Computer Models for Environmental Fate of Chemical Pollutants: SPARC

Why Are Computer Models Needed?

In light of recent trends in environmental regulatory strategies, the U.S. EPA will have to rely more heavily on predictive models when performing the increasingly complex exposure and risk assessments. These are needed to develop scientifically defensible regulations that protect human health and safeguard the environment. As the complexity and scale of exposure and risk assessments increase, the complexity and scale of predictive models also increase. The pressing need for multimedia (water, air, and soil), multistressor (pollutants, nutrients, etc.), multipathway (inhalation, ingestion, and dermal contact) assessments, from both the human and ecological perspectives, over broad spatial and temporal scales, places a high priority on the development of new modeling tools. These new models will necessarily require huge arrays of input data, and many of the required inputs are neither available in the published literature nor easily measured. The SPARC model will provide much of this data.

What is SPARC?

SPARC (SPARC Performs Automated Reasoning in Chemistry) is a computer modeling system that calculates a large number of physical and chemical properties for chemical pollutants from their molecular structure and from basic information about the environment such as media, temperature, pressure, and pH. SPARC research involves an integrated effort by scientists and modelers to explain and model the physical, chemical, and biological processes that describe what happens to organic pollutants, nutrients, and other stressors in environmental systems. These models, along with estimation algorithms for reactivity constants, are incorporated into SPARC. Models developed through SPARC can be used in exposure and risk assessments.

Major Products

The SPARC system has been under development for several years and currently calculates a wide array of physical and chemical reactivity properties. Current and future research will focus on extending, refining, and testing of current SPARC models. Completed SPARC models are available on the Internet to modeling clients.

SPARC

Benefits
- This research is important in developing multimedia modeling technologies to carry out an increasingly complex array of exposure and risk assessments. These assessments are necessary in developing scientifically defensible regulations.

Purpose
- Development of SPARC supports the U.S. EPA's goal of Sound Science through greater innovation to address environmental concerns.

Selected Milestones
- Upgrades of SPARC will include prototype models for abiotic reduction in sediment suspensions, microbial reductive transformations in sediment systems, phyto-enzymatic processes, and oxidative transformations in soil systems.

Participants/Affiliations
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To use the online SPARC Calculator, visit the UGA Website
http://ibmlc2.chem.uga.edu/sparc/

For more information on this and other NERL science projects, visit our Website
http://www.epa.gov/nerl/