

# NUMERICAL MODELING OF ADSORPTION DYNAMICS THROUGH ACTIVATED-CARBON-FIBER CLOTH

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## Introduction

Activated-carbon-fiber cloth (ACFC) [1-5] has promising characteristics as an adsorbent, and potentially as a molecular sieve, a catalyst, or a catalyst support for a wide range of concentrations and chemical species. This is mainly because ACFC can be prepared with different and controlled pore size distributions, total pore volumes, specific surface areas and surface chemistries. ACFC can be > 95% by mass carbon, with the balance being hydrogen, oxygen, and nitrogen. Surfaces of ACFC can be modified to be acidic, basic, neutral or polar surfaces [6-7]. Risk of side reactions, poisoning and sintering in a zero ash content ACFC is minimal. Due to the ACFC physical structure and electrical resistance properties, it can be efficiently regenerated by electro-thermal regeneration [1,2,8]. Adsorbate retentivity in ACFC regenerated electro-thermally is less than in other carbon adsorbents regenerated by conventional methods. The high affinity of ACFC for certain adsorbates and rapid adsorption, desorption and heat transfer rates can reduce the required process cycle time, and increase the working capacity by reducing the length of the mass transfer zone. ACFC can be installed in different configurations providing desired heat, mass and momentum transfer. Therefore, use of ACFC in many new applications is promising for the near future.

To take advantage of ACFC properties fully in the design of a separation, purification or catalytic conversion system, it is important to simulate transport processes through it. Simulation of these processes can be used to perform sensitivity studies that describe the performance of a proposed system. Results can then be used to find the optimum process conditions for a certain objective such as reducing the cost. Because ACFC is inhomogeneous and has different degrees of periodicity and characteristic lengths in three dimensions, coupling of heat, mass, and momentum transfer processes affect the ACFC local adsorption equilibrium and kinetics. With recent advancements in computer hardware and computational algorithms, these complexities can be resolved to provide a general predictive tool.

## Numerical Modeling Efforts

### Equilibrium & Non-equilibrium Properties

The ACFC equilibrium adsorption surface (modeled in a multi-variable space) provides local and instantaneous thermo-chemical characteristics of an adsorbate in contact with an individual activated-carbon-fiber (ACF). From the

equilibrium characterization results, other ACF properties such as pore size distribution and connectivity are derived. These results in combination with the first principles of gas kinetics are then used to predict some of the needed non-equilibrium parameters such as the effective diffusion and conductivity coefficients. These derived coefficients can then be used to describe the adsorption kinetics of an individual ACF.

### Adsorption Kinetics

The characteristic time for physical adsorption at the surface of an adsorbent particle is generally high,  $> 10^{-9}$  s (e.g. see [9]). Therefore, the adsorption kinetic is a heat transfer and mass diffusion limited process. Assuming a known concentration and temperature profile at the surface of an ACF, diffusion and heat conduction equations can be solved to provide the concentration profile and mass uptake of adsorbate to the fiber. A semi-analytical-numerical method is used for this purpose.

### Adsorption Dynamics

Adsorption kinetics of an individual fiber are not sufficient to describe adsorption transient characteristics of the ACFC. This is because ACFC is inhomogeneous and has different degrees of periodicity and characteristic lengths in three dimensions that can affect film diffusion and local heat transfer characteristics. Also, there exists coupling between transport equations in the gas and solid phases. Due to these complexities, adsorption dynamics through inhomogeneous structured adsorbents have not yet been quantitatively analyzed. In order to fully model the adsorption dynamics at the bulk pore level, we should simultaneously solve equations of continuity, momentum, species in the gas phase, species in the solid phase, energy in the gas phase, and energy in the solid phase. This requires an extensive amount of computational time. A simpler approach is to develop an effective medium approximation for a unit cell of ACFC. For this purpose, we simulate heat, mass and momentum transfer through a unit cell of ACFC to determine the cell transport properties such as effective conductivity, gas permeability, and diffusivity.

Simulation of gas dynamics through a unit cell of ACFC provides the information we need for the distribution of flow through the inter-yarn and intra-yarn spacings of the ACFC. In the absence of adsorption, the distinguished phenomena that contribute to the dispersion through a fiber bed are: 1) diffusion in the gas phase and in the adsorbent, 2) hydrodynamic dispersion caused by velocity fluctuations

induced by the fluid flow and the presence of the fibers, and 3) concentration gradients that are generated by the boundary layers and hold-up regions [10]. A multi-component gas flow simulation is used to describe the effective diffusivity that arises from the above phenomena. The effective pure conductances are derived from the simulation of diffusion through the unit cell.

Conventional numerical methods such as finite elements or finite difference that have been used to solve the Navier-Stokes equations for simple physical domains, require a huge computational power due to the complicated boundaries that exist in the pore structures. Therefore, a different numerical approach is required to resolve the fluid dynamics at the scale of the ACF's pores. We are formulating and using the Lattice Boltzmann method (LBM) for the simulation of the transport processes in the unit cell of structured woven adsorbent.

### Lattice Boltzmann Method

LBM was recently developed to solve fluid transport quite efficiently for complex domains [11]. LBM in a simple sense, can be considered as a finite difference simplification of the *Generalized Boltzmann Equation* (GBE) in a Lagrangian space. The GBE equation can be written in the form of:

$$\partial(F_p)/\partial t + c_p \cdot \nabla(F_p) + \mathbf{A} \cdot \partial(F_p)/\partial \mathbf{c} = \int (F_p^* F_{1q}^* - F_p F_{1q}) c_{pq} \sigma_{pq} d\omega d\mathbf{c}_{1q}$$

where subscripts p and q are used as the index of species, c is the velocity of gas molecules, A is the external body force, F and F\* are the distribution functions in the velocity space before and after the molecular collision, c<sub>pq</sub> is the reduced mass, and σ<sub>pq</sub> dω is the collision differential cross-sectional area, and t is time [12]. In the Lagrangian system of reference, and absence of the body force, the GBE can be written in a simplified form of

$$\partial F_p / \partial t = \Omega_p$$

where Ω<sub>p</sub> represents the collision integral in the GBE. The normalized finite difference form of this equation can be written as

$$F_{p,ij,k}(\mathbf{x} + \mathbf{c}_{p,ij,k}, t+1) - F_{p,ij,k}(\mathbf{x}, t) = [F_{p,ij,k}^e(\mathbf{x}, t) - F_{p,ij,k}(\mathbf{x}, t)]$$

where the collision operator is approximated by the first order term of Taylor expansion around an equilibrium distribution function, F<sub>p,ij,k</sub><sup>e</sup>(x,t). F<sub>p,ij,k</sub>(x,t) is the mass, momentum, or enthalpy portion of species p that moves in the direction ij at the nodal point k and at the normalized time t and space x. F<sub>p,ij,k</sub>(x+c<sub>p,ij,k</sub>, t+1) is the distribution function at space x+c<sub>p,ij,k</sub> and time t+1. At each time step, physical variables such as component densities, velocities, and enthalpies are determined from the zeroth moment of their respective distribution functions. The shape functions for F<sub>p,ij,k</sub> are selected such that after a multi-dimensional Chapman-Enskog and Taylor expansions the simulation equations result in the conservation equations. For example, if [F<sub>p,0,k</sub>, F<sub>p,1,k</sub>, F<sub>p,2,j,k</sub>] = [(4ρ<sub>p,0,k</sub>/9), (ρ<sub>p,1,k</sub>/9), (ρ<sub>p,2,j,k</sub>/36)] is selected, pure diffusion can be simulated through a d2q9 square lattice (d2q9 denotes a 2-D square lattice that has nine mass velocities [13], and ρ is the density at each nodal points). These shape functions result in a lattice diffusion coefficient equal to 5/36. The physical diffusion coefficient (D<sub>p</sub>) is related to the lattice diffusion coefficient (D<sub>l</sub>) by

D<sub>p</sub> = D<sub>l</sub> · (dx)<sup>2</sup>/dt, where dx and dt are the space and time intervals.

Certain concentration gradients are imposed across the ACFC unit cell and the diffusion processes are simulated. Then, the directional effective diffusivities are calculated from the ratio of the directional mass fluxes over the concentration gradients of the same directions.

### Summary

Lattice Boltzmann method is being developed to simulate mass, momentum and heat transfer processes through complex adsorbent geometries such as activated-carbon-fiber cloth. The physical geometry of such inhomogeneous structured adsorbents are modeled mathematically and discretized numerically. The LBM is used to determine effective properties of the ACFC unit cell. Then, the effective properties are used in a macro-scale numerical modeling to provide a more efficient simulation tool for design applications. Results of the numerical modeling will be presented and discussed as they are related to adsorption of organic compounds from gas streams with ACFC.

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