Chemical Engineering Science 187 (2018) 117–126

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

# The development and numerical modelling of a Representative Elemental Volume for packed sand

Ashraf Thabet, Anthony G. Straatman *

*Department of Mechanical & Materials Engineering, Western University, London N6A 5B9, Canada*

## HIGHLIGHTS

- Idealized geometric model introduced to characterize packed sand in pore-level computations.
- Geometric model has spherical particles packed randomly, but with spatial periodicity.
- Comparisons show that idealized model gives predictions similar to actual sand REV.
- Particle size variation shown to not be important in computational model.
- Influence of temperature on properties shown to be important in interstitial exchange.

## ARTICLE INFO

*Article history:*
Received 6 February 2018
Received in revised form 21 April 2018
Accepted 23 April 2018
Available online 30 April 2018

*Keywords:*
Computational modelling
Packed bed
Porous media
Convective heat transfer

## ABSTRACT

This article describes a comparison between a packed-sand geometric model derived from experimental digitization of a small volume of sand and from a mathematical model (Yet Another Development Engine, YADE) that produces a random packing of spherical particles. As the application of the model is towards smoldering combustion, the comparison focuses on the pressure drop and convective heat transfer at very low Reynolds numbers and a wide range of high temperatures. The comparison shows that the YADE geometric model gives results that are in good agreement with the digitized packed-sand model in the range of Reynolds numbers considered, which, given the cost and time saving of using a mathematical model, is an extremely useful result. The geometric model was also used to explore the influence of particle size variation and temperature dependence of air properties affects the flow and convective exchange at temperatures relevant to smouldering combustion. A correlation is presented to demonstrate how the heat transfer results can be put into a compact form for use in computations using a porous continuum approach.



## 1. Introduction

Significant progress has been made with respect to understanding the behavior of fluid flow, heat and mass transfer, and chemical reaction in permeable porous media. Fluid flow and heat transfer in porous materials is prevalent in numerous applications in science and engineering. For example, in chemical engineering, transport in porous media is related to filtering and drying applications, packed bed reactors, catalytic converters and fuel cells. In mechanical engineering, applications of porous materials include enhanced heat transfer, evaporative cooling, insulation and heat sinks. In environmental applications, porous media provide context for the study of groundwater flows and contaminant transport in groundwater.

Another important environmental application of porous media is in smoldering combustion phenomenon, which is characterized as an oxygen-limited flameless form of combustion with a slow propagation rate and a relatively low temperature (in the context of combustion). The phenomenon is extremely complex and includes heterogeneous chemical reactions and transport of heat, mass, and momentum of multiple phases (Rein, 2009). Motivation for the study of smoldering combustion has arisen primarily from the possible economic and pollution-related impact of this phenomenon. In the USA, it has been reported that an estimated 31,200 smoldering fires that occurred during 2001 caused property losses of about US$400 million (Rein, 2009). In Canada, since 1990, "wildland fires" have consumed an average of 2.5 million hectares a year, especially during prolonged periods of drought (NRC). Such fires can smolder underground all winter and then re-emerge at the surface in the spring. In this respect, the potential for significant economic damage and losses provides motivation for better

* Corresponding author.
*E-mail address:* astraatman@eng.uwo.ca (A.G. Straatman).

https://doi.org/10.1016/j.ces.2018.04.054

**Nomenclature**

| | | | |
|---|---|---|---|
| $a_{fs}$ | specific interfacial surface area of porous media, $m^2/m^3$ | $C_E$ | form drag coefficient for porous medium |
| $A_{fs}$ | interfacial surface area of porous media, $m^2$ | $P$ | pressure, Pa |
| $C_p$ | specific heat capacity, J $kg^{-1}$ $K^{-1}$ | $R$ | specific gas constant of air, J $kg^{-1}$ $K^{-1}$ |
| $d$ | particle diameter, m | v | Darcy velocity, m $s^{-1}$ |
| $L$ | length scale of porous medium or REV length, m | u | fluid velocity vector, m $s^{-1}$ |
| $g$ | acceleration of gravity, m $s^{-2}$ | $\dot{m}$ | mass flow rate, kg/s |
| $h_{fs}$ | interstitial heat transfer coefficient between the solid and gas phases, W $m^{-2}$ $K^{-1}$ | $T_f$ | temperature of fluid constituent of porous media |
| $k$ | thermal conductivity, W $m^{-1}$ $K^{-1}$ | $T_s$ | temperature of solid constituent of porous media |
| $k_{fe}$ | effective conductivity of fluid phase, W $m^{-1}$ $K^{-1}$ | $Pr$ | Prandtl number |
| $k_{se}$ | effective conductivity of solid phase, W $m^{-1}$ $K^{-1}$ | $\rho$ | density, kg $m^{-3}$ |
| $K$ | permeability of the medium, $m^2$ | $\mu$ | dynamic viscosity, Pa s |

understanding the smoldering process and development of preventative strategies, which can minimize its harmful effects on climate, the environment and human and animal life.

A second motivation for better understanding smoldering combustion is to explore the feasibility of its use as a remediation technique. To this end, a recent application called Self-sustaining Treatment for Active Remediation (STAR) has been developed based on in-situ controlled smoldering combustion of contaminated soils or sands. The source of fuel for this technology is the contaminant in the porous soil or sand, which is ignited and then slowly oxidized using hot air, which is delivered through a well to the target contaminated zone. Following ignition – and provided a sufficient amount of ambient or combustion air is supplied – the process is self-sustaining, without the need for external injected fuel (Savron Smoldering Solutions).

Critical to developing an understanding of smoldering combustion phenomenon is knowledge and characterization of heat and mass transfer (at combustion-level temperatures) in packed sands and soils, and these processes can be investigated both experimentally and computationally. Experimental studies can provide the insight into the fundamental processes, which can then be modelled mathematically and included in computer codes that can be used to conduct parametric studies. Numerical modelling can be done at both the pore-level and the porous-continuum (volume-averaged) level. In this manner, detailed information can be established by conducting highly-resolved simulations on representative volumes of porous media, which can then be used to develop parameters required to mathematically close the volume-averaged transport equations, which can be used to study large porous domains. A critical element required to conduct useful and accurate pore-level simulations is a geometric model that correctly mimics the porous structure in which the phenomenon occurs. Such a geometric model is called a Representative Elemental Volume (REV), which is defined as a small volume that is representative of the larger domain (which can be comprised of millions or billions of particles). Thus, one goal of the present article is to address the specific task of identifying a suitable REV for packed sand that can be used to conduct simulations to understand the pore-level activity associated with flow, convection, reaction and mass transfer at conditions associated with smoldering combustion.

In general, permeable porous media are heterogeneous materials comprised of a solid microstructure (or matrix) and a fluid that fills the space unoccupied by the matrix. The structure and material of the porous media play an important role in the physical behavior of the media and in the interaction of the matrix with the fluid phase (Khan et al., 2015). The matrix can take a wide variety of forms, including networks of interconnected ligaments, interconnected spherical voids and packed beds of particles. The specific type of porous structure affects the amount of internal interfacial area between the solid and fluid phases (interstitial area) and the way in which the fluid flows through the medium. A packed bed is a heterogeneous system composed of solid particles and a fluid flowing in the interstitial space between the particles. Packed beds represent a particular type of permeable porous structure and its geometric properties are affected by particle size, particle size variation and particle shape.

Studies on fluid flow and convective heat transfer in packed particle beds has received extensive attention in the last century, particularly during the 1970s. Empirically-derived correlations show that the heat transfer coefficient is dependent on the porosity, particle size, and shape of the packed bed as well as on the Prandtl number of the fluid and the Reynolds number derived from the range of the particle diameters (Vafai, 2015). Dimensionless analysis of the problem suggests that a general correlation for the interstitial Nusselt number of the form (Wakao and Kaguei, 1982):

$$Nu_d = \frac{h_{sf}d}{k_f} = a + cPr^m Re_d^n \qquad (1)$$

can be used to capture the convective exchange, where $h_{sf}$ is the interstitial convective exchange coefficient, $d$ is the particle diameter and $k_f$ is the fluid conductivity. $a$, $c$, $m$ and $n$ are unknowns that require experiments or pore-level computation to determine. Wakao et al. (1979) published their well-known correlation for packed beds of spheres:

$$Nu_d = 2 + 1.1Pr^{1/3}Re_d^{0.6} \qquad (2)$$

which is valid over the range $0.7 < Pr < 1$ and $15 < Re < 8500$, and was established from packed beds of particles with diameters in the range 10–130 mm (Wakao and Kaguei, 1982; Wakao et al., 1979). This correlation has been widely used in studies of packed beds reported in the literature and has been extended to include consideration of exchange at lower Reynolds numbers and of particles with small diameters and geometric shapes other than spheres. Kar and Dybbs (1982) proposed:

$$Nu_d = 0.004\left(\frac{d_v}{d}\right)^{0.35} Pr^{1/3}Re_d^{1.35} \qquad (3)$$

where $d_v = 4\varepsilon/a_{sf}$ is the average void diameter, and $d$ is the particle diameter. This correlation is valid for $Re < 75$, but it underestimates the interfacial heat transfer at low Reynolds numbers. Another option is for the second term $(Pr^m Re_d^n)$ of the equation to be multiplied by the porosity ($\varepsilon$). For spherical particles whose porosity is within the range of $0.7 < \varepsilon < 0.95$ this leads to (Nakayama et al., 2009):