# User manual ACC-HUMANsteady 1.0

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## **About ACC-HUMANsteady**

ACC-HUMANsteady is a steady state (fugacity based) model of the bioaccumulation of organic contaminants developed at the Department of Applied Environmental Science, Stockholm University. The basic inputs to the model are two of the three partition coefficients between air-water, octanol-water and octanol-air, the corresponding heats of phase transfer, degradation rates, and chemical concentrations in air, water, soil and sediment. It also has a built in Level I environmental fate model. This model is coded in Visual Basic for Applications (VBA) and runs within Microsoft Excel. The model has been developed and tested on a 32-bit version of Excel 2007 and on a 64-bit version of Excel 2010.

This document is a guide to installing, starting and using ACC-HUMANsteady. For a detailed description of the model structure, the input parameters and the process descriptions in the model, please see the report “Model description for ACC-HUMANsteady 1.0” which may be downloaded from <http://www.osiris.ufz.de/index.php?en=17129>.

## **Download and installation**

The model can be downloaded from <http://www.osiris.ufz.de/index.php?en=17129>. The program is free software. You are free to modify the source code, which is readily accessible through the Visual Basic Editor of Excel. The program is distributed with the hope that it will be useful, but without any warranty. The model does not require any type of installation, but when the Excel file is opened you need to enable the macros.

## **Start up**

1. Download the model and save the Excel file somewhere on your hard drive.
2. To be able to run the model, the decimal separator must be “.” (i.e. not “,”). The separator may be changed in Excel, but to run the VB code correctly it must be changed from the Control panel. In Windows 7 this is defined under the Regional and Language Settings available under Control Panel: Control Panel 🡪 Clock, Language and Region 🡪 Change the date, time, or number format. Click on Additional settings button. This will display the Customize Format window where the Decimal Separator is defined. For instructions for other versions of Windows, search the Internet for “Change decimal separator in Windows”.
3. Launch the ACC-HUMANsteady model by double clicking the file. This should automatically start Excel. At start-up you may receive some warnings that the file contains Visual Basic macros. You must enable macros in Excel (either before opening the ACC-HUMANsteady model or at start-up) in order to run the model (To do this in Office 2007: Microsoft Office Button 🡪 Excel Options 🡪 Trust Center 🡪 Trust Center Settings 🡪 Macro Settings. Office 2010: File Menu (Office Backstage) 🡪 Options 🡪 Trust Center 🡪 Trust Center Settings button. Or simply search for “Enable macros Excel” at the web for detailed instructions).
4. When the model opens, the “InitializeModel” sheet should automatically be displayed. If not, click the “InitializeModel” tab. To start the model, click the “Initialize model” button. (The model will not work properly if you do not initialize the model first). After a few seconds, the “Model Input and results” sheet is displayed. If an error occurs (e.g. the Visual Basic editor opens and an error message is displayed) just click the stop button (or go to Run 🡪 reset), and then try initializing again by clicking the “Initialize model” button in the Initialize model sheet.

The “Model Input and results” sheet is the main page where you run the model and changes any settings. Here you can:

* 1. Select a chemical for which to run simulations
  2. Select scenario properties (i.e. environmental and food chain characteristics)
  3. Define concentrations or fugacities in the environmental media (air, water, sediment and soil)
  4. Access forms for Chemical Properties and Scenario Properties
  5. See the results of the simulations.

## **How to make a simulation**

### Select and/or define the chemical

This may be done in two ways. One way is to select a chemical from the drop list (the first entry is “Hypothetical 1”). This list contains the chemicals in the built in chemical database. By clicking the “Chemical Properties” button, a form appears where the physical chemical properties of the selected chemical are displayed.

Click the “Partition Coefficients” tab to display/change the molecular weight and partition coefficients between air-water (KAW), octanol-air (KOA) and octanol-water (KOW). Note that only two of the three partition coefficients are required, since the third is calculated from the two others. You must select which two to use in the calculations. Partition coefficients between aerosol-air (Kq) and organic carbon-water (KOC) are calculated from the octanol-air-water partition coefficients by default, but you may overwrite the default values by unchecking the box to the right and enter a value manually.

The “metabolism rate constants…” tab allows you to enter the metabolism rate constants, gut absorption efficiencies and feces-blood partition coefficient. The biotransformation rates and feces-blood partition coefficient are not calculated by the model; these must be defined by the user. The absorption efficiencies are calculated by the model, but may be overwritten by the user (uncheck the boxes as appropriate).

Any changes made in the “Chemical Properties” form may be saved by clicking “Save”. Note that this will overwrite the values in the chemical database (found in the “Chemical database” sheet), except for the hypothetical 1 chemical which cannot be changed in this way. (To change the properties of the default hypothetical chemical 1, simply change the values in the chemical database). If you do not click “Save”, but make changes and then click “OK”, the manually entered values will be used in the simulations, but the chemical database will not be changed. Next time you open the model, or if you click the “Initialize model” button, the values in the chemical database will appear in the form again.

The second way to define the chemical is to add another entry in the chemical database. To do this, click the “chemical database” tab to display the chemical database sheet. In the first empty cell below the list of chemicals in the database, write the name of your chemical. Then fill in the physical chemical properties in the same row. To make sure that the formatting is correct, you may choose to copy and paste the last row of the database and then change all values either directly in the chemical database or by returning to the “Chemical properties” form to enter the correct values for the new chemical from there. Minimum data required are MW, logKAW, log KOA, log KOW, KNLOM:Koct and KFB(human), and the heats of phase transfer ∆UAW, ∆UOA, ∆UOW. Note that you have to indicate which two of the octanol/air/water partition coefficients and heats of phase transfer that should be used manually before starting the simulation, this information cannot be saved in the database. To make the new chemical appear in the drop list in the “Model Input and results” sheet, go to the “Initialize Model” sheet and click the “Initialize Model” button. The new chemical may then be selected from the drop list, and the physical chemical properties entered in the database will also appear in the “Chemical Properties” form. If you want to keep your new chemical in the database, save the Excel file before you close the program.

### Select and/or define the scenario

A default scenario is coded into the ACC-HUMANsteady, which is based on environmental conditions and typical food chains in Southern Sweden. You may select a different scenario from the Scenario Properties drop list (below the drop list for Chemical Properties). The parameter values for each scenario are recorded in the scenario database (see the “scenario database” sheet). Similarly to the chemical database, you may create your own scenario, this time by adding parameter values to the first empty column in the database (again, you may choose to copy and paste the last column and then make your changes directly in the database or via the Scenario Properties form). You may change the values of existing scenarios (except the default scenario) by changing values in the Scenario Properties form, which will appear if you click the “Scenario Properties” button. Saving the changes by clicking “Save” will overwrite the corresponding values in the scenario database. Note that you cannot change the order in which parameters are listed, or delete any empty rows. The entries in the database are read by the program in the order specified when the model was developed. There are also hidden rows in the database (these rows cannot be removed from the sheet, but contains no information that is used in the calculations).

The Scenario Properties form shows all parameters describing the abiotic environment and the various organisms. Text boxes that are enabled and without a check box next to them indicate that the value is given by the user. Disabled text boxes (with grey text in them) indicate that the default value is calculated from other parameters. The default calculated value may be overwritten by the user by unchecking the box next to the text box and typing a new value. This value will then be used in the calculations. If you also click “Save”, the value you entered will be stored in the scenario database. By checking the box again, the default value will appear, and will be used in the simulations.

### Environmental concentrations

The default setting is a fugacity of 1 pPa in each of the environmental compartments (air, water, soil and sediment). The user may define the concentrations or fugacities by checking the box “Change input concentrations or fugacities”, and then enter the new values. By checking the “Unit world” box, the model calculates the concentrations and fugacities in each compartment from the emissions which are entered in the emissions text box. By clicking “Save fugacities” you overwrite the fugacities stored in the scenario database.

### Run a simulation and view the results

When all settings are made, you have to click the “StartSimulation...” button to make the calculation (i.e. no calculations of concentrations/fugacities are made when you change parameter values in the forms). The results (concentrations, fugacities, BCFs, BMFs etc) are then displayed in the sheet “Model Input and Results”. The D-values are displayed in the “D values” sheet, and a number of graphs in the “Charts” sheet. Note that the charts are updated only when you run a simulation, not when a change is made in the “Model Input and Results” sheet.

### Saving the changes and results

Note that Excel will not ask you whether or not you want to save any changes if you close the program by clicking the X in the upper right corner (this function is disabled in the model). End the program by clicking the “End” button instead. In general, it is better to save any changes before ending the program.

## **General advice**

Clicking and changing values in the forms may sometimes cause an error or empty text boxes to appear in the forms. If this happens, simply click the “Initialize Model” button and try all over again. Note that when clicking “Initialize Model”, you will lose any unsaved data entered in the forms.

The forms coded into the model are helpful to get to know the model and to get an overview of the parameters that are used in the calculations. It is recommended that you save any new chemical and scenario in the corresponding databases to make sure that you always know exactly which parameter values that are used in the calculations. For parameters that are calculated by default, you have to leave the corresponding cells in the databases empty (i.e. do not enter “0”) if you want the default calculated value. The model will check if a number is entered in the database before making the default calculation. If a number is entered, this will be used in the simulation. Note that for parameters that must be user defined, an empty cell will be interpreted as “0” by the model.