum_{k=1}^{l} \dot{\omega}_{k,i} \qquad (4)$$

$$\frac{\partial (\rho c_p T)}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n \lambda_{eff} \frac{\partial T}{\partial r}\right)$$
$$+ \sum_{k=1}^{l} \dot{\omega}_k H_k \qquad (5)$$

where $\vec{v}$, D_i, $\dot{\omega}$, ρ, c_p, T, and λ denote gas velocity in the pore space, diffusion coefficient, reaction rate, density, specific heat capacity, temperature and heat conductivity. The exponent n defines the geometry of a slab (n=0), cylinder (n= 1) or sphere (n=2). Boundary conditions are given by heat and mass transfer between the particle surface and state of the gas in the proximity of the respective particle. Hence, the following convective boundary conditions for heat and mass transfer are applied.

$$-\lambda_{eff} \frac{\partial T}{\partial r}\Big|_R = \alpha(T_R - T_\infty) + \dot{q}_{rad} + \dot{q}_{cond} \quad (6)$$

$$-D_{i,\text{eff}} \frac{\partial c_i}{\partial r}\Big|_R = \beta_i(c_{i,R} - c_{i,\infty}) \qquad (7)$$

where T_∞, $c_{i,\infty}$, α and β denote ambient gas temperature, concentration of specie i, heat and mass transfer

coefficients, respectively. Additionally, a radiative heat flux $\dot{q}_{rad}$ and a conductive flux $\dot{q}_{cond}$ between particles in contact is taken into account.

The thermodynamic 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 both gas velocity and composition in space and time are resolved accurately by Computational Fluid Dynamics (CFD) [37, 38, 39].

2.3 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 as a flow though a porous media for which the transient and 3-dimensional differential conservation equations for mass, momentum and energy are solved. The current approach has the advantage that the distribution of particles with their volumes is known by predictions of the motion module, so that the distribution of porosity within the flow field in particular near walls is readily available. Therefore, no further correlations for porosity distributions are required. This feature of the current approach leads to an accurate prediction of velocity and temperature distributions of the flow field, of which the temperature and composition of the gas in the vicinity of the particles determine heat and mass transfer by appropriate transfer coefficients.

3 Predicted Results and Discussion

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

3.1 Flow Characteristics of a Randomly Packed Bed

A classical continuous representation of particulate matter requires either experimental data or empirical correlations to determine both total surface of the particles and the distribution of void space between them. These disadvantages are omitted by the current approach. XDEM evaluates the available surface for heat transfer and void space influencing the flow distribution. Of particular interest is the distribution of void space in near wall regions and its effect on flow, heat and mass transfer. For this purpose a cylindrical reactor was randomly filled with particles and the final arrangement allowed assessing local heat and mass transfer conditions. In particular the the distribution of void space and axial velocity are shown in fig. 2 and 3, respectively.

An important characteristic of packed beds is the wall effect, this is manifested by an increased porosity around
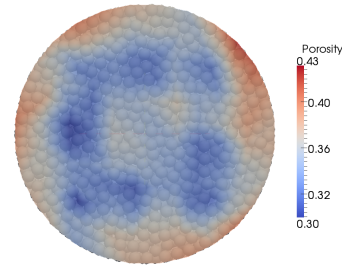

Figure 2. Distribution of void space in a cross-sectional area of a randomly packed bed
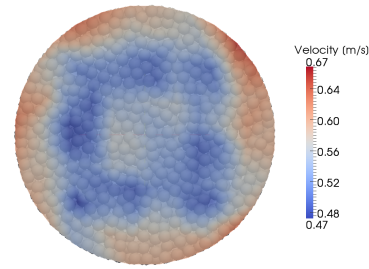

Figure 3. Distribution of axial velocity in a cross-sectional area of a randomly packed bed

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. 3. It contributes to an increased heat transfer to the walls, and thus may causes increased thermal losses of the entire reactor.

3.2 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. 7 shows the drying process in form of an integral loss of moisture versus the drying period of 160 minutes for two temperatures of the incoming gas of T = 408 K and T = 423 K.

(a) t = 1000 s   (b) t = 2000 s
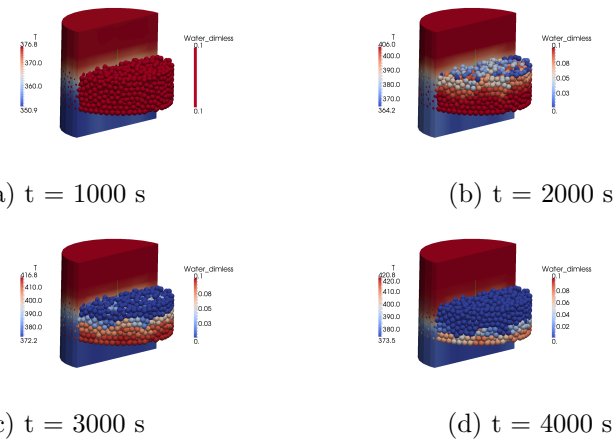
(c) t = 3000 s   (d) t = 4000 s

Figure 4. Temperature distributon of the gas phase and moisture content of individual particles during drying of a packed bed.

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. 7.
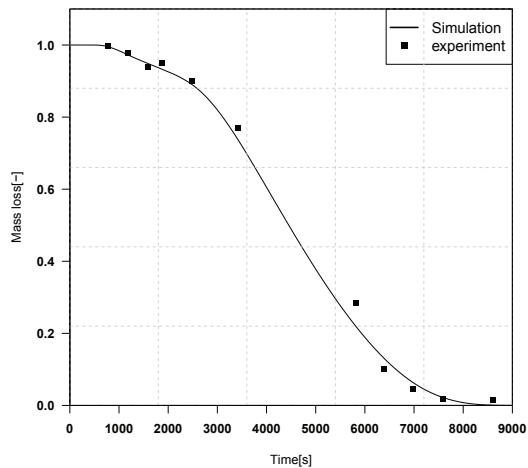
(a) $T_{in} = 573$ k
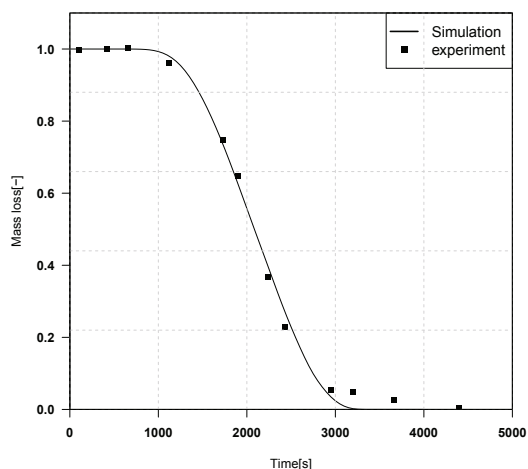
(b) $T_{in} = 803$ k

Figure 5. Comparison between measurements and predictions for pyrolysis of a randomly packed bed

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. 4 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. 4 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. 4, 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 and 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. 4 and is not comparable to a drying front propagating through a bed as often assumed by many authors.

According to the experiment, initially inlet gas temperature is lower than initial particle temperature and it increases gradually to final temperature. This temperature variation can be seen in fig. 6 which present the gas temperature at the centre line and different heights. At $z = 160 \ mm$, approximately from $t = 1200 \ s$ until about $t = 2200 \ s$ the temperature profile shows a deviation from the expected exponential profile. Instead an almost straight line with a smaller slope is observed. This deformation occurs due to drying of particles around that point ($z = 160 \ mm$). however as soon as those particles are dried, the gas temperature increases and its profile returns again to an exponential form. A similar behaviour occurs at different positions along the height of bed.
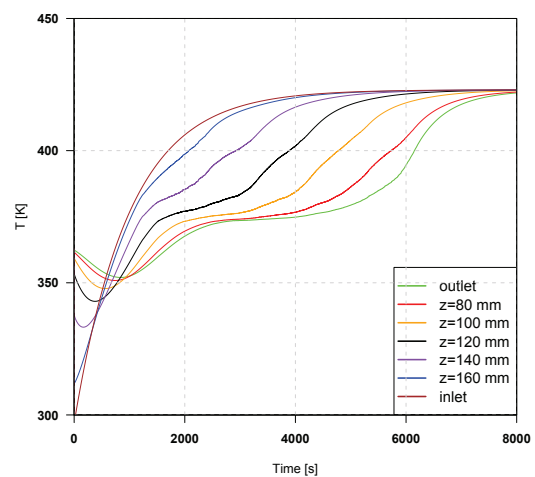

Figure 6. Gas temperature at different heights of the reactor

3.3 Pyrolysis of a Randomly Packed Bed

Similar to drying, pyrolysis of wood particles in a packed bed was predicted and compared to measurements. Fig. 5 presents the mass loss of the packed bed due to pyrolysis of wood particles for two different inlet temperatures for both experiment and predictions. A good agreement between measurement and numerical predictions for both low and high inlet temperatures has been achieved.

Thermal degradation of wood particles in absence of an oxidizing agent, leads to the formation of char, gases and tar. Each of these products may be the desired result of the pyrolysis. Fig. 8 illustrates that the tar mass fraction in the gas phase and the degree of conversion of particles at different times. In order to show the species distribution inside the reactor, only a quarter of the gas

phase is depicted and half of the particles have been shown in in fig. 8 to illustrate the heterogenous reaction progress inside the bed. The hot gas entering from the top of the bed, the conversion of the wood particles also starts from top. Fig. 8 shows clearly that reaction progesses from the top of the bed to the bottom. At t=1000 s few particles on the top of the bed start decomposing, and therefore the small amount of tar appears in the gas phase. As time proceeds more particles degradate and larger amounts of tar is produced and transferred to the gas phase.
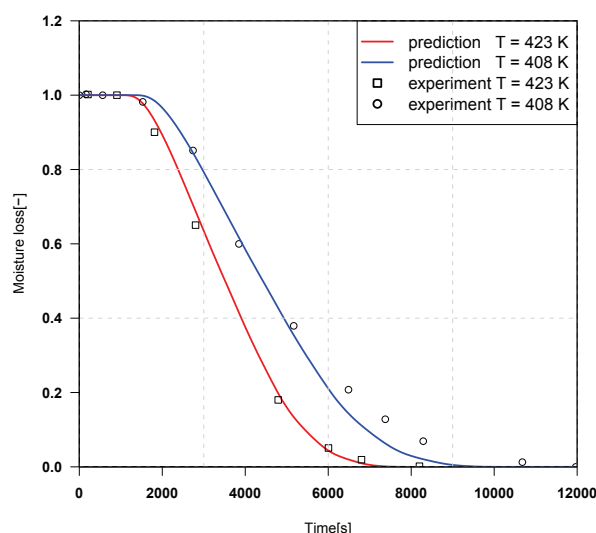

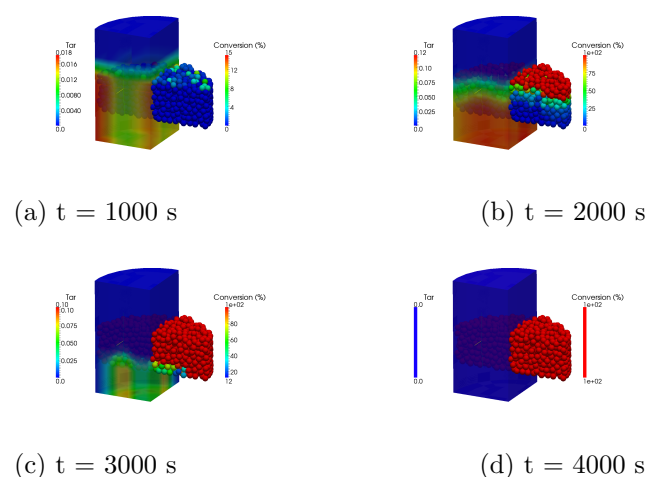**Figure 7.** Comparison between measurements and predictions for drying of a randomly packed bed

(a) t = 1000 s   (b) t = 2000 s

(c) t = 3000 s   (d) t = 4000 s

Figure 8. Mass fraction of tar and particle conversion at different times.

4   Summary

The current contribution introduces the Extended Discrete Element Method (XDEM) and applies to thermal conversion of packed beds as often encountered in process engineering. The proposed concept couples effectively the particulate phase with a gas streaming through the void space of a packed bed reactor. For this purpose, the particulate phase is resolved discretely by solving one-dimensional and transient differential conservation equations for mass and energy for each particle individually by fast and efficient algorithms. Hence, the thermodynamic state of each particle is determined taking into account heat and mass transfer between the particle surface and the surrounding gas phase. The latter is described by solving the conservation equations of classical Computational Fluid Dynamics (CFD). This concept was employed to predict both drying and pyrolysis of a packed bed, that yielded detailed results of a large range of length scales between the particles dimensions and the global length scales of the reactor. A comparison of predictions with measurements for global mass losses of the packed bed agreed very well.

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