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Nowadays hydrogen demand represents a crucial point for deeper liquid fuel hydro-refining. It is well known that prospective process for hydrogen production is based on a common utilization both renewable natural and fossil waste sources by partial oxidation (POX) and gasification of biomass materials and/or heavy petrochemical wastes.

The goal of this work was to develop numerical model of experimental POX pilot plant reactor of UNIPETROL RPA to test application of different raw materials.

Process performance was compared with results of its simulation by Aspen Plus software. Both chemical equilibrium and kinetic of pyrolysis and soot formation were taking into account. Also sensitivity of POX product composition depending on properties of different raw materials and reaction condition were analysed by mathematical modelling approach.

Mathematical model development made in the study consisted of several steps:

First of all, complex chemical composition was predominantly solved by concept of representative chemical compounds resulting in the same elemental composition as the raw material used in experiments.

Next, simulation model of the process was created using simulator Aspen Plus, supposing pseudo-homogeneous CSTR and fitting reaction kinetics and chemical equilibrium of complex reactions on experimental data. Physical non ideal behaviour was treated by Peng-Robinson equation of state, chemical equilibrium composition was evaluated by minimization of Gibbs energy and optimization procedure using Marquardt or Nelder –Mead methods.

Finally, CFD simulation model was developed in COMSOL Multiphysics environment (PDE solver by finite element method) to find steady state gas velocity, temperature and concentration profiles inside of POX reactor.

Hydrogen production depends both on oxygen and water steam ratio to carbon content in raw material. From a hydrodynamic point of view process efficiency depends also on flow characteristics and internal mixing inside the reactor. Residence time distribution reaction mixture in the reactor affects selectivity of consecutive reaction steps: pyrolysis, water gas shift and steam reforming reactions. Due to different reaction rates CFD modelling approach can help to understand complex heat, mass and momentum transfer phenomena in the POX reactor.

Literature

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