# microReport

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# Adding a custom model to the NLDFT library - a CO_2 GCMC model for carbons

New models for determining the pore volume and pore size distribution of porous solids may be easily added to MicroActive. These kernels developed using NLDFT, GCMC and other variants have been available for more than 20 years. Traditionally instrument manufacturers have supplied these proprietary models. To introduce new powerful capabilities for users, Micromeritics has developed a simple program to convert model isotherms (a kernel) to a model file that can be easily used with MicroActive. This provides users the full capabilities of the MicroActive user interface and advanced deconvolution techniques. A full description of the model requirements and conversion process are provided below and include an example using a GCMC kernel for carbon slit-shaped pores and CO_2 adsorption. The GCMC kernel used in this example was developed by Inmondo Tech. For user calculated kernels the following general specifications should be observed:

1. Each model isotherm should be calculated using a common pressure table and the minimum pressure should be less than 5e-9 atmospheres (or relative pressure),
2. A minimum of 15 points per decade of pressure and the pressures should be logarithmically spaced and the vector or pressures should be saved in a text file as **pVector.txt**,
3. Pore widths may start at a minimum of 0.32 nm and may have a spacing of 0.01 nm. The vector of pore widths should be saved in a text file as **width.txt**,
4. The kernel shall contain isotherms with each column corresponding to the pore width found in the file **width.txt** and adsorption densities in each row corresponding to pressures in **pVector.txt**. The kernel should be saved in text file as **kMatrix.txt**.

Using the three files, **width.txt**, **pVector.txt**, and **kMatrix.txt** a kernel compatible with MicroActive may be created using Python 3.x and a custom library from Micromeritics (dftmodel.py). The example kernel, CO2 adsorption and carbon slit-shaped pores is shown below.
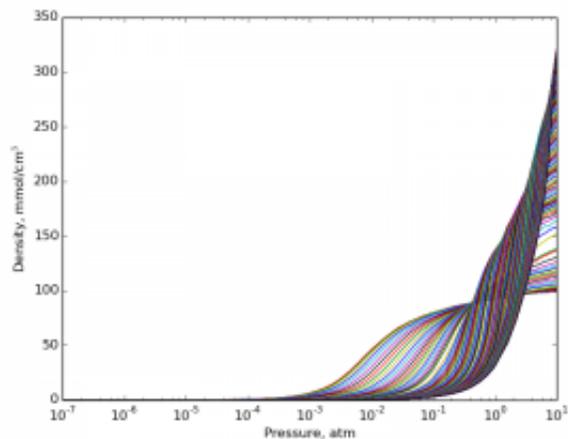
The new model may be copied to the **models** directory in MicroActive and is immediately available for use. Simply open a file containing adsorption data and select DFT pore size and the new model appears in the selection list as shown below.
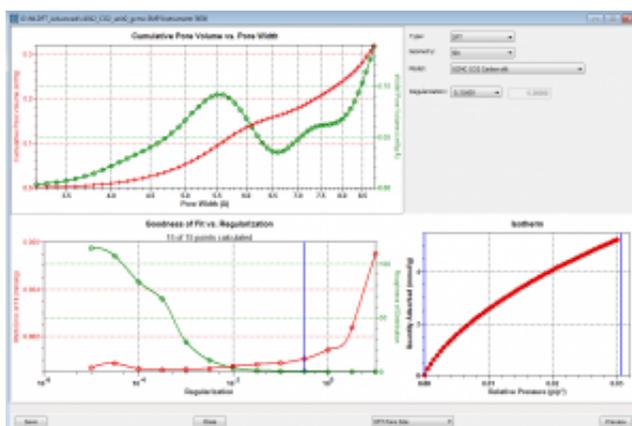
For a additional information on adding new models to MicroActive or a copy of the example used to create the GCMC kernel please contact your local Micromeritics representative.

This entry was posted in Articles on November 11, 2014 [http://micro-report.com/adding-a-custom-model-to-the-nldft-library-a-co2-gcmc-model-for-carbons/] by Jeff Kenvin.