27th LCA Discussion Forum, 17 November 2005

ecosolvent: A tool for waste-solvent management in chemical industry

Christian Capello, Stefanie Hellweg,

Christina Seyler, Konrad Hungerbühler

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

www.sust-chem.ethz.ch

Safety and Environmental Technology Group

Contents

- Introduction to the waste-solvent management in Swiss chemical industry
- Project goals
- Inventory models
- Uncertainty quantification
- The *ecosolvent* tool
- Case Study application
- Final conclusions

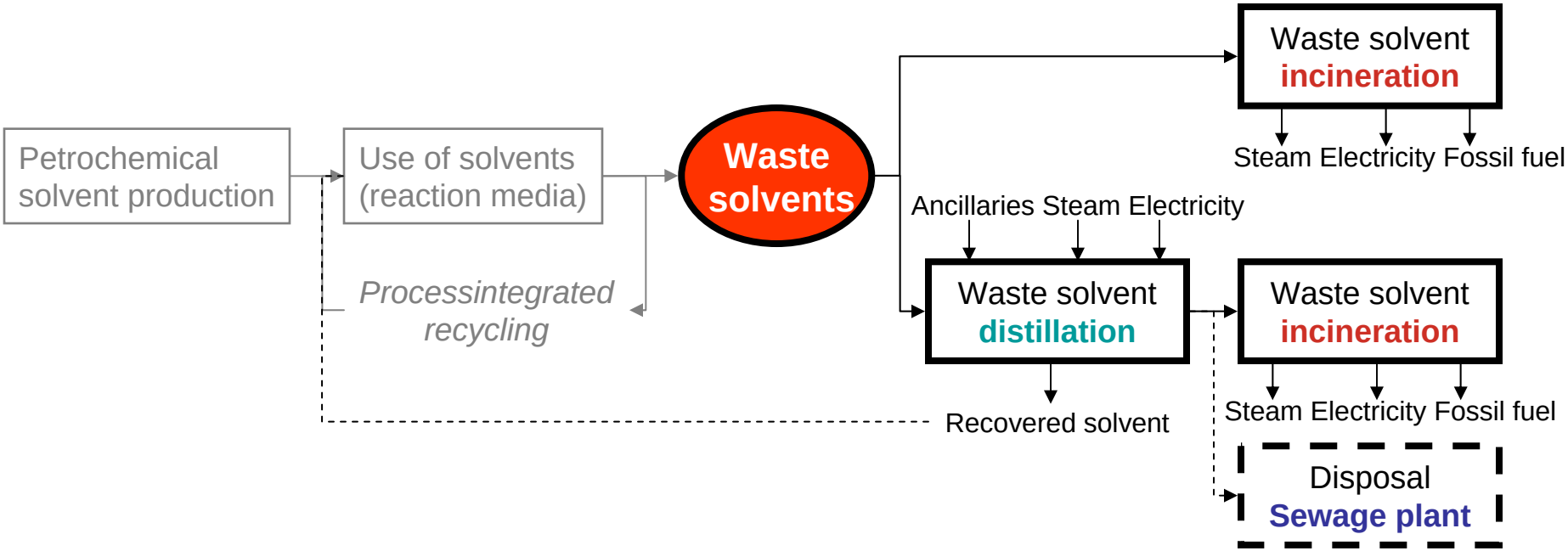
Waste solvent in Swiss chemical industry

- Swiss chemical industry operates mainly in the field of pharmaceutical and specialty chemicals (>90% of the total turnover)
- High consumption of organic solvents (~250'000 tonnes of fresh solvents / year)
- 45 organic solvents were identified to be important (industry survey)
- Waste-solvent management is controlled by economic and logistic factors
- So far, no instruments are available for quantifying the environmental impact of waste-solvent treatment

Project goals

- Development of an easy usable tool for the comparative environmental assessment of waste-solvent treatment technologies for specific, user-defined waste-solvent mixtures
- Environmental assessment using the LCA methodology
- Close collaboration with industry (data and requirements)

Model overview



- Incineration ➡ Avoidance of fossil fuels
- Distillation ➡ Avoidance of petrochemical solvent production
- Both treatment options enable a reduction of the demand of non-renewable resources

LCI-models incineration: Multi-input allocation models

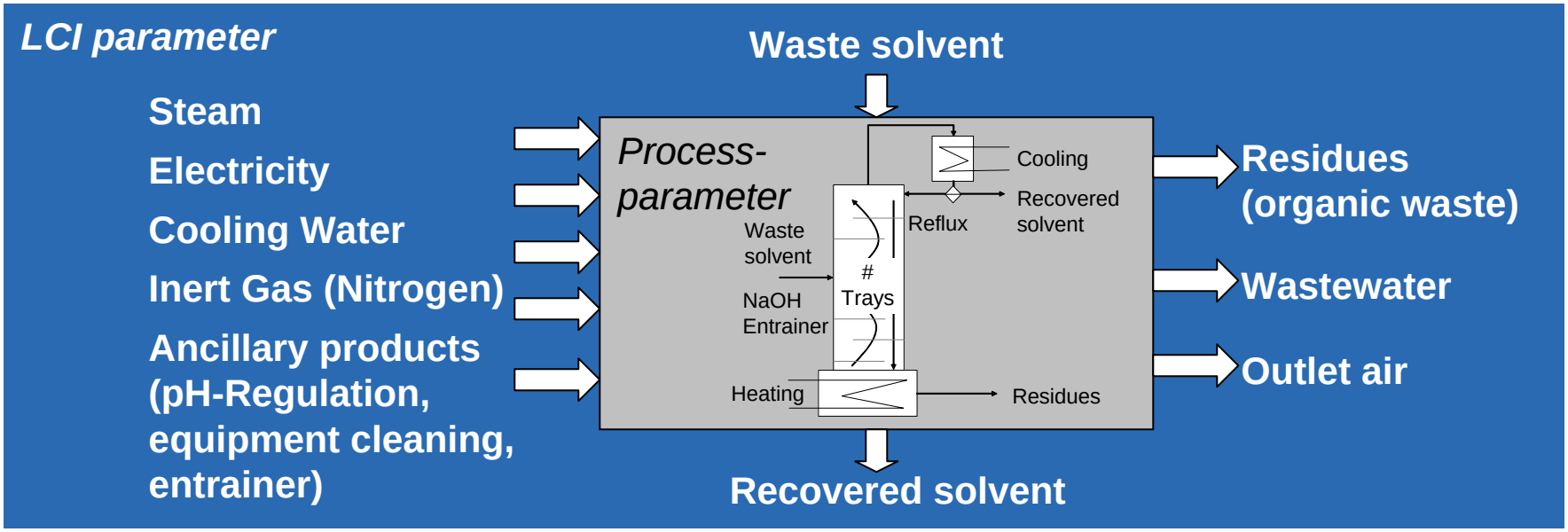
- Allocation:
  - Elemental composition (e.g. NaOH consumption)
  - Net calorific value (e.g.process steam as co-product)
  - Waste-solvent mass (e.g.electricity consumption)
- Models:
  - Waste-solvent incineration plant (capacity 35'000 t/a)
    (Seyler et al. 2005, J. of Cleaner Production 13, 1211-1224)
  - Incineration in cement kilns (Swiss average, 8 plants)
    (Seyler et al. 2004, Int. J. of LCA 10 (2), 120-130)
- Input information needed:
  - Elemental waste-solvent composition and water content

LCI-model wastewater treatment plant: Multi-input allocation model

- Currently:
  - Allocation based on TOC-content
  - All consumption and emission factors are based on industry data
  - Differentiation between well degradable alcohols (e.g. methanol and ethanol) and other solvents.
- Planned improvement:
  - More comprehensive model, including various technologies and allocations

    (A. Köhler, Dissertation ETH)

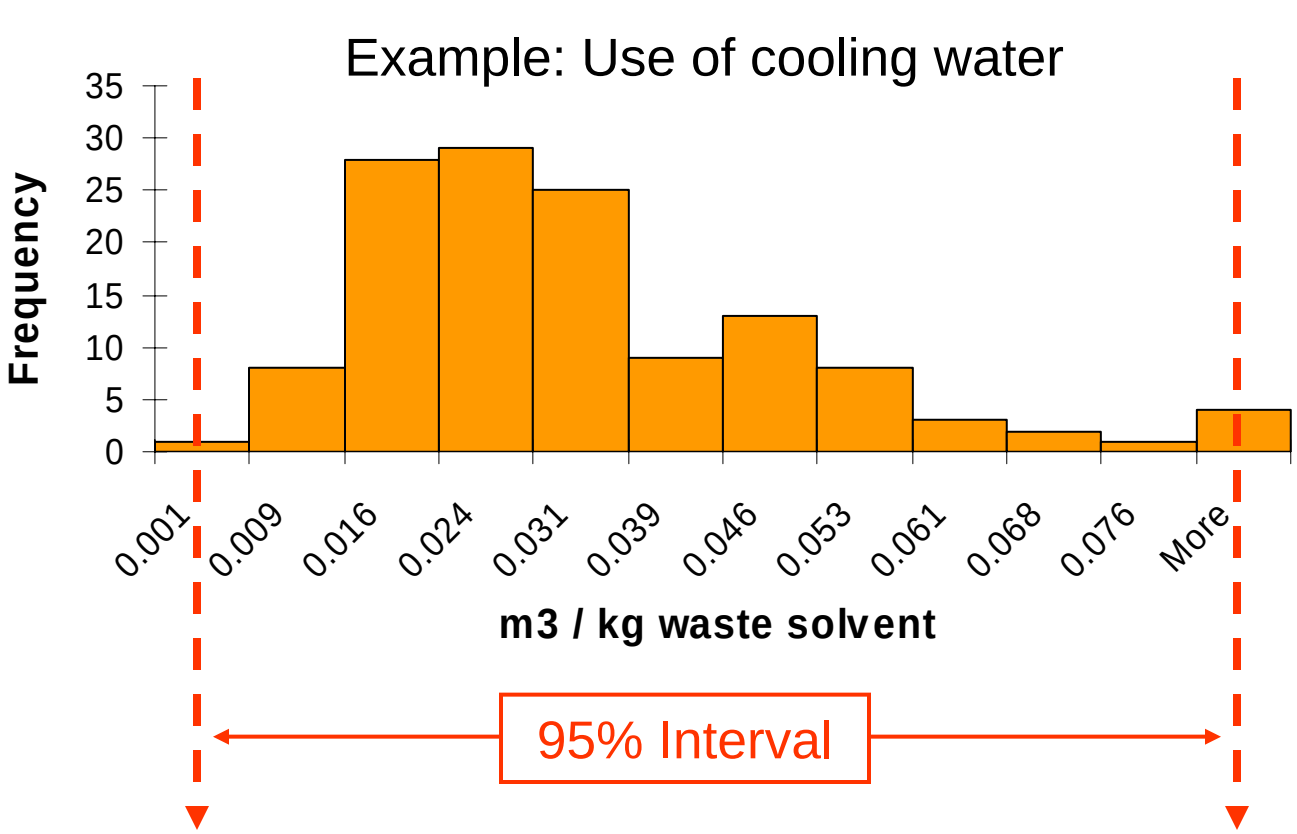
LCI-model distillation: A statistical approach



- Problem: Every distillation process is unique (waste composition, distillate purity, technology)
- Solution: Statistical analysis of 150 industrial waste-solvent distillations
- Results: Generic data ranges for each LCI parameter
  (Capello et al. 2005, ES&T 39 (15),5885-5892)

LCI-model distillation: Case 1

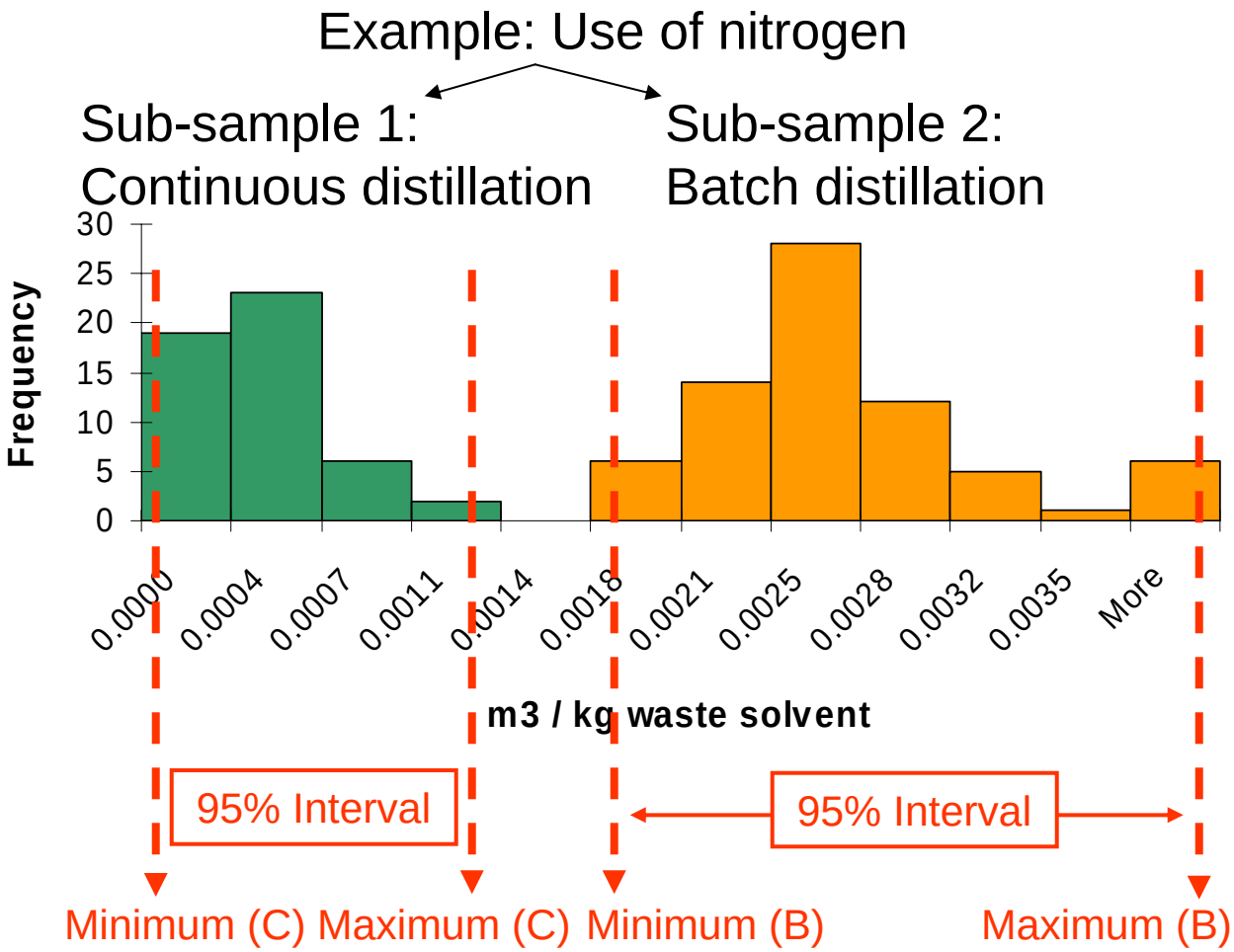
Generic data ranges I: Data ranges based on full sample



Generic data range I:
First approximation in case no information is available (no primary data, no measurements)

LCI-model distillation: Case 2

Generic data ranges II: Data ranges based on sub-samples



Generic data range II:

More accurate approximation in case little information is available (distillation technology, use of ancillaries)

LCI-model distillation: Model overview

Required Information	Additional Information	
•Waste solvent composition •Recovered solvent	•Distillation technology (batch/continuous) ➢ Solvent recovery ➢ Steam consumption ➢ Nitrogen consumption ➢ Amount of outlet air • Ancillaries (purpose) ➢ pH regulation ➢ Entrainer (azeotrop) ➢ Cleaning agents	•User defined values for • Solvent recovery • Steam consumption • Electricity consumption • Nitrogen consumption • Ancillary consumption • Amount of outlet air • Amount of wastewater • Amount of cooling water
Generic data ranges I	**Generic data ranges II**	**Precise user data**
(Case 1)	**(Case 2)**	**(Case 3)**

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

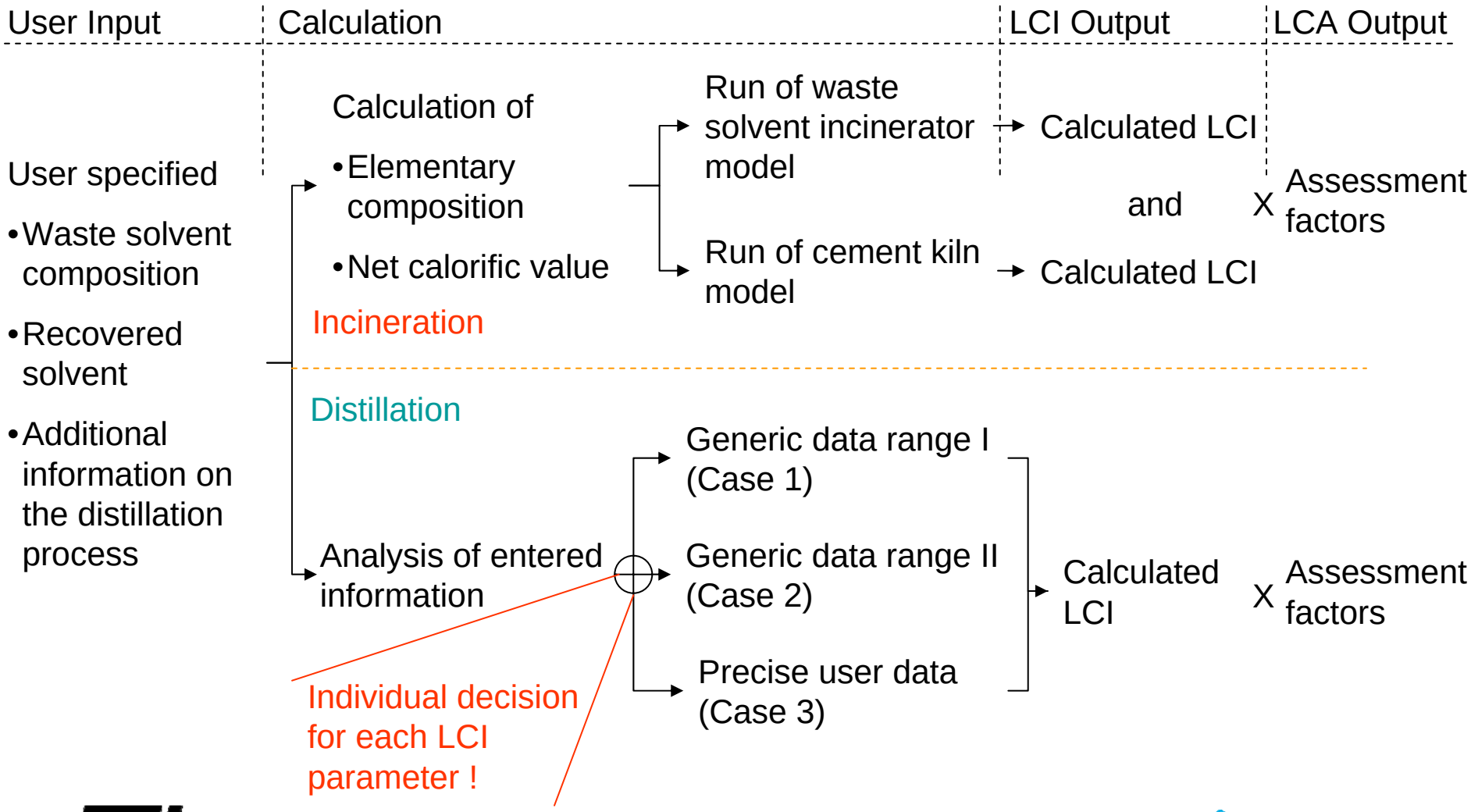
www.sust-chem.ethz.ch

Safety and Environmental Technology Group

Methods of uncertainty quantification

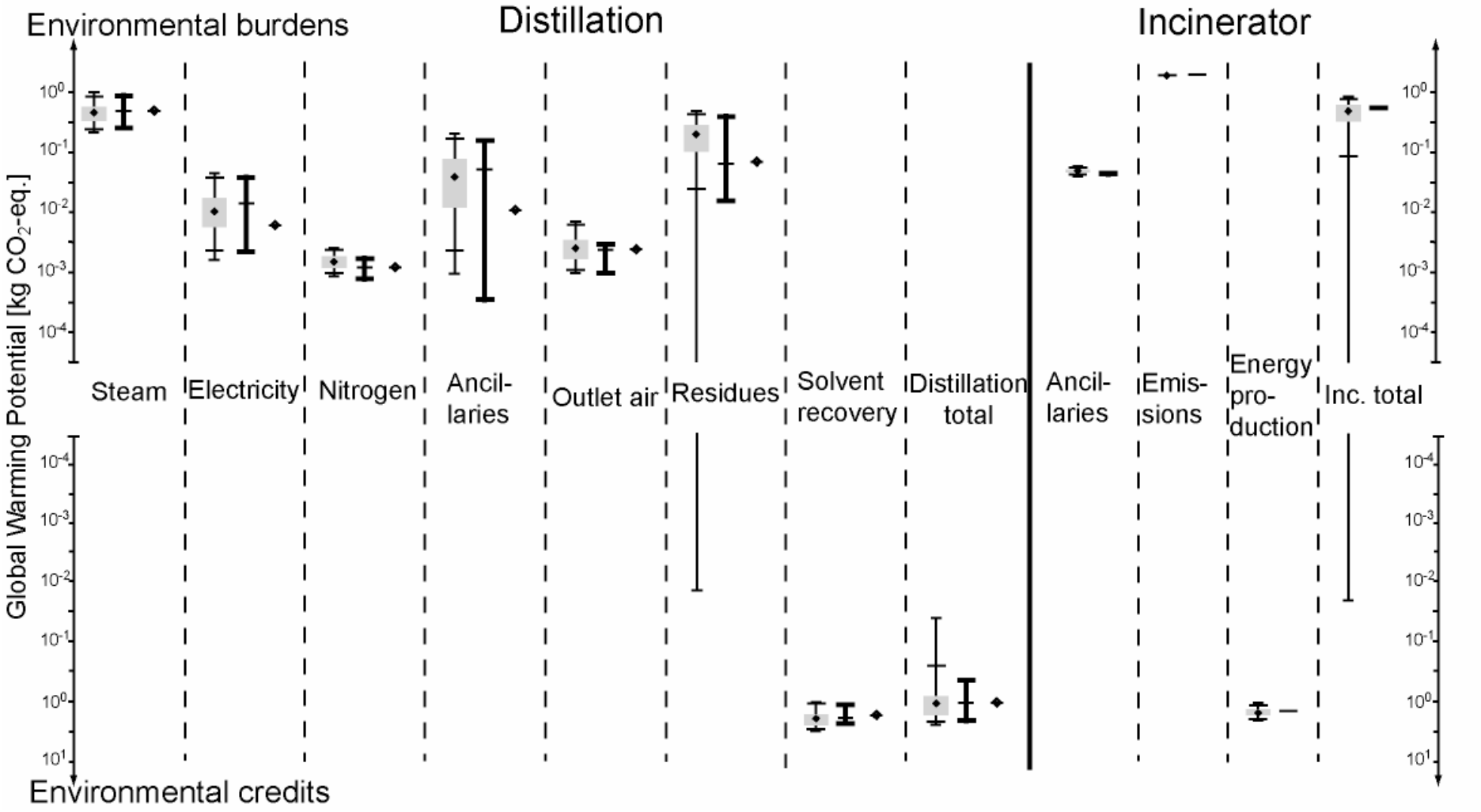
- Method 1: “Bounding analysis”
  - Total minimum / maximum values based on minimum / maximum values of all consumption and emission factors (incineration) and 95% interval (LCI-parameter distillation)
- Method 2: Stochastic modelling (Monte Carlo)
  - Fitted probability functions for all model parameters (incineration and distillation)
  - Uncertainty of the background-inventories (ecoinvent database or generic uncertainty factors)

The ecosolvent tool: Schematic overview



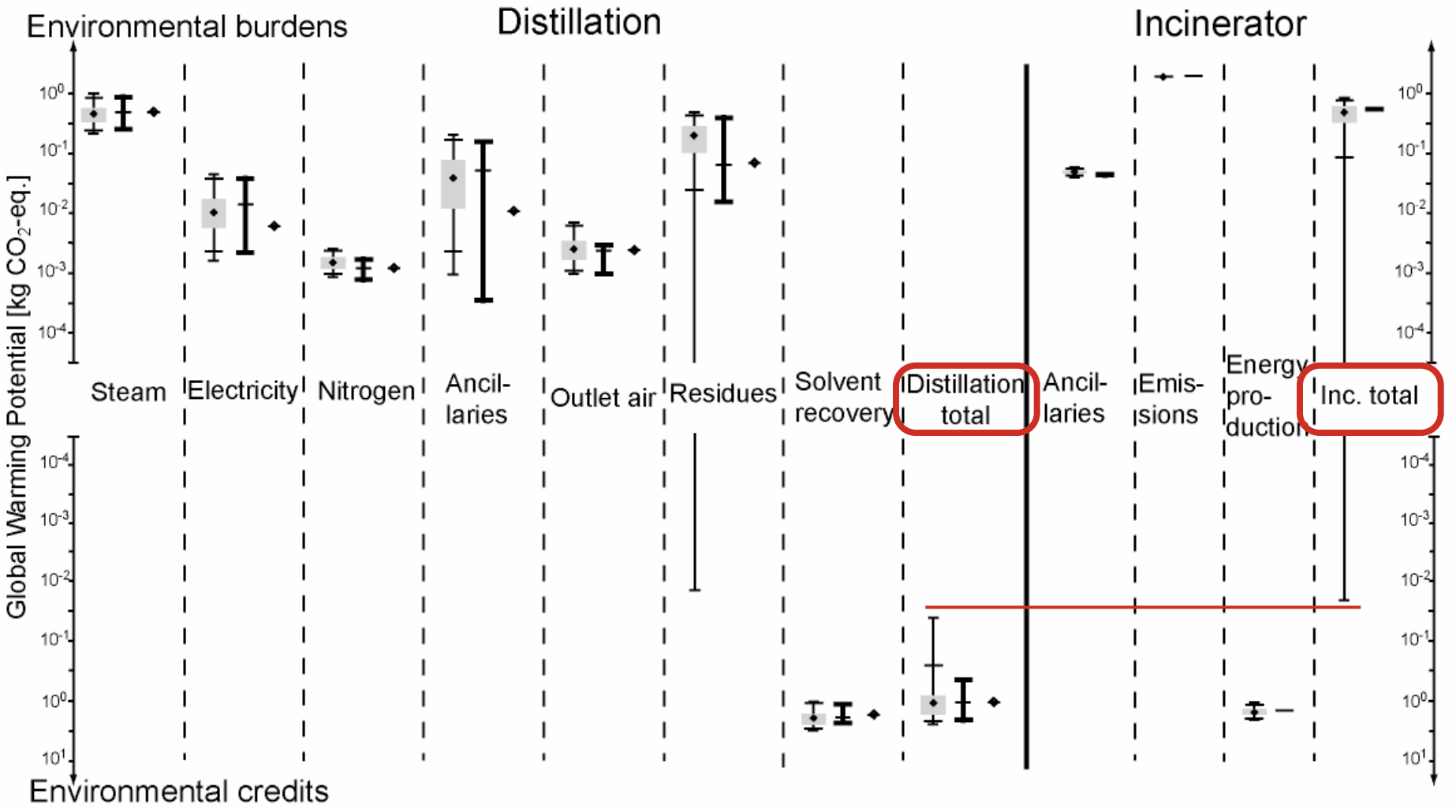
Case study 1: Ethyl acetate mixture

- 1 kg waste solvent: Ethyl acetate (92 wt%), ethanol (1 wt%), water (1 wt%), organic solids (6 wt%)

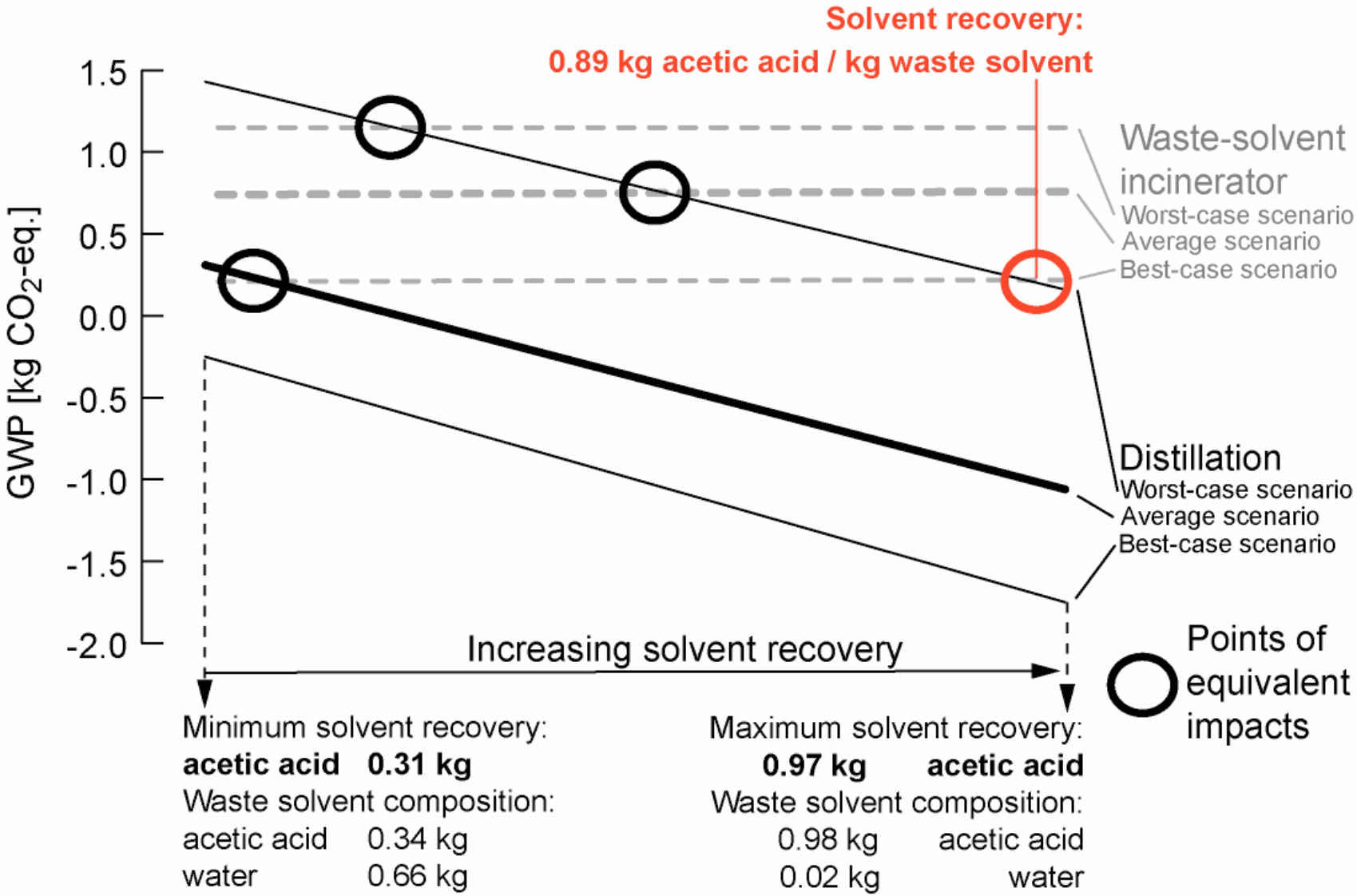


Case study 1: Ethyl acetate mixture

- **Distillation is the environmentally superior treatment option**



Case study 2: Acetic acid / water mixture



Summary & Conclusions

- The *ecosolvent* tool enables to calculate the environmental impact of thermal treatment as well as recovery of specific, user-defined waste solvents
- All models are based on industry data
- Only few input information is needed (waste solvent composition and solvent to be recovered)
- Increasing completeness of information leads to more accurate results
- Due to its flexibility in terms of information needed, the *ecosolvent* tool can be used for the environmental assessment
  - of already operating processes (retrofit) as well as
  - in the stage of process design

Software release

- Scheduled software release is **Juli 2006**
- Information available under http://www.sust-chem.ethz.ch

Acknowledgment

- Financial support:
  - Swiss Federal Office of Energy (Project No. 100065)
- Financial support and data support:
  - Ciba Specialty Chemicals AG
  - Ems-Dottikon AG
  - Lonza Group Ltd.
  - Novartis Pharma AG
  - Hoffmann-La Roche AG
  - Sigfried Ltd.
  - Valorec Services AG

Thank you for your attention!

- Further information:
  - christian.capello@chem.ethz.ch
  - http://www.sust-chem.ethz.ch/research/lifecycle/solvents.html
- References:

  - Capello, C, Hellweg, S, Badertscher B, Hungerbühler, K (2005): Life-cycle Inventory of Waste Solvent Distillation: Statistical Analysis of Empirical Data, ES&T 39 (15), 5885-5892
  - Seyler, C, Hofstetter, T-B, Hungerbühler, K (2005): Life-Cycle Inventory for Thermal Treatment of Waste Solvent from Chemical Industry: A Multi-Input Allocation Model, J. of Cleaner Production 13, 1211-1224
  - Seyler, C, Hellweg, S, Monteil, M, Hungerbühler, K (2004): Life-Cycle Inventory for of Waste Solvent as Fuel Substitute in the Cement Industry: A Multi-Input Allocation Model, Int. J. of LCA, 10 (2), 120-130

The 45 solvents included in the *ecosolvent* tool

Alcohols
- Amyl alcohol
- Benzyl alcohol
- Butanol (-1)
- Butanol (-2)
- Butanol (-Iso)
- Ethanol
- Methanol
- Pentanol
- Propanol (-1)
- Propanol (-2)

Aldehydes
- Benzaldehyde
- Formaldehyde
- Propionaldehyde

Aromatic hydrocarbons
- Ethyl benzene
- Toluene
- Xylene

Aliphatic hydrocarbons
- Heptane
- Hexane
- Isohexane
- Pentane

Carbon Acids
- Acetic acid
- Formic acid

Cycloaliphatic hydrocarb.
- Cyclohexane
- Methylcyclohexane

Chlorinated hydrocarb.
- Dichloromethane
- Monochlorbenzene

Esters
- Butyl acetate
- Ethyl acetate
- Isoamyl acetate
- Isobutyl acetate
- Isopropyl acetate
- Methyl acetate
- Methyl formate

Ethers and glycol ethers
- Butylene glycol
- Diethyl ether
- Dioxane
- Methyl-tert. butyl ether
- Tetrahydrofurane

Ketones
- Acetone
- Cyclohexanone
- Methyl ethyl ketone
- Methyl isobutyl ketone

Miscellaneous Solvents
- Acetic Anhydride
- Acetonitrile
- Dimethylformamide

LCIA methods included in the *ecosolvent* tool

- Aggregated scores:
  - Eco-Indicator 99
  - Method of Ecological Scarcity (UBP'97)
  - Cumulative Energy Demand
- Midpoints:
  - Global Warming Potential
  - Respiratory Inorganics, Climate Change, Fossil Fuels
  - CML Fresh Water Aquatic Toxicity, extended with a characterization factor for TOC from chemical industry
- Elementary flows:
  - CO2