Notes for specific chemical databases

A user can add properties of compounds to the databases. Default data is available as well in several databases. These databases can be downloaded separately and used in CapSim version 3 and higher. There are specific chemical database files for PAHs, PCBs, metal-related compounds, pesticides and other common compounds. Data comes from a variety of sources (listed below). Every effort is made to ensure that the data is accurate but users are cautioned that the data is only as good as they original source. They are provided as an aid to the user and the numbers should be verified by independent assessment for critical calculations.

These databases can be saved into the default database subdirectory in the Capsim directory. By launching CapSim and selecting “edit chemical database” from the main menu and then “import database file”, you can import data from these databases. Prior to importing these databases it would be a good idea to save a backup copy of the default database file, “capsim3\_chemicaldatabase”, by copying it to a new name (e.g. default capsim3\_chemicaldatabase”). The file can be found in the default Capsim directory in the database subdirectory. Whatever you have imported will be saved in this database file automatically unless you save them under another name. We suggest giving them a new name thus you can make your own databases and go back to them easily. Since we have included hundreds of compounds in the present databases, it’s not recommended to import after choosing “select all” into the default database due to the resulting large size of the database will make it more difficult to work with. If you wish to restore the original database you can delete the modified database and restore the saved copy of the original database.

The temperature shown in this database is based on the diffusion coefficient in water, which is calculated via SPARC, a program for computation chemistry (<http://archemcalc.com/sparc.html> ).

Reference abbreviations in the databases used for basic parameters except isotherm parameters are described below

\*LookChem - lookchem.com, which provides molecular formulas, molecular weights and density of some compounds.

\*TCEQ – Texas Commission on Environmental Quality chemical database, which includes physical, chemical and toxicological properties of compounds. Dwat and LogKow are found here. (<http://www.tceq.texas.gov/remediation/trrp/trrppcls.html>)

\*F300-Freundlich parameters with Carbon type--F300

\*Mackay 2006 - Mackay, D. (2006). Handbook of physical-chemical properties and environmental fate for organic chemicals (2nd ed.). Boca Raton, FL: CRC/Taylor & Francis.

\*SPARC - SPARC calculator (<http://archemcalc.com/sparc.html>), which is used for calculating water diffusivity at specific temperature.

\*Hawker 1988 - Hawker D W, Connell D W. Octanol-water partition coefficients of polychlorinated biphenyl congeners[J]. Environmental science & technology, 1988, 22(4): 382-387.

\*WIKI - Wikipedia, formula, molecular weight and density can be found here.

Reference abbreviations used specifically for activated carbon isotherm parameters are listed below (due to the lack of space, they are not shown in Capsim)

PAHs isotherm parameters reference

\*Walters and Luthy 1984 - Walters R W, Luthy R G. Equilibrium adsorption of polycyclic aromatic hydrocarbons from water onto activated carbon[J]. Environmental science & technology, 1984, 18(6): 395-403.

\*Dobbs and Cohen 1980- Dobbs, R.A. and Cohen, J.M., “Carbon Adsorption Isotherms for Toxic Organics”, EPA-600/8-80-023, U.S. Environmental Protection Agency, Cincinnati, Ohio, 1980.

PCBs isotherm parameters reference

\*Azhar 2015 - "Evaluation of Sorbing Amendments for In-situ Remediation of Contaminated Sediments" by Wardah Azhar, B.S.E.; M.S.E. 2015

\*McDonough et al 2008 - McDonough K M, Fairey J L, Lowry G V. Adsorption of polychlorinated biphenyls to activated carbon: Equilibrium isotherms and a preliminary assessment of the effect of dissolved organic matter and biofilm loadings[J]. Water Research, 2008, 42(3): 575-584.

Metal-related compounds isotherm parameters reference

\*G. McKay, et al 1985- McKay, G., M.J. Bingo, and A.R. Altanemi, “The Adsorption of Various Pollutants from Aqueous Solutions on to Activated Carbon,” Wat. Res., 1985, 19:4, 491-495.

Pesticides & Other common compounds isotherm parameters reference

\*Dobbs and Cohen 1980- Dobbs, R.A. and Cohen, J.M., “Carbon Adsorption Isotherms for Toxic Organics”, EPA-600/8-80-023, U.S. Environmental Protection Agency, Cincinnati, Ohio, 1980.

\* Westvaco Isotherms and Speth 1990-Speth, T.F. and R.J. Miltner, “Technical Note: Adsorption Capacity of GAC for Synthetic Organics,” Journal AWWA, Research and Technology, February 1990, 72-75.

\* Speth, et al 1988-Speth, T.F., Miltner, R., Crittenden, J.C., and Hand, D.W., “An Evaluation of GAC Adsorption Capacities for SOCs,” submitted to Journal AWWA, 1988.