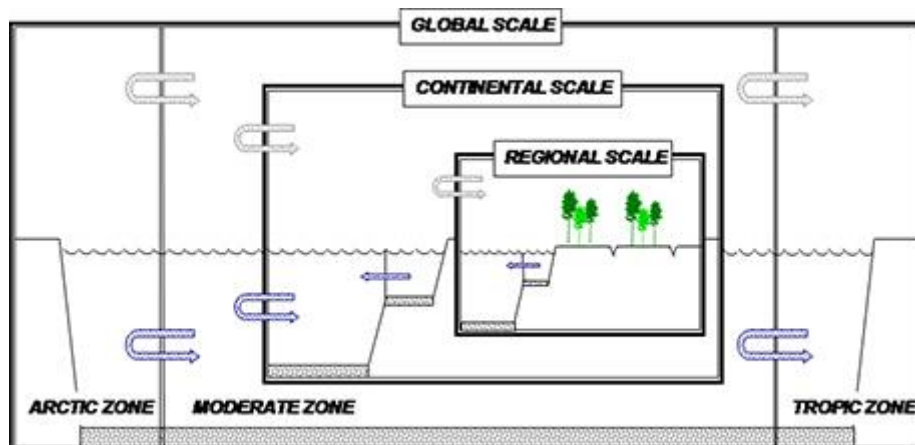


For the most recent info go to: www.rivm.nl/simplebox

About



SimpleBox is a multimedia mass balance model of the so-called 'Mackay type'. It simulates environmental fate of chemicals as fluxes (mass flows) between a series of well-mixed boxes of air, water, sediment and soil on regional, continental and global spatial scales.

Method

SimpleBox does so by simultaneously solving mass balance equations for each environmental compartment box in the model. SimpleBox is a first-principles model in the sense that it internally derives mass flow rates from physical and chemical substance properties, and characteristics of the environment modeled. It takes user-specified release rates as input, producing exposure concentrations in the environment as output.

Model code

SimpleBox is operated as Microsoft Excel spreadsheet, supported by numerical computations in R, which are linked to the spreadsheet via RExcel. Documentation has been published for model versions 1-4 in various technical RIVM documents [[1](#), [2](#), [3](#), [4](#)].

Framework

SimpleBox has served as 'regional distribution module' in the European Union System for the Evaluation of Substances (EUSES). It is currently used as part of the CHESAR tool, hosted by the European Chemicals Agency [[5](#)] to demonstrate possibilities for 'safe use' of chemicals, which is required for registration of chemical substances under REACH. SimpleBox also serves as fate module in Life Cycle Impact Assessment models [[6](#)].

Designed originally as a research tool, SimpleBox has proven most useful in dedicated environmental fate studies, focused at understanding and predicting environmental fate from fundamental physical and chemical substance properties.

Availability

The SimpleBox spreadsheet model and its documentation files are freely available for non-commercial use [8]. In order to [download the tool](#) you will be requested to fill in a short registration form. After submitting the form, you can download the tool immediately. For more information, please contact joris.quik@rivm.nl.

Performing quasi-dynamic ('level IV') calculations

- Note that SimpleBox uses R-based numeric calculations to produce quasi-dynamic ('levelIV') solutions; R/Rstudio installation necessary. SimpleBox calculates steady-state ('levelIII') output, using Excel only; no R tools are required.
 - Required: [R](#) and packages [deSolve](#) and [openxlsx](#).
 - Use the provided R script notebook for [Rstudio](#).
 - See 'Dynamic_SB4_Rnotebook.Rmd'Updates to this template might be available on [github](#).