NEXT GENERATION CB HAZARD PREDICTION AND CONSEQUENCE ASSESSMENT WITH MULTI-ECHELON DECISION SUPPORT APPLICATIONS

Automated Property Prediction And Material File Generation For Hazard Prediction Using Propcast

Stephen Houghton SRC Inc. **Heather Carlson-Lynch** SRC Inc. **Julie Melia** SRC Inc. **Emily Golden** SRC Inc. **Lauren Cassidy** SRC Inc. **Lauren Volles** SRC Inc. **Mario Citra** SRC Inc. **Nathaniel Stemmler** SRC Inc.

SRC, Inc is working with DTRA's Operational Technical Reachback Division's (RD-OPR) Chemistry Team to develop the PropCast software module. This module will enable a more efficient process for assessing new and emerging chemical threats. PropCast provides a mechanism to automatically generate properties required as inputs to run a transport and dispersion model of a chemical threat in the Hazard Prediction and Assessment Capability (HPAC) system. This new capability allows analysts to generate an input file from only a chemical structure. PropCast leverages the experimentally measured chemical property data and computational tools developed and implemented in the CLEARR application. This significantly expands the ability of Reachback analysts to rapidly generate modeling results for new and emerging threat chemicals using Quantitative Structure Activity Relationships (QSARs) and extrapolation of available human and animal toxicity data across routes and severity categories using source for structural analog identification (ID).

Some of the core calculations that are produced in PropCast fall into three property categories 1) physicochemical, 2) thermodynamic, and 3) toxicological/effects. Physicochemical properties estimated or provided from databases by PropCast include Antoine coefficients, gas density, liquid viscosity, liquid surface tension, gas/liquid specific heat, atmospheric reactivity with hydroxy or nitrate radicals. Thermodynamic properties estimated include heat of vaporization, fusion temperature, heat of combustion, ignition temperature as well as some assigned defaults for other properties based on physical state. Toxicological and effects values are derived based on commonly used approaches in toxicological assessments such as in silico (QSARs), extrapolation from animal studies, or structural/toxidromic read-across. The result is a toxicity derivation workflow that has been implemented to provide LCt50 and ECt50 values for inhalation exposure and LD50 and ED50 values for percutaneous exposure as well as first-order estimates of probit slopes and toxic load exponents (TLEs). Additional techniques will be explored such as new approach methodologies (NAMs), and in vitro-in-vivo extrapolation (IVIVE) processes using other datasets available in CLEARR.

This capability is being deployed in HPAC via the CLEARR – PropCast module to enable analysts to develop these new material files on demand. This will allow DTRA to develop the toxicity effects material files for FXCODA more rapidly for HPAC modeling runs of new and emerging threats. The strategy employs a tiered approach to providing a quick screening level assessment that can be used when time is essential. The generated input files can then be fully validated via a more rigorous approach and SME review when more time for vetting is available.

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