**Computational fluid dynamics model of internally cooled bubbling fluidized-bed reactor for CO2 methanation process**

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**Highlights**

* A CFD model was proposed for CO2 methanation in bubbling fluidized-bed (BFB).
* An internal helical heat exchanger was employed to the BFB reactor.
* Heterogeneous reaction kinetics and multiphase heat transfer were applied.
* Temperature, solid holdup, gas composition and reaction heat were analyzed.

**1. Introduction**

Power-to-gas (PtG) processes are being considered as one of the most promise alternatives to integrate renewable energy resources into a current energy grid [1] via CO2 methanation process. Computational fluid dynamics (CFD) has become a suitable tool for design and hydrodynamics evaluation of chemical processes [2,3]. Kopyscinski et al., [4] did the first attempt to apply the fluidization technology for CO methanation. Recently, Sun et al., [5] evaluated the full-loop circulating fluidized-bed using CFD for CO methanation. However, few CFD studies on bubbling fluidized-bed (BFB) reactor have been done for CO2 methanation with H2.

This study focuses on the design of an internally-cooled BFB (IC-BFB) reactor for CO2 methanation with H2 using CFD model. A heterogeneous reaction kinetics from the literature and gas-solid heat transfer model are employed to the CO2 methanation with a Ni-based catalyst. The CFD model results on pressure, velocity, temperature, solid volume fraction, CH4 composition, and reaction heat are presented.

**2. CFD model and boundary condition**

The IC-BFB includes the two domains: (1) fluidized-bed reactor with diameter of 80 mm and height of 500 mm, where the catalyst bed height is about 250 mm; (2) helical coil heat exchanger (HCHE) with a tube diameter of 6 mm and a center diameter of two coils of 30 and 60 mm, respectively.

A commercial CFD code ANSYS Fluent R19 (ANSYS Inc., USA) was used, the reaction kinetics from Xu and Froment [6] was employed via a user-defined function. The material properties and boundary conditions are summarized in Table 1. The 2D CFD domains were discretized into 39,000 cells. The time step of the unsteady-state gas-solid Eulerian two-fluid flow model was set to 1×10-4 s. The CFD domains and mesh structure are shown in Figure 1a.

Table 1. Material properties and boundary conditions.

|  |  |
| --- | --- |
| Material type | Properties |
| Diameter [µm] | $ρ$ [kg/m3] | $λ$ [W/m/K] | $C\_{p}$ [J/kg/K] | Diff. [m2/s] | Viscosity [kg/m/s] |
| Catalyst  | 100 | 2350 kg/m3 | 0.67 | 880 | - | 1.789e-5 |
| Gas mixture  | - | SRK real gas | Ideal-gas mixing-law | Mixing law | Kinetic-theory | Ideal-gas mixing-law |
| BC name | Boundary conditions |
| BC type | T [K] | HTC [W/m2/K] | P [Pa] | Velocity [m/s] | CO2/H2/N2 [mole %] |
| Inlet  | Velocity inlet | 673 | - | 5e5 | 0.13 m/s | 0.2/0.8/0 |
| Outlet | Pressure outlet | 673 | - | 5e5 | - | 0/0/1 |
| Reactor wall | Wall | 353 | 0.3 | - | - | - |
| Coil wall | Wall | 470 | 135 | - | - | - |

**3. Results and discussion**

The snapshots at t = 60 s for the contours of pressure, velocity, solid volume fraction, temperature, CH4 mole fraction, and heterogeneous reaction heat are displayed in Figure 1b, c, d, e, f and g. Reactions are more intensive at the core of the reactor, while gas-solid mixing is enhanced by HCHE to become almost even distribution of temperature in the whole catalyst bed. The product dry gas compositions of CO2/H2/CH4 = 0.079/0.329/0.592 are similar to literature [7].



**Figure 1.** CFD domain and meshing, and CFD results.

**4. Conclusions**

An IC-BFB was modeled using a 2D Eulerian two-fluid CFD model for CO2 methanation. The CFD model demonstrated the excellent heat and mass transfer capability of the IC-BFB reactor.

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