About

SimpleBox4.0-nano is a variant of the SimpleBox model, which is designed such that it simulates the specific environmental behaviour of nanomaterials. The main adaptation consists of adding three particulate chemical species[1] to the dissolved species already included in SimpleBox. SimpleBox4.0-nano calculates mass flows of nanomaterials by simultaneously solving mass balance equations for 4 different chemical species for each environmental compartment in the model.

Documentation on the model definition that is added to simplebox to include the three particulate chemical species and make the model fit for nano has been published [link]. The main input parameters related to nanomaterial fate are the size and density of the nanomaterial, the size, density and concentration of natural particles and the transformation rates from emitted nanomaterial to the heteroagglomerate or dissolved species.
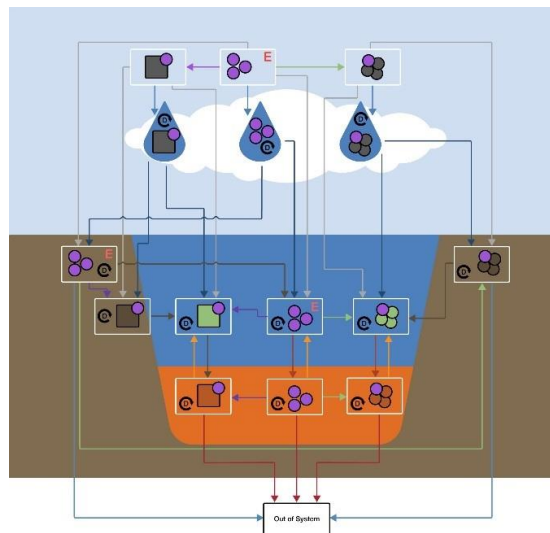
Model code

SimpleBox is operated as Microsoft Excel spreadsheet, supported by numerical computations in R. This can be attempted with the embedded macro linked to the spreadsheet via RExcel. The preferred option is reading in the spreadsheet model into R and performing further analysis in R. This can be done using the simple R script provided.

Running dynamic with RExcel and rtools?

0. Note that SimpleBox uses R-based numeric calculations to produce quasi-dynamic ('levelIV') solutions; R and RExcel installation necessary. SimpleBox calculates steady-state ('levelIII') output, using Excel only; no R tools are required.
    0.1. Required: R and package deSolve.

1. Install RExcel
    1.1. See: http://rcom.univie.ac.at/download.html

2. Run SimpleBox dynamicR routine
    3.1. Start Excel and open the SimpleBox spreadsheet.

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[1] The three particulate chemical species consist of: i) the emitted nanomaterial, ii) smaller heteroagglomerates (<450 nm) consisting of nanomaterial and natural colloids or aerosols and iii) bigger heteroagglomerates (>450 nm) consisting of nanomaterials and other particulates found in air, water and soil.

3.2. Start up R via Add-Inns -> Rexcel -> Start R. Excel is now set to execute the dynamicR routine for making quasi-dynamic model calculations. Make sure that Excel is set to use the RExcel add-in.

3.3. From SimpleBox4|dynamicR, execute the 'dynamicR' macro by pressing the button 'SIMULATE''