

Accepted Manuscript

Mean Field Treatment of Heterogeneous Steady State Kinetics

Nadav Geva, Valerie Vaissier, James Shepherd, Troy Van Voorhis

PII: S0009-2614(17)30681-4

DOI: <http://dx.doi.org/10.1016/j.cplett.2017.07.011>

Reference: CPLETT 34937

To appear in: *Chemical Physics Letters*

Received Date: 20 April 2017

Accepted Date: 4 July 2017



Please cite this article as: N. Geva, V. Vaissier, J. Shepherd, T.V. Voorhis, Mean Field Treatment of Heterogeneous Steady State Kinetics, *Chemical Physics Letters* (2017), doi: <http://dx.doi.org/10.1016/j.cplett.2017.07.011>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Mean Field Treatment of Heterogeneous Steady State Kinetics

Nadav Geva¹, Valerie Vaissier¹, James Shepherd, Troy Van Voorhis*

*Department of Chemistry
Massachusetts Institute of Technology
77 Massachusetts Ave.
Cambridge, MA 02139 USA*

Abstract

We propose a method to quickly compute steady state populations of species undergoing a set of chemical reactions whose rate constants are heterogeneous. Using an average environment in place of an explicit nearest neighbor configuration, we obtain a set of equations describing a single fluctuating active site in the presence of an averaged bath. We apply this Mean Field Steady State (MFSS) method to a model of H_2 production on a disordered surface for which the activation energy for the reaction varies from site to site. The MFSS populations quantitatively reproduce the KMC results across the range of rate parameters considered.

Introduction

Beneath the ensemble average common to macroscopic observations, heterogeneity plays an astonishing role in chemical kinetics. From light harvesting [1] to chemical catalysis [2] to signaling [3] to enzyme function [4] there is a common theme: chemical function is not determined by the typical or average member of the ensemble. Rather, the rate of a given process can be strongly influenced by outliers.

*Corresponding author

Email address: tvan@mit.edu (Troy Van Voorhis)

¹These authors contributed equally to the work.

Download English Version:

<https://daneshyari.com/en/article/5377586>

Download Persian Version:

<https://daneshyari.com/article/5377586>

[Daneshyari.com](https://daneshyari.com)