User Guide

The ecosolvent tool

About the ecosolvent tool:

Ecosolvent Version 1.0.0

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Introduction: Scientific Background

The ecosolvent tool is a generic life-cycle assessment tool that allows for the environmental comparison of various waste-solvent treatment technologies for specific, user-defined waste-solvent mixtures. The environmental impact is quantified using the Life-Cycle Assessment (LCA) methodology [4]. The functional unit is defined as the comparison of the treatment of a certain amount of waste solvent with two different treatment technologies (e.g. waste-solvent distillation vs. incineration).

The technologies are represented by so called life-cycle inventory (LCI) models that are all based on industry data. With these models, waste-solvent specific life-cycle inventory data, such as emissions flows, ancillary uses, and generation of co-products are calculated. The ecosolvent tool comprises comprehensive models of a hazardous waste-solvent incineration plant, an average Swiss cement kiln, industrial distillation (rectification) processes, and an industrial wastewater treatment plant.

The *incineration models* of the tool calculate inventory data of solvent combustion as a function of the elemental solvent composition and technology used. Causal relationships between the consumption of ancillaries and energies, the generation of co-products and the emissions of pollutants, and their causing components within the waste solvent were modeled with the help of consumption and emission factors and transfer coefficients The resulting multi-input allocation model allows for the calculation of life-cycle inventory (LCI) data for specific waste solvents. Two different multi-input allocation models for the incineration are implemented in the tool: The first model describes a large waste solvent incineration plant where liquid wastes including spent organic solvents, distillation residues, mother liquors, waste oils and highly organically charged wastewaters are disposed off. Co-products of this incineration plant are steam and electricity. This model is based on data of an incineration plant located within a large chemical production site in Switzerland and with a capacity of about 35'000 tonnes per year [11]. The second model represents the incineration of waste solvents in cement kilns. The use of waste solvents as fuel in cement production saves fossil fuels such as coal and heavy fuel oil. This model was established similarly to the above one, based on average technology used in Switzerland [10].

The *model of distillation processes* is based on empirical relationships that are used as approximation if precise information (measured values) is missing. Such empirical relationships have been established by collecting and analyzing LCI data of 150 industrial waste-solvent distillation processes in collaboration with the Swiss chemical industry. The LCI data contain values for the demand of steam, electricity, cooling water, inert gas (nitrogen), and ancillary products as well as for the amount of recovered solvent, residues, wastewater, and outlet air. These data were used to derive two empiric data ranges (empiric average, minimum, and maximum values) for each LCI parameter. The first generic data range is based on the entire sample and thus gives a rough estimation. This data range is applied in the LCI-model when no information about the distillation process is given. The second generic data range is based on sub-samples (e.g. batch or continuous distillation) and is thus a more precise estimation. It is used if information about the distillation, such as distillation technology or use of ancillaries, is available [1].

The *model of the wastewater treatment plant* enables the calculation of inventory parameters as a function of the wastewater composition (e.g. TOC content) and the technologies applied. For this purpose, data on energy and auxiliaries consumption, wastewater composition and process parameters from chemical industry have been collected and they have been allocated according to physical relationships. Generic and site-specific data ranges for LCI parameters, respectively, are provided for the processes mechanical-biological treatment, reverse osmosis and extraction. The input-dependent process inventories help to bridge data gaps when primary data is not available [9].

Finally, the calculated inventory data of all models is linked to background inventory data (production of ancillaries, fuels, and energy) taken from the ecoinvent database [3] or from industry data. In the ecosolvent tool, the full life-cycle inventory is presented as result as well as it can be assessed with various life-cycle impact assessment methods (Global Warming Potential [7], Cumulative Energy Demand [8], Eco-indicator 99 (H/A) [5], and Method of Ecological Scarcity (UBP'97) [6]).

Chapter 1: Getting started

The ecosolvent tool can be downloaded from

www.sust-chem.ethz.ch/tools/ecosolvent

Download and run the ecosolvent tool:

1. Download the ecosolvent.zip file from the given link on the website.

2. Unzip the .zip file (e.g. use winzip tool for windows (http://www.winzip.com)). Now you have a folder "ecosolvent" with all necessary files in it.

3. To run ecosolvent:

   For windows: double click "ecosolvent.exe" in the folder ecosolvent

   For mac and unix: execute the script "startEcosolvent.bat" in the terminal:
   cd pathToEcosolvent
   ./startEcosolvent.bat
   (where pathToEcosolvent stands for the complete path to the file startEcosolvent.bat)
   Note that it might be necessary to change the executable rights for the file startEcosolvent.bat which can be done by executing the following command in the terminal:
   chmod 777 startEcosolvent.bat

For further information follow the instructions given on the website.

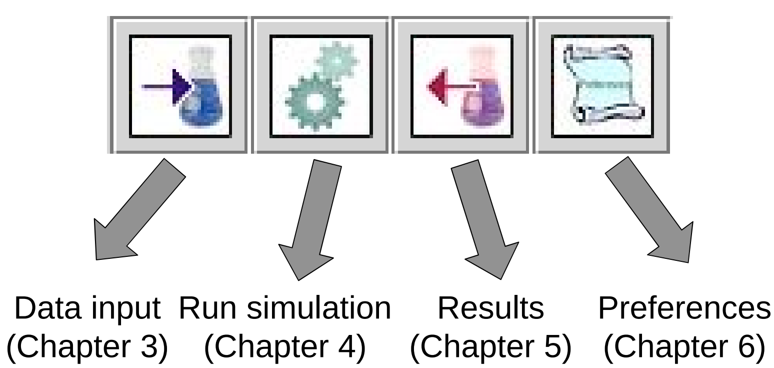
Please note that the ecosolvent tool needs a lot of random access memory (RAM). This might slow down your computer significantly if other applications are running at the same time.

Chapter 2: Overview

This chapter gives an overview on the functionality of the ecosolvent tool and shows how to use the software in order to perform environmental comparisons of waste-solvent treatment options.

The ecosolvent tool is subdivided into 4 sections. In the section "Data input", the waste-solvent composition and the waste-solvent treatment technologies to be compared is specified. Additionally, information on the treatment technologies can be entered (e.g. distillation or incineration technology, solvent recovery, TOC elimination or transport distances). This section is described in detail in Chapter 3. The section "Run simulation" is used to start the actual calculation of the environmental impact for the selected waste-solvent composition and technologies. This section is described in detail in Chapter 4. The "Results" section shows the calculated results. Various life-cycle impact assessment methods may be chosen to analyze the environmental impact of the specified waste-solvent treatment, such as "Global Warming Potential", "Cumulative Energy Demand", CO2-balance, "Method of Ecological Scarcity (UBP '97), and "Eco-Indicator 99". A variety of reports are provided as well as the option to export the results to MS Excel. This section is described in detail in Chapter 5. Finally, in the section "Preferences" (Chapter 6), default data ranges (e.g. use of steam and electricity, yield) that are used as approximation in the distillation model in case no precise information is available are shown as well as the solvents that are available in this tool. All sections are directly accessible on the main navigation bar.

Main navigation bar and indication of the Chapters in this user guide that describe the sections in detail.

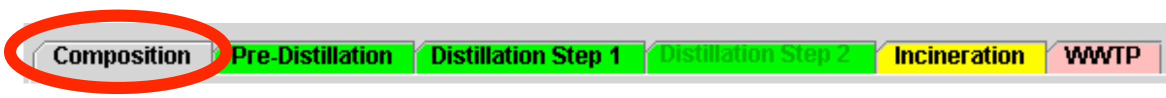


Chapter 3: Data input

This chapter describes how to specify the waste-solvent composition and the technologies used for the waste-solvent treatment. The ecosolvent tool is designed with a tiered structure. You can enter precise information on the treatment technologies, such as measured steam consumption of a distillation process. If such precise information is entered, the calculated results show a relatively small uncertainty ranges. However, the ecosolvent tool may also be used if such precise information is missing. In that case generic data are used to abridge the lack of information. But using generic data results in larger uncertainty ranges of your results.

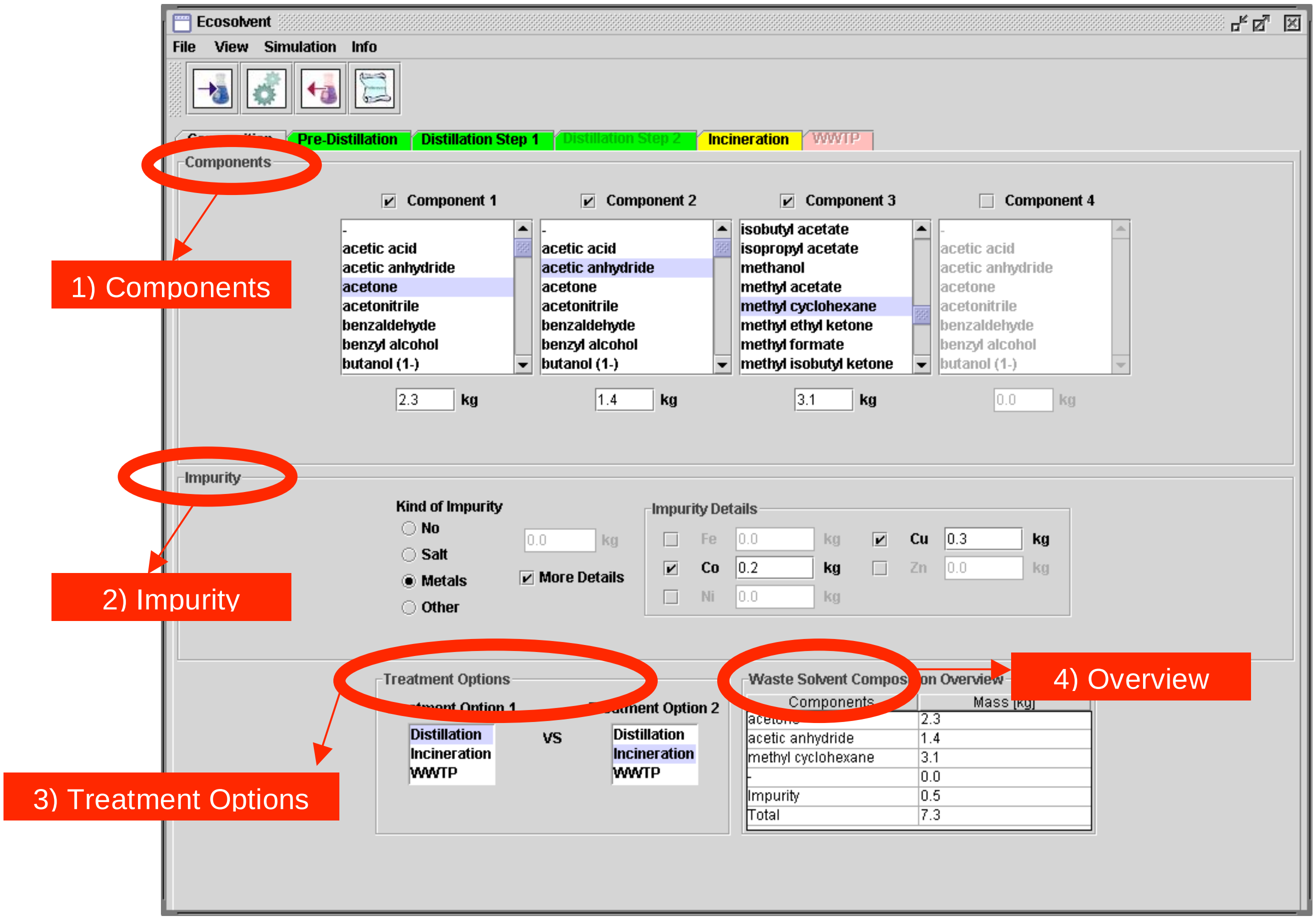
Waste-solvent composition and treatment technologies

In a first step, the waste solvent and the waste-solvent treatment options have to be specified. To this end, the tab "Composition" in the menu bar has to be selected.



Menu bar in the section "Data input".

In window "Composition", the components (1) and impurity (2) of the waste solvent have to be specified as well as the treatment technology for this specific waste solvent (3). The waste solvent may consist of up to 4 solvent components (1). 45 organic solvents and water may be chosen from the list and their amount has to be specified. In case a waste-solvent mixture is composed of other solvents than the 45 solvents, a generic organic solvent may be selected as an approximation. In addition to these components, the waste solvent may also show impurities (2), such as salt, metals or other (organic) solids. In case metals are present in a waste-solvent mixture, they may be specified specifically because metals cause individually different impacts to the environment. In addition to the waste-solvent mixture, the treatment options to be compared have to be specified (3). Finally, an overview on the selected components, impurities and the corresponding amounts is given (4).



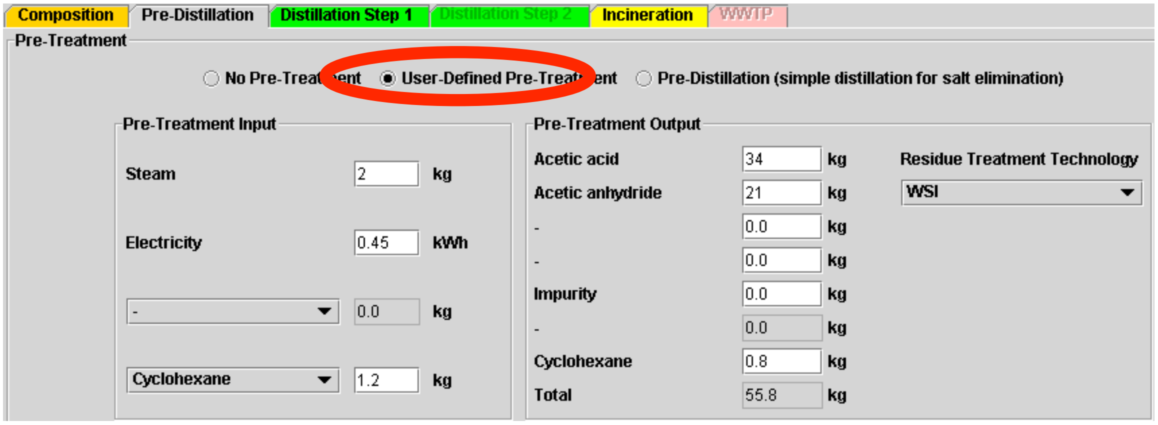
Window "Composition" in the "Data input" section.

Waste-solvent distillation: Pre-distillation

If distillation has been selected as waste-solvent treatment option, a potential pre-treatment of the waste-solvent mixture may be specified. To this end, the tab "Pre-Distillation" in the menu bar has to be selected.

Menu bar in the section "Data input".

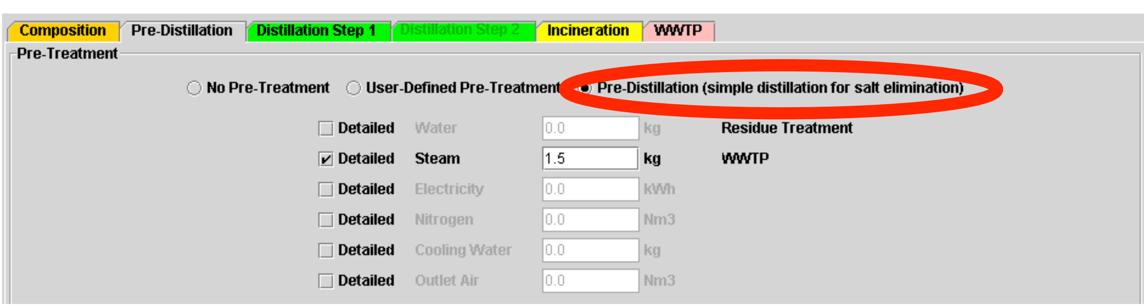
In the ecosolvent tool, two different pre-treatment processes may be specified: A user-defined pre-treatment and a simple pre-distillation step.



User-defined pre-treatment of the waste-solvent mixture.

The *user-defined pre-treatment* is designed as a "black-box" process. You can specify an energy input (steam, electricity) and material input (ancillaries, e.g. solvents, water or sodium hydroxide). Additionally, the product (output) has to be specified as well as the treatment technology of the residue. The output is treated subsequently in the distillation step 1. With such a "black-box", unit processes may be modeled that are used to purify the waste-solvent mixture before distillation (e.g. liquid-liquid extraction).

The *simple pre-distillation* represents a simple batch distillation step without reflux in order to separate organic compounds from water and dissolved salt particles. Therefore, this pre-treatment option can only be selected if the waste solvent contains a water fraction and salt as impurity. Detailed information on the simple distillation can be entered (e.g. steam or energy use, nitrogen and cooling water consumption, and the amount of outlet air). If such information is not available, generic data is used as approximation. The distilled organic components are distilled (distillation step 1) and the aqueous residues are treated in the wastewater treatment plant.



Simple pre-distillation of the waste-solvent mixture.

Waste-solvent distillation: Distillation step 1

Information on the distillation process itself can be entered selecting the tab "distillation step 1" in the menu.

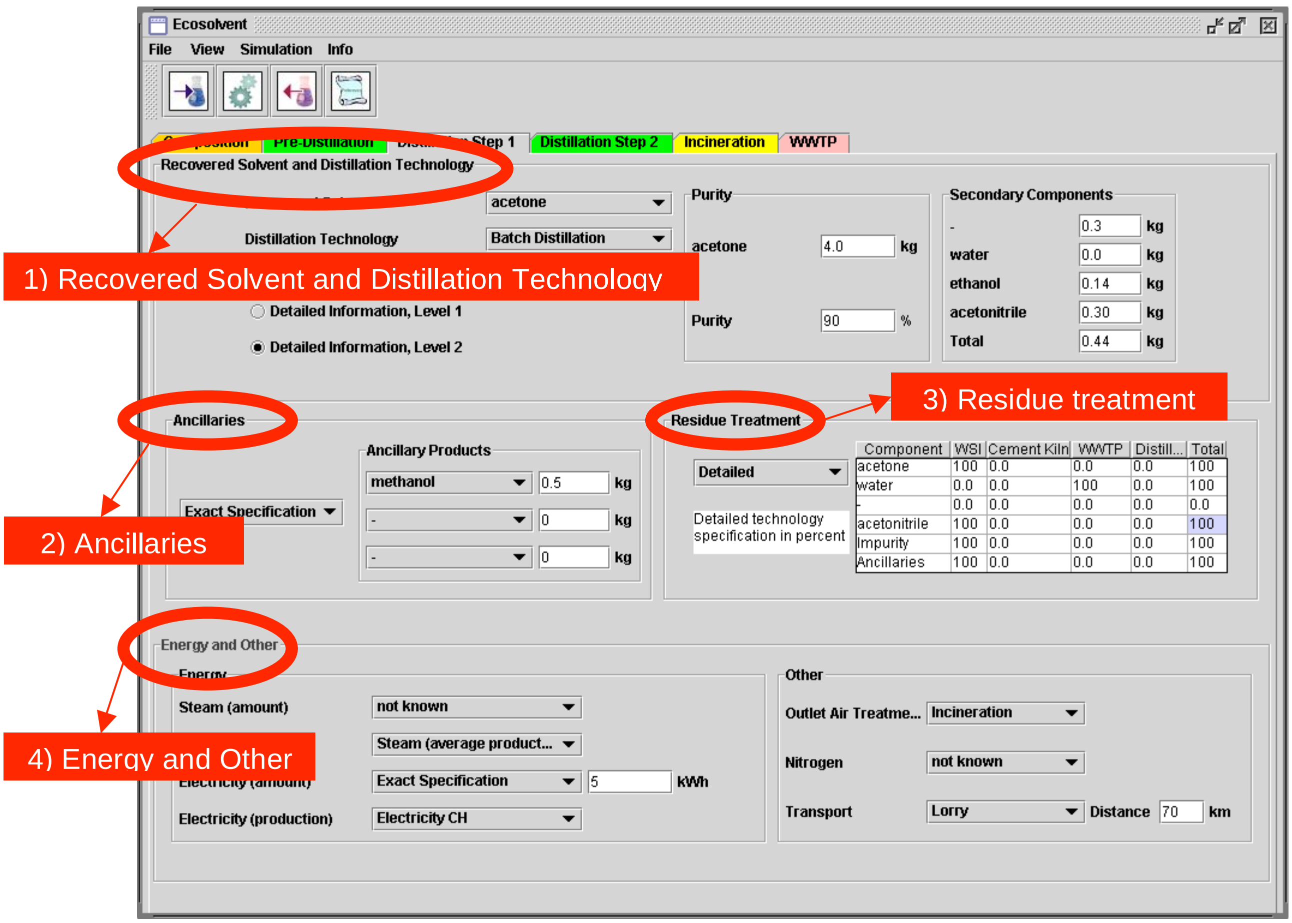
Menu bar in the section "Data input".

In the first section of the window "distillation step 1" the solvent to be recovered out of the waste-solvent mixture and its amount can be specified (1). If precise information on the recovered amount of solvent is not available, generic data on solvent recovery may be used as approximation either for a specific distillation technology (batch or continuous) or for waste-solvent distillation processes in general, if the technology is not known. In case the solvent recovery is known, the amount and the purity of the solvent can be specified exactly (detailed information level 1). Additionally, the secondary components present in the product may be specified (detailed information level 2). This is important for products with relatively low purities (below 95%).

The use of ancillaries can be specified in the second section (2). If no information is available, generic data for the use of ancillaries in waste-solvent distillation processes in general is used as approximation. In case the use of ancillaries for specific purposes is known, such as entrainer in case of azeotropic mixtures or cleaning agents for equipment cleaning, more accurate generic data can be used as approximation. Finally, up to 3 chemicals can be specified to determine the use of ancillaries exactly.

In the next section, the distillation residue treatment can be specified (3). Possible residue treatment options are the incineration in either a special waste-solvent incinerator (WSI) or in cement kilns (Cement Kiln), the treatment of the residue in a wastewater treatment plant (WWTP) or a subsequent distillation of the residue in order to recover a second component as product (Distillation Step2). However, with regard to complex distillation processes this choice may not be sufficient because multiple residue streams arise that require individual treatment technologies. For example, water from a decanter is treated in a wastewater treatment plant, the distillate output of the start-up phase is incinerated, and the residue remaining in the batch is distilled in a second step in order to recover another solvent. In order to cover such complex distillation processes, the residue treatment can be specified for all components present in the waste-solvent mixture specifically (Detailed).

In the last section, the energy consumption and production can be specified as well as the use of nitrogen, the outlet air treatment, and transport processes from the origin of the waste solvent to the distillation column (4). With regard to the amount of used energy and nitrogen, generic data are used as approximation in case no information is available. The consumption of steam may alternatively be calculated if the reflux ration is known (e.g. based on the operating instruction of the distillation process). Considering the production of steam and electricity, various production scenarios may be chosen (e.g. average European production, Swiss production or production from waste-solvent incineration).



Window "Distillation step 1" in the "Data input" section.

Waste-solvent distillation: Distillation step 2

The window "Distillation step 2" can only be selected if a subsequent distillation has been specified as (partial) residue treatment in the first distillation step. This window shows the same options than for the first distillation step. The only exception is that no subsequent distillation step may be selected for the residue treatment.

Waste-solvent incineration

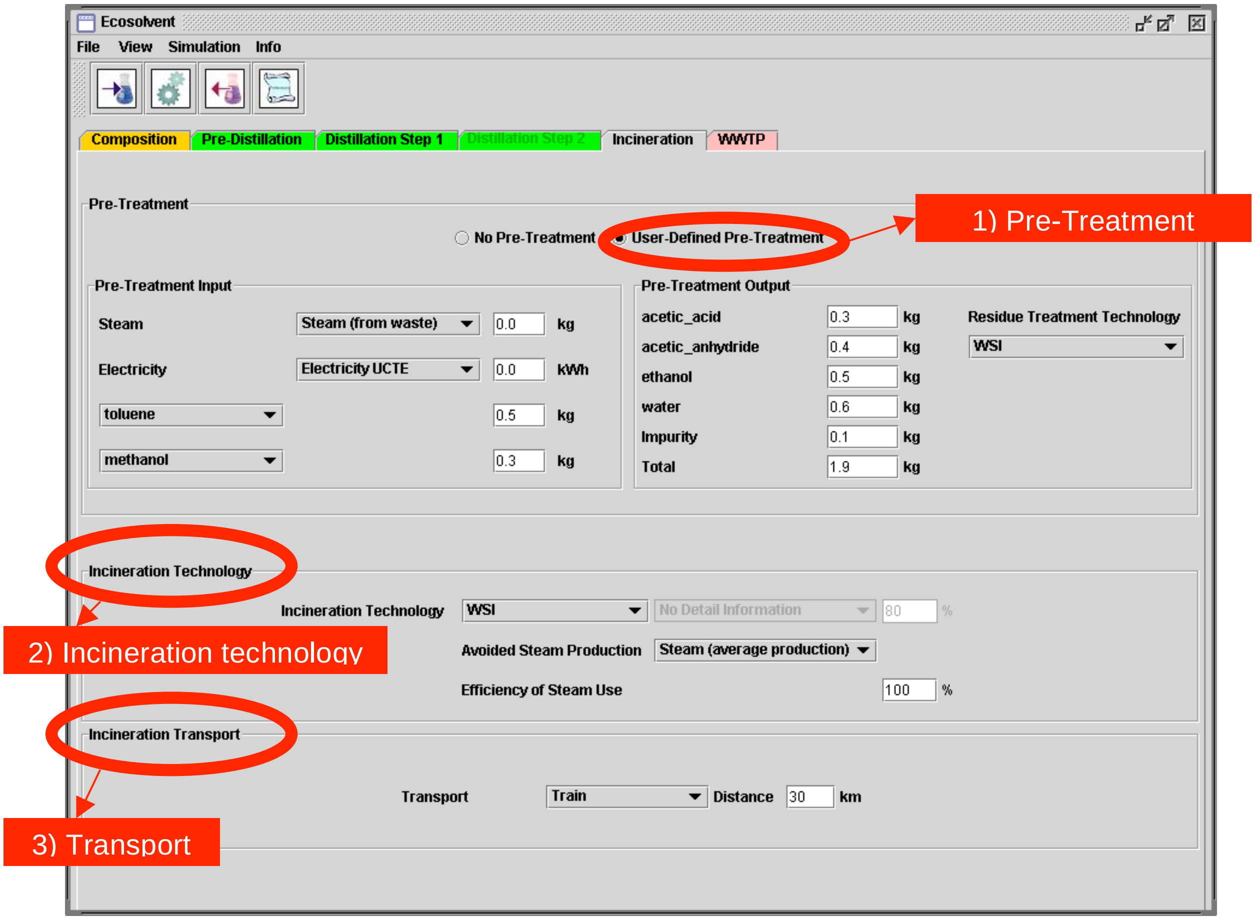
If incineration has been selected as treatment option, information on the incineration process has to be specified. To this end, select the tab "Incineration" in the menu bar.

Menu bar in the section "Data input".

The waste solvent may also be pre-treated before the incineration, analogue to the distillation process,. Therefore, it is also possible to specify a user-defined pre-treatment (1) that corresponds to the user-defined pre-treatment used for distillation processes (see section "Waste-Solvent Distillation: Pre-Treatment"). The only difference is that the output is subsequently incinerated.

In the second section, the waste-solvent incineration technology has to be specified (2) (special waste-solvent incinerator "WSI" or cement kiln). Moreover, additional information on the incineration processes may be given: Regarding the cement kiln, the efficiency of the NOx reduction facility may be specified since it depends of the plant and the operating settings (it is also possible that no NOx reduction facility exists). Regarding the special waste-solvent incinerator, the alternative technology for steam production may be specified. Additionally, the percentage of the produced steam may be determined that is effectively used in the chemical plant.

Finally, transport processes from the origin of the waste solvent to the incineration plant can be specified (3).



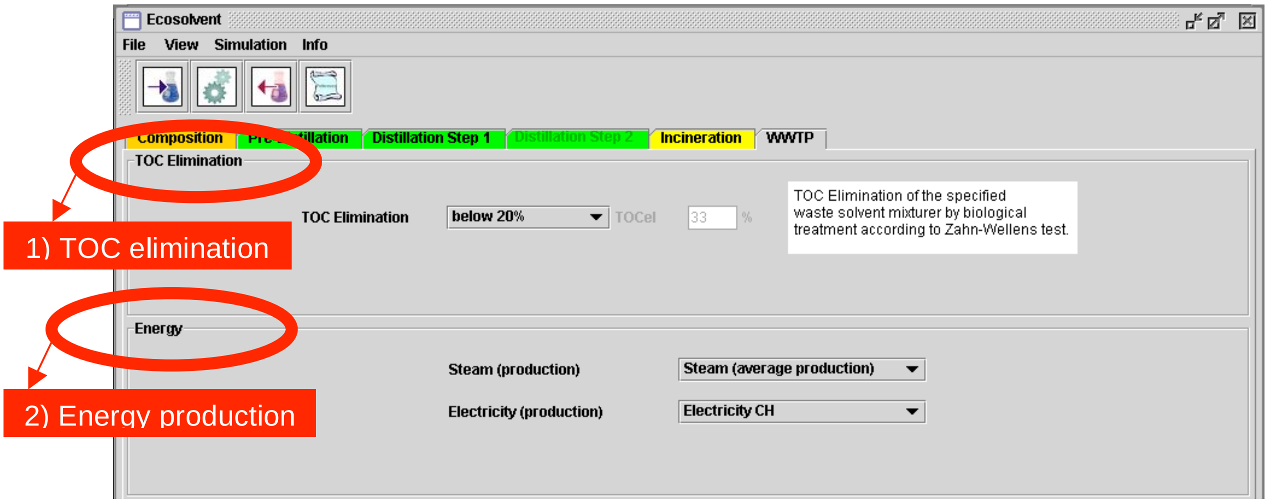
Window "Incineration" in the "Data input" section.

Waste-solvent treatment in wastewater treatment plant

If incineration has been selected as treatment option, information on the incineration process has to be specified. To this end, select the tab "Incineration" in the menu bar.

Menu bar in the section "Data input".

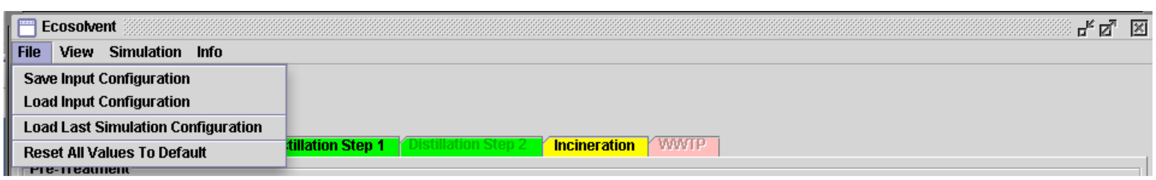
To calculate inventory data of the wastewater treatment plant, information on the TOC-elimination by biological treatment in Zahn-Wellens [2] test is required for the specified waste-solvent mixture (1). The TOC elimination determines what wastewater-treatment technologies are used (Extraction, Reverse Osmosis, Mechanical-biological wastewater treatment). If the TOC-elimination cannot be specified in detail, ranges can be selected (e.g. TOC-elimination between 20% and 90%). This leads to larger uncertainties of the calculated inventory parameters. In addition to the TOC-elimination, the energy production scenario can be specified (2).



Window "Wastewater Treatment Plant" in the "Data input" section.

Load / save / reset files

Once the data input has been finished, the configuration can be saved. The save / load function is located in the File menu. If a new waste-solvent mixture has to be specified the function “Reset All Values To Default” can be used to clean all prior modifications and start with a new waste-solvent mixture.

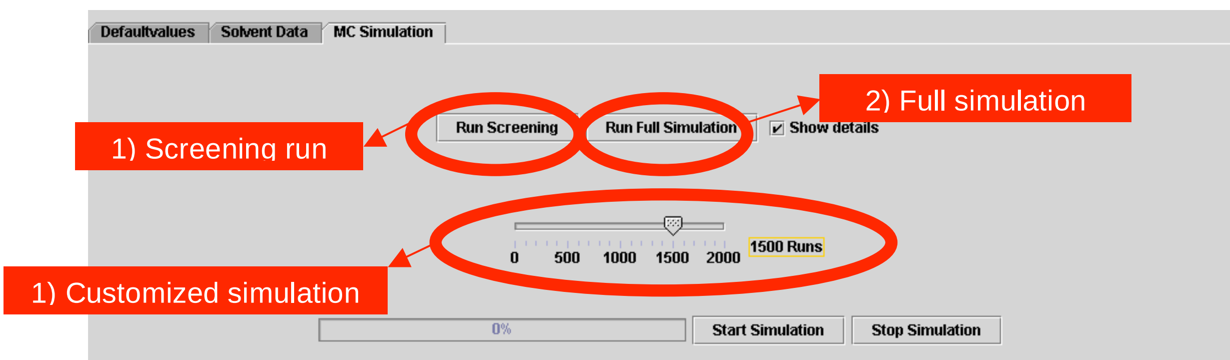


Save, load, and reset function in the "File" menu.

Chapter 4: Run simulation

The calculation of the results fully takes the parameter uncertainty of input and model parameters into account using stochastic modeling (Monte Carlo Analysis) to quantify the uncertainty. Therefore, the results are presented under uncertainty and not as exact values. Note that only uncertainty arising from the life-cycle inventory analysis is quantified whereas uncertainty of impact assessment factors cannot be considered.

Stochastic modeling may be time-consuming depending on the complexity of the waste-solvent treatment. Therefore, various options are available to perform the calculation. The screening run (1) gives a preview on what results can be expected with the full simulation. Since only 200 itineration steps are calculated, results are available quickly. However, for reliable conclusions on environmentally favorable treatment technologies, more itineration steps are needed in order to reduce the variability of the results. For this purpose, the full simulation (2) has to be performed where 2'000 itineration steps are calculated. Finally, the user also has the option to customize the number of runs of the simulation (3).



Chapter 5: Results

Quantifying the environmental impact

Within the framework of life-cycle assessment various methods for the quantification of the environmental impact have been developed (life-cycle impact assessment). In the ecosolvent tool the following methods are implemented:

Eco-indicator 99:
This complex method for life-cycle impact assessment aims to quantify all emissions and resource uses as damages [5]. In the ecosolvent tool, we used the average hierarchic perspective (H/A). The eco-indicator 99 score is expressed as **eco-indicator 99 points**.

Method of ecological scarcity (UBP'97):
The method of ecological scarcity – also called UBP'97 method - allows for a comparative weighting and aggregation of various environmental interventions by use of so-called eco-factors". All these factors are calculated from the present pollution level (current flows) and on the pollution considered as critical (critical flows). The latter ones are thereby deduced from the scientifically supported goals of the Swiss environmental policy [6]. The score is expressed as **UBP.**

Global warming potential:
Calculates the global warming potential according to IPCC guidelines [7]. A hundred year perspective has been chosen. The global warming potential is expressed as **CO2-equivalents**.

Cumulative energy demand:
Calculates the primary energy demand [8]. The cumulative energy demand is expressed as **MJ-equivalents**.

Total CO2:
Complete CO2 balance.

CO2 without waste emissions:
CO2 balance without CO2 emissions from waste such as CO2 emissions from the incineration of waste solvent.

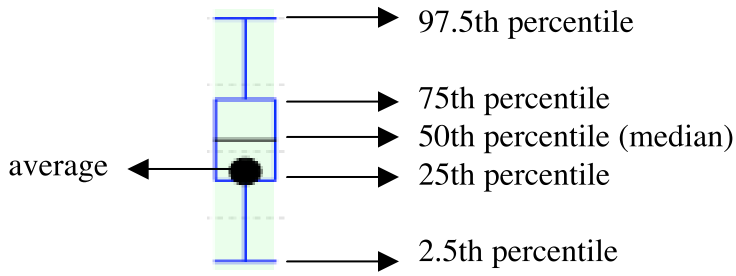
Graphical presentation of the results (result plot)

The "Result Summary (Plot)" gives an overview of the results for one selected environmental indicator. Single contributions to the environmental impact are summed up to intuitively understandable parameters. The same parameters are also used in the "level 2 impact assessment report" (see next paragraph). The parameters are explained in detail in the following table:

parameter	**includes environmental contributions from:**
general parameter	
production	petrochemical production of organic solvents
transport	waste-solvent transport from origin to distillation column or incineration plant
pre-treatment	pre-treatment of the waste solvent either by the user-defined pre-treatment or simple distillation
distillation-specific parameters	
energy	use of steam and electricity for distillation
ancillaries	use of ancillaries (entrainer, cleaning agent etc.) for distillation
residue treatment	treatment of the distillation residue and outlet air
solvent recovery	recovery of solvents (environmental credits for the avoidance of solvent production)
incineration-specific parameters	
ancillaries	use of ancillaries in the incineration plant (e.g. use of sodium hydroxide, electricity, hydrochloric acid etc.)
direct emissions	direct emissions from the incineration or changes in emissions
energy production	recovery of energy out of the waste-solvent incineration (environmental credits for the avoidance of fossil fuel based energy)
parameters specific for the wastewater treatment plant	
MBTP	use of ancillaries and electricity in the mechanical-biological treatment and emissions to air and water
sludge	use of ancillaries and electricity in the sludge treatment and emissions to air
reverse osmosis	use of ancillaries and electricity for the reverse osmosis and emissions to air
extraction	use of ancillaries and electricity for the extraction and emissions to air

Parameters used in the reports "Result Summary (Plot)" and "Level 2 Impact Assessment Report" in the section "Results".

The "Result Summary (Plot)" shows the results graphically as box-whisker plots. The span between the minimum and maximum value represents the 95% interval.

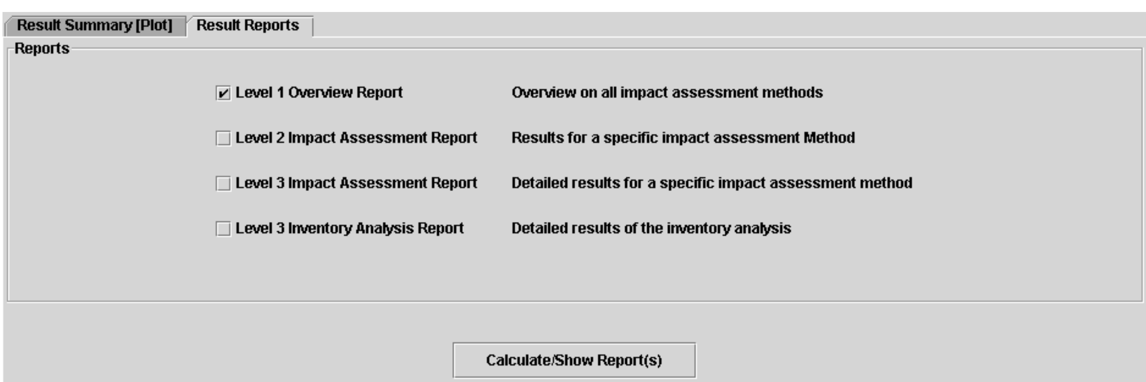


Box-whisker plot used in report " Result Summary (Plot)" in the section "Results".

Results greater than 0 represent environmental burdens (e.g. due to the use of steam in the distillation process) and results less than 0 denote environmental credits due to the avoidance of virgin solvent production (credits for solvent recovery) or fossil fuels (credits for the energy use of the waste solvent).

Result Reports

This section describes the 4 reports provided in the ecosolvent tool to analyze the environmental impact of the specified waste-solvent treatment in different levels complexity. All reports are structured equally. First, the selected waste-solvent composition is shown. Second, the results are presented, and third, a summary of the data input (configuration) is given.



The 4 reports provided by the ecosolvent tool that can be selected in the result section.

The report **"Level 1 Overview Report"** is valuable for a quick decision-support. In this report, the comparisons of the total environmental impacts of the waste-solvent treatment technologies are shown for all environmental indicators (CO_2, Global Warming Potential, Cumulative Energy Demand, Method of Ecological Scarcity, and Eco-Indicator 99). Only if the assessments of all single environmental indicators end up with the same result a treatment technology is considered environmentally superior to another. Otherwise none of the treatment technologies can be considered as environmentally favourable. The advantage of this report is that decisions can be made without going into details of the interpretation of LCA output. But the various characteristics of all environmental indicators have therefore to be involved in the assessment in order to guarantee a reliable result.

The report **"Level 2 Impact Assessment Report"** shows the same results as the Result Summary Plot" presented as table. The minimum and maximum values shown in the table denote the 2,5th and 95th percentiles, respectively. As an addition compared to the box-whisker plot, this report also shows for all parameters the inventory parameter with the highest contribution to its environmental impact (e.g. steam contributes to 90% of the environmental impact of the distillations' energy consumption).

The **"Level 3 Impact Assessment Report"** shows every contribution to the environmental impact of the complete life-cycle inventory for a selected impact assessment method. Thus, this report allows for a comprehensive interpretation of the obtained LCA results.

The **"Level 3 Inventory Analysis Report"** shows the complete life-cycle inventory of the two selected treatment options. The data are not linked to environmental indicators. The data are arranged in the sections "mass flows", "energy flows", "emissions to air", and "emissions to water". Also, the source of the material and energy flows is indicated in the result table as percentage. This report serves as basis for interpretation without considering the life-cycle impact assessment stage.

Export results to MS Excel

All data presented in the reports can be exported to MS Excel or saved as pdf-files. These options are located in the menu in the reports.

Important remark to the results

Please note that the Total and Subtotal values presented in the reports and the plot are extracted of a calculated probability distribution (2,5th, 25th, 50th, 75th, and 97.5th percentile). Thus, they are not the result of the addition of the percentiles (2,5th, 25th, 50th, 75th, and 97.5th percentile) of the single contributions. Such an addition would be made with a minimum/maximum analysis that results in much higher uncertainty ranges. An example is given below.

Level 2 Distillation Results

	Contribution	P 2.5	P 97.5	Mean	Important Parameter	[%]
Solvent Production	Total	452.397	1,835.649	980.746	Toluene	99
Pretreatment	Total	0	0	0		0.0
Distillation Step 1	Energy	24.718	150.509	66.032	Steam (from natural gas)	99
Distillation Step 1	Ancillaries	124.768	427.858	242.557	Total Ancillaries	100
Distillation Step 1	Residue Treatment	-460.872	-129.734	-259.103	Steam (average prod)	87
Distillation Step 1	Solvent Recovery	-1,508.936	-266.033	-726.333	Toluene	100
Distillation Step 1	Transport	0	0	0		0.0
Distillation Step 1	Subotal	-1,339.396	-283.974	-676.848		

The presented Subtotal is not calculated as addition of the single contributions (Energy, Ancillaries, Residue Treatment, Solvent Recovery). It is extracted from the calculated probability distribution of the Subtotal in the Monte Carlo Analysis. Only the Mean values (50th percentile) deviate little and could therefore be added as an approximation.

Log files

With every simulation log files are created in the folder “ecosolvent/log”. These log files store error messages that might occur during a simulation. Although the size of a single log files is small, these files (not the folder!) should be deleted from time to time in order to save memory on your hard disk.

Chapter 6: Preferences

The default values used in the distillation model and a detailed description of the solvents available in this tool are shown in the section "Preferences". The default values are generic uncertainty distributions that are used as approximation of missing data in the distillation process. The various types and the parameterization of these distributions are summarized in the following.

Parameterization of the generic distributions used in the distillation model.

Distribution type	Parameter 1		Parameter 2	
	Symbol	Description	Symbol	Description
Normal	μ	Mean value	σ	Standard deviation
Log-normal	μ	Mean value	σ	Geometric standard deviation
Exponential	λ	Degradation rate	Not used	Not used
Uniform	α	Start interval	β	End interval

Shift: general shift of the x-axis

IsTruncated: False if the distribution is not truncated, True if the distribution is truncated

TruncateStart: Starting value of the truncated distribution

TruncateEnd: End value of the truncated distribution

Chapter 7: Edit background data and impact assessment factors

Edit the generic uncertainty distributions

The parameterization of the generic uncertainty distributions is saved in the file "bgDefault.dat" that is located in the ecosolvent folder. This file may be edited using any text edit application. In this file, all parameters of the distribution are listed as described above and may be adapted according to specific conditions. Only the file name must not be changed. After editing the "bgDefault.dat" the ecosolvent tool has to be restarted.

Edit the solvent names and solvent properties

The solvent names and chemical properties are saved in the file "bgOrganicSolvents.dat" that is locacted in the ecosolvent folder. This file contains all properties of the organic solvents, such as name, CAS-number, elemental composition, heat of vaporization, and heating value. These properties may be edited using any text edit application. Only the file name must not be changed. After editing the "bgOrganicSolvents.dat" the ecosolvent tool has to be restarted.

Edit impact assessment factors

Background data link the calculated inventory data of the treatment technology models (incinerator, distillation process, wastewater treatment plant) to production chains (e.g. production of 1 kg sodium hydroxide). The impact assessment factors are needed to quantify the environmental impact of such a production chain or the emissions of the waste-solvent treatment technologies.

The impact assessment factors of the solvent production and the other production chains (e.g. production of 1 kWh electricity) are saved in the files "bgAssessmentEI99.dat" (Eco-indicator 99 assessment factors), "bgAssessmentCED.dat" (Cumulative energy demand assessment factors), ”bgAssessmentCO2.dat.orig”(CO2 assessment factors), ”bgAssessmentGWP.dat”(Global warming potential assessment factors), and ”bgAssessmentUBP.dat”(UBP’97 assessment factors) and are located in the ecosolvent folder. These files may be edited using any text edit application. Only the file name must not be changed. After editing the "bgAssessment.XXX(X).dat" files the ecosolvent tool has to be restarted.

References

[1] Capello, C, Hellweg, S, Badertscher, B, and Hungerbühler, K: 2005. Life-Cycle Inventory of Waste Solvent Distillation: Statistical Analysis of Empirical Data. Environmental Science & Technology. 39. (15). 5885-5892.

[2] DIN EN ISO 9888: 1999. Water quality - Evaluation of ultimate aerobic biodegradability of organic compounds in aqueous medium - Static test (Zahn-Wellens method). Brussels, Belgium: European Comitee for Standardisation.

[3] ecoinvent Centre: 2004. ecoinvent data v1.1, Final Reports ecoinvent 2000 No. 1-15, CD-ROM. Swiss Centre for Life Cycle Inventories. Dübendorf.

[4] EN ISO 14040: 1997. Environmental management - Life cycle assessment - Principles and framework. Brussels, Belgium: European Comitee for Standardisation.

[5] Goedkoop, M and Spriensma, R: 2000. The Eco-Indicator 99: A Damage Orientated Method for Life-Cycle Impact Assessment. Methodology report 2000a. Pre Consultants.

[6] Hischier, R: 2004. The Method of Ecological Scarcity (Umweltbelastungspunkte, UBP'97). LCIA Implementation. CD ROM. Final Report ecoinvent 2000 No. 3. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories. Dübendorf, CH.

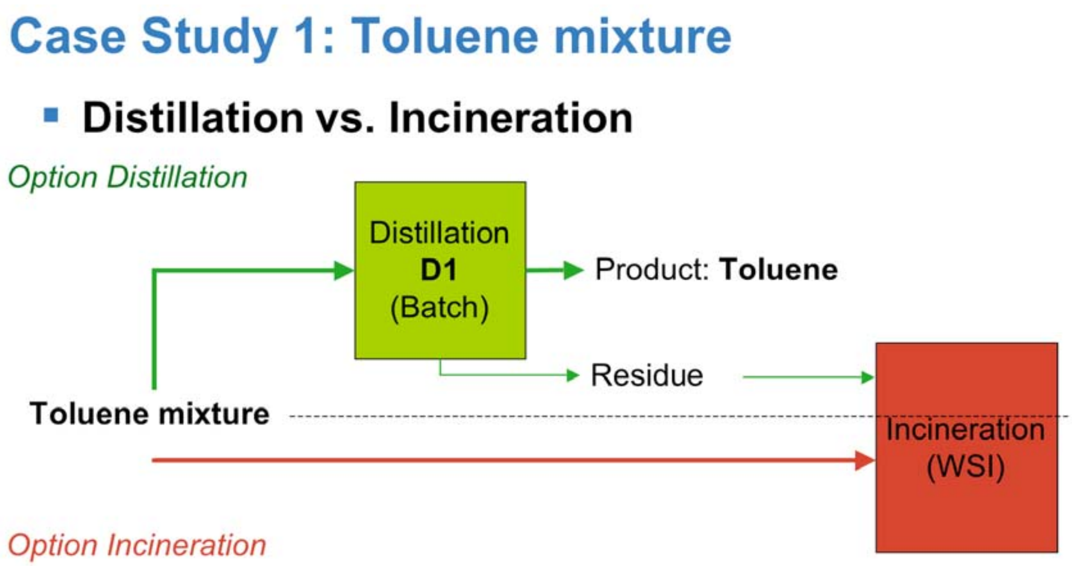
[7] IPCC (2001): 2001. Climate Change 2001: The Scientific Basis. In: Third Assessment Report of the intergovernmental Panel on Climate Change (IPCC). Cambridge University Press. Cambridge.

[8] Jungbluth, N and Frischknecht, R: 2004. Cumulative Energy Demand. LCIA Implementation. CD ROM. Final Report ecoinvent 2000 No. 3. EMPA Dübendorf, Swiss Centre for Life Cycle Inventories. Dübendorf, CH.

[9] Köhler, A, Hellweg, S, Recan, E, and Hungerbühler, K: 2006. Input-Dependent Life-Cycle Inventory Model of Industrial Wastewater-Treatment Processes in the Chemical Sector. Submitted to ES%T.

[10] Seyler, C, Hellweg, S, Monteil, M, and Hungerbühler, K: 2004. Life Cycle Inventory for Use of Waste Solvent as Fuel Substitute in the Cement Industry: A Multi-Input Allocation Model. International Journal of LCA. 10. (2). 120-130.

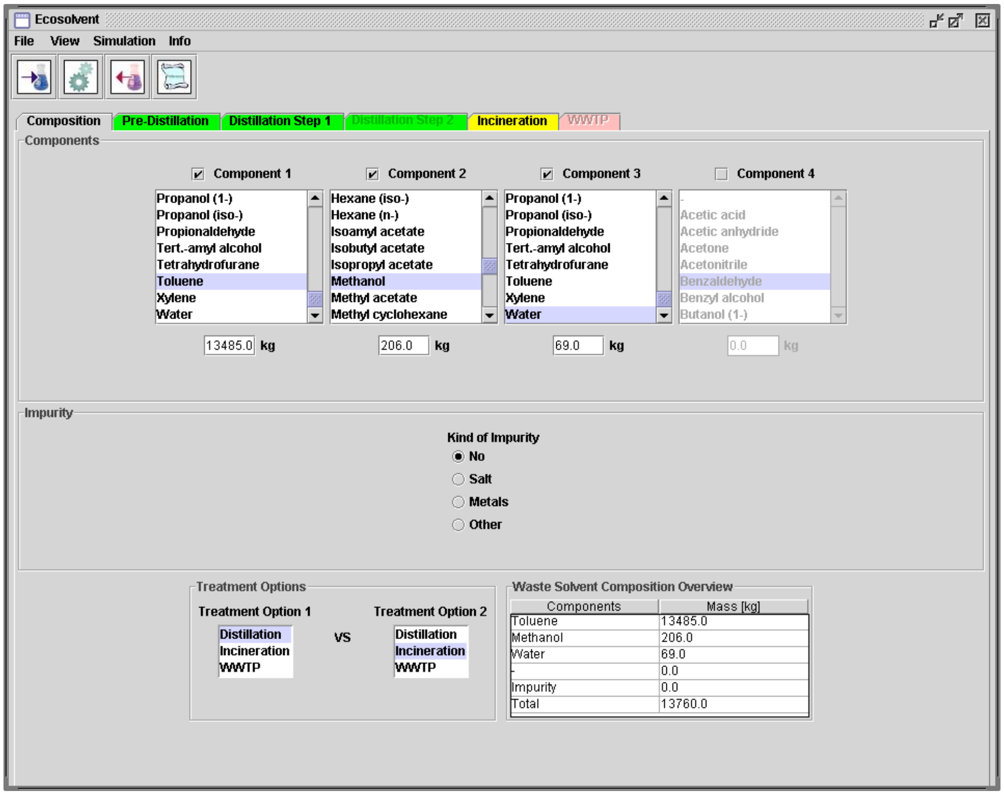
[11] Seyler, C, Hofstetter, TB, and Hungerbühler, K: 2005. Life Cycle Inventory for Thermal Treatment of Waste Solvent from Chemical Industry: A Multi-Input Allocation Model. Journal of Cleaner Production. 13. (13-14). 1211-1224.



Mass and Energy flows in Distillation D1

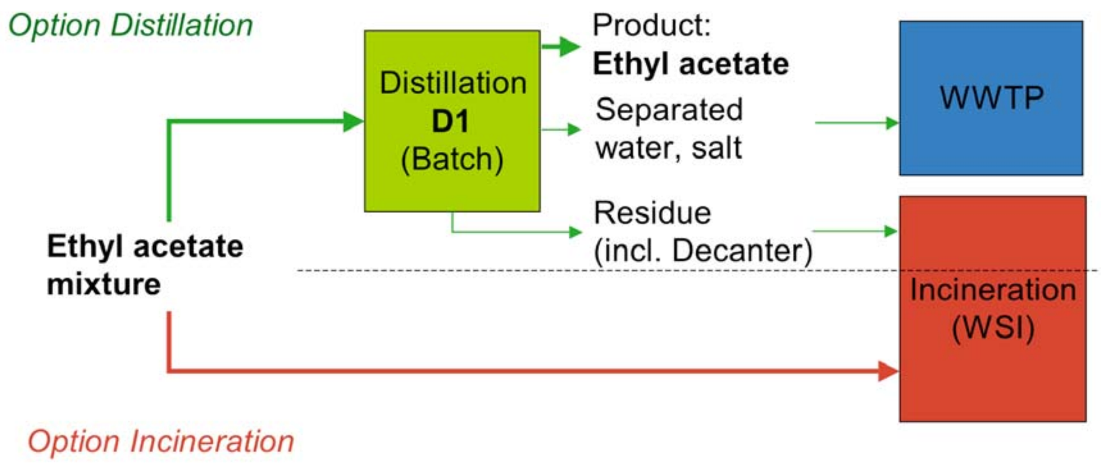
Input D1 (Batch)			Output D1		
WS	Toluene	13485 kg	**Product**	**Toluene (99.5%)**	**11610 kg**
	Methanol	206 kg		*Toluene*	*11552 kg*
	Water	69 kg		*Methanol*	*46 kg*
				Water	*12 kg*
Ancillaries	Methanol (cleaning)	500 kg			
			Residue -> WSI		
Energies	Electricity (amount)	not known		*Toluene*	*1933* kg
	Electricity (prod)	Swiss mix		*Methanol*	*160* kg
	Steam (amount)	unbekannt		*Water*	*57* kg
	Steam (prod)	from waste			
Transport		no			

Specification of the Toluene mixture in ecosolvent



Specification of the Distillation D1 in ecosolvent

Case Study 2: Ethyl acetate mixture

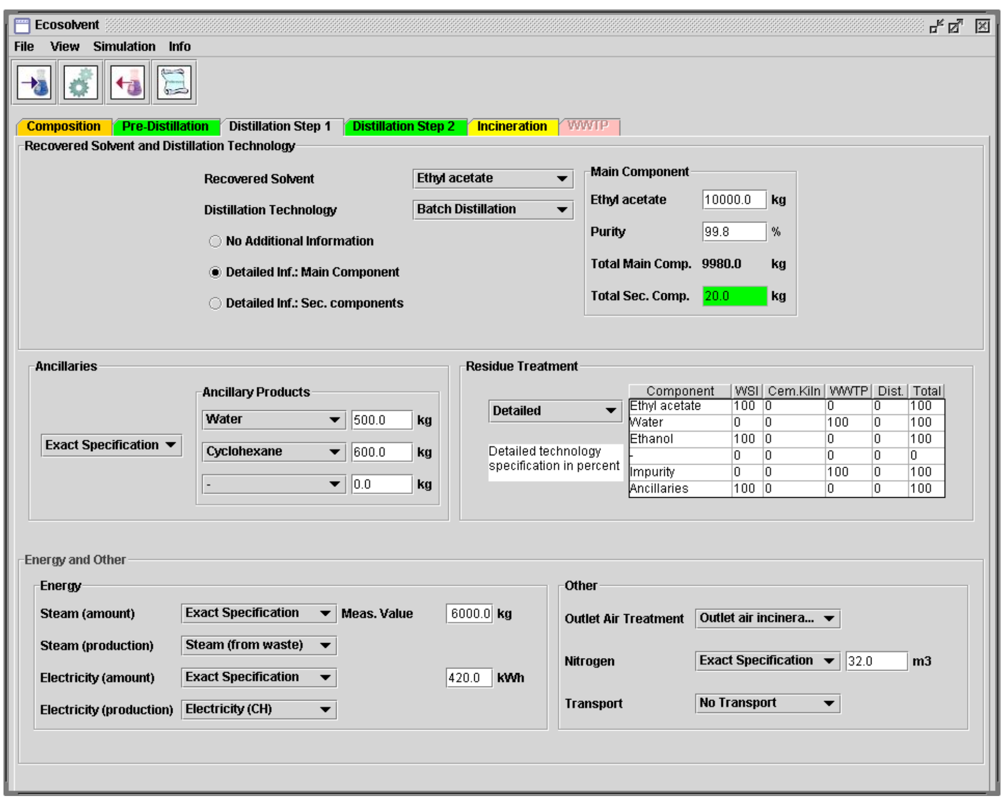


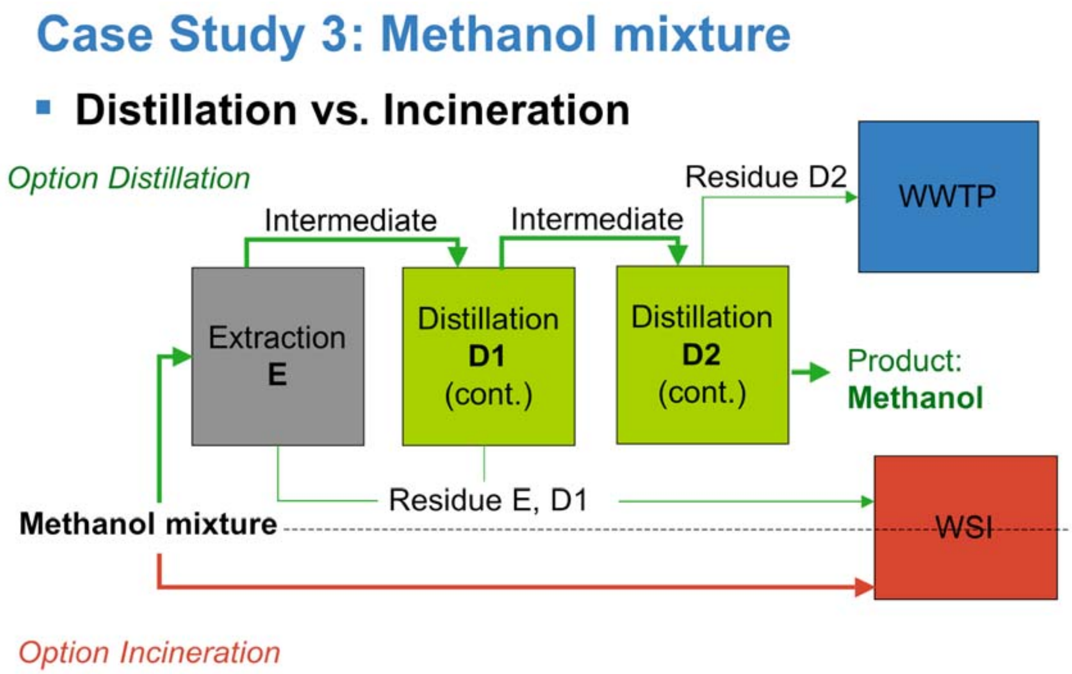
Mass and Energy flows in Distillation D1

Input D1 (Batch)			Output D1		
WS	Ethyl acetate	13081 kg	**Product**	**Ethyl acetate (99.8%)**	**10000 kg**
	Water	550 kg			
	Ethanol	137 kg	*Residue (incl. Decanter) -> WSI*		
	Salt	2 kg		*Ethyl acetate*	*100 %*
Ancillaries	Water (decanter)	500 kg		*Ethanol*	*100 %*
	Cyclohexane (entrainer)	600 kg		*Ancillaries*	*100 %*
Energies	Electricity (amount)	420 kWh			
	Electricity (prod)	Swiss mix	*Residue (Separated Water and Salt) -> WWTP*		
	Steam (amount)	16000 kg		*Water*	*100 %*
	Steam (prod)	from waste		*Salt*	*100 %*
	Nitrogen	32 m3			

Specification of the Ethyl acetate mixture in ecosolvent

Specification of the Distillation D1 in ecosolvent

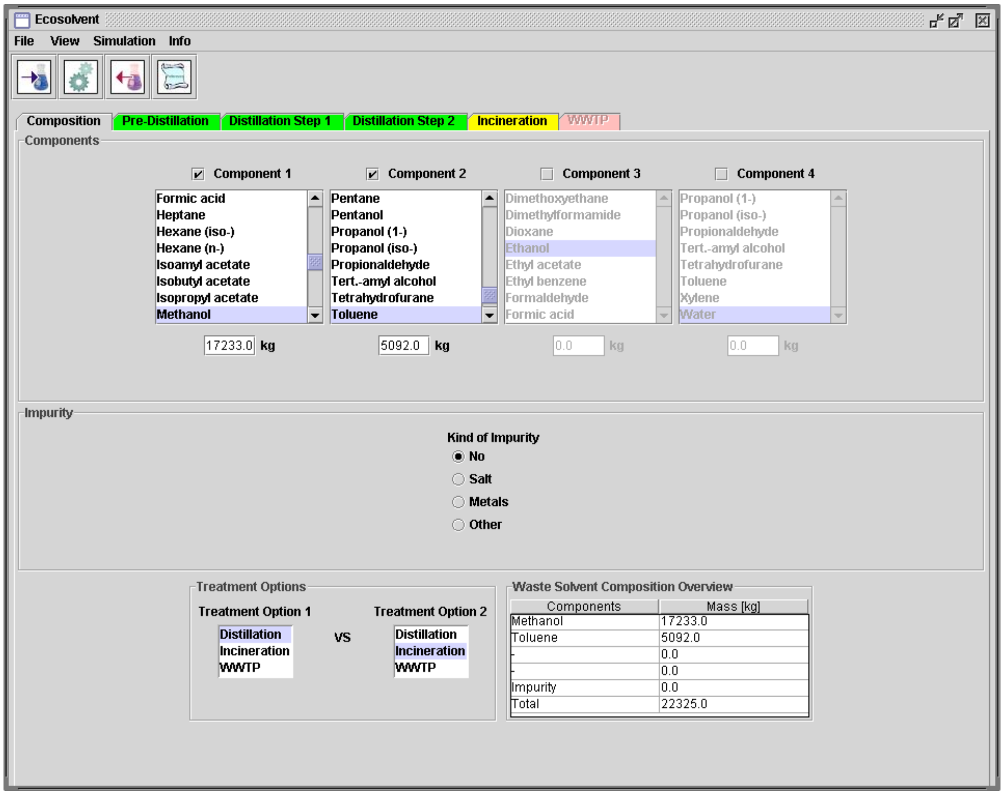




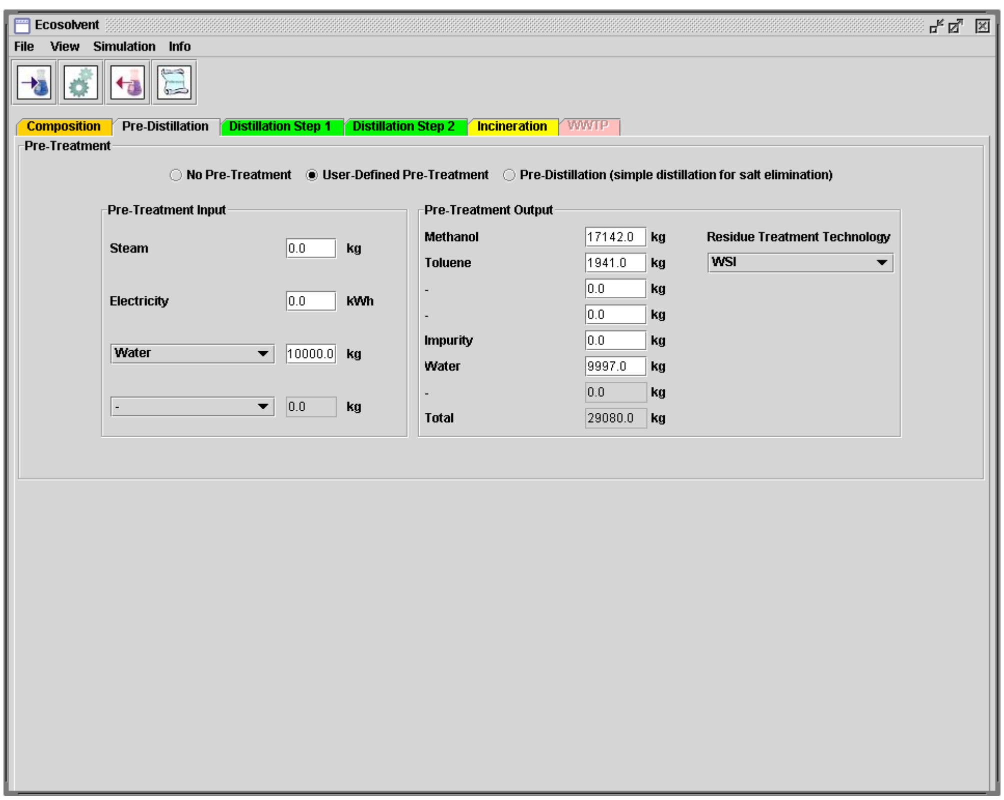
Mass and Energy flows in Extraction E

Input Extraction			Output Extraction		
WS	Methanol	17233 kg	*Intermediate -> Distillation 1*		
	Toluene	5092 kg		*Methanol*	*17142 kg*
				Toluene	*1941 kg*
				Water	*9997 kg*
Ancillaries	Water	10000 kg	*Residue -> WSI*		

Specification of the Methanol mixture in ecosolvent



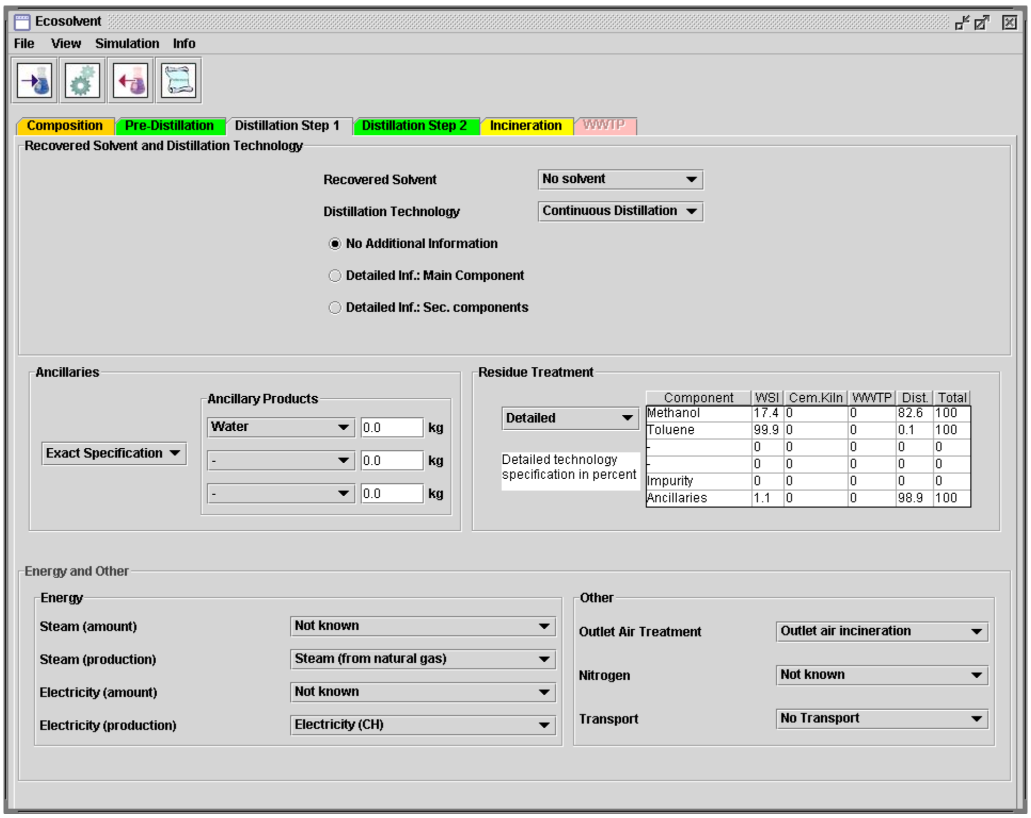
Specification of the Extraction E in ecosolvent



Mass and Energy flows in Distillation D1

Input D1 (Cont. Distillation)			Output D1		
WS	Methanol	17142 kg	Product	no	0 kg
from **Extr.**	Toluene	1941 kg			
	Water	9997 kg	*Intermediate -> Distillation 2*		
				Methanol	*82.6 %*
				Toluene	*0.1 %*
				Water	*98.9 %*
Energies	Electricity (amount)	not know			
	Electricity (prod)	Swiss mix	*Residue -> WSI*		
	Steam (amount)	not known		*Methanol*	*17.4 %*
	Steam (prod)	natural gas		*Toluene*	*99.9 %*
				Water	*1.1 %*

Specification of the Distillation D1 in ecosolvent



Mass and Energy flows in Distillation D2

Input D2 (Cont. Distillation)			Output D2		
WS	Methanol	14166 kg	**Product**	**Methanol (99.7%)**	**14201 kg**
from **D1**	Toluene	2 kg			
	Water	9888 kg	*Residue -> WWTP*		
				Methanol	*9 kg*
Energies	Electricity (amount)	not know		*Water*	*9844 kg*
	Electricity (prod)	Swiss mix		*Toluene*	*2 kg*
	Steam (amount)	not known			
	Steam (prod)	natural gas			

Specification of the Distillation D2 in ecosolvent