SimaPro 6: what is new?

1.1 Introduction

This document describes what is new in SimaPro 6. The most important improvements are:

- A new range of SimaPro versions
- The ecoinvent database available in SimaPro 6 database format
- New substance nomenclature
- Advanced Monte Carlo Uncertainty analysis
- Inclusion of subcompartments for raw materials and emissions

Details on these and many more improvements are described below.

We hope you will enjoy working with the new SimaPro 6 and like all the new features. Should there be any questions, or suggestions for further improvements, feel free to contact us.

1.2 New SimaPro versions

With SimaPro 6, we introduce a range of new SimaPro versions:

SimaPro 6 Analyst
The standard version with all advanced analytical features, including Monte Carlo analysis. It is available as single user and multi user network version. An ecoinvent database is included for new orders.

Existing users of the SimaPro 5.1 Analyst versions are updated to this version and will receive the ecoinvent database if they ordered it separately.

SimaPro 6 Compact
A SimaPro focused on creating quick results using the LCA Wizard and ecoinvent database. This database is included with new orders.
Not all features are available: most notably it has reduced analytical features (no Monte Carlo analysis) and import/export options. It is available as single user and multi user network version.

Existing users of the SimaPro 5.1 Light versions are updated to this version and will receive the ecoinvent database if they ordered it separately.

SimaPro 6 Developer
A new version that is similar to the Analyst, with the added ability to create Wizards (formerly scripts). On request a COM interface is available to develop interfaces with other tools.

The Developer version is available as single user and multi user network version. An ecoinvent database is included for new orders.

SimaPro 6 Educational versions
SimaPro educational versions are based on the SimaPro versions as described above. The ecoinvent database is not automatically included and should be ordered separately.

- SimaPro multi user licenses are updated to the SimaPro 6 Classroom version, comparable to the SimaPro Compact in multi user version.

- SimaPro campus licenses are updated to the SimaPro 6 Faculty version, comparable to the SimaPro Compact in single user version.

- SimaPro educational single user licenses are updated to the SimaPro 6 PhD version, comparable to the SimaPro Analyst in single user version.

1.3 New libraries

Ecoinvent unit and system processes
For SimaPro 5.1 users who ordered an ecoinvent database license, the ecoinvent unit and systems are included in the SimaPro database.

Unit processes describe the inputs and outputs of a process in detail. They have links to other processes and contain uncertainty information to be used by Monte Carlo analysis. As a unit process often is a part of a large, interlinked matrix of processes, the total calculation time can be quite long.

Systems processes represent the inventory results and as such only show the raw material inputs and emissions. They do not have any links to other processes. They also do not contain any uncertainty information. This means system processes can be used for quick calculations where no detailed information is needed.

The conversion is made based on ecoinvent database version 1.01. The ecoinvent update to version 1.1 in SimaPro format is expected end 2004. As SimaPro does not have all the fields as specified in the EcoSpold format used by ecoinvent, not all meta-information is included. However, all important documentation fields are included.

Support on the ecoinvent data is given by the ecoinvent centre. You can contact the centre via support@ecoinvent.ch. Detailed background reports are available on the ecoinvent CD-ROM which is sent to licensed ecoinvent database users.

USA Input Output Database 98
This Input Output Database is developed by Dr Sangwon Suh at CML of the University of Leiden. It consists of a 500x500 commodity matrix with economic flows, linked to a large database of environmental interventions collected from various sources. Note that the impact assessment methods have not yet been fully updated to be compatible with this library.

1.4 New substance nomenclature

In SimaPro 6.0 many of the substances from 5.1 have been given a new name. The substance names are newly defined according to the guidelines of SETAC and EcoSpold (the format used by ecoinvent). CAS numbers, formulas and synonyms have been added as much as possible to make searching easier.

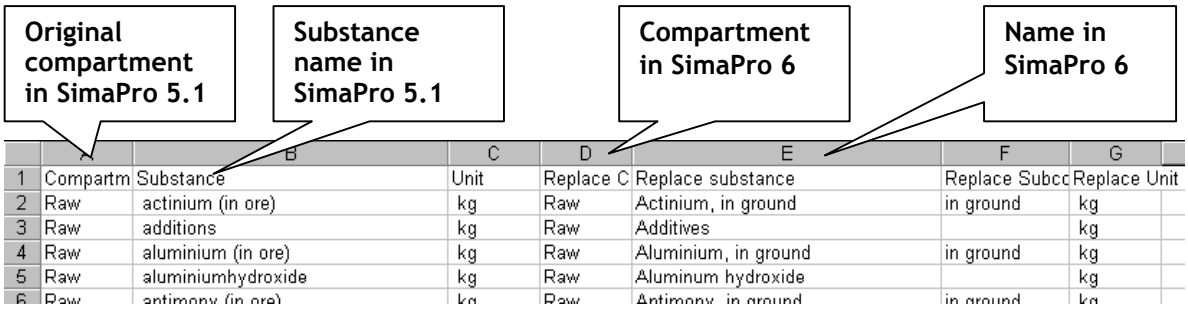
The following reasoning and hierarchy was followed to develop the new substance names in SimaPro 6:

- Ecoinvent name including CAS number and comment as default.
  If a substance name is not available in ecoinvent:
  - SETAC substance name and CAS number. Formula and synonyms are added based on information from chemfinder (www.chemfinder.com).
    If not available in the SETAC list:
    - Substances with a short chemical name: written in the same way as chemicals are written in ecoinvent and SETAC. Meaning:
      - first the main chemical structure, followed by appendices. For example 1,2,3-trichlorobenzene becomes Benzene, 1,2,3-trichloro-
      - Full names (no chemical formulas). CO2 becomes carbon dioxide.
      - 'Commercial name' for pesticides
      - unspecified for substance groups, except for groups with a specification to avoid long ugly names (for example chlorinated alkanes)
    - Substances with a long chemical name: as written default in chemfinder
    - Raw materials in ground, like ores and fossil resources, have 'in ground' in their name to prevent confusion with materials from technosphere.

The category 'Solids' is changed into the category 'Final waste'. The amount of substances in this category has been limited. Most are provided with 'waste' in the name, to prevent confusion with products from technosphere.

The append file, delivered with SimaPro 6.0 is the exact documentation of all replaced substance names. You can open this file in Excel if you want to see what has changed in SimaPro 6. Please do not make any changes in this file.

You also need this append file if you want to update your previous 5.1 standard database to SimaPro 6, as described the update instructions.



	A	B	C	D	E	F	G
1	Compartm	Substance	Unit	Replace C	Replace substance	Replace Subcc	Replace Unit
2	Raw	actinium (in ore)	kg	Raw	Actinium, in ground	in ground	kg
3	Raw	additions	kg	Raw	Additives		kg
4	Raw	aluminium (in ore)	kg	Raw	Aluminium, in ground	in ground	kg
5	Raw	aluminiumhydroxide	kg	Raw	Aluminum hydroxide		kg
6	Raw	antimony (in ore)	kg	Raw	Antimony, in ground	in ground	kg

Most substances from the compartment *Non material* are moved to other compartments:

- All 'substances' related to land-use, are moved from *Non-material* to the category *Raw*
- Radiation and emission from heat are moved to their related category. For example the non material emission 'U234 to air' from SimaPro 5.1 is moved to air and became 'Uranium-234' as written in ecoinvent.

A few additional remarks can be made on some of the substances:

	Substance in SimaPro 5.1	**New substance name in SimaPro 6**	**Comments**
air	1,2,5-trimethylbenzene	Benzene, 1,2,4-trimethyl-	EDIP gives deviating characterisation factors for both substances, but to our knowledge 1,2,5-trimethylbenzene does not exist.
air	odorous sulfur	Mercaptans, unspecified	Odorous sulfur is not used by processes or methods in SimaPro 5.1 and therefore appended to Mercaptans (which is a group of sulfuric chemicals)
air	Sox Sox as SO2	Sulfur oxides	Formula: SOx as SO2 Ecoinvent is followed above SETAC (Sulfur oxide)
air	NOx Nox as NO2	Nitrogen oxides	Formula: NOx as NO2 Ecoinvent is followed above SETAC (Nitrogen oxide)
air	2 butanone	methyl ethyl ketone	This is deviating from the SETAC suggestion ('Butanone, methyl-ethyl-ketone) because this was thought to be confusing since butanone and methyl ethyl ketone are the same substance (and it is not referring to a combination of these two)
Raw	methane (kg) ETH	Gas, mine, off-gas, process, coal mining/kg	methane (kg) ETH is only used in unit processes for coal mining.
Raw	F	Fluorine, in ground	CAS: 14762-94-8, Formula: F The raw material 'F' in ecoinvent (Fluorine, 4.5% in apatite, 1% in crude ore, in ground) has CAS-number 7782-41-4. According to Chemfinder this is the CAS number for F2, therefor we did not copy this CAS number for 'Fluorine, in ground'

1.5 Changes in existing libraries

New process category structure
The inclusion of the ecoinvent database with over 2500 processes as well as changes in the SimaPro Wizards made it necessary to create a new process category naming structure. All existing libraries have been updated. Existing SimaPro 5.1 users can update the structure by following the SimaPro update procedures.

New substance nomenclature
All existing libraries have been updated with the new substance nomenclature. Existing SimaPro 5.1 users can update their nomenclature by following the SimaPro update procedures.

Adapted impact assessment methods
The impact assessment methods in SimaPro have been updated with the new substance nomenclature. Furthermore, they have been partially modified to be compatible with the new ecoinvent data. Note that not all methods have been updated to be compatible with the ecoinvent and USA Input Output database 98 libraries. See the comment fields in the methods for detailed information.

The impact assessment methods in SimaPro have been renamed to avoid overwriting your old methods. They now include a version number.

1.6 Summary of new software functionality

Monte Carlo Uncertainty analysis
SimaPro 6 can make advanced Monte Carlo uncertainty analysis calculations. In order to make this possible, the process and product stage records have been extended so that distributions can be entered for any flow. Only the new ecoinvent unit processes library currently contains a full set of distributions.

With this input, SimaPro calculates the uncertainty in the inventory results. The Monte Carlo calculations are made on the full system, i.e. each flow for which an uncertainty distribution is defined is taken into account. Starting Monte Carlo will give a setup window where you can change the amount and unit and the impact assessment method that must be used.

They uncertainty is displayed in impact assessment results as high-low ranges. On substance level the actual sampling distribution can be shown. Tables with extensive statistical information are available.

Monte Carlo Uncertainty analysis can also compare 2 systems. As often these systems are using the same processes, a method called process correlation is used to make sure that the variation in the sampling is the same. No high-low graphics are available for these comparisons, as they may lead to misinterpretations. Instead we show the chance that process A is better than process B.

All graphs and tables can be copied and pasted to other applications.

Activation
Apart from registration, it may be required to activate SimaPro. This can be done online or offline. Activation means a hardware (PC) dependent registration code is created so that unauthorized installations are not possible. In this process no personal data are collected. Please contact us if you are not allowed to install SimaPro anymore, for example when you install SimaPro on a new PC.

Substances
The substance definitions are extended with a CAS number and comment field. The category "Solid emissions" is changed to "Final waste flows". New categories are added for economic issues and social issues; no "issues" (substances) have yet been defined.
Furthermore, you can now choose from prédefined subcompartments (e.g. groundwater, lake, ocean, river for emissions to water) in the process and method editor. This means that more detailed impact assessment methods can be used.

Better substance appending
Appending substances could only be done one at a time. This was a time consuming job and had to be repeated with each new import of the same substance names. In SimaPro 6, you can append multiple substances in batch mode, which makes the process about 50 times faster. You can now save your append list as an Excel file which makes you have a archive of your changes. This file can be reused in later append actions. Append has furthermore been adjusted to allow change of compartment, as well as the appending of a substance to a subcompartment.

Improved method editor
The method editor has been adjusted to work with the new subcompartments. An important calculation choice has been made so that you will get meaningful results, even if the impact assessment method is not compatible with the use of subcompartments. If a substance in a process is defined with a subcompartment, but the selected method has no specific characterisation factor for this subcompartment, SimaPro will use the characterisation factor for the "unspecified" substance.

Characterisation and damage factors are now shown with their complete units, created from the unit of the impact or damage category and the unit of the selected substance. For example, the characterisation factor for methane in global warming is now shown as "methane 62 kg CO2/kg" rather than "methane 62 kg".

Find Text
In processes, product stages and methods you can now quickly search for (parts of) words, substance names and units. Use CTRL+T or the right mouse button to activate this function. You must be in the edit or view mode.

Calculation setup
When you now start a calculation (analysis, network, tree or compare) a calculation setup window is shown. Here you can change the amount and unit of the item(s) to be calculated as well as the method to be used. Furthermore you can indicate if the inventory should be shown per subcompartment. If you do not select this option the totals of all subcompartments for each substance are shown.
In the Developer version you can also indicate if infrastructure processes should be excluded from the calculation. Infrastructure processes are defined in both the ecoinvent and ETH-ESU libraries using a special option in the process.

Improved calculations
We have increased the speed of the network calculations; it is about 50 times faster. As a result, the gravity button is not needed anymore as the perturbation algorithm is directly included in the calculation. Note however that the increase in calculation speed is compensated by increasing complexity of the database.

New navigation in network and process tree
The navigation bar in the network has been divided in a navigator part and a flow part. These can be switched on or off using the toolbar button.

Display images in network and process tree
Images added to a process or product stage can be shown in a network and process tree. Use the toolbar button to switch images on or off. A small set of images was added to the ecoinvent libraries as example.

Hints on results tables
A mouse-over hint is now given in the inventory and impact assessment result tables if a result is not available. If no result is available because a substance is not defined in a method, this will be specified.

New network options
Using the right mouse button on a process in a network or process tree, you will find a number of layout options. New options are the Font size option, where you can choose the font size used in the boxes, and the Display name option, where you can choose between process names or product names. A process name is the definition of the process, or the default name as it was always shown in previous versions of SimaPro. The product name is defined in a process, in the field "Name" in the documentation tab. Here you can define a short name that is used instead of the often very long process names. Note that existing libraries have not yet been adjusted for this feature.

Improved graph layout options
SimaPro now has an extensive module to layout your results graphs. It is possible to make 3D graphs, add background colors, use gradients, etc. To change the settings of your graphs, click on the Chart settings button in the result windows.

Save Analyse/Compare as report
The calculation setup chosen to make an analysis or comparison can now be saved as a report setup, using the right mouse button in the impact assessment or inventory results.

Save Inventory as system process
The inventory results of a calculation can now be saved as a process. This allows you to aggregate complex or confidential data as a system in one process record. Use the right mouse button on a result column in inventory results to activate this function.

Associated assembly visible in product stages index
The index of the product stages now shows to which assembly a life cycle, disposal scenario, disassembly or reuse refers. This will help you in selecting the correct product stages when you are modelling complex products.

Faster import SimaPro database
As SimaPro databases become larger and larger, an improvement in the import speed was needed to make the import times acceptable. Still, import can take a long time.

EcoSpold import in SimaPro 6 Developer
Import of XML files in EcoSpold format is possible in the SimaPro Developer version. To make sure the data are implemented in a way that is compatible with the SimaPro 6 database structure, additional work is needed. You can contact our helpdesk (support@pre.nl) to learn more about the EcoSpold import procedure.

Wizard development in SimaPro 6 Developer
It is now possible to show a network in wizards and to activate external programs or websites. Forms have been renamed to "Product systems" and are now integrated in the Wizard window. These options will work in all SimaPro versions. Furthermore, a new manual on developing wizards is available.

Wizard start up screen in Compact version
The SimaPro Compact, Classroom and Faculty versions will start up with the LCA Wizard window.