

## Accepted Manuscript

A compact formula for the effective diffusivity of two-dimensional, anisotropic porous media with surface diffusion and interacting phases

Marziye Mirbagheri, Amir Akbari, Reghan J. Hill

PII: S0009-2509(17)30599-7  
DOI: <https://doi.org/10.1016/j.ces.2017.09.045>  
Reference: CES 13822

To appear in: *Chemical Engineering Science*

Received Date: 3 April 2017  
Accepted Date: 22 September 2017

Please cite this article as: M. Mirbagheri, A. Akbari, R.J. Hill, A compact formula for the effective diffusivity of two-dimensional, anisotropic porous media with surface diffusion and interacting phases, *Chemical Engineering Science* (2017), doi: <https://doi.org/10.1016/j.ces.2017.09.045>

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.



# A compact formula for the effective diffusivity of two-dimensional, anisotropic porous media with surface diffusion and interacting phases

Marziye Mirbagheri<sup>a\*</sup>, Amir Akbari<sup>b</sup>, Reghan J. Hill<sup>a</sup>

<sup>a</sup>*Department of Chemical Engineering, McGill University,  
Montreal, Quebec, H3A 0C5, Canada*

<sup>b</sup>*Process Systems Engineering Laboratory, Massachusetts Institute of Technology,  
Cambridge, MA 02139, USA*

---

## Abstract

The effective diffusivity of two-dimensional, anisotropic porous materials with surface diffusion is studied. The continuum model of Albaalbaki and Hill (2012), which couples diffusion in the bulk and surface domains via interfacial exchange fluxes, is implemented to couple the phases. Using a cell model, a new analytical solution is developed for aligned fibres with elliptic cross-sections and arbitrary orientation with respect to the mean gradient. The anisotropic boundary-value-problem is solved using an isotropic approximation to furnish concentration distributions in the three phases. Therefore, the model is more accurate near the isotropic limit and at lower inclusion volume fractions. When surface diffusion is significant, the present anisotropic model reproduces the isotropic model of Albaalbaki and Hill (2012) for unit aspect ratio and a variety of physical parameters. For a sphere with negligible surface flux, the model agrees with Maxwell's theory, and reproduces the model of Akbari et al. (2013) with various aspect ratios. To test the model for several parameters and other aspect ratios, direct numerical computations of the effective diffusivity, using spatially periodic unit cells, are undertaken, and a comparison with experimental data is presented. This model serves as a two-dimensional solution for the effective diffusivity of dilute anisotropic structures with surface diffusion.

*Keywords:* effective diffusivity, porous media, surface diffusion, anisotropy, analytical model

---

## 1. Introduction

The effective diffusivity, which combines the effects of different diffusion types, such as void, solid and surface diffusion, is important for many applications. It determines the reaction rate in catalytic monoliths [15]. Reactant- and product-diffusion in porous catalysts are controlled by void diffusion through a network of irregular shaped pores, the structures of which are commonly characterized by the pore-size distribution. Gas diffusion in polymer electrolyte fuel cells plays an important role in electrochemical reactions and affects power density [11, 29]. In nano-structured materials, which have a

---

\*Corresponding author

*Email addresses:* marziye.mirbagheri@mail.mcgill.ca (Marziye Mirbagheri<sup>a</sup>), aakbari@mit.edu (Amir Akbari<sup>b</sup>), reghan.hill@mcgill.ca (Reghan J. Hill<sup>a</sup>)

Download English Version:

<https://daneshyari.com/en/article/6588911>

Download Persian Version:

<https://daneshyari.com/article/6588911>

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