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A METHODOLOGY FOR INTEGRATING SUSTAINABILITY CONSIDERATIONS INTO PROCESS DESIGN

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Designing more sustainable processes is one of the key challenges for sustainable development of the chemical industry. This is by no means a trivial task as it requires translating the theoretical principles of sustainable development into design practice. At present, there is no general methodology to guide sustainable process design and almost no practical experience. In an attempt to contribute to this emerging area, this paper proposes a new methodology for integrating sustainability considerations into process design. Underpinned by life cycle thinking, the methodology guides the process designer through different design stages to enable integration of technical, economic, environmental and social criteria. The approach is illustrated on a design case study of the vinyl chloride monomer process. The case study shows how to identify relevant sustainability criteria, how to assess the level of sustainability and how to use the obtained information to make the design more sustainable.

Keywords: process design; sustainability; systems approach; life cycle assessment; VCM.

INTRODUCTION

Traditionally, process design has been guided by technical and micro-economic decision criteria to ensure that plants are 'fit for purpose' and that the financial returns are maximized. However, it is now becoming increasingly obvious that modern plants can no longer be designed using these two types of considerations alone and that the other two dimensions of sustainability—environmental and social—must also become an integral part of process design (Azapagic *et al.*, 2004a).

Some of the environmental and social criteria (e.g., emissions from the plant and health and safety, respectively) are already integrated into traditional design procedures. For example, some design and flowsheeting packages, such as ChemCAD (Chemstations, 2003) enable calculation of environmental impacts from a process, including global warming, ozone depletion, acidification and so on. However, both environmental and social impacts are still often considered as an 'after-thought', once the technical and economic components of the design have been finalized. Such an approach can lead to a sub-optimal performance of the plant, because design choices are more limited in the latter stages of design and may not allow consideration of more sustainable process alternatives. Moreover, even if included in the design stage, environmental and social criteria are usually satisfied at the minimum level required by the relevant legislation and are almost invariably related to direct interventions from the plant without considering the upstream or downstream impacts. Thus, the designer can design a plant which reduces the impacts from that particular process, but leads to an increase in impacts further upstream, perhaps through a choice of unsustainable raw materials and energy sources, or downstream, for example, through waste management and disposal.

Therefore, designing sustainable processes requires a systems approach whereby sustainability is systematically integrated into process design rather than considered as an 'add on'. Process and chemical engineers are familiar with the systems approach because this is the approach that underpins design. However, traditionally the system boundary is drawn around the process itself, usually without considering any upstream and downstream activities. For example, while material inputs, energy use, emissions and wastes from the process are considered in considerable detail, their origin upstream and destination downstream are usually not included within the system boundary. As already mentioned, this can lead to a design which optimises the performance inside the system boundary but is sub-optimal outside it.

Design is often focused on the operation stage and is usually not concerned with the other stages in the life cycle of the plant, i.e., construction and decommissioning (see Figure 1). However, these stages can often have significant economic, environmental and social impacts—not accounting for the full life cycle of the plant during design can potentially lead to much higher economic, environmental and social costs at the end of the plant's useful life. Furthermore, the drive for broader corporate

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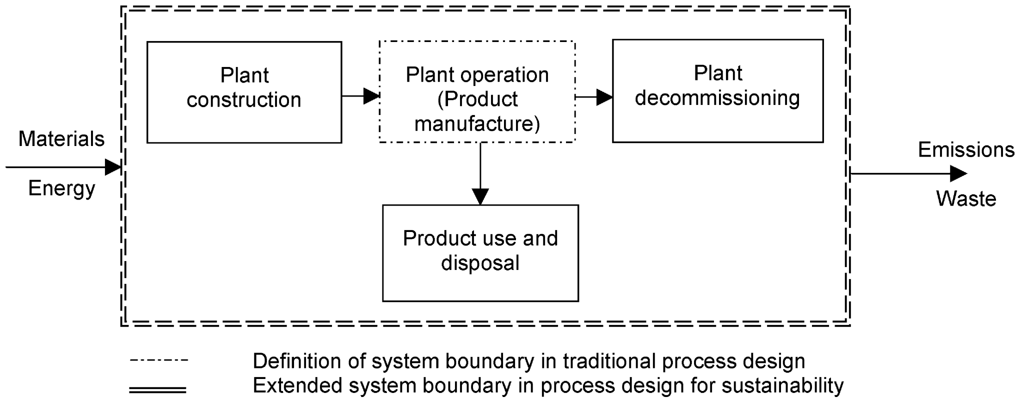


Figure 1. Process design for sustainability requires considering the life cycles of both the process and product(s).

social responsibility (Azapagic, 2002, 2003) also demands consideration of the life cycle of the product to be produced by the plant, including its use and subsequent disposal (Figure 1). For example, optimizing product formulation at the process design stage (known as 'concurrent engineering') can lead to less costly or environmentally polluting disposal of the product after its use. The application of life cycle approach and Life Cycle Assessment (LCA) are now increasingly being required by EU legislation, for example through the Directive on Integrated Pollution Prevention and Control (IPPC) (EC, 1996) and within the Integrated Product Policy (IPP) (EC, 2003).

However, integrating sustainability criteria into process design is by no means a trivial task as there are a number of challenges associated with that, including:

- the extended system boundary and the need to consider both process and product life cycles;
- the need to assess the system on all three components of sustainability (economic, environmental, social) and an increased number of decision criteria compared to conventional design; and
- identification of the relevant sustainability indicators and the need to compare and trade-off often disparate criteria.

Currently, there is no standardized methodology and almost no practical experience in integrating sustainability criteria into process design. Therefore, in an attempt to contribute towards developments in this filed, this paper proposes a general methodology for process design for sustainability (PDfS). The approach is illustrated on a design of a vinyl chloride monomer (VCM) plant.

METHODOLOGY FOR PROCESS DESIGN FOR SUSTAINABILITY

The methodology for integrating sustainability considerations into process design proposed here follows the usual stages in process design, i.e.,

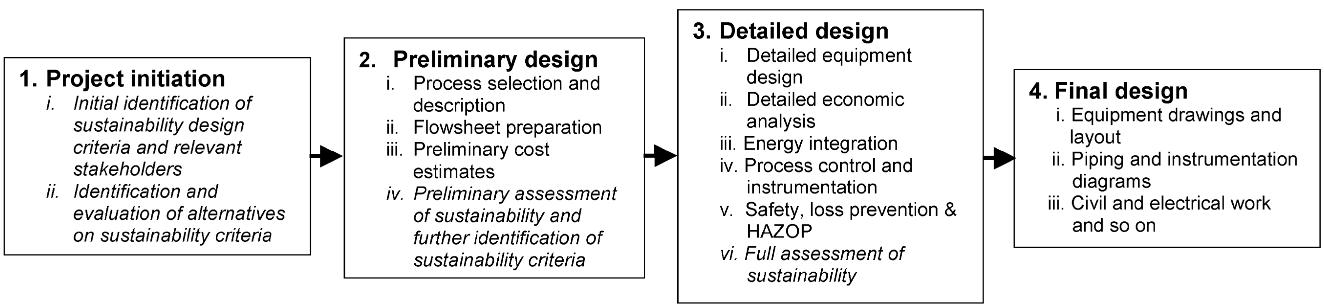
- project initiation;
- preliminary design;
- detailed design; and
- final design.

As shown in Figure 2, each of these four stages consists of a number of steps. Detailed explanation of the design procedure is beyond the scope of this paper; the interested reader can find excellent descriptions in e.g., Ulrich (1984), Douglas (1988), Ray and Johnston (1989), Sinnott (2000) and Seider *et al.* (1999). Instead, this paper concentrates on the design stages where consideration and integration of sustainability criteria are required.

Project Initiation

Initial identification of sustainability design criteria and relevant stakeholders

Traditional process design normally starts by considering alternative processing routes, technologies, raw materials, energy sources and so on, which are evaluated mainly



Text in italics—design stages related to sustainability; normal text—stages in traditional design

Figure 2. Stages in process design for sustainability (adapted from Azapagic *et al.*, 2004a).

using technical and a limited number of economic criteria (e.g., capital and operating costs). However, the starting point in PDfS is identification of sustainability criteria on which the alternatives, and later the whole design, will be assessed. As argued in the preceding section, PDfS requires a systems approach based on life cycle thinking. Thus, sustainability design criteria must include all activities in the system from 'cradle to grave' (see Figure 1). At this initial stage of the project specification, when it is still not clear what design alternatives exist and which sustainability issues may be relevant for each alternative, particularly when designing completely new processes, the designer can only identify and use sustainability design criteria that are generally applicable to most processes. Some examples of these criteria that can be used to evaluate and screen the alternatives are listed in Table 1. For example, typical economic criteria relevant for process design include the usual micro-economic factors such as capital and operating costs and profits but also macro-economic criteria such as value added, taxes paid and ethical investments. Environmental criteria include emissions and wastes from the process and environmental impacts they cause, such as global warming, acidification, human toxicity and so on. The social criteria listed in Table 1 take into account both the interests of employees and those of the neighbouring communities by addressing health and safety issues associated with the construction, operation and decommissioning of the plant as well as with the product use and post-use waste management. Furthermore, they also take into account potential nuisance that the plant can cause to neighbouring communities through odour, noise and visual impact. Associated with these criteria is the public acceptability of the plant and the product and the so-called 'social licence to operate'. Further detail on various process-related sustainability criteria can be found in e.g., Azapagic (2003), Azapagic and Perdan (2000) and IChemE (2003).

In identifying the specific sustainability criteria, the designer must be aware of the relevant groups of stakeholders and their sustainability concerns in relation to the proposed plant. Typically, the stakeholders will include employees of the company which will own and operate the plant, investors, neighbouring communities and citizens, non-governmental organizations (NGOs) and government. Each stakeholder group will potentially be interested in a number of specific sustainability issues; these should be taken into account in the development of further specific sustainability criteria and indicators.

Identification and evaluation of alternatives on sustainability criteria

Evaluation of alternatives at this stage is carried out on a qualitative basis by identifying advantages and disadvantages of different alternatives with respect to the sustainability criteria identified in the previous step. Ideally, the outcome of this stage should be identification of the most promising processing route, raw materials, energy sources and so on; however, in practice, it is more likely that there will be several feasible and potentially sustainable alternatives. In that case, further, quantitative, assessment of the alternatives is necessary—this is carried out in the next, preliminary, design stage.

Preliminary Design

In traditional process design, this stage normally involves selection of the most appropriate processing route, flowsheet preparation and a preliminary economic evaluation, to enable a more detailed development of the process. In PDfS, in addition to the economic evaluation, the system is also assessed on environmental and social sustainability (see Figure 2). To enable this, the qualitative sustainability criteria identified during project initiation need to be translated into the appropriate economic, environmental and social indicators or metrics. The indicators will be largely quantitative, although some will be expressed as qualitative statements. For example, the profitability criterion (see Table 1) is usually translated into the economic indicators such as cash flow and net present value and expressed in monetary units. On the other hand, the criterion 'public acceptability' is normally represented by a set of qualitative indicators which describe the concerns raised by neighbouring communities, NGOs and other stakeholders. Some examples of economic, environmental and social indicators are shown in Table 1. Further examples are provided by IChemE (2003) who have developed a set of sustainability indicators specifically for the chemical and process industry.

Preliminary assessment of sustainability and further identification of sustainability criteria

Assessing economic sustainability: Economic evaluation in traditional design is normally based on the micro-economic indicators, such as net present value, discounted cash flow analysis, returns on capital invested and so on.

Table 1. Examples of sustainability design criteria and indicators.

Economic	Environmental	Social
Micro-economic, e.g.,	Raw materials	Provision of employment
Capital costs	Energy	Health and safety of:
Operating costs	Emissions to:	Employees/contractors
Profitability	Air, water and land	Customers
Investments (e.g., decommissioning, health & safety and so on)	Environmental impacts, e.g.,	Citizens
	Global warming	Nuisance
Macro-economic, e.g.,	Ozone depletion	Odour
Value added	Acidification	Noise
Taxes paid	Human toxicity	Visual impact
Other investments (e.g., ethical)	Eco-toxicity	Public acceptability
Environmental liabilities	Summer smog	Process
	Eutrophication	Product

These indicators are also used in PDfS; however, as shown in Table 1, the additional economic indicators should also be considered, including value added and investments in, for example, pollution prevention and decommissioning. In many cases these costs will be difficult to estimate, particularly decommissioning and environmental liability costs. Nevertheless, it is important that they are considered at this stage as this analysis may help to improve the economic sustainability of the plant.

In traditional process design, if the preliminary economic evaluation is favourable, the project is then authorized either on the basis of that information or after further, more detailed estimates. However, in PDfS, before the project can proceed to detailed design, it is necessary to evaluate the process on the other two dimensions of sustainability: environmental and social.

Assessing environmental sustainability: Environmental sustainability of a process can be assessed by two types of quantitative indicators: environmental burdens and impacts. The former include consumption of materials and energy and emissions to air, water and land and are obtained directly from the flowsheet and material and energy balances. These can be translated into potential environmental impacts by multiplying the burdens by their 'potency' factors. For example, the global warming potency factor for methane, expressed relative to CO_2, is 21 $kg_{CO_2eq.}/kg_{CH4}$. The potency factors for a number of environmental burdens can be found in e.g., IChemE (2003).

As discussed earlier, in PDfS the environmental burdens and impacts are calculated within an extended system boundary, drawn from 'cradle to grave' (as shown in Figure 1). LCA is nowadays used routinely to estimate and evaluate the burdens and impacts from 'cradle to grave'. The environmental burdens and impacts listed in Table 1 are usually included in LCA studies. By quantifying a range of environmental burdens and impacts, LCA enables evaluation of the overall level of environmental sustainability, but also helps to identify the most significant impacts for a particular process design. Furthermore, it helps to determine the 'hot spots' in the system, i.e., the parts of the system which contribute most to the environmental impacts and should be targeted for maximum improvements. An LCA software and database will normally be required for the assessment of environmental sustainability. A more detailed account of using LCA for process design can be found in Azapagic (1999).

Assessing social sustainability: Social sustainability criteria (see Table 1) can be translated into both quantitative and qualitative indicators. For example, provision of employment can be expressed in quantitative terms as 'number of employees'. Other criteria can normally only be expressed qualitatively; for example, visual impact of the plant. Dealing with qualitative information can be challenging in process design, where most information and decisions are based on quantitative data. However, for most of the socially-related criteria that are relevant to process design, various quantitative methods have been developed. For example, the LD50[1] values or occupational exposure limits (OEL) are used to evaluate a health hazard from raw materials used in the process; Dow Fire and Explosion Index (Sinnott, 2000) is used to calculate a potential safety risk from fire and explosion, and so on.

Like environmental analysis, evaluation of social sustainability also enables identification of the most significant social impacts and the 'hot spots'. This information is then fed to the next, detailed, stage of design.

Detailed Design

Full assessment of sustainability

Detailed design involves detailed equipment design; detailed economic analysis; energy integration; process control and instrumentation; safety assessment and HAZOP. In PDfS, however, one additional step must be carried out before commencing the work on the final design: a full assessment of sustainability of the proposed design. This involves an integrated assessment of economic, environmental and social performance and is aimed at ensuring that all relevant sustainability criteria have been identified so that they can be addressed appropriately to improve the level of sustainability of the design.

As the full assessment is based on the preliminary assessment already carried out, it will normally not involve much more additional work. Detailed economic assessment and some aspects of the social assessment will have been carried out as part of the traditional detailed design (e.g., steps ii. and v. in Figure 2, respectively). The environmental assessment will require a more detailed LCA study which, once carried out, requires only marginal additional effort, particularly if an LCA software is used.

DEMONSTRATION OF THE METHODOLOGY: VCM CASE STUDY

The PDfS methodology is now demonstrated on a design case study of VCM. The case study aims to illustrate what kind of sustainability criteria are relevant and should be considered in process design; how to carry out sustainability assessment of the system; how to identify 'hot spots'; and how to improve the overall level of sustainability of the system.

It should be noted that the main purpose of the case study is an illustration of the PDfS approach so that some of the assumptions and design choices presented here may not necessarily be realistic or practical. For the same reason, the case study goes only as far as the preliminary design with some discussion of the detailed design related to the full sustainability assessment. As in the previous section, the emphasis is on the design steps that are concerned with sustainability rather than on the traditional design stages as it is assumed that the reader is familiar with the latter.

Project Initiation

This case study is based on the design capacity of 15 000 kg h^{-1} or 130 000 tonne y^{-1} of VCM. The VCM processing route is well established: as shown in Figure 3, VCM is produced first by reacting ethylene and chlorine by direct and oxy-chlorination to produce ethylene dichloride (EDC). This is followed by EDC cracking to obtain VCM and HCl. The VCM product is then purified by separating out HCl and uncracked EDC which are recycled back into the process. The process is carried out

[1]LD50: Lethal dose at which 50% of the test animals are killed.

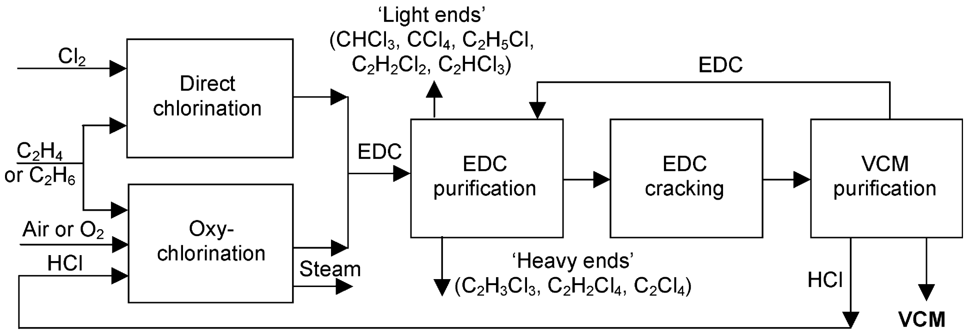


Figure 3. Simplified flow diagram of the VCM process.

according to the following summary reaction:

$$\begin{array}{ccc} C_2H_4 + Cl_2 \longrightarrow & C_2H_4Cl_2 \longrightarrow & C_2H_3Cl + HCl \\ \text{Chlorination} & \text{EDC} & \text{Cracking} \end{array}$$

The majority of VCM worldwide is used to produce PVC; in this case study the assumption is that the VCM will be sold to a nearby PVC plant.

Initial identification of sustainability design criteria and relevant stakeholders

The first step in PDfS is identification of initial sustainability criteria that will enable a preliminary assessment of the process and the related alternatives. As explained in the previous section, the general sustainability criteria listed in Table 1 can be used for these purposes; these criteria will be refined further and translated into appropriate sustainability indicators in the preliminary design stage. In the case considered here, the main stakeholders are investors and insurers, company employees, contractors, suppliers, the PVC customer and neighbouring communities. As shown in Table 2, they will have differing and potentially conflicting interests in a number of sustainability issues (Azapagic, 2004). For example, investors and insurers will have a strong interest in the economic aspects of sustainability, particularly those related to the return on investments and potential future environmental liabilities. Employees and contractors are likely to have a strong interest in the economic performance of the plant and safe and healthy working conditions; increasingly, employees are also interested in a responsible environmental approach to business. The customer will be interested in purchasing VCM at minimum cost and environmental, health and safety risks. Local communities, on the other hand, while interested in the employment opportunities that the new plant may offer, will also be concerned about the environmental and social impacts of the future plant. As most of these concerns could be alleviated if considered during design, it is important that they are addressed appropriately at an early stage, starting with the choice of design alternatives.

Table 2. The main VCM stakeholders and their potential interest in sustainability issues (adapted from Azapagic, 2003).

	Sustainability interests and concerns		
Stakeholders	Economic	Environmental	Social
Investors and insurers	☑	✓	✓
Employees and contractors	☑	✓	☑
Suppliers	☑	×	×
Customer	☑	✓	✓
Local communities	✓	☑	☑

Notation:
☑ strong interest/concern.
✓ some interest/concern.
× little or no interest/concern.

Identification and evaluation of alternatives on sustainability criteria

Although the VCM processing route is well established, several process alternatives are used or are being investigated with the aim of improving production efficiencies, costs, health, safety and environmental performance. Here, for illustration, we concentrate on the feedstock and process alternatives.

Feedstock alternatives: One of the feedstock-related alternatives would be to replace the more expensive ethylene with a relatively inexpensive ethane feedstock in the direct chlorination stage (Clegg and Hardman, 1998; Marshall *et al.*, 2001). However, this alternative can lead to a loss of ethane, mainly through its oxidation and the formation of CO_2 (Clegg and Hardman, 1998). Another alternative here would be to source either feedstock from renewable sources, e.g., from biomass.

A further feedstock-related alternative would be to use air instead of pure oxygen in the oxy-chlorination stage. Using air could be advantageous economically because, unlike oxygen, it is available (almost) free of charge. On a life cycle basis, using air is also favoured environmentally as air separation to produce oxygen is energy intensive and generates various emissions to the environment (Azapagic *et al.*, 2004b). However, there are certain advantages to using pure oxygen, including smaller equipment size, lower energy use, lower operating temperature, higher process efficiencies and product yield.

Processes alternatives: One of the problems in direct chlorination is that EDC can be contaminated easily, either by iron (from the $FeCl_3$ catalyst) or through the formation of β-trichloroethane (generated in further chlorination of EDC). To control this contamination, two different processes can be used:

- sub-cooling, where EDC is maintained below its normal boiling temperature (at 60°C);

Table 3. Summary of advantages and disadvantages of the alternatives (only selected criteria relevant for the alternatives considered here are shown).

	Economic criteria			Environmental criteria			Social criteria
Alternatives	Capital costs	Operating costs	Profits	Materials & energy	Emissions & solid waste	Env'l impacts	Health & safety
Ethylene	=	−	−/+	=	+	+	=
Ethane	=	+	−/+	=	−	−	=
Oxygen	+	−/+	+	−/+	−	−	−
Air	−	+/−	−	+/−	+	+	+
Sub-cooling	+	=	=	+	−	=	=
Boiling	−	=	=	−/+	+	=	=

Notation:
+ the alternative is better for that criterion.
− the alternative is worse for that criterion.
−/+ the alternative has both advantages and disadvantages for that criterion.
= no significant difference between alternatives for that criterion.

- boiling, where EDC is maintained at the normal boiling point (84°C).

The sub-cooled process produces EDC with less β-trichloroethane but is iron-contaminated. The boiling process generates more β-trichloroethane but EDC can, in principle, be obtained iron-free. The boiling process would eliminate the need to wash and dry the EDC stream, which must be done before cracking if it contains iron. However, because of the higher proportion of β-trichloroethane in the boiling process, the reactor needs to be constructed from a material that is resistant to erosion and corrosion, as opposed to the sub-cooled process where the carbon steel can be used.

The advantages and disadvantages of these alternatives with respect to the above sustainability issues and criteria are summarized in Table 3. As can be seen from this summary, the choice is not easy as neither of the alternatives has a clear overall advantage over the other. Therefore, depending on the preferences of the stakeholders and importance they place on various sustainability criteria (as discussed in the section on Project initiation), either of the alternatives could be selected for preliminary design. Some multi-criteria decision analysis may need to be applied here to help trade off the sustainability criteria and identify the most sustainable alternatives (Azapagic and Perdan, 2005a, b). However here, again for the illustration purposes, we choose ethylene (sourced from a conventional rather than biomass source), oxygen and the sub-cooling process as the most promising alternatives for preliminary design.

Preliminary Design

The initial process specification and the assumptions used for preliminary design in this case study are given in Table 4. The flowsheet of a preliminary design simulated by ChemCAD[2] is shown in Figure 4. To simplify the analysis for the purposes of the illustration of the PDfS methodology, this flowsheet is shown as a simplified process flow diagram (PFD) in Figure 5. The summary mass balances and energy requirements in the system are shown in Table 5; they correspond to the PFD in Figure 5. A summary of the input materials and utilities and gaseous and liquid discharges from the process is shown in Table 6. The overall capital and operating cost estimates are given in Table 7.

In addition to the assumptions given in Table 4, the following assumptions have been made regarding the discharges from the process:

- gaseous emissions: the chlorinated hydrocarbons, including dioxins and furans, are destroyed completely by incineration. The HCl and NOx formed during incineration are scrubbed by sodium hydroxide;
- liquid discharges: the HCl stream from EDC purification is neutralised by sodium hydroxide;
- solid waste: spent catalysts is landfilled;
- as specified in Table 4, all the regulated discharges must be IPPC-compliant.

These assumptions and the results summarized in Tables 5–7 provide a basis for assessing the level of economic, environmental and social sustainability of the proposed design, as illustrated subsequently.

Assessment of economic sustainability

As shown in Table 1, the assessment of micro-economic sustainability of the plant involves calculation of the capital and operating costs and profitability analysis. These results are given in Table 8. As shown in the table, it will cost around £35 700 000 to build the plant and around £31 875 000 y^{-1} to operate it. Assuming the sale price of 315 £ t^{-1} VCM, the projected income is 41 050 800 £ y^{-1}. The profitability analysis using net present value (NPV)[2], shows that, at the assumed interest rate of 6%, the plant has a pay-back time of just over 10 years and after 18 years it will have made a cumulative profit of £24 240 000.

With respect to the other investments, it has been assumed that over the life cycle of the plant approximately 1% of the capital will be invested in the environmental protection and 2% in health and safety; the costs of decommissioning have been assumed at 10% of capital investments

[2]For calculation of NPV, the following assumptions have been made: The design and construction will take three years; the total fixed capital for the plant will be spent at a rate of 10% in the first year, 30% in the second and 60% in the third year. Also spent in the third year is the working capital for the project, which is spent on items like stocks of raw materials and for building up a product inventory and as such, this money is recoverable at the end of the project. This figure is assumed at 15% of the fixed capital. The plant will start producing VCM at the beginning of year four, incurring the operating costs but also bringing income from the sales of the product. The profit from this income is subject to a corporate tax at a rate of 30%.

Table 4. Design specification and assumptions.

Feeds	C_2H_4	8.0 bara and 20°C with <400 ppm v/v ethane	
	Cl_2	At 3.0 bara containing: O_2: 2.0% v/v; N_2: 0.5% v/v; H_2: 0.1% v/v;	
	O_2	CO_2: 0.15% v/v Purity >99% v/v	
Product	VCM	Impurities: <100 ppm w/w	
Intermediate streams	EDC	As cracker feed: purity >99% w/w	
		Impurities:	
		C_1 lights: <2000 ppm w/w	C_2 heavies: <1000 ppm w/w
		C_2 lights: <4000 ppm w/w	C_4 heavies: <50 ppm w/w
		C_4 lights: <100 ppm w/w	β-trichloroethane: <500 ppm w/w
		Water: <0.002 mole%	Fe: <1 ppm w/w
	HCl	Separated from cracked gas: <200 ppm w/w VCM	
	EDC	Separated from cracked gas: <200 ppm w/w VCM	
Utilities	LP steam	3.1 bara and 155°C	
	IP steam	15.0 bara and 225°C	
	HP steam	42.4 bara and 270°C	
	Natural gas	4.5 bara and 35°C with: 94% v/v CH_4; 4% v/v ethane; 2% v/v N_2	
	Towns water	8.0 bara and 20°C	
	Cooling water	4.0 bara and 22°C	
Costs	Feeds	Cl_2:	£76/t
		C_2H_4:	£305/t
		O_2:	£32/t
	Utilities	Electricity:	£38/MWh
		Heat (natural gas):	£1.37/GJ
		NaOH (50% solution):	£60/t
		Nitrogen:	£23/t
		Water:	£0.37/m^3
		Cooling water:	£0.07/m^3
	Product	VCM:	8% of equipment costs
	Other cost information	Equipment shipping cots:	£315/t
		Tankage investment:	20% of on-site investment costs
		Off-site investment:	10% of on-site investment costs
		Corporation tax rate:	30%
		Depreciation allowance:	100% in 1st year of operation
		Operating personnel:	5 shifts
		Labour cost (one shift):	£300 000 (incl. overheads)
		Annual maintenance cost:	3% of capital costs
		Other annual costs:	2.6% of capital costs
Emissions, effluents and solid waste		All gaseous emissions, liquid effluents and solid wastes must be below the limits prescribed by EU legislation. Best Available Technique (BAT) should be used for the prevention and control of environmental pollution	

[normally ranging from 5–17% (Hicks *et al.*, 2000)]. Therefore, the total additional investment required is around £4.6 million, bringing the total investment costs to just over £40 million.

The results of the macro-economic evaluation of sustainability are also summarized in Table 8. The indicators used for these purposes include value added[3] (Azapagic, 2003), a 'green' tax such as Climate Change Levy (CCL) and potential environmental liabilities. For this design the value added is estimated at approximately £12 377 000 y^{-1}, or £95 per tonne of VCM produced. Per unit sales, the value added is £0.30 $£^{-1}$.

The corporate tax paid on the profits at the rate of 30% is equal to £2 753 000 y^{-1}. The cost of the CCL, which taxes the industrial users in the UK for the use of fossil-fuel derived energy, is estimated at around £600 000 per year. However, the design incorporates a combined heat and power plant (CHP) and is therefore exempt from the CCL. This will represent a significant saving to the operating company and therefore increase the economic sustainability of the plant. In addition to the CCL, the cost of landfill tax is also calculated; at £10 000 this is a relatively small cost, reflecting a relatively small amount of solid waste (catalysts) being landfilled.

Thus, based on these findings, it could be argued that the proposed design is economically (just) sustainable. Further improvements to the design to reduce costs and improve profitability will be carried out in the detailed design.

Assessment of environmental sustainability

LCA has been used to assess the environmental sustainability of the system. Figure 6 shows a simplified flow diagram of the life cycle of VCM, encompassing the production of raw materials, energy, VCM and PVC; however, PVC disposal or recycling are not considered in this case study. Considerations of construction and decommissioning of the VCM plant are limited to the amount of steel used to construct the plant, which is assumed to be recycled after the decommissioning; the other environmental impacts associated with these two stages are not included here.

To help distinguish between the contribution to the environmental impacts of different parts of the system, the system is divided into the 'direct' and 'indirect' activities. The environmental impacts from the former are related to the operation of the VCM plant and have been calculated using the design data; the impacts from the latter are from the life cycles of raw materials and energy as well as from the production of PVC and

[3]Value added by the operation is the value of sales less the cost of goods, raw materials (including energy) and services purchased. It shows how much the operation of the plant increases the value of purchases such as raw materials, energy, goods and services.

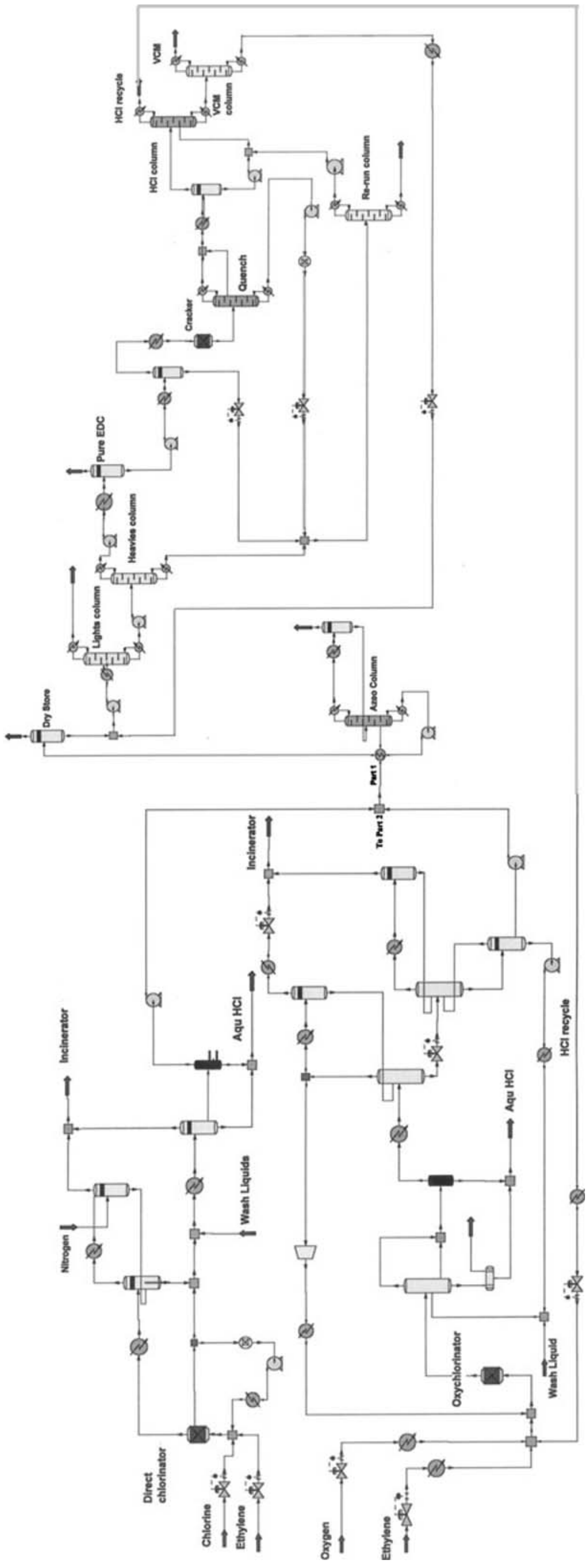


Figure 4. Flowsheet of the preliminary design of the VCM plant.

they have been calculated using an LCA database (Pira, 2000). The basis for analysis (or in the LCA terms, the functional unit) is production of 130 000 t y^{-1} of VCM.

The LCA results are summarized in Figure 7. The environmental burdens and impacts shown in the figure correspond to the environmental criteria and indicators listed in Table 1. In addition to these, two further environmental indicators have been identified for the VCM system: emissions of heavy metals and carcinogenic effect of VCM (as discussed in the section on social sustainability below) and other substances. These results are also shown in Figure 7. For example, producing 130 000 t y^{-1} of VCM would, on a life cycle basis, consume around 3 million GJ of energy per year and generate 180 000 tonnes of $CO_{2eq.}$ Total emissions of heavy metals would be around 10 t $Pb_{eq.}$; these and other toxic substances, including VCM, could lead to approximately nine DALYs (disability adjusted life years) caused by their carcinogenic potential. Furthermore, as shown in Figure 8, polymerization of VCM to PVC would increase all the impacts on average by 30%. This increase is mainly due to the energy used for polymerisation and the associated life cycle impacts of energy sources (natural gas and fuel oil).

These results can be used to assess if the design is environmentally sustainable. However, unlike economic sustainability, it is much more difficult to evaluate environmental sustainability just by looking at the results, without having a reference point for comparison. The fact that the plant is IPPC compliant is helpful to a certain extent, but in PDfS that is only a part of the whole picture: the designer should be able to assess whether the proposed design is environmentally sustainable on a life cycle basis and if not, what could be done to improve its sustainability. This question could be addressed in several ways, e.g., by:

- identifying the 'hot spots' to find out which parts in the system contribute most to the impacts and targeting these for maximum improvements;
- optimizing on environmental objectives of interest (e.g., energy use, global warming or toxicity) to minimize the impacts from the whole system;
- comparing the proposed design with an existing VCM plant or industry average;
- comparing the proposed design with other chemical plants in the same or a related sector.

Further discussion of all of the above options is beyond the scope of this paper; however, for illustration, two of the above options are considered briefly here: the identification of 'hot spots' and comparison with an average VCM plant in Europe. For the methodology and examples on environmental process optimization see e.g., Azapagic and Clift (1999).

Identification and targeting of 'hot spots': These results are given in Figure 9, which indicates that the 'hot spots' are mostly related to the indirect activities and mainly stem from the life cycles of chlorine, ethylene and generation of electricity and heat. The impacts from the direct activities (i.e., operation of the plant) are relatively small as there are few direct discharges from the process. This points to a conclusion that further improvement of the design should be directed towards the indirect activities rather than the operation of the plant as the latter would lead to small improvements in the overall environmental performance. This analysis also shows that there would

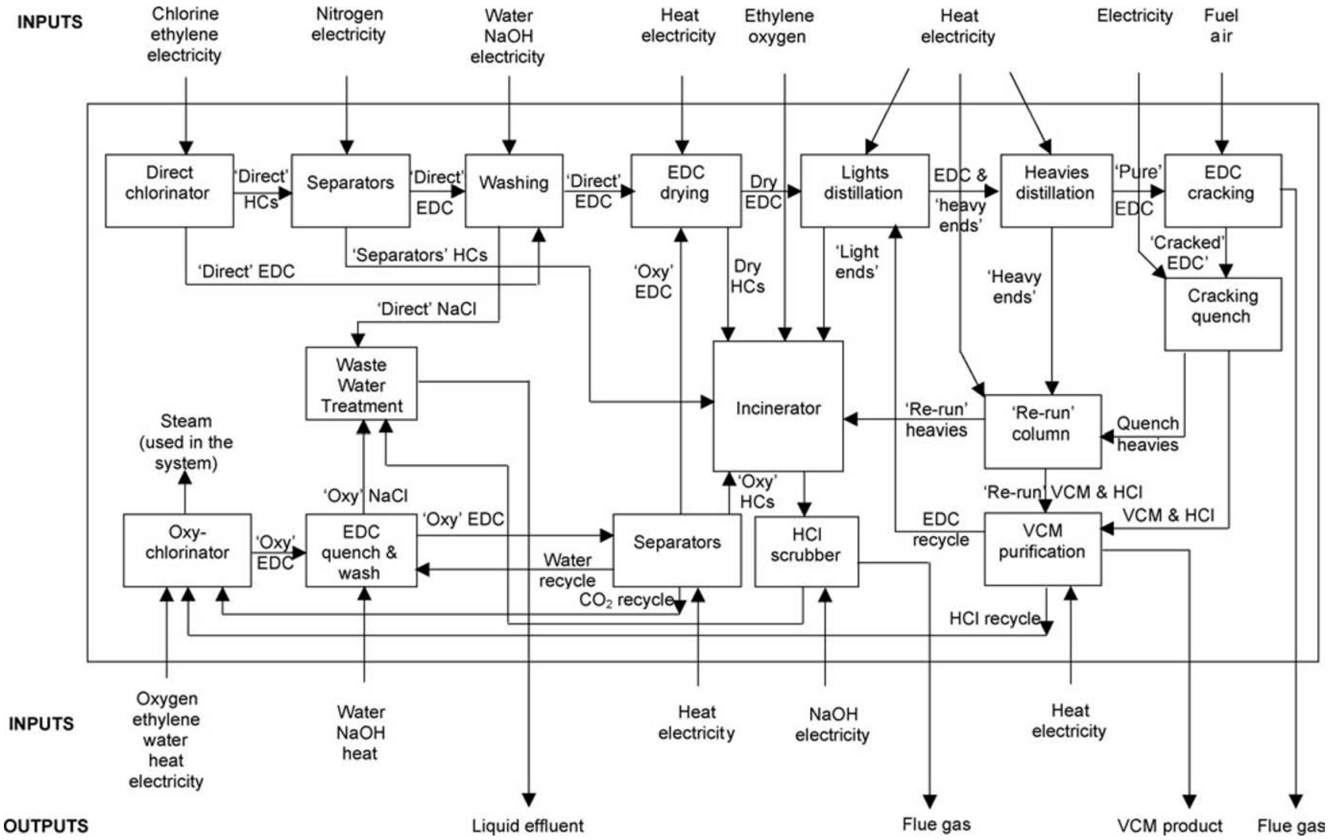


Figure 5. Simplified process flow diagram of the VCM plant.

be little environmental advantage in using air instead of oxygen, one of the alternatives discarded previously, since the contribution of oxygen to the total environmental impacts is negligible (grouped under 'other' in Figure 9) and it offers significant process advantages. On the other hand, replacing ethylene and chlorine by more sustainable feedstocks could lead to a significant environmental improvement. As discussed earlier, the only other feasible alternative to ethylene is ethane—since its source and the production process are normally the same as for ethylene, again, very little environmental advantage would be gained in this way. However, sourcing ethylene from biomass may offer some environmental advantages. Finally, as there is currently no feasible alternative to chlorine, replacing this feedstock is not a feasible option.

Thus, based on this assessment, it would appear that this design has gone as far as it could to minimize the environmental impacts in the whole life cycle of the VCM production so that it could be argued that this design is as environmentally sustainable as possible given the system constraints. However, before reaching this conclusion, it would be interesting to compare this design with an average European VCM plant.

Comparison with an average VMC plant: These results, displayed in Figure 10, show that, for most impacts, the proposed VCM design is environmentally more sustainable than an average European VCM plant. The exception to this is energy use whereby the proposed plant would use around 3% more energy and generate around 7% more greenhouse gases. A much more significant difference is noted for the water discharge: while the proposed plant is using around 30% less water than the average plant, it is discharging into the environment almost twice as much as the average plant. The proposed plant also has higher carcinogenic potential, through a higher release of toxic substances. Therefore, these are the areas where further improvements could be investigated in the detailed design.

Finally, it is interesting to integrate the findings of the environmental and economic assessments to gain further insights in the level of sustainability of this design. For these purposes, the LCA impacts of the VCM plant have been expressed per tonne of VCM produced and per unit value added (as shown in Table 8, value added has been calculated at £95 t^{-1}). These results are shown in Table 9. They indicate that, for example, for each tonne of VCM, 62.5 GJ of energy are used, depleting 1.5 tonnes of abiotic resources (i.e., fossil fuels, expressed as oil equivalents) and generating 2 tonnes of CO_{2eq}. Linking the environmental and economic performance, for every pound of value added per tonne of VCM, 658 MJ of energy and 15.8 kg of oil eq. are consumed and 34 kg of CO_2 are emitted. To make these results more meaningful, they could be compared with other plants in the same or related sector. For illustration, a comparison with the production of poly-olefins is given in Table 10. It is interesting to note, that although the systems are quite different and produce different products, per unit value added, their environmental performance is quite comparable. The IChemE (2003) approach to evaluating sustainability of process industries is also based on value added as a 'normalisation' factor to enable sustainability comparisons across different sectors.

Table 5. Material balances and energy use for the VCM plant (basis: production of 15 000 kg h^{-1} VCM; reference: Figure 6).

	Material in	kg h^{-1}	Material out	kg h^{-1}	Energy use (MJ)
Oxy-chlorination					
Oxy-chlorinator	Oxygen	2493	'Oxy' EDC	19 792	5664
	Ethylene	3479			
	HCl recycle	8959			
	CO_2 recycle	4861			
Direct chlorination					
Direct chlorinator	Chlorine	9204	'Direct' EDC	12 530	746
	Ethylene	3625	'Direct' HCs	299	
EDC purification					
Separators (direct chlorinator)	'Direct' HCs	299	'Direct' EDC	108	73
	Nitrogen	840	'Separators' HCs	1032	
Washing (direct chlorinator)	'Direct' EDC	12 638	'Direct' NaCl	353	10
	NaOH (as 100%)	1	'Direct' EDC	12 646	
	Water	360			
EDC quench & wash (oxy-chlorinators)	'Oxy' EDC	19 792	'Oxy' EDC	20 857	1155
	Water	90	'Oxy' NaCl	2778	
	NaOH (100%)	176			
	Water recycle	3577			
Separators (oxy-chlorinator)	'Oxy' EDC	20 857	'Oxy' EDC	11 899	324
			'Oxy' HCs	519	
			Water recycle	3577	
			CO_2 recycle	4861	
EDC Drying	'Direct' EDC	12 646	'Dry' HCs	5	3808
	'Oxy' EDC	11 899	'Dry' EDC	24 522	
'Lights' distillation	'Dry' EDC	24 522	'Light ends'	247	29 499
	EDC recycle	24 842	EDC & 'heavy ends'	49 118	
'Heavies' distillation	EDC & 'heavy ends'	49 118	'Pure' EDC	48 270	49 878
			'Heavy ends'	848	
EDC Cracking					
EDC cracker	'Pure' EDC	48 270	'Cracked' EDC	48 270	33 192
Cracking quench	'Cracked' EDC	48 270	'Quench' heavies	750	611
			VCM & HCl	47 520	
'Re-run' column	'Quench' heavies	750	'Re-run' heavies	283	1020
	'Heavy ends'	848	'Re-run' VCM & HCl	1315	
VCM purification	VCM & HCl	47 520	VCM	15 034	20 535
	'Re-run' VCM & HCl	1315	EDC recycle	24 842	
			HCl Recycle	8959	
Wastewater treatment					
	'Direct' NaCl	352	Treated wastewater	3130	n/a
	'Oxy' NaCl	2778			
Incinerator					
	'Oxy' HCs	519	Flue gas containing:	2672	n/a
	'Separators' HCs	1032	HCl	443	
	'Dry' HCs	5	CO_2	1153	
	'Light ends'	247	Chlorine	3	
	'Re-run' heavies	283	Chlorinated HCs	Traces	
	Oxygen	576	NOx	$8.5 \cdot 10^{-3}$	
	Ethylene	10	Water vapour	110	
			Nitrogen & oxygen	963	

Assessing social sustainability

The final step PDfS within the preliminary design stage is social sustainability assessment. The findings of the quantitative and qualitative assessment for the VCM plant are shown in Table 11 and discussed below. Some of these preliminary findings will serve as a starting point for safety, loss prevention and HAZOP studies in the detailed design stage.

It is envisaged that the proposed VCM plant would provide full time employment to 20 operators over the life time

Table 6. Summary of raw materials and energy used by the VCM plant (basis: 15 000 kg h^{-1} VCM).

	Direct chlorination	Oxy-chlorination	EDC purification	Cracking & purification	Total
Cl_2 (kg h^{-1})	9204				9200
C_2H_4 (kg h^{-1})	3620	3470	10		7000
O_2 (kg h^{-1})		2495	575		3070
NaOH (as 100%) (kg h^{-1})	1	176			177
N_2 (kg h^{-1})	840				840
Water (kg h^{-1})	360	90			450
Electricity (MJ h^{-1})	745	475	1835	7450	10 505
Heat (as natural gas) (MJ h^{-1})		5190	82 440	47 900	135 530

Table 7. Summary of the total capital and annual operating costs (basis: 130 000 t y^{-1} VCM).

Capital costs (£)	
Total delivered cost of equipment (incl. shipping costs at 8% of the equipment costs)	6 000 000
Estimated capital costs (Lang factor = 4.56)	27 500 000
Total capital costs (incl. tankage and off-site investments)	35 710 000
Operating costs (£ y^{-1})	
Fixed costs (labour, maintenance and other)	3 200 000
Raw materials	25 755 000
Utilities	2 920 000
Total operating costs	31 875 000

Table 8. Assessment of economic sustainability of the VCM preliminary design (basis: 130 000 t y^{-1} VCM).

Economic indicators	Value
Micro-economic analysis	
Total capital costs	£35 700 000
Operating costs	£31 875 000 y^{-1}
Profitability (as NPV):	
Break-even point	10 years
Profit after 18 years	£24 240 00
Additional investments (as % of capital costs)[4]	
Pollution prevention (~1%)	£357 000
Employee health and safety (~2%)	£714 000
Decommissioning (10%)	£3 570 000
Macro-economic analysis	
Value added	£12 377 000 y^{-1}
Value added per unit value of sales	£0.30 £$^{-1}$
Value added per unit amount of product	£95 t^{-1}
Taxes:	
Income tax (@30%)	2 753 000 £ y^{-1}
Climate change levy tax	CHP plants exempt
Landfill tax	~10 000 £ y^{-1}
Potential costs of environmental liability	Uncertain, potentially large

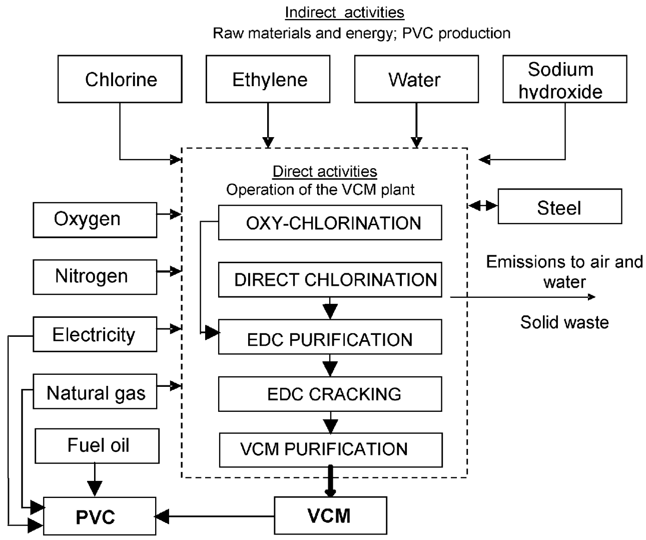


Figure 6. Simplified life cycle diagram of VCM and PVC production.

of the plant. In addition to this, an estimated 25 full-time contractors would be employed during the construction phase which is projected to last for 3 years.

Occupational health and safety is an important issue for any chemical plant, but particularly in the case of VCM. In addition to the usual health and safety concerns such as injuries, fatalities, exposure to noise and vibration, there are several other issues that need to be considered here. Firstly, production of VCM requires the use of hazardous materials, such as chlorine, ethylene, sodium hydroxide and oxygen; as shown in Table 11, the Dow Fire and Explosion Index for the oxy-chlorinator is 206 which indicates a severe fire and explosion hazard; the plant is also classified as top-tier site according to the COMAH regulations and will require an on-site emergency evacuation plan. Therefore, the associated risks must be minimized by design. Secondly, exposure to VCM has been linked to liver and other types of human cancer (Rahde, 1992). For this reason, the occupational exposure limits for VCM have been reduced significantly over the years to the current value of 2.6 mg m^{-3} or 1 ppm (expressed as 8 h time-weighted average). Furthermore, the short-exposure limit (15 min) must not exceed 5 ppm; direct contact with liquid VCM must be avoided. Although these are operational issues, the preliminary and then later the detailed design must ensure that the exposure to and contact with VCM are minimized as far as possible.

In addition to protecting the employees from exposure to VCM, the design must minimize or prevent exposure to VCM of the general public living in the vicinity of the plant. Some studies suggest that daily VCM inhalation rates range from 4 μg to more than 100 μg per person per day for populations living in the immediate vicinity of VCM plants (ECETOC, 1988).

Dioxins and furans are another health and safety concern associated with the production of VCM as exposure to these substances can cause cancer and other toxicological effects. In this design, it is proposed to incinerate the waste streams with chlorinated hydrocarbons and dioxins. However, incineration can generate further amounts of dioxins through *de novo* synthesis so that the design and operating conditions in the incinerator must be such that the formation of dioxins is prevented (e.g., by controlling temperature and residence time).

Finally, health and safety of customers must also be taken into account in assessing social sustainability of process plants. Since VCM is a human carcinogen and the majority of VCM is used for PVC production, it is important that PVC contains as little residual monomer as possible (<5 ppm).

The design must also ensure that noise, odour and visual impact of the plant are minimized to avoid causing nuisance to the neighbouring public. These and the other social issues discussed above will have a direct impact on the public acceptability of the plant which can ultimately determine whether an industrial installation gets a planning permission. It is therefore important that the above issues are addressed adequately in the design, so that the objections to the

[4]The HSE costs shown here in addition to the usual costs taken into account when designing a new plant, and include both the process integration measures and 'end of pipe' solutions, e.g., incineration. The usual HSE costs have already been accounted for in the total capital costs.

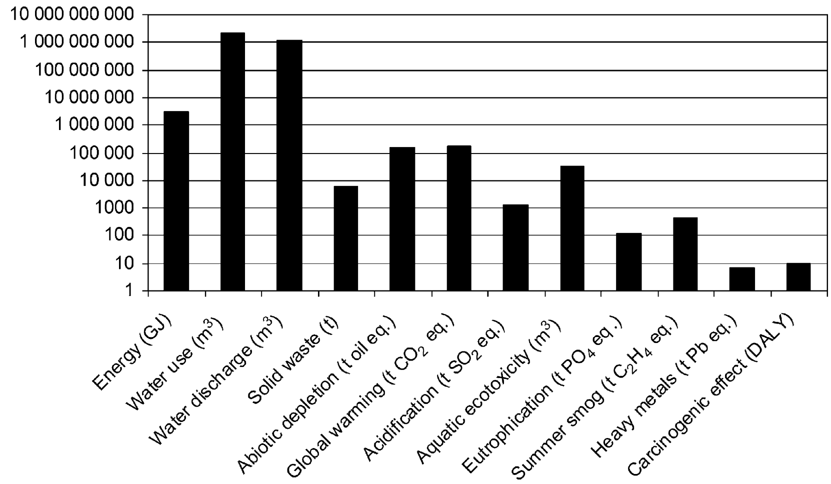


Figure 7. The LCA results showing the environmental burdens and impacts of the proposed VCM design from 'cradle to gate' [Notes: All burdens and impacts expressed per 130 000 t y^{-1} VCM produced; DALY: Disability Adjusted Life Years calculated using the Ecoindicator 99 method (Goedkoop and Spriensma, 2001); all other environmental impacts calculated using CML Problem oriented method (Heijungs *et al.*, 1992)]

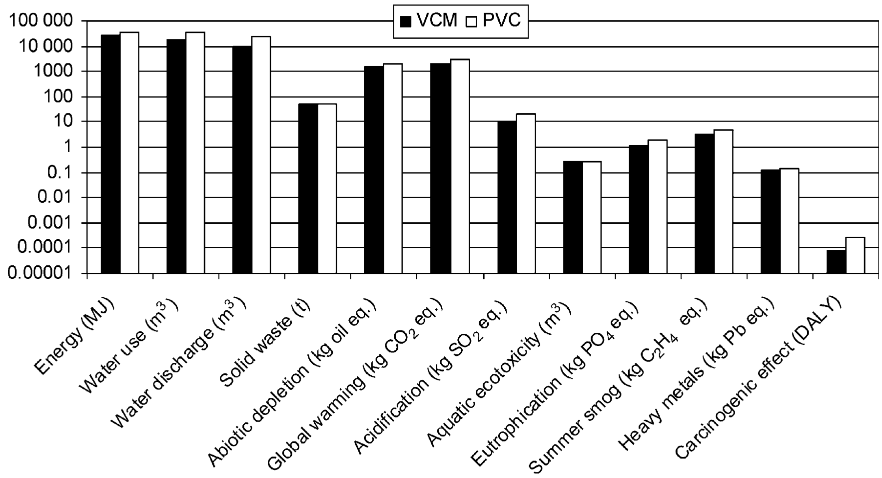


Figure 8. Comparison of life cycle impacts of VCM and PVC (all impacts expressed per 1000 kg of product).

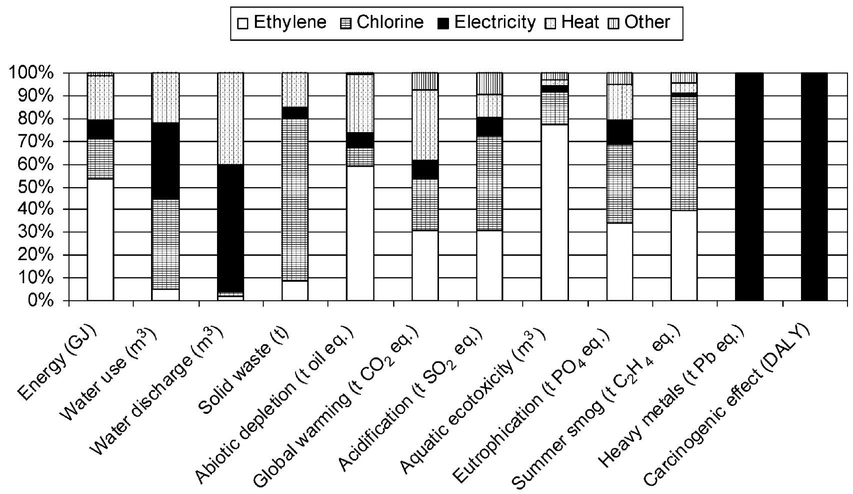


Figure 9. Contribution of different parts of the VCM plant to the total environmental impacts from 'cradle to gate'. [Notes: 'Chlorine', 'ethylene', 'electricity' and 'heat' represent the life cycles of chlorine, ethylene, electricity and heat; 'other' includes direct activities (operation of the plant) and the life cycles of all other parts of the VCM system shown in Figure 6, apart from chlorine, ethylene, electricity and heat; PVC production is not included in these results.]

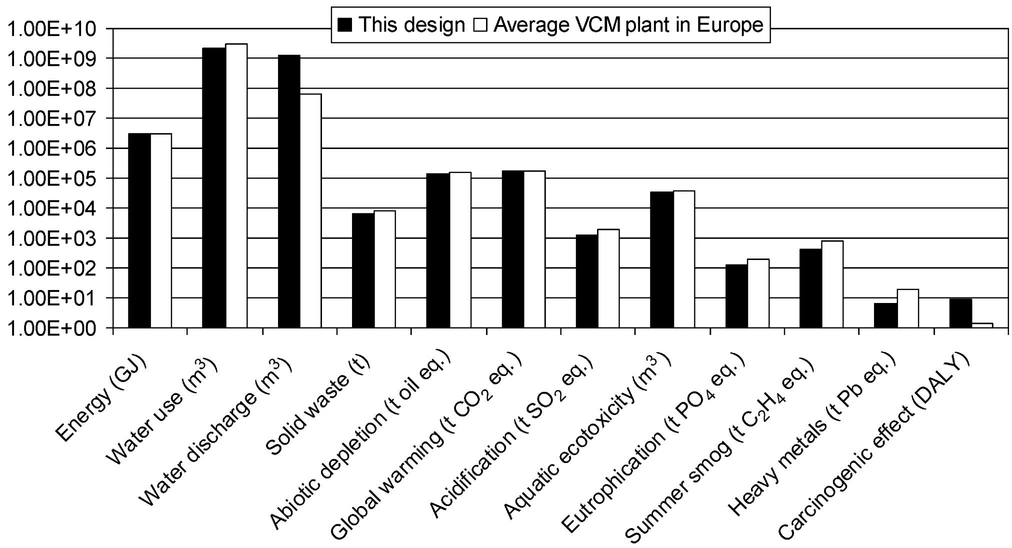


Figure 10. Comparison of environmental sustainability of the proposed design and an average European VCM plant [LCA data for the average European VCM plant obtained from APME (Pira, 2000)].

Table 9. Linking environmental and economic sustainability assessments.

Environmental indicators	Expressed per tonne of VCM	Expressed per value added
Energy use	62 484 MJ t^{-1}	658 MJ £$^{-1}$
Water use	19 474 m^3 t^{-1}	205 m^3 £$^{-1}$
Water discharge	11 254 m^3 t^{-1}	118 m^3 £$^{-1}$
Solid waste	53 kg t^{-1}	0.6 kg £$^{-1}$
Abiotic depletion	1502 kg oil eq t^{-1}	15.8 kg oil eq £$^{-1}$
Global warming	2029 kg CO_2 eq t^{-1}	34 kg CO_2 eq £$^{-1}$
Acidification	11 kg SO_2 eq t^{-1}	0.1 kg SO_2 eq £$^{-1}$
Eutrophication	1 kg PO_4 eq t^{-1}	0.01 kg PO_4 eq £$^{-1}$
Summer smog	3 kg C_2H_4 eq t^{-1}	0.03 kg C_2H_4 eq £$^{-1}$
Aquatic ecotoxicity	0.3 m^3 t^{-1}	$3.2 \cdot 10^{-3}$ m^3 £$^{-1}$

Table 10. Comparison of economic and environmental sustainability of VCM with another plant in the related sector.

Environmental indicators	VCM	Poly-olefins
Energy use	658 MJ £$^{-1}$	668 MJ £$^{-1}$
Global warming	34 kg CO_2 eq £$^{-1}$	58 kg CO_2 eq £$^{-1}$
Acidification	0.1 kg SO_2 eq £$^{-1}$	1 kg SO_2 eq £$^{-1}$
Eutrophication	0.01 kg PO_4 eq £$^{-1}$	0.02 kg PO_4 eq £$^{-1}$
Summer smog	0.03 kg C_2H_4 eq £$^{-1}$	0.1 kg C_2H_4 eq £$^{-1}$
Aquatic ecotoxicity	$3.2 \cdot 10^{-3}$ m^3 £$^{-1}$	$3.07 \cdot 10^{-3}$ m^3 £$^{-1}$

(Assumptions for the poly-olefin plant: Results based on the preliminary design of the process to produce 450 000 t y^{-1} of a mixture of products from a propylene/butane stream fed from a catalytic cracker. The product split: heptene: 76 545 t y^{-1}; higher olefins: 175 770 t y^{-1}; LPG: 134 510 t y^{-1}; C_2: 31 990 t y^{-1}; motor gasoline: 22 680 t y^{-1}; fuel oil: 8505 t y^{-1}; value added = £91 t^{-1}.)

proposed plant are minimized. Furthermore, there are also public acceptability issues further downstream in the life cycle of the VCM product, related to the manufacture and use of PVC. Many people object to PVC because of the potential formation of dioxins and furans during its post-use incineration. Additives used to improve PVC characteristics, such as phthalate plasticizers and stabilisers which contain heavy metals are also an issue of public concern because of their potential to reach the environment. One of the ways to deal with these objections would be to build into the design a possibility for feedstock recycling of PVC (Azapagic *et al.*, 2003; Vinyl 2010, 2004).

Detailed Design

Following this preliminary sustainability assessment, detailed design is carried out to further improve and optimise economic, environmental and social performance of the plant. A full sustainability assessment should then be carried out to ensure that all relevant sustainability issues

Table 11. Assessment of social sustainability of the VCM preliminary design.

Social indicators	Value
Provision of employment	20 plant operators and 25 contractors
Employee health and safety	
Dow Fire and Explosion Index	Direct chlorination = 123 Oxy-chlorination = 206 Cracking = 166
COMAH	Higher threshold: 2.2; Lower threshold: 8.7
VCM exposure	<2.6 mg m^{-3} or 1 ppm (as 8 hours time weighted average) <5 ppm (15 min exposure) Direct contact with liquid VCM must be avoided
Citizens′ health and safety	
Emissions of VCM, dioxins, furans and other toxic substances	Must be prevented or minimized
Customer health and safety	
VCM exposure	<5 ppm
Nuisance	
Odour, noise, visual impact	Must be minimized
Public acceptability	All of the above (plus possibly further specific concerns by local communities) must be satisfied to minimise objections to the plant

have been addressed appropriately before proceeding to the final design step. The procedure for a full sustainability assessment is similar to that illustrated for preliminary design so that detailed design is not discussed here.

CONCLUSIONS

This simplified case study illustrates how sustainability considerations could be integrated into process design from project initiation through preliminary to detailed design. It has been argued that this requires a systems approach whereby sustainability is not considered as an 'add on' but is systematically integrated into process design taking into account the whole life cycle of the plant and the product. The proposed methodology enables identification of relevant sustainability criteria and indicators, comparison of alternatives, sustainability assessment of the overall design and identification of 'hot spots' in the life cycle of the system. In this way, it is possible to arrive at a design configuration that would ensure the most sustainable performance of the plant and product over their whole life cycles. This could be achieved in various ways, for example:

- by identifying and choosing the alternatives that would not normally be considered in conventional design (due to the 'we have always done it this way' syndrome);
- by identifying and addressing at an early stage important environmental or social issues that would have otherwise remained hidden until the plant is in operation;
- by targeting the 'hot spots' in the life cycle for maximum improvements rather than concentrating on the plant operation stage alone, which may have only a marginal contribution to the overall sustainability of the system (as for example, shown in the case study of VCM with respect to environmental sustainability);
- by avoiding economic and other costs associated with the above.

Today, process plants are largely designed with the plant operation in mind alone; applying the PDfS principles would help to move away from that narrow approach and improve the level of sustainability of future processes and products. However, currently, there is little experience in applying these principles in practice. Amongst other enabling factors, incorporation of sustainability considerations into commercially available flowsheeting packages would be a step forward in promoting a wider uptake by practitioners of process design for sustainability.

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