Role of Chemical Reaction Engineering in Sustainable Process Development*
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1. Introduction

Achieving sustainable processes, that allow us at present to fully meet our needs without impairing the ability of future generations to do so, is an important goal for current and future engineers. In production of new materials, chemicals, and pharmaceuticals sustainable processes certainly require the most efficient use of raw materials and energy, preferably from renewable sources, and prevention of generation and release of toxic materials. Advancing the state of the art of chemical reaction engineering (CRE) is the key element needed for development of such environmentally friendly and sustainable chemical processes.

Current chemical processes depend heavily on the non-renewable fossil-based raw materials. These processes are unsustainable in the long run. In order to make them sustainable, chemical technologies must focus on employing renewable raw materials as well as preventing and minimizing pollution at the source rather than dealing with end-of-pipe treatments. New technologies of higher material and energy efficiency offer the best hope for minimization and prevention of pollution. To implement new technologies, a multidisciplinary taskforce is needed. This effort involves chemical engineers together with environmental engineers and chemists since they are predominantly in charge of designing novel chemical technologies.

Pollution prevention problem can be attacked via a hierarchical approach based on three levels as outlined in the book by Allen and Rosselot1. Each level uses a system boundary for the analysis. The top level, (the macro-level) is the largest system boundary covering the whole manufacturing activity from raw material extraction to product use and eventually disposal. These activities involve chemical and physical transformation of

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* Chapter submitted to Sustainable Engineering Principles book.
raw materials creating pollution or wastes as shown schematically in Figure 1. The scope of the macro-level analysis is mainly in tracking these transformations, identifying the causes of pollution and suggesting the reduction strategies.

The next level is the plant level or the meso-scale which is the main domain of chemical engineers. The meso-level focuses on an entire chemical plant, and deals with the associated chemical and physical transformations of non-renewable resources (e.g. petroleum and coal, etc.) and renewable resources (e.g. plants and animals) into a variety of specific products. These transformations can result in a number of undesirable products which, if not checked, can result in pollution of the environment. The challenge then for modern chemical engineers is to improve the efficiency of existing processes, to the extent possible, and design new cleaner and more efficient processes. While in the past the effort was focused on end of the pipe clean-up and remediation, the focus now is on pollution prevention and ultimately on sustainability. Mass and energy transfer calculations as well as optimization of processes that result in less pollution can be performed at this level. This plant scale boundary usually consists of raw material pretreatment section, reactor section, and separation unit operations. (See Figure 2.) Although each of these sections are important, the chemical reactor forms the heart of the process and offers considerable scope for pollution prevention. The present paper addresses the scope for pollution prevention in the reactor unit and sustainable development. It may however be noted that the reactor and separator sections are closely linked and in some cases, improvements in the reactor section may adversely affect the separation section leading to an overall increase in pollution. Hence any suggested improvement in the reactor section has to be reevaluated in the overall plant scale context.

The third level indicated by Allen and Rosselot is the micro-level that deals with molecular phenomena and how it affects pollution. Analysis at this scale includes synthesis of benign chemicals, design of alternative pathways to design a chemical, etc. CRE plays a dominant role at this level as well and some applications of CRE at the micro-level pollution prevention are also indicated in the paper.

Waste reduction in chemical reactors can be achieved in the following hierarchical manner: (i) better maintenance, (ii) minor modifications of reactor
operation, (iii) major modifications or new reactor concepts and (iv) improved process chemistry, novel catalysts and use of these in suitable reactors. The items (i) and (ii) are usually practiced for existing plants while items (iii) and (iv) above are more suitable in the context of new technologies or processes. Also items (iii) and (iv) involve a multi-disciplinary R&D activities which can be costly. But since long-term sustainability is the goal this is a worthwhile effort and increasing activities are expected in this direction in the future. The items (i) and (ii) are addressed in a paper by Dyer and Mulholland\textsuperscript{2} and this paper focuses mainly on (iii) and (iv).

It is also appropriate at this point to stress the multi-scale nature of reaction engineering. Figure 3 shows the multi-level CRE approach. We have at the tiniest scale the catalytic surface up to macro-scale of huge 10m high chemical reactor and hence the task of pollution prevention in chemical reactor is a formidable task and has to address phenomena at all these scales. At the molecular level, the choice of the process chemistry dramatically impacts the atom efficiency and the degree of potential environmental damage due to the chemicals produced. We will first review how some micro-level concepts such as atom efficiency (Section 2) and optimum catalyst development (Section 3) affect reactor choice and pollutants generated. At the meso-level, optimizing the catalyst properties (Section 3) and choosing the right media (Section 4) significantly reduces the adverse environmental impact of chemical processes. Clearly, proper understanding and application of the principles of multiphase reaction engineering are very important for proper execution of truly environmentally benign processes since almost all processes involve more than one phase. At the macro-level, it is crucial to estimate the hydrodynamic effects (Section 5) on reactor performance as this will lead to the selection of the right reactor. Furthermore, novel approaches to reactor design using process intensification concepts (Section 6) can be implemented to improve efficiency and minimize pollution. In addition, environmental impact analysis (Section 7) of the developed process has to be evaluated to see if green chemistry conditions are met and to assess the overall global impact of these changes. As can be seen, CRE is a marriage of multidisciplinary and multi-scale efforts with the aim of operating at sustainable green chemistry conditions to reduce pollution and maximize efficiency. The summary of these efforts and conclusions are given in Section 8.
2. Raw Materials Selection

The aim of benign synthesis is to reduce the amount of side reactions generating undesired by-products, i.e. waste. Alternative direct synthetic routes are therefore advantageous from the point of waste reduction and have an economic advantage. The organic chemistry is rich with reactions where large quantities of inorganic salts are generated as wastes that lead to poor atom efficiency. These can be avoided by selecting raw materials appropriately. Therefore, using environmentally benign raw materials can make a big impact on pollution prevention and thus enhance sustainability. Atom and mass economy calculations, that measure how efficiently raw materials are used, are the key decision-making concepts in selection of raw materials for a given process.

To give an example, two raw materials, benzene and n-butane can be employed in the production of maleic acid. The following reactions are possible routes to maleic anhydride (the first step to produce maleic acid).

**Benzene route:**

\[
2C_6H_6 + 9O_2 \xrightarrow{V_2O_5, MoO_3} 2C_4H_2O_3 + H_2O + 4CO_2
\]

**n-butane route:**

\[
C_4H_{10} + 3.5O_2 \xrightarrow{(VO)_2P_2O_7} C_4H_2O_3 + 4H_2O
\]

In the benzene route, there are four carbon atoms in product maleic anhydride per 6 carbon atoms in benzene. Therefore, the atom efficiency for the carbon atom is \(\frac{4}{6} \times 100\% = 66.7\%\). In the n-butane route, there are four carbon atoms in n-butane per four carbon atoms in maleic anhydride thus giving 100% atom efficiency.

If mass efficiency is considered, then the mass of the product is compared to the mass of the raw materials. The molecular weight of maleic anhydride is 98. For the n-butane route, we need 1 mole of n-butane (molecular weight 58) and 3.5 moles of oxygen (total mass of 3.5 x 32 = 112.) Thus the total mass of raw materials needed is 170. The mass efficiency of the n-butane route is therefore \(\frac{98}{170}\) or 57.6%. By a similar calculation, we can show that the mass efficiency of the benzene route is only 44.4%.
As can be seen, n-butane is favorable to benzene in comparison of both atom and mass economy. In addition, benzene is expensive and toxic. Therefore n-butane has replaced benzene in maleic anhydride production since the 1980s. A detailed case study comparing the two routes is given in the Green Engineering book\textsuperscript{3}.

Choosing benign and efficient raw materials is the first step in designing environmentally friendly processes. Once the process route is selected, the process yield and efficiency can be further improved and pollution can be minimized more effectively by the proper choice of catalyst and solvents used. Issues related to catalyst selection and development are discussed next.

3. **Catalyst Selection, Development and Reactor Choice**

Catalysts are being used extensively in chemical and fuel industries. Hence, selecting and developing the right catalyst has a huge impact on the success of a proposed process route. However, it may be noted that the development of novel catalyst has to be often combined with novel reactor technology for the process to be economically viable and environmentally beneficial. Hence catalyst development and reactor choice often have to be considered in unison.

As a general heuristic rule, the processes that replace liquid routes by solid catalyzed routes reduce pollution significantly especially when the some of the liquid reactants are toxic. For example, many liquid acids such as H\textsubscript{2}SO\textsubscript{4} and HF used as catalysts in petroleum refining industry impose a significant environmental hazard as they are highly corrosive and toxic. Therefore, based on environmental concerns these catalysts are now being replaced by solid-acid catalysts.

Once selected, to further tailor the catalyst to get optimum yield and selectivity, physical properties of the catalyst have to be determined and improved. Experimental methods, namely NMR, spectroscopy, kinetic measurements are available to study important properties such as the surface topology of the catalyst, the adsorption sites and how the molecules are adsorbed on the catalyst surface. Computer simulations of pore structure are also becoming increasingly popular to study the transport behavior of the catalysts. Detailed micro-kinetic modeling using molecular dynamic simulations are also useful to guide the design of a new catalyst.
Examples of catalyst development and appropriate reactor selection are illustrated in the following discussions by consideration of oxidation and alkylation which are two common reaction types in organic synthesis.

**Oxidation:**

Oxidation reactions are important in producing many fine chemicals, monomers and intermediates. \( \text{O}_2, \text{H}_2\text{O}_2 \) and \( \text{HNO}_3 \) are common oxidants used in these reactions, with oxygen being the most benign oxidant. We will particularly talk about n-butane oxidation to maleic anhydride in this section and discuss the reactor choice for vanadium phosphorous oxide (VPO) catalyst.

Initially, fixed bed reactor configurations were used for this process. Fixed bed catalytic reactor is one of the most utilized reactors in the petrochemical and petroleum refining industry. These reactors use solid catalysts in pellet or granular form and they can be visualized as shell and tube heat exchangers. There are several limitations in employment of fixed bed catalytic reactors. The reactors are expensive and only up to 2 % n-butane can be used in the feed\(^4\). Yield is around 50 % with 70-85 % conversion and 67-75 % molar selectivity to maleic anhydride\(^4\). Moreover, since the reaction is exothermic, hotspot formation must be avoided. Reactor designs have advanced to a point where some of these issues can be addressed effectively. Catalyst development has also progressed and the yield and selectivity have improved over the years by controlling the chemical composition and morphology of the catalyst. However, it may be noted that, the mechanical properties of the catalyst is equally important. The catalysts used in packed beds are usually supported metals from 1 to 10 mm in size. These must have adequate crushing strength to carry the full weight of a packed bed.

In order to minimize hotspots, fluidized catalyst beds are preferred over fixed catalyst beds. The advantages of fluidized catalyst beds include the ease of temperature control, superior heat transfer and lower operating temperatures compared to fixed catalyst beds. In a fluidized catalyst bed, higher butane concentrations (up to 4%) are handled reducing operating costs\(^4\). The disadvantage of the fluidized catalyst bed is the rapid reduction of the catalyst surface, catalyst attrition and carry over of fines leading to air pollution. Again the mechanical properties of the catalyst play an important role. In
fluidized beds, much smaller (compared to packed bed) catalyst particles on support (20 to 150 μm) are used and these must exhibit outstanding attrition properties. Hence, extensive catalyst development was required to move butane oxidation from fixed to fluidized beds.

In the mid 1990s, another improvement by DuPont de Nemours\textsuperscript{5} in reactor design introduced circulating fluid bed (CFB) technology to maleic anhydride production. The incentive for this change was provided by the realization that much higher productivity and selectivity can be obtained by using the catalyst in transient rather than steady state operation. CFB provides an ideal reactor set-up for such cyclic transient operation. In this reactor configuration, the chemistry is executed in a fluid bed-riser combination to accommodate successive oxidation and reduction of the catalyst. In the riser, n-butane gets converted to maleic anhydride while the catalyst gets reduced from V\textsuperscript{+5} to V\textsuperscript{+3} given by the scheme as:

\[
V^{+5} \xrightarrow{HC} V^{+4} \xrightarrow{HC} V^{+3}
\]

The reduced catalyst then circulates to the regenerator where it contacts air and gets oxidized back to V\textsuperscript{+5} given by the scheme as:

\[
V^{+3} \xrightarrow{O_2} V^{+4} \xrightarrow{O_2} V^{+5}
\]

In this way, n-butane and oxygen are not in direct contact and this leads to minimizing side reactions and higher maleic anhydride selectivity (up to 90 %) is therefore obtained\textsuperscript{4,6}. Figure 4 shows the circulating fluid bed reactor configuration. Again, to enable the use of CFB extensive catalyst development took place to introduce a highly porous but extremely attrition resistant shell on the VPO type catalyst.

VPO catalyst has also been subject to detailed investigation to further optimize its physical properties. For example, Mota\textit{ et al.}\textsuperscript{7} investigated modifying VPO catalyst by doping with Co or Mo to operate under fuel-rich conditions (i.e. O\textsubscript{2}/C\textsubscript{4}H\textsubscript{10} = 0.6). The authors state that Co-doped VPO catalyst performed better than the Mo-doped VPO catalyst and did not deactivate as the original VPO catalyst.

\textit{Alkylation:}

Hydrocarbon alkylation reactions are important in petroleum industries for producing high octane gasoline stocks. Traditional routes use liquid phase acids such as
HF or H₂SO₄ or Lewis acid metal halides such as AlCl₃ and BF₃. In these reactions, stoichiometric quantities of acids and/or halides are often needed and generate massive corrosive and toxic effluents. Alkylation reactions are, therefore, excellent targets for new cleaner chemistry.

There has been a significant development in the reactor design in liquid phase processes to lessen the environmental risks. In the original process, stirred tanks (mixer settlers with heat exchanger), operated in parallel to keep olefin concentration low, were used with HF being the catalyst. Figure 5 shows the schematics where HF is recycled with an external pump. Due to HF use and leaky seals on the pump and reactor mixing shafts, this process is environmentally unfriendly. The newer reactor solved this problem by utilizing an HF internal recycle. This design accomplished mixing by utilizing the buoyancy force created in the mixture of a heavy (HF) and light phase (hydrocarbon paraffin-olefin mixture). Unfortunately, the process is still environmentally unfriendly due to presence of HF. The challenge is to develop a stable solid catalyst that will be effective and regenerable as the conventional HF/H₂SO₄ catalyst that is still employed worldwide.

Common types of solid acids are the Beta zeolites, ion exchange resins, such as silica, supported nafion and heteropoly acids such as tungsto-phosphoric acids. However, these catalysts are easily deactivated and must be reactivated each time. Hence, complex reactor types must be designed so that the reaction and regeneration activities can be combined. Circulating fluid beds, packed beds with periodic operation, stirred tanks with or without catalyst baskets and chromatographic reactors are types of reactors that have been considered. Figure 6 shows a circulating fluid bed which is similar in concept to the reactor used in maleic anhydride production.

In order to select the best reactor among these reactor types, reactor models based on hydrodynamics, kinetics and pore diffusion must be accounted for since transport resistances may play a significant role in reactor performance. Therefore, proper understanding of these factors is a must to interpret the product selectivity and extent of formation of waste products. An additional discussion of transport resistance is in Section 5.
4. Solvent selection

As a general guideline, for an improved process reactor design, the use of solvents should be reduced and benign solvents should be employed if necessary. With these guidelines in mind, much attention has been given to “green” solvents such as supercritical CO₂ (scCO₂) and ionic liquids with the hope that they will replace the current solvents that cause pollution.

scCO₂ is environmentally friendly as it is non-toxic, unregulated, and non-flammable. It is also preferable as it is ubiquitous and inexpensive. scCO₂ has been extensively used in oxidation reactions. However, scCO₂ based oxidations are limited by low reaction rates. Further the homogeneous catalysts needed in the reaction have limited solubility in scCO₂. Hence, the use of expanded advents is being advocated for homogeneous catalytic oxidations and currently there has been a shift in the research to use the CO₂-expanded solvents for many organic processes. Advantage of CO₂-expanded solvents is that the process pressure can be significantly lower compared to scCO₂. By changing the amount of CO₂ added, it is possible to generate a continuum of media ranging from the neat organic solvent to pure CO₂. Wei et al. have studied the solubility of O₂ in CO₂-expanded CH₃CN and found that it was two times higher compared to neat CH₃CN, resulting in maximizing oxidation rates. The authors also reported that conventional organic solvent was replaced up to 80%. Hence CO₂-expanded solvents look promising in replacing the current solvents that are not environmentally friendly. More research is still needed in this area to enable scale-up and commercialization.

Ionic liquids are solvents that have no measurable vapor pressure. They exhibit Brønsted and Lewis acidity, as well as superacidity and they offer high solubility for a wide range of inorganic and organic materials. The most common ones are imidazolium and pyridinium derivatives but also phosphonium or tetraalkylammonium compounds can be used for this purpose. Classical transition-metal catalysed hydrogenation, hydroformylation, isomerisation, dimerisation can be all performed in ionic liquid solvents. The advantages of ionic liquid solvents over conventional solvents are the ease of tuning selectivities and reaction rates as well as minimal waste to the environment. As with scCO₂, more research is needed in scale-up and
commercialization as well as in investigating different types of ionic liquid solvents for other catalytic reactions.

5. **Reactor Design**

Choice of reactor type should be made in the early stages of process and catalyst development. It should consider the kinetic rates achievable and their dependence on temperature and pressure, the transport effects on rates and selectivity, the flow pattern effect on yield and selectivity as well as the magnitude of the needed heat transfer rates. Then plug flow or perfect mixing is identified as ideal flow pattern that best meets the process requirements in terms of productivity and selectivity. The final reactor type is chosen so as to best approach the desired ideal flow pattern and provide the needed heat transfer rates. The reactor should not be overdesigned to reach the desired product selectivity and to minimize waste generation. Therefore, sophisticated reactor models have been developed as essential tools for reactor design and scale-up. For these models to be accurate, information on volume fraction (holdup) distribution, velocity and mixing of the present phases has to be known. This hydrodynamic information is then coupled with kinetics of the reaction and deactivation to develop a sophisticated reactor model.

There are several experimental measurement techniques to get information on velocity and turbulence parameters in gas-solid, gas-liquid, liquid-solid, and gas-liquid-solid systems. Computed Tomography (CT) and Computer Automated Radioactive Particle Tracking (CARPT) are non-invasive measurement methods well suited for providing information needed for validation of CFD codes and reactor model development. Figure 7 gives the schematics of these experimental techniques. CT experiments are used to obtain density distribution and CARPT experiments to obtain the velocity field and mixing information\textsuperscript{12,13}.

Hydrodynamic information obtained from CT and CARPT experiments can then be applied to reactor models. For example, for a liquid-solid riser, there are four reactor models at different sophistication levels: heterogeneous plug flow model (as the simplest), 1-D axial dispersion model, core annulus model and 2-D convection-dispersion model as the most complex. Each model requires an appropriate set of hydrodynamic parameters. The CT and CARPT provide these and combining this data
with the kinetics of reactions and deactivation of the catalyst, one can develop detailed models to guide the selection and design of catalytic riser reactors.

6. **Process Intensification**

Process intensification involves design of novel reactors of increased volumetric productivity and selectivity. The aim is to integrate different unit operations to reactor design, meanwhile operating at the same or better production rates with minimum pollution generation. To meet these goals, the practice involves utilization of lesser amount of hazardous raw materials, employing efficient mixing techniques, using microreactors, catalytic distillation, coupling of exothermic and endothermic reactions and periodic operations. As examples consider catalytic distillation and coupling of exothermic and endothermic reactions.

* Catalytic distillation:

Catalytic distillation has been employed successfully for ethylacetate, H₂O₂, MTBE, and cumene production. The catalytic distillation unit consists of rectifying and stripping sections as well as a reaction zone that contains the catalyst. The column integrates separation and catalytic reaction unit operations into a single unit therefore reducing capital costs. It is also beneficial in the fact that separation reagents that are toxic are no longer required. Since unreacted raw materials are recycled, less amount of feed is converted to products, thus reducing the use of harmful raw materials and waste generation. Significant energy savings due to utilizing the heat released by exothermic reaction for distillation is also another factor that contributes to this unit being environmentally friendly.

An application to ketimine production scheme using a catalytic distillation unit is illustrated in Figure 8. Condensation of ketones with primary amines results in the synthesis of ketimines given by the reaction scheme:

\[
\text{R-NH}_2 + \text{O} \quad \leftrightarrow \quad \text{R-N} + \text{H}_2\text{O} 
\]
The reaction is reversible and therefore equilibrium limited. In the conventional process, the reversible reaction can be pushed forward to products by employing drying agents such as TiCl$_4$, BuSnCl$_2$, Al$_2$O$_3$ and molecular sieves which remove the product water. By using catalytic distillation, ketones and amine react to produce ketimine. Excess ketones are recycled back and product water is separated via in situ separation. No drying agents are needed thereby making the process cost efficient and environmentally friendly.

**Coupling of exothermic and endothermic reactions:**

Using heat integration is another important guideline for improved reactor design and is another example of process intensification. Exothermic and endothermic reactions can be combined together in a reactor configuration to maximize energy conversation in the process. As an example, steam reforming of methane, an endothermic reaction (Reaction 1) can be combined with partial oxidation of methane, an exothermic reaction (Reaction 2).

\[
CH_4 + H_2O \leftrightarrow CO + 3H_2 \quad \text{(Reaction 1)}
\]

\[
CH_4 + \frac{1}{2}O_2 \rightarrow CO + 2H_2 \quad \text{(Reaction 2)}
\]

The coupled reactions can be carried out in a shell and tube exchanger design that improves the energy efficiency of the process. This leads to a compact design. By contrast conventional steam reforming require huge furnaces leading to large capital cost and loss of energy.

Additional examples of process intensification such as microreactors, disk and plate reactors and reactive membranes can be found at Tsouris *et. al.* and Reaction Engineering for Pollution Prevention book.
7. Environmental Impact Analysis

Once new chemical processes are developed, catalyst, solvent and reactor type selected using CRE methodology, the impact on the environment of the new chemical processes must be compared with the impact of conventional processes before implementation of the new process. Several tools such as Waste Reduction Algorithm (WAR)\textsuperscript{20,21}, Life Cycle Analysis (LCA)\textsuperscript{22} and Environmental Fate and Risk Assessment Tool (EFRAT)\textsuperscript{23} are available for environmental impact analysis. Much research is devoted to improve the accuracy of these tools and to develop a standard methodology.

The WAR algorithm is used for determining the potential environmental impact of a chemical process based on 9 different impact categories listed in Table 1.

Table 1. Potential environmental impact categories

<table>
<thead>
<tr>
<th>Physical Potential Effects</th>
<th>Acidification</th>
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<td></td>
<td>Greenhouse Enhancement</td>
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<td></td>
<td>Ozone Depletion</td>
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<tr>
<td></td>
<td>Photochemical Oxidant Formation</td>
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<td>Human Toxicity Effects</td>
<td>Air</td>
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<td></td>
<td>Water</td>
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<td>Soil</td>
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<td>Ecotoxicity Effects</td>
<td>Aquatic</td>
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<td></td>
<td>Terrestrial</td>
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Potential environmental impact is a conceptual quantity that arises from energy and material that the process takes from or emits to the environment\textsuperscript{24}. The impact categories listed in Table 1 are weighted according to local needs and policies, and the scores are normalized to eliminate bias within the database. The WAR is particularly useful for comparison of different existing processes but does not provide modifications that would minimize the waste. Application examples of WAR studies include methyl ethyl ketone production from secondary butyl alcohol\textsuperscript{24,25}, ammonia production from synthesis gas\textsuperscript{25}, and reactive distillation for butyl acetate production\textsuperscript{26}.
The LCA has been developed to understand and characterize the range and scope of environmental impacts at all stages within a product or process\textsuperscript{27}. LCA basically evaluates the process based on the boundaries of the assessment. Life cycle inventories for the inputs, products and wastes are evaluated for the system boundary. The results then can be compared for different chemical processes. LCA is very useful for global analysis shown in Figure 1.

EFRAT is a simulation package developed by the EPA. It is used to estimate the environmental and health impacts of chemical process design options through a combination of screening-level fate and transport calculations and risk assessment indices\textsuperscript{23}. EFRAT is a powerful simulation tool as it provides the process design engineer with the required environmental impact information, so that environmental and economic factors may be considered simultaneously\textsuperscript{23}.

CRE together with green engineering principles\textsuperscript{28} provide the key concepts in designing and operating chemical processes at sustainable conditions. The improved process, however, must also be examined under close scrutiny by using the tools mentioned above. The results must be compared to conventional processes to see if the overall environmental impact has been reduced.

8. **Summary and Conclusions**

In our road to achieving sustainability in production of materials and chemicals we must strive to eliminate pollution at the source, improve material and energy efficiency of our processes and use renewable resources. The best way to prevent pollution is at the source. Thus, if we want to have high tech processes that are “sustainable” and “green”, we must use chemical reaction engineering concepts to the fullest extent. The days when the chemist found a magic ingredient (catalyst) for a recipe and the chemical engineer tried in earnest to get its full potential expressed in an available ‘kettle’, must be replaced by the coordinated effort of the chemist to select the best catalyst and the chemical engineer to provide the best flow pattern and reactor. This effort requires the multi-scale CRE approach consisting of molecular, particle/eddy and reactor scale considerations.
Since the last decade, the chemical reaction engineers have been re-focusing on developing new technologies that prevent or minimize pollution rather than dealing with ‘end of pipe’ treatments. In order to develop such technologies, a quantitative understanding of reaction systems and transport properties on the reaction rates is a must. Furthermore, the physical properties of the catalyst and media are also determining factors in choosing the “right” reactor for an environmentally benign process. Hence, it is a multidisciplinary task combining chemistry, reaction engineering, environmental impacts and economics. This chapter outlined the multi-scale nature of the CRE approach starting from the molecular level at the atom efficiency to the process level at the scale-up of a reactor. Each scale is important in design and operation of a sustainable process. The combination of CRE approach with “green processing” principles should lead to the development of a sustainable chemical industry with minimal waste production.

Acknowledgements

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REFERENCES:


FIGURES

Figure 1. Schematic of chemical and physical transformations causing pollution or wastes.
Figure 2. Schematic of system boundaries. The first figure shows the global scale and the second one shows the plant scale. The reactor itself constitutes another boundary that chemical reaction engineers focus on.
Figure 3. Schematic of integrated multi-level CRE approach. All the above levels are important in design and operation of a successful reactor.
Figure 4. Circulating Fluid Bed reactor used for maleic anhydride production.

Figure 5. Reactor types for liquid phase alkylation process
Figure 6. Novel reactor type for solid acids.
Computer Tomography (CT) Provides Solids Density Distribution

Radioactive Particle Tracking (CARPT) Provides Solids Velocity and Mixing Information

Figure 7. Computer Automated Radioactive Particle Tracking (CARPT) and Computer Tomography (CT) experiments
Figure 8. Ketimine production by catalytic distillation.
MIBK: Ketones
EDA: Amine