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Abstract Formulary

Presentation type: **Oral** ☐ **Poster** ✔

Title: Combined Diffusion Limited Cluster Aggregation/Lattice Boltzmann Model for Simulating the Catalytic Behavior of Aerogel Materials

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ABSTRACT (Space limited to 2200 characters)

Aerogel materials have high surface area, high porosity and good thermal stability which makes them attractive in a variety of catalysis applications. One application of particular interest is in automotive pollution mitigation which requires the use of three-way catalysts to simultaneously convert nitrogen oxides, carbon monoxide and a variety of unburned hydrocarbon species. Experimental research has shown the promise of using aerogels in this area [1, 2].

We have developed a two-dimensional computational model to study the effect of aerogel structure and catalyst loading on overall catalytic potential. The model includes four primary components: development of an aerogel structure, distribution of a catalyst in the structure, modeling flow into and through the structure and determination of fluid-catalyst interactions.

The Diffusion Limited Cluster Aggregation method is employed in the development of the aerogel structure [3] and is tied to a pore distribution calculator that allows us to achieve a specified pore distribution, density and porosity in the simulated material. Catalyst particles are then randomly distributed throughout the simulated aerogel with control over the amount of catalyst and the catalyst particle diameter. A D2Q9 Lattice-Boltzmann (LB) method is implemented to model flow into and through the aerogel structure and monitor the number of fluid-catalyst interactions as a measure of catalytic potential. Future work will focus on development of three-dimensional models and implementation of catalytic reaction models. This poster will describe the implementation of the four components to assess catalytic potential, present several aerogel structures with LB flow results and include preliminary results on the overall catalytic potential as a function of aerogel structure and catalyst distribution.

References:

(1) Anderson, et al., 2022. J Sol-Gel Sci Technol, 102(2), 422-436.
(2) Anderson et al., 2020. Emission Contr Sci Technol 6(3), 324-335.
(3) Abdusalamov et al., 2021. J Phys Chem B, 125(7), 1944-1950.