

# MODELLING OF THE THERMOCHEMICAL PROCESSES IN POROUS MEDIA WITH PHASE TRANSITION USING XDEM AND FVM METHODS

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## 1. Introduction

The fluid flow through the porous media with phase transition is an important technical issue that is common in the power industry, and is also an interesting research problem. The task described and analyzed in the following work is derived directly from the thermal conversion of solid fuel. It refers for example to a process of gasification/combustion in the packed bed or even the conversion of single fuel particles. Thermal conversion of solid fuels plays an important role in energy generation. In Poland still over 80% of electrical energy is produced from coal. The combustion of fossil fuels gives Poland high energy independence, while providing relatively low cost of the electricity and heat produced from coal. Unfortunately, the combustion of coal, mostly in small scale old domestic boilers, causes high concentration of PM2.5 in the surrounding air and the highest level of benzopyrene in the European Union [1] which is one of the most toxic components of smog. Therefore, an analysis of thermal conversion of solid fuels has a practical meaning. Moreover flow through a porous packed bed of solid particles with mass loss phenomenon is interesting from research reasons.

The main goal of this work is to investigate the possibility of different numerical methods (eXtended Discrete Element Method - XDEM, Finite Volume Method - FVM) to simulate the behavior of solid fuel particles during the gasification process that is performed in the Institute of Fluid-Flow Machinery PAsci (IMP).

## 2. Thermochemical processes in packed bed and single fuel particle

The XDEM method aims at resolving the particulate phase with its various processes attached to the particles [3]. The main assumption of numerical modelling is that each particle undergoes a sequence of thermodynamic processes that are described by a set of one-dimensional and transient conservation equations for mass, momentum and energy using Discrete Particle Method (DPM) [2]. XDEM practically extends the dynamics of particles described by the classic DEM. In the analyzed solid fuel conversion problem the simplified geometry of the IMP "INKA" reactor was used. In Figure 1 the XDEM/CFD numerical results are presented. The propagation of the heating front and the moisture content in each particle can be observed. As can be seen, the hot gas flows into the cylinder from the top wall to the bottom wall. Due to the heat transfer from hot air to cold biomass, the central temperature of each particle is increasing.

For comparison the numerical analysis of single particle heating obtained from 1D in-house code is presented (Figure 2). The numerical code is based on the finite volume method (FVM) and includes the mass, momentum and energy balance equations with the source terms. Main assumption is the structure of the solid particle which consists of the solid, gas and water phase and has an ideal spherical shape. Additional simplification is that the thermochemical properties may change only in the radial direction, what gives simpler form of the partial differential equations. The cold particle is heated by the stream of hot nitrogen. Due to the heat transfer from the surrounding gases, the structure of particle is changing and the moisture and volatiles are released. The mass source terms for moisture and volatiles, the porosity change and the particle thermophysical properties variation were implemented basing on the appropriate temperature relationships [4].

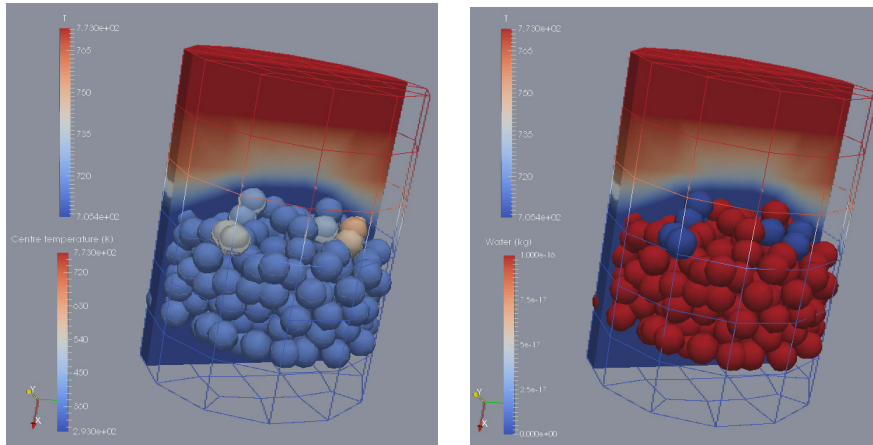


Figure 1: Temperature distribution and particle water content in a simplified reactor geometry

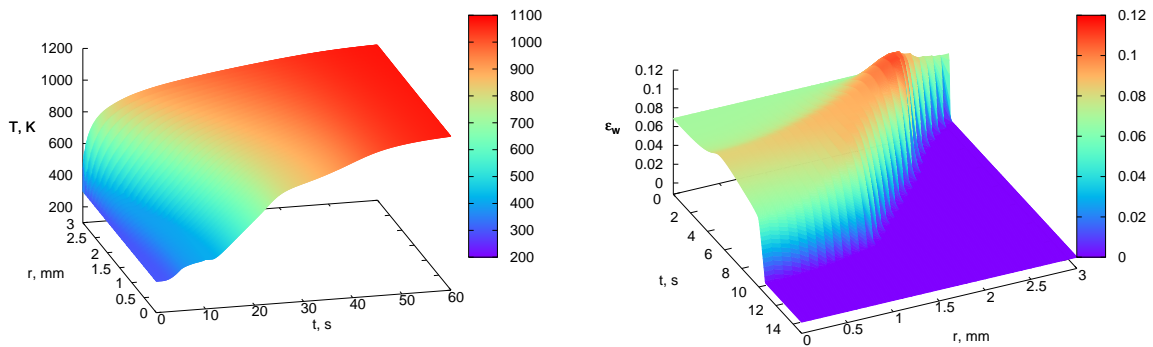


Figure 2: Temperature distribution and particle water volume content in the solid single fuel

### 3. Conclusions

The main goal of this work was to investigate the possibility of the XDEM/1D FVM programs to simulate the behavior of the solid fuel particles during the thermochemical conversion process that was performed in the real gasifier called "INKA" (IMP). Basing on the test case calculations of the analyzed reactor, the following conclusions can be made: (I) the XDEM method can be used to simulate heat and mass transfer processes in the packed bed reactors, (II) the numerical results obtained using both programs show propagation of the heating front and the change of the moisture content in particles, (III) the time of conversion depends on the type of the fuel, its structure, size and physical parameters.

### References

- [1] Polycyclic aromatic hydrocarbons air pollution at urban background stations in 2016 - in Polish. *Główny Inspektorat Ochrony Środowiska, Warszawa, 2017.*
- [2] A. A. Estupinan Donoso and B. Peters. XDEM used for predicting tungsten-oxide reduction. *CAPE Forum 2015, Computer Aided Process Engineering, University of Paderborn, April 27-29, Paderborn, Germany, 2015.*
- [3] B. Peters, X. Besseron, A. Estupinan, F. Hoffmann, M. Michael, and A. Mahmoudi. Enhanced thermal process engineering by the extended discrete element method (XDEM). *Univ. J. Eng. Sc.*, 1(4):139–145, 2013.
- [4] I. Wardach-Świącicka. *Modelling of physicochemical processes in a solid fuel particle in a stream of hot gases, PhD Thesis - in Polish.* IMP, Gdańsk, 2016.