An Advanced PBPK Model Input System and Data Repository for Complex Models with Export for the ACSL Model Engine

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Introduction

Preparing the inputs for a multi-chemical, multi-exposure modeling system such as the Dose Estimating Exposure Model (DEEM) is a daunting task. The Advanced Front End for DEEM (AFED) was developed in order to aid the user in preparing model inputs. DEEM has been written using ACSLTOX (Pharsight Corporation) and AFED is written using Power Builder and the SQL AnyWhere database system (Sybase).

General

The user can specify the version of DEEM to run, the units of the inputs and the outputs. Scaling of the DEEM input variables by body volume is an optional feature with the user supplying the scaling exponent to be used (not shown). The user may have many different Model Data Sets saved within AFED. If desired, a Model Data Set can be exported to an ACSL command file and ACSL can then be executed (using the ACSL Viewer). A new export module would have to be written for export to another modeling engine.

The user must proceed through the menu items in order. For instance, data cannot be input for a compartment unless that compartment has been chosen as active for the simulation.

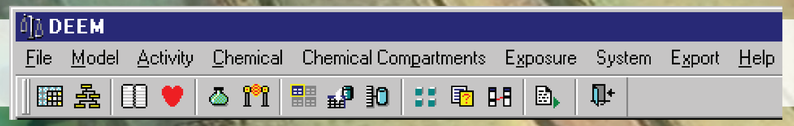
Details

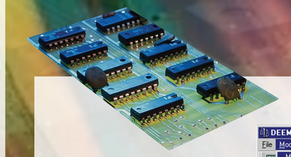
The screens in AFED are presented for five menu options: Model Menu, Activity Menu, Chemicals Menu, Chemical-Compartment Menu, and the Exposure Menu. The system menu options are not shown but include a list of available sub-systems, compartments, chemicals, and exposures with descriptions of each. Also not shown is the description of each input variable that is displayed when the user passes the mouse over the input label. Units are shown being added to the input variables.

Also not shown are screens for the user to specify:

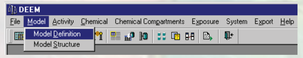
- *Output variables for which a time history will be saved,*
- *The absolute error limit for specified state variables,*
- *One or more variables and their values for which the Model Data Set inputs are not included,*
- *A list of variables to be printed while the simulation is running,*
- *A list of variables whose time history is to be printed when the simulation is completed,*
- *Multiple plot statements with multiple variables plotted in each plot.*

Main Menu

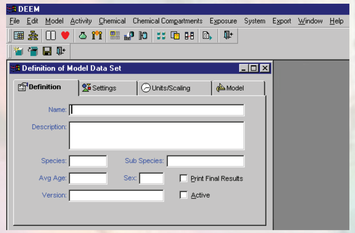


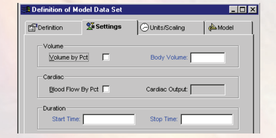


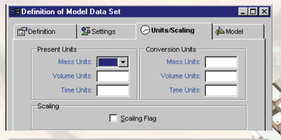
Model Menu

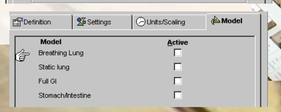


Model Definition

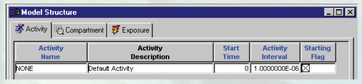


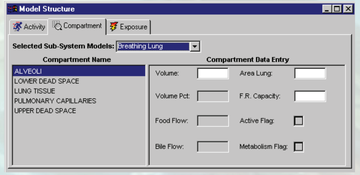


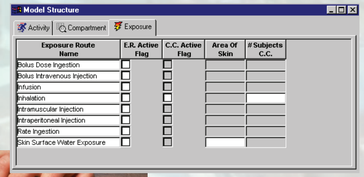




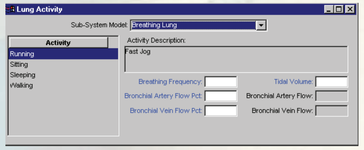
Model Structure

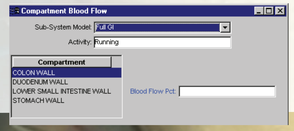




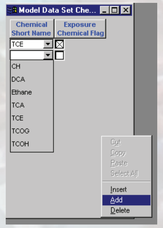


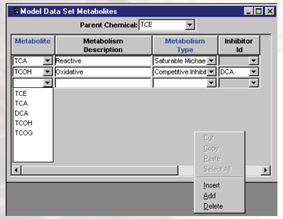
Activity Menu



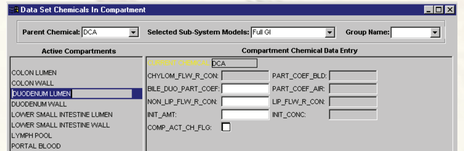


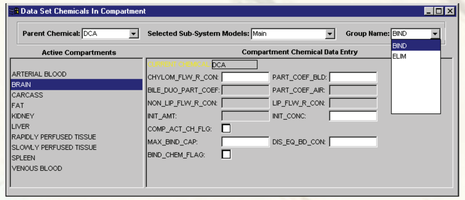
Chemicals Menu

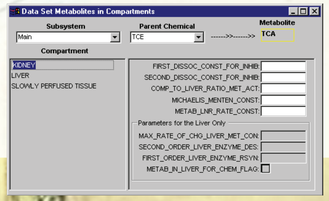


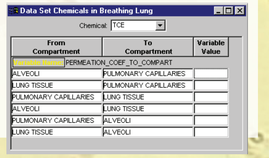
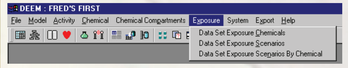
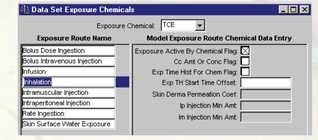
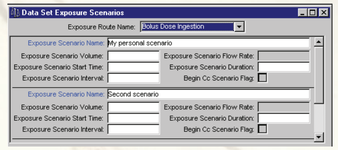


Chemical-Compartment Menu









Exposure Menu