



## Ecosolvent: A Tool for the Environmental Assessment of Waste-Solvent Treatment in Chemical Industry

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The software tool “*ecosolvent*” is presented that allows for comparative environmental assessment of treatment technologies for specific, user-defined, waste-solvent mixtures. The *ecosolvent* tool is comprised of models for waste-solvent distillation, thermal treatment in hazardous waste-solvent incinerators and cement kilns as well as for industrial wastewater treatment. The life-cycle assessment method is used to quantify the environmental impact. The *ecosolvent* tool is valuable for practical decision-support in chemical industry due to its easy application and its high level of flexibility for informational needs. On the one hand, it can be used in order to assess the environmental impact of waste-solvent treatment processes in retrospect. On the other hand, generic data ranges enable the application of the *ecosolvent* tool in the early phase of process development.

**Keywords:** Life-cycle assessment (LCA), generic life-cycle inventory (LCI) model, distillation, hazardous waste-solvent incinerator, cement kiln, wastewater treatment, stochastic modeling.

## 1 Introduction

In the chemical industry, organic solvents are used in large amounts for a range of products (paints, coatings, adhesives), as raw material for product syntheses, as reaction media, and for equipment cleaning. About 250'000 tonnes of fresh organic solvents are used annually in Swiss pharmaceutical and specialty chemicals industry. Therefore, solvents belong to the most important industrial chemicals. Since many solvents are highly volatile, considerably persistent, and highly toxic, the handling of solvents in the chemical industry represents a high priority environmental issue. After their use in the chemical production process, solvents often cannot be reused in the original process due to residual contaminations, quality requirements and/or legal restrictions, such as regulations imposed by good manufacturing practices of the US Food and Drug Administration. Such solvents become waste solvents. Waste solvents in the chemical industry are mostly liquid at ambient temperature and vary largely with respect to their chemical composition. Mainly two different waste solvent treatment options are applied: (1) thermal treatment in hazardous waste solvent incinerators and the cement industry and (2) solvent recovery. The most important technology for solvent recovery is distillation (rectification). From an environmental perspective it is not known to date, whether waste-solvent incineration or recovery is the preferable treatment option. Both treatment options enable a reduction of the demand of non-renewable resources. Solvent incineration, on the one hand, substitutes fuel for steam and electricity production or coal and heavy fuel oil in cement kilns. Waste-solvent recovery, on the other hand, avoids petrochemical solvent production. Both types of avoided products correspond with the avoidance of environmental impacts.

## 2 Goal

The goal of our work was to develop an integrated software tool that enables the identification of environmentally preferable waste-solvent treatment options in industry. This tool, entitled "ecosolvent", combines Life-cycle inventory (LCI) models of the most important technologies, such as distillation and thermal treatment. With this tool, a full Life-cycle assessment (LCA) of various waste-solvent treatment options can be calculated for specific, user defined waste-solvent compositions without much effort.

## 3 The *ecosolvent* tool

The *ecosolvent* tool was developed in close collaboration with experts from 7 chemical companies. The tool is publicly available for download and use at no cost:

<http://www.sust-chem.ethz.ch/tools/ecosolvent>

The *ecosolvent* tool is structured hierarchically. The waste-solvent composition and the solvent to be recovered need to be specified by the user as a minimal input (tier I).

Additionally, the user has the option of entering further information on the incineration technology (cement kiln or special waste-solvent incinerator) as well as on the distillation technology (batch or continuous mode) and use of ancillaries in the distillation process (pH-regulation, entrainer) (tier II). If additional information is missing or only partially available (tier I or tier II), generic data ranges are used as approximations to bridge this informational gap. Finally, the user can specify the inventory data precisely, e.g. based on measured values such as steam consumption per kg waste solvent (tier III). Generally, the more complete the user information, the more accurate the calculated inventory.

*Further information are presented in:*

*Capello C, Hellweg S, Badertscher B, Betschart H, Hungerbühler K. 2007: Environmental Assessment of Waste-Solvent Treatment in the Pharmaceutical and Specialty Chemicals Industry. Part 1. The ECOSOLVENT Tool. Journal of Industrial Ecology, in press.*

### **3.1 Life-cycle inventory models of incineration**

With the implemented models of solvent incineration, inventory flows of solvent incineration (e.g. direct emissions to air or ancillaries needed) are calculated as a function of the elemental solvent composition and technology used. To represent the relationship between inventory flows and waste solvent, consumption factors (amount of ancillaries and energy needed for the treatment of 1 kg waste solvent) and process-dependent emission factors (amount of emissions resulting from the treatment of 1 kg waste solvent) as well as transfer coefficients (specific elemental emission flow per kg elemental input) were defined. Two sub-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 organic charged waste waters are disposed. Co-products of this incineration plant are steam and electricity. This model is based on data from an incineration plant located within a large chemical production site in Switzerland (capacity: 35'000 tonnes per year).

*Further information are presented in:*

*Seyler C, Hofstetter T. B., Hungerbühler K. 2005: Life Cycle Inventory Thermal Treatment of Waste Solvent from Chemical Industry: A Multi-Input Allocation Model. Journal of Cleaner Production, 13 (13-14), 1211-1224.*

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. In this model, changes in the emissions as a consequence of substituting fossil fuels with waste solvents are calculated. The model is based on 5 cement kilns with rotary kiln

technology (3 dry and 2 semi-dry processes), which represents the technology mix used in Switzerland.

*Further information are presented in:*

*Seyler C, Hellweg S, Monteil M, 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.*

### **3.2 Life-cycle inventory model of distillation**

The model for solvent recovery focuses on solvent distillation, which is the most important technology for solvent recovery. Input parameters that can be specified by the user comprise the waste-solvent composition, solvent recovery rate, ancillary products, process specifications (e.g. reflux ratio), and the technology used for the treatment of the residues. If such process information is not available, generic data ranges are provided. To determine these generic data ranges, statistical methods were applied. In collaboration with Swiss chemical industry, we collected over 150 data for input and output variables from different waste-solvent distillation processes. The statistical evaluation of these data provides empirical average, minimum, and maximum values. In order to calculate uncertainty ranges probability distribution for each parameter were statistically fitted. With increasing completeness of information from the user (e.g. used technology, yield, energy demand, etc.) these uncertainty ranges decrease.

*Further information are presented in:*

*Capello C, Hellweg S, Badertscher B, Hungerbühler K. 2007: Life Cycle Inventory of Waste Solvent Distillation: Statistical Analysis of Empirical Data. Environmental Science and Technology, 39 (15), 5885-5892.*

### **3.3 Life-cycle inventory model of the wastewater treatment plant**

Waste-solvent treatment in wastewater treatment plants is limited to aqueous mixtures and is subject to strict regulatory restrictions. This treatment option plays a minor role for organic waste solvents except for few well degradable alcohols such as methanol or ethanol and some residues from distillation processes. The model we implemented in the *ecosolvent* tool calculates 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.

*Further information are presented in:*

*Köhler A. 2006: Environmental Assessment of Industrial Wastewater Treatment Processes and Waterborne Organic Contaminant Emissions. Ph.D. thesis ETH No. 16367.*

### **3.4 Uncertainty quantification**

In the *ecosolvent* tool, the uncertainty of calculated inventory data is quantified with stochastic modeling (Monte Carlo Analysis). To this end, probability distributions for all model parameters are used to describe their variability. As output, probability distributions of the environmental impact scores are determined for all inventory parameters.

## **4 Conclusions**

The *ecosolvent* tool is valuable for practical decision-support in chemical industry due to its easy application and its high level of flexibility for informational needs. On the one hand, it can be used in order to assess the environmental impact of waste-solvent treatment processes in retrospect. Such assessments are particularly important in case a set of multi-purpose distillation columns are used: processes can thus be optimized with respect to their environmental performance, without much effort, by changing the column. Retrospective assessments often have the advantage of accurate data (measured data) being available. On the other hand, the generic data ranges enable the application of the *ecosolvent* tool in the early phase of process development, in which a change in the waste-solvent treatment option as a consequence of environmental considerations is easier practicable than in already established processes. Thus, the *ecosolvent* tool also facilitates decision-making regarding change in a production campaign and, with it, change in the waste solvent. In this case, existing waste-solvent treatment equipment can be adapted and optimized to the new waste solvent. Finally, the *ecosolvent* tool can be used to promote strategic investment decisions when new production processes are developed or production volume is increased and, as a consequence, new waste-solvent treatment capacity is needed.