Abstract:

The effectiveness of energy conversion and carbon dioxide sequestration in Integrated Gasification Combined Cycle (IGCC) is highly dependent on the syngas composition and its further processing. Water gas shift membrane reactor (WGSMR) enables a promising way of syngas-to-hydrogen conversion with favourable carbon dioxide sequestration capabilities. This paper deals with a numerical approach to the modelling of a water gas shift reaction (WGSR) in a membrane reactor which promotes a reaction process by selectively removing hydrogen from the reaction zone through the membrane, making the reaction equilibrium shifting to the product side. Modelling of the WGSR kinetics was based on Bradford mechanism which was used to develop a code within Mathematica programming language to simulate the chemical reactions. The results were implemented as initial and boundary conditions for the tubular WGSMR model designed with Aspen Plus software to analyze the broader system behaviour. On the basis of selected boundary conditions the designed base case model predicts that 89.1...