Abstract: The advances in material synthesis and modification require methods that provide capabilities to evaluate the resulting texture of the material. Three areas influencing the characterization of porous materials are examined: 1) fluid interactions with microporous materials, 2) the complete pore size distribution from nanometers to micrometers, and 3) understanding the pore window and pore size distribution of porous materials.

Sorption of fluids such as argon or nitrogen is frequently used to quantify the pore volume and pore size distribution. In this work, we examine the use of thermodynamics to assess the suitability of nitrogen, argon, and oxygen for the characterization of zeolites. From the thermodynamic assessment, the adsorption potential distribution provides clear trends that are observed with respect to the chemistry of the zeolite (cation and silica to alumina ratio) and fluid sorption induced material deformation. The thermodynamic assessment was also used to examine sorption interactions of nitrogen, argon, ethane, and ethane with MOFs. The adsorption potential for these materials clearly distinguishes strongly interacting sorbates (nitrogen and ethene) from weakly interacting fluids (argon and ethane). A non-parametric technique for calculating the heats of adsorption is also used to further emphasize the importance of a thermodynamic assessment in addition to the modeling of traditional textural descriptors (porosity and pore size distribution).

Porous materials provide a network of macro, meso, and micropores, the resulting texture is designed to provide greater access to active sites and reduce the transport limitations inherent to microporous materials. Traditionally, the textural characterization employed during new material synthesis and in particular porous materials has relied upon adsorption and mercury intrusion to determine parameters such as surface area and porosity. These techniques are often used separately to assess the pore volume and pore size distribution. For example, it is quite common to use sorption isotherms for micro- and meso pore characterization and complement the analysis by using mercury porosimetry for describing the meso- and macropores. A generalized approach to modeling the pore size distribution is presented to
determine the complete distribution of macro, meso, and micropores. Rather than using a fragmented approach of simple overlays from individual techniques, a unifying approach that utilizes a kernel constructed from model isotherms and model mercury intrusion curves is used to calculate the complete pore size distribution and the total pore volume of the catalyst. The resulting pore size distribution has the benefit of satisfying both the adsorption (or desorption) isotherm and the mercury porosimetry.

A variety of modeling approaches has been employed to characterize the texture of porous materials using adsorption isotherms. These models typically assume geometrically uniform pores and from that a theoretical isotherm may be calculated for a given pore width. Unfortunately, many naturally occurring, or synthetically produced materials do not have a uniform pore system. These geometrically heterogeneous materials also exhibit significant isotherm hysteresis, and this often leads to an erroneous or questionable calculation of the pore size and area distribution. In this work, we use both the adsorption and desorption branches of the isotherm to calculate the size distribution of pore throats and cavities.

**Biography:** Dr. Kenvin received his B.S. degree in Chemical Engineering from Drexel University in Philadelphia, Pa. He received his Ph.D. degree in Chemical Engineering from the Georgia Institute of Technology in Atlanta, Ga. His areas of expertise are in the characterization of porous materials and catalysts using physical and chemical adsorption and in mercury porosimetry.

While employed by the Mobil Research and Development Company as a member of the Mobil Lubes - Process and Products Research Division, Dr. Kenvin managed research and development projects involving the commercialization of new hydrotreated base oils. He was the innovator of the use of chemometrics to define base oil quality standards. These chemometric models subsequently led to the development and implementation of novel techniques for characterizing composition and optimizing refinery lube operations, and the technology was successfully implemented in all Mobil lube refineries. In 1994, Dr. Kenvin received the Products Division - Technology Award for his contribution to the Mobil Corporation.

Later, as a member of the Hoechst A.G. North America Next Generation Process-Polymer Group, Dr. Kenvin directed leveraged-research at the Georgia Institute of Technology. His research involved the identification of new technologies for the process and development of low-cost terephthalic acid and novel monomers for improving the properties of PET (polyester terephthalate), including the application of super-acid catalysis for the carbonylation of toluene.

Dr. Kenvin has been invited to present scientific lectures at more than 100 seminars and regularly participates in short courses on particle technology. He also serves on international advisory boards and is an officer of the ASTM D-32 committee on catalysis.