Title: Agent-Based Modeling – Proof of Concept Application to Membrane Separation and Hydrogen Storage in a MOF

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PII: S0098-1354(17)30116-3
DOI: http://dx.doi.org/doi:10.1016/j.compchemeng.2017.03.004
Reference: CACE 5754

To appear in: *Computers and Chemical Engineering*

Received date: 3-11-2016
Revised date: 27-2-2017
Accepted date: 8-3-2017

Please cite this article as: McCarthy, Rachael., & Achenie, Luke E.K., Agent-Based Modeling – Proof of Concept Application to Membrane Separation and Hydrogen Storage in a MOF.*Computers and Chemical Engineering* http://dx.doi.org/10.1016/j.compchemeng.2017.03.004

Agent-Based Modeling – Proof of Concept Application to Membrane Separation and Hydrogen Storage in a MOF

(*For submission to Special Issue of Computers & Chem. Eng.,*

Festschrift in honor of Rafiqul Gani)

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Highlights

- Agent-based modeling (ABM) is a powerful modeling paradigm that can be used to model complex systems.
- ABM offers the possibility of scale bridging between different length scales. Time scale bridging may be a possibility that needs to be resolved.
- ABM can be computationally more efficient than molecular dynamics and could act as a first step before a full blown MD.
- The successful application to hydrogen capture in metal-organic frameworks and to membrane separation builds confidence in applying the ABM approach in molecular modeling in general.

Abstract

Modeling techniques such as molecular dynamics are often complicated and computationally expensive. This paper discusses agent-based modeling (ABM) as an alternative modeling approach that allows for any level of modeling complexity at a reasonable computational effort. The ABM framework is generally applicable for modeling complex systems. More specifically, ABM makes it possible to impose simple behaviors on individual "agents" which interact to produce an overall complex system behavior, thus facilitating the modeling of complex systems. To demonstrate the feasibility of ABM, we apply the approach to two problems: gas separation in an inorganic-organic membrane and hydrogen capture in a Metal-Organic Framework (MOF). The data collected from the models is consistent with experimental data suggesting that ABM is an effective modeling tool.

Keywords: agent-based modeling; ; ; ; , molecular dynamics, metal-organic framework, membrane, separation

1. Introduction

1.1. Background on Agent Based Modeling

Agent-based modeling (ABM) is a modeling paradigm for environments with "actors" or "agents" of different shapes and sizes, ranging from molecular scale to continuum or macro scale. Each agent acts autonomously according to a model that could be in the form of deterministic constructs (algebraic, differential and integro-differential equations) or a set of rules with stochastic elements [1, 2]. The inputs to the agent behavior models come from interactions of a given agent with other