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Supplementary Material

Entrained-flow Coal Gasification Process Simulation with the Emphasis on Empirical Char Conversion Models Optimization Procedure

Jakub Mularski * and Norbert Modliński

Department of Energy Conversion Engineering, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland; norbert.modlinski@pwr.edu.pl
* Correspondence: jakub.mularski@pwr.edu.pl; Tel.: +48-71-320-21-81

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4. Reactor. Computational Domain

The geometry of the reactor was discretized applying a 2-D axisymmetric grid consisting of 101777 elements. The minimum orthogonal quality was equal to 0.86, while the average one was equal to 0.9973. The mesh density was increased near the inlet and the symmetry axis. The minimum mesh sizes for the axial and radial directions were equal to 2 mm and 0.2 mm, respectively (Fig. 1).

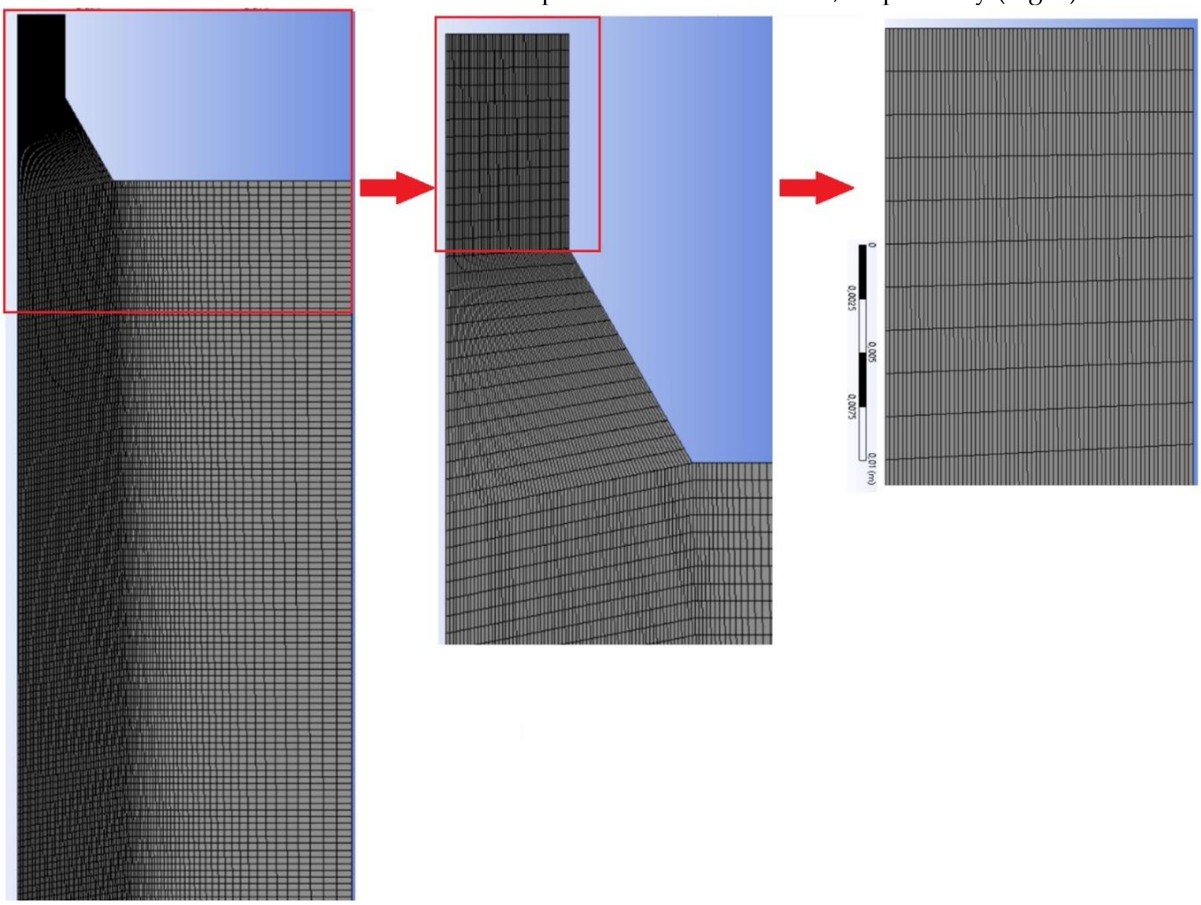

Figure 1. Mesh of the reactor

As regards the boundary conditions, the mass flow rates were presented in the manuscript in Table 3. Inlets were defined as mass-flow-inlets, reactor wall as a wall-type condition with the temperature of 1500 K, while outlet as a pressure outlet.

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The solution was monitored by means of the residuals and specific variables at the outlet and in the flame region (e.g. temperature, CO mole fraction, H_2 mole fraction). DPM iteration interval was equal to 60. In order to obtain stable calculations, under-relaxation factor for the discrete phase was set to 0.005. The simulation required approximately 90 000 iterations to converge.

Exemplary results from the mesh independence study:

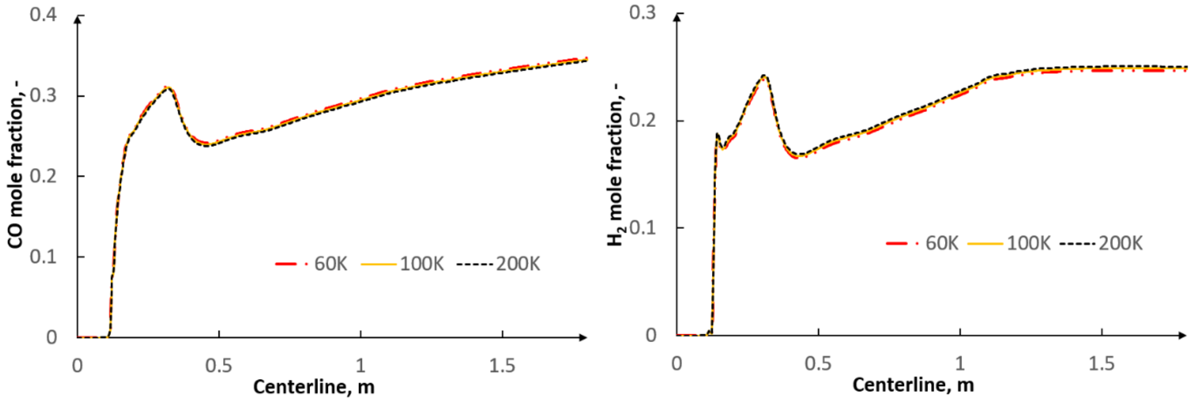

Figure 2. Exemplary mesh independence study results for CO and H_2 mole fractions.