

MODELING PHARMACEUTICALS AND ORGANIC WASTEWATER CHEMICALS

Nicole Whittier *

ABSTRACT: A wide variety of pharmaceuticals and other organic wastewater chemicals are continuously being discharged in our streams and rivers. It is important to understand how the water quality will be effected from such discharges, how far will the chemical be transported as well as what are the potential concentrations in the water. To help address these needs, the three-dimensional chemical dispersion model CHEMMAP is used to estimate the fate and concentrations of selected organic wastewater chemicals, as well as the potential human health and ecological hazards from the discharged wastewater. CHEMMAP uses environmental data forcing (currents and wind) and physical-chemical properties to simulate fate processes over time after the release, including: (1) slick spreading, transport, and entrainment of floating materials, (2) transport of dissolved and particulate materials in three dimensions, (3) evaporation and volatilization, (4) dissolution and adsorption, (5) sedimentation and resuspension, (6) and degradation. The physical-chemical properties include density, vapor pressure, water solubility, environmental degradation rates, adsorbed/dissolved partitioning coefficients (K_{ow} , K_{oc}), viscosity, and surface tension. The chemical fates model estimates the distribution of chemical (as mass and concentrations) on the water surface, on shorelines, in the water column and in the sediments. The model is three-dimensional, separately tracking surface slicks, entrained droplets or particles of pure chemical, chemical adsorbed to suspended particulates, and dissolved chemical. CHEMMAP may be run as a single scenario (forecast or hindcast) or in stochastic mode to estimate the probable distribution and concentrations resulting from wastewater discharges. Select pharmaceuticals and organic wastewater chemicals, contained in the Pharmaceuticals in the Environment, Information for Assessing Risk database maintained by the National Centers for Coastal Ocean Science, Center for Coastal Environmental Health and Biomolecular Research, are evaluated using CHEMMAP. Based on model outputs, it is possible to select chemicals that would have the highest human health and ecological hazards when discharged. The model results can then be used to indicate the volume of water that may be contaminated above toxicity thresholds provided in the Pharmaceuticals in the Environment, Information for Assessing Risk database.

* Chemical Engineer/Project Manager, Applied Science Associates, 70 Dean Knauss Drive, Narragansett, RI 02882, USA, Phone: 401-789-6224, Fax: 401-789-1932, Email: nwhittier@appsoci.com