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Uncertainty Analysis and Toxicity Classification in Life-Cycle Assessment Using the Case-study of Gas Purification Systems

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Abstract. This comprehensive thesis structures the decision-making process for making a choice of the most adequate gas purification system (GasPS). Various gas purification technologies (biofilter, activated carbon filter, catalytic oxidation, thermoreactor) have been evaluated based on an industrial case-study for waste gas streams. The ecological performance was quantified using the life-cycle impact assessment methods Eco-Indicator 95 and Swiss Ecopoints (environmental scarcities). Both life-cycle impact assessment methods have been improved by a new classification method for volatile organic compounds (VOCs) which considers the environmental fate and exposure as well as the toxicity of these compounds. For life-cycle assessment, a detailed quantitative uncertainty analysis was carried out using Monte Carlo simulation. Based on the uncertainty analysis, developing statements about the significance of the results and of relative differences between various GasPS alternatives has been possible. The eco-efficiency of the investigated GasPSs was finally characterised based on four indicators: Net Ecological Benefit (NEB_N), Ecological Yield Efficiency (lgEYE), Net Present Value (NPV), and Ecological-Economic Efficiency (EEE).

Keywords: Chemical industry; clean air legislation; decision-making; eco-efficiency indicators; Eco-Indicator 95; gas purification system; Life-cycle assessment; Swiss Ecopoints; toxic substances; uncertainty analysis

Introduction

Over the last few years, the chemical industry has begun to implement the ideas of sustainable development by applying the concept of integrated product and process development (IPPD). Even if this concept is fully implemented, however, end-of-pipe technologies will remain necessary for reducing the remaining environmental impacts. Therefore, given the socio-political, technical, ecological and economic contexts that have motivated IPPD, there is a critical need for the integrated evaluation of these end-of-pipe technologies.

In this thesis, an extensive study was carried out to develop an integrated evaluation methodology for gas purification systems (GasPSs). The purification of an industrial waste gas stream, consisting of a mix of twenty different volatile organic compounds, was used as a case study. The decision-making process for the choice of the *most adequate* GasPS may be divided into two "decision levels" (**Fig. 1**). Based on their compliance with clean air legislation and their technical feasibility (first decision level), four GasPSs were chosen for in-depth evaluation: a biofilter, an activated carbon filter (AC), a catalytic incinerator (CatOx), and a thermoreactor (Thermo). The second decision level evaluates the alternatives with respect to their economic and ecological performance. Economic evaluation was based on the Net Present Value (NPV) of the costs during construction, operation and disposal of the GasPSs. Ecological performance of GasPSs was evaluated using life-cycle assessment methodology (LCA). Life-cycle impact assessment was performed using the methods Eco-Indicator 95 and Swiss Ecopoints.

With respect to LCA and to ecological evaluation in general, three major innovations were made in this study: the addition of a quantitative uncertainty analysis, a new classification for toxic substances, and the definition of eco-efficiency indicators.

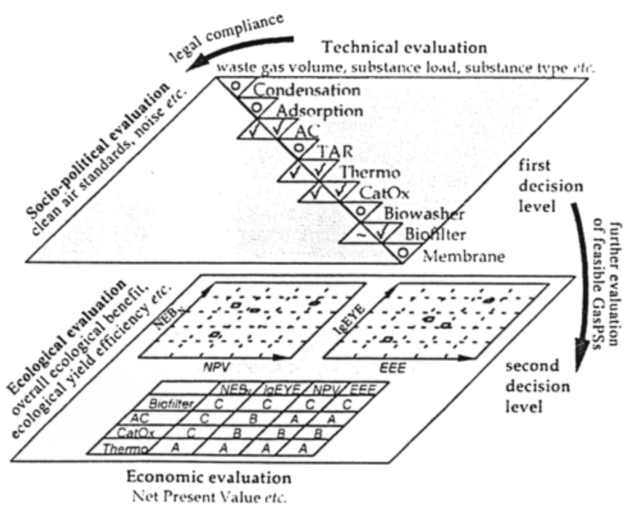

Fig. 1: Overall decision-making process for an adequate GasPS in the chemical industry, structured on two decision levels (first level: technical and socio-political evaluation; second level: ecological and economic evaluation).

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1 Quantitative Uncertainty Analysis

Decision making in real life must occur under uncertainty. After an LCA was performed on the four GasPS alternatives, detailed uncertainty and imprecision analyses of the results were performed using Monte Carlo simulations with Latin Hypercube sampling. In a first step, nine different quantifiable uncertainties in Eco-Indicator 95 were identified (others were found for Swiss Ecopoints):

(1) Measurement of site-specific process data (d_1),

(2) age of the foreground data (temporal variation, d_2),

(3) choice of background data modules (d_3),

(4) emission measurements (d_4),

(5) averaging background data over space and time (d_5),

(6) non-consideration (ignorance) of emissions (d_6),

(7) determination of classification factors (w_1),

(8) determination of the normalisation factors (w_2), and

(9) determination of the reduction factors (d_3).

Uncertainties were quantified based on the analysis of the actual foreground and background data, literature, and expert judgement. The distribution of the uncertainty was modelled either with the normal or log-normal distribution. Fig. 2 summarises the results from the uncertainty quantification as well as the uncertainty propagation throughout the LCA aggregation.

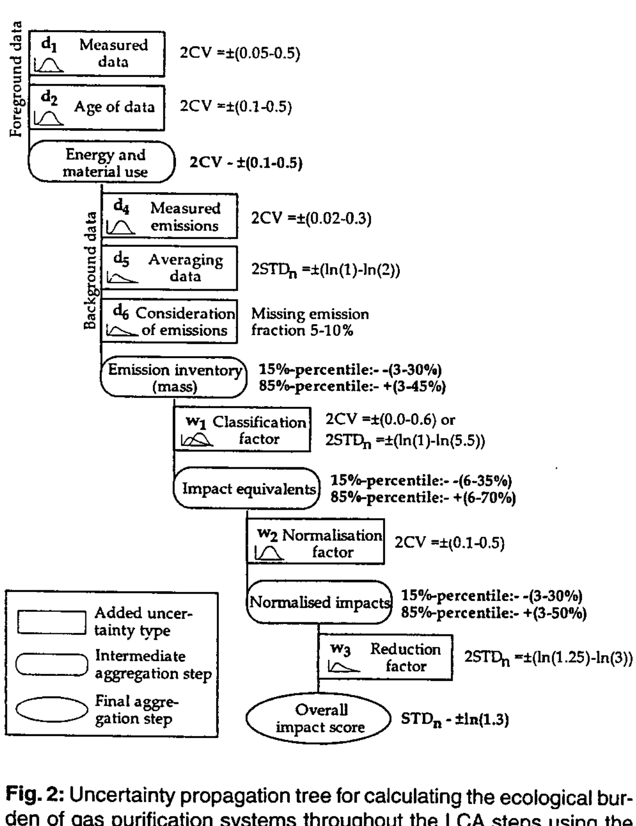

Fig. 2: Uncertainty propagation tree for calculating the ecological burden of gas purification systems throughout the LCA steps using the modified Eco-Indicator 95 (STD: Standard deviation of the corresponding normal distribution; CV: coefficient of variation).

Based on the uncertainty analysis, the following findings were possible for the LCA results:

(1) Distribution of the overall effect score,

(2) evaluation of the significance of the different effects scores on the level of impact categories and overall score,

(3) significance of the relative ranking of various GasPSs alternatives,

(4) identification of major contributions to the overall uncertainty range, and

(5) analysis of the influence of data correlation on the uncertainty range.

2 Classification of Toxic Substances

Neither Eco-Indicator 95 nor Swiss Ecopoints account for the toxicity of volatile organic compounds found in industrial waste gas streams, such as the one in this case study. Thus, a new toxicity classification method had to be developed in the thesis and integrated into both methods. The classification method was developed based on fate-and-exposure modelling similar to the EU-risk assessment of chemicals. The volatile organic compounds were classified on the basis of a "critical discharge flow" into a unit world. The critical discharge flow is the discharge flow leading to an impairment of either humans or ecosystems and is related to an adequate reference substance. Finally, the strengths and weaknesses of the proposed classification method and the fate-and-exposure modelling were reviewed with respect to the following issues: (1) quality of toxicological data, (2) complexity of the applied unit world model, (3) impacts of degradation products, (4) sensitivity of toxicity classification to uncertainties of input variables, (5) time to steady-state for fugacity models, and (6) the choice of appropriate reference substances.

3 Definition of Eco-Efficiency Indicators

For an integrated evaluation of end-of-pipe GasPS technologies, four appropriate performance indicators have been defined in the thesis. The eco-efficiency indicators complement one another and describe the system's performance adequately. The performance indicators assist the decision-making process in choosing *adequate* GasPSs. Net Ecological Benefit (NEB_N) measures if, and how much of, an overall ecological benefit is reached. It is a measure of *effectiveness*. Ecological Yield Efficiency (lgEYE) measures how the invested ecological costs compare to the particular ecological benefits achieved. It is a measure of *efficiency*. Economic costs are measured using NPV. Finally, Ecological-Economic Efficiency (EEE) provides the ratio of NEB_N to NPV.

Fig. 3 shows the indicators NEB_N and lgEYE for the four investigated GasPSes. The indicators allow a ranking and prioritising of the various GasPSes. Due to the comprehensive uncertainty analysis, the significance of the ranking can be determined. For instance, the probability that NEB_N of the activated carbon filter (AC) is higher than for the catalytic incinerator (CatOx) is 68.9%.

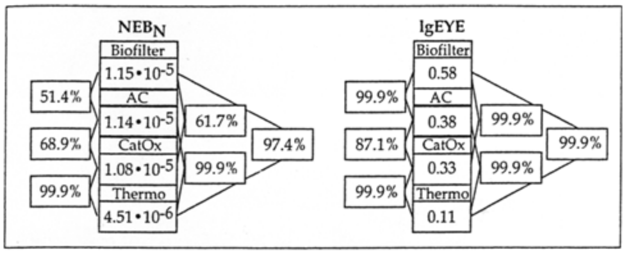

Fig. 3: Ranking and significance diagrams of the investigated GasPSes (NEB_N [Pts./m³ gas] and IgEYE [-] as median; modified Eco-Indicator 95). The middle column shows the ranking with the corresponding indicator value. The significance is indicated for each comparison as the probability of the actual ranking (P(X>0) in %).

4 Summary

The defined performance indicators and the adapted evaluation methods allow an integrated evaluation of gas purification systems with respect to their effectiveness and efficiency. Based on these indicators, various optimisation approaches and their potentials could be identified for the investigated GasPSes. In addition, the ability of the GasPSes to adapt to changes in the pollutant load or waste gas volume was discussed. Finally, the clean air legislation was analysed with respect to their effectiveness and efficiency. A simplified LCA for the evaluation of GasPSes was proposed in the thesis.

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New LCA Theses: Announcement

Spatial Differentiation in Life Cycle Impact Assessment
A Framework, and Site-Dependent Factors to Assess Acidification and Human Exposure*

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*Josepha Maria Barbara (José) Potting got her doctorate at the University of Utrecht, March 8th, 2000, 15.30 o'clock.