Scale-Resolved Prediction of Pyrolysis in a Packed Bed by the Extended Discrete Element Method (XDEM)

B. Peters, X. Besseron, A. Estupinan, F. Hoffmann, M. Michael, A. Mouhmadi, and M. Mohseni
University of Luxembourg, Faculty of Science, Technology and Computer Science, 6, rue Coudenhove-Kalergi, L-1359 Luxembourg, Luxembourg, tel.: +352 46 66 44 54 96, fax: +352 46 66 44 52 00; e-mail: bernhard.peters@uni.lu

Many engineering applications in particular process engineering deal with a particulate phase and a fluid phase such as liquids or gases simultaneously. Predominant applications are 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. These applications commonly span a large spectrum of length and time scales that need to be resolved to predict relevant phenomena accurately. Only recently a novel and innovative technique referred to as Extended Discrete Element Method (XDEM) has emerged, that is based on an Euler-Lagrange concept. 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 characterization of the reaction progress on the scale of the particles in a packed bed. The distribution of particles in a packed bed defines the interstitial space between them that is available for the fluid to flow through the packed bed. The flow in the void space is described by well-established Computational Fluid Dynamics and is coupled to the particulate phase through heat and mass transfer. Thus, the proposed methodology provides a high degree of resolution ranging from scales within a particle to the continuum phase as global dimensions. These superior features as compared to traditional and pure continuum mechanics approaches are applied to predict pyrolysis of wood particles in a packed bed as shown in fig. 1.

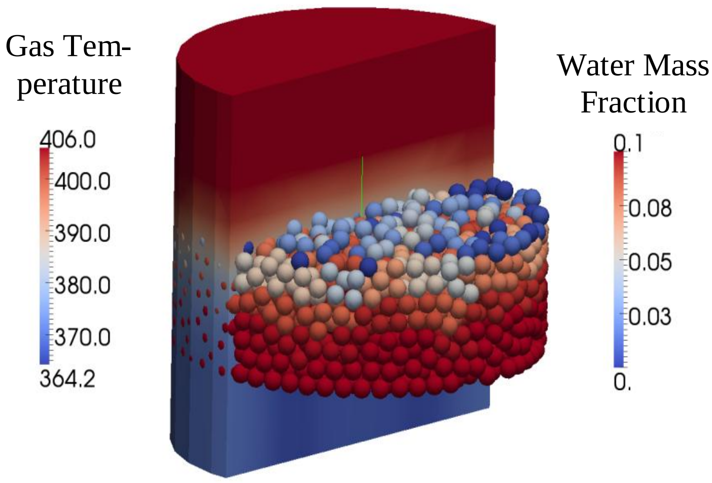

Figure 1: Gas and particle resolved temperature during pyrolysis of a packed bed

Fig. 1 shows the rather inhomogeneous drying process in the upper part of the reactor with higher temperatures around the circumference of the inner reactor wall. The latter is due to increased porosity in conjunction with higher mass flow rates than in the centre of the reactor, and thus, augmented heat transfer. Hence, the Extended Discrete Element Method offers a high degree of resolution avoiding further empirical correlations and extends the knowledge into the underlying physics.