World Academy of Science, Engineering and Technology
International Journal of Environmental and Ecological Engineering
Vol:11, No:11, 2017

Multiscale Computational Approach to Enhance the Understanding, Design and Development of CO_2 Catalytic Conversion Technologies

Authors : Agnieszka S. Dzielendziak, Lindsay-Marie Armstrong, Matthew E. Potter, Robert Raja, Pier J. A. Sazio

Abstract : Reducing carbon dioxide, CO_2, is one of the greatest global challenges. Conversion of CO_2 for utilisation across synthetic fuel, pharmaceutical, and agrochemical industries offers a promising option, yet requires significant research to understanding the complex multiscale processes involved. To experimentally understand and optimize such processes at that catalytic sites and exploring the impact of the process at reactor scale, is too expensive. Computational methods offer significant insight and flexibility but require a more detailed multi-scale approach which is a significant challenge in itself. This work introduces a computational approach which incorporates detailed catalytic models, taken from experimental investigations, into a larger-scale computational flow dynamics framework. The reactor-scale species transport approach is modified near the catalytic walls to determine the influence of catalytic clustering regions. This coupling approach enables more accurate modelling of velocity, pressures, temperatures, species concentrations and near-wall surface characteristics which will ultimately enable the impact of overall reactor design on chemical conversion performance.

Keywords : catalysis, CCU, CO_2, multi-scale model
Conference Title : ICCD 2017 : International Conference on Carbon Dioxide
Conference Location : Venice, Italy
Conference Dates : November 13-14, 2017