The Extended Discrete Element Method (XDEM) for Multi-Physics Applications

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ABSTRACT

A vast number of engineering applications include not solely physics of a single domain but consist of several physical phenomena, and therefore, are referred to as multi-physics. As long as the phenomena considered are to be treated by either a continuous i.e. Eulerian or discrete i.e. Lagrangian approach, a homogeneous numerical solution concept may be employed to solve the problem. However, numerous challenges in engineering exist and evolve, that 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 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].

2 Extended Discrete Element Method (XDEM)

Contrary to a continuum mechanics concept, the Extended Discrete Element Method (XDEM) 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).

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 [11], Haff [12], Herrmann [13] and Walton [14]. For a more detailed review the reader is referred to Peters [15].

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. 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.

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 a flow through 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 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 porosity in near wall regions and its effect on flow, heat and mass transfer. 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.
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.

### 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. 2 shows the drying process in form of an integral loss of moisture versus the drying period of $\sim 160$ minutes for two temperatures of the incoming gas of $T = 408 \, K$ and $T = 423 \, K$. 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. 2.

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. 3 at different instances of time for which both water content of the
During the initial period of 1000 s as shown in fig. 3a 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. 3b, 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. 3 and is not comparable to a drying front propagating through a bed as often assumed by many authors.

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Figure 2: Comparison between measurements and predictions for drying of a randomly packed bed
Figure 3: Comparison with experiment data a) inlet temperature equal to 408 K b) inlet temperature equal to 423 K
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5 References


