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Environmentally conscious design of chemical processes and products: Multi-optimization method

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ABSTRACT

This paper presents an environmentally conscious integrated methodology for design and optimization of chemical process especially for separation process, whose energy consumption occupies more than 70% of the whole process. The methodology incorporates environmental factors into the chemical process synthesis at the initial design stage, which is totally different with the traditional end-of-pipe treatment method. Firstly, one rigorous model for simulation of multi-stages and multi-components separation process was developed, and based on our proposed environmental impact assessment method, the calculation methods of the reasonable economic and environment objective are constructed. Then one multi-objective mixed integer non-linear mathematical model was established by considering environmental and economic factors. Finally, the high non-linear model was solved by multi-objective evolutionary algorithm (non-dominated sorting genetic algorithm).

It is often difficult to find an optimum for a process that satisfies both economic and environmental objectives simultaneously. Normally, an arrangement of optimal solutions is obtained, which forms a non-inferior set. Identifying the optimum from this non-inferior set is subjective, depending on the preference of decision makers. In this paper, technique for order preference by similarity to ideal solution (TOPSIS) for identifying the set of optimal parameters is developed and used at the decision-making step, in which the preference relation for the decision-maker over the objectives is adopted by trade-off information between objectives.

The proposed methodology was highlighted through two industrialized processes, dimethyl carbonate production processes by pressure-swing distillation and extraction distillation process, respectively.

Keywords: Environmentally conscious; Process integrated; Multi-objective; Model; Green design

1. Introduction

Traditional process design and optimization often pay much attention to the economic profit, such as fixed capital investment, net present value, operation cost, and pay back period. The environmental impacts of process design have been given a lower priority, and generally are incorporated into traditional design as end-of-pipe treatment. Over the past decade, as a result of escalating environmental control costs and newly issued environmental regulations, industries are showing increasing interests in minimizing environmental impacts of process design and development. So the environmentally conscious design (ECD) methodology of a chemical process is imperative (Allen and Shonnard, 2001).

How can we incorporate environmental perspectives into the process design and optimization? In general, there are two main ways. The most common one is to treat environmental consideration as constraints on economic optimization, or

Abbreviations: TOPSIS, technique for order preference by similarity to ideal solution; NSGA-II, non-dominated sorting genetic algorithm; DMC, dimethyl carbonate; EHI, environmental hazards index; LCA, life cycle assessment; AHI, atmospheric hazard index; EIM, environmental impact of material flow; EIE, environmental impact of energy; EIP, environmental impact potential; GWP, global warming potential ozone; ODP, depletion potential acidification; PCOP, photochemical oxidation potential; AP, potential; NEP, nutrient enrichment potential; ETP, ecological toxicity potentia; HTPI, human toxicity potential by ingestion; HTPE, human toxicity potential by dermal exposure; PSD, pressure-swing distillation.

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treat environmental incentives as main objectives in process selection and design but overlook the economic feasibility. For example, Dantus and High developed an economic-based methodology to minimize waste and reduce energy consumption for the chemical industry by modifying existing processes while satisfying all of the environmental, product specification, and profitability constraints (Dantus and High, 1996). Soorathep and Masahiko presented a procedure to synthesize economically efficient separation process considering environmentally factors as constraint by hierarchical design method (Soorathep and Masahiko, 2004). Recently Cave developed the environmental hazards index (EHI) for the process selection (Cave and Edwards, 1997). But these approaches are mainly used in early stage design, cannot provide the detail design and assure the design to obtain a global optimal result (Chen et al., 2002). Another approach for environment benign design is to treat environmental requirements as objectives together with other objectives such as max profit, min operation cost and so on, to form multi-objective problem. For example, Ciric and Jia proposed a multi-objective optimization scheme for simultaneously minimizing waste generation and maximizing profits (Ciric and Jia, 1994). Although the latter approach is obviously more reasonably and powerful, however, it is difficult to find a suitable mathematical algorithm because of the highly complex nature of the process and the difficulty solution of the complexity model. The final solving strategy is often simplifying the model by some strategy or transferring multi-objective optimization (MO-O) model into a single objective optimization problem, for example, Ramzan and Witt proposed one systematic and effective procedure for solving multi-objective decision-making problems, which consists of four stages/layers. This method simplified the problem scale effectively, which provides the new ideal for the solution of complexity and conflicting nature of multi-objective decision-making (Ramzan and Witt, 2006; Ramzan et al., 2008). For example, AHP (Chen and David, 2004), concept of relative importance degree (Sun et al., 2004) and so on were used. Lou developed hierarchical Pareto optimization methodology, which provides a systematic and flexible framework to solve multi-scale, multi-dimensional problems, and also provides clear guidance for improving process sustainability (Lou and Singh, 2006). Recently, a multi-objective evolutionary algorithms (NSGA-II) was used for multi-optimization of crude distillation unit (Inamdar et al., 2004), which provides the possibility for solution of complex model, but in the study the environmental impact was not considered.

So another key problem for the latter approach is how to find a suitable environmental objective that can reflect the whole environmental impact of the process. Minimizing waste generation, environmental penalties (global emission) (Cabezas and Douglas, 1999), mass of pollutant of concern, total mass of waste (Ahmad and Barton, 1995) and so on are often adopted as environmental objective in the early stage especially in 1990s. Recently, several systematic methodologies are available for the detailed characterization of the environmental impacts of chemicals, products, and processes, which include life cycle assessment (LCA) (Lou et al., 2004), the environmental fate and risk assessment tool (Achour et al., 2005), the atmospheric hazard index (AHI) (Gunasekera and Edwards, 2003), thermodynamic analysis method (emergy and exergy) (Hau et al., 2007; Yi and Bakshi, 2007; Bakshi, 2002). In fact, the environmental impact of a chemical process not only contains the material involved in the process, but also the energy consumption, the effect of flow recycle, percent conversion and so on. So the assessment of environmental impact is a complexity problem, it has not a uniform criteria till now (Daniel et al., 2004; Michael and Julian, 2004).

In this study, the impact assessment methodology is presented based on our environmental impact indices database. Detailed characterization of environmental impacts of chemicals and energy is proposed, which provides a guidance in design and optimization of environmental benign process design. Based on our developed rigorous simulation model and environmental impact assessment method, one multi-objective mixed integer non-linear mathematical model was established, then was solved by multi-objective evolutionary algorithm (non-dominated sorting genetic algorithm). A range of optimal solutions is obtained. The technique TOPSIS for identifying the set of optimal is used and developed at the decision-making step, in which the preference relation for the decision-maker over the objectives is adopted as trade-off information between objectives. Lastly, the proposed methodology was highlighted through two dimethyl carbonate production processes.

2. Framework of the integrated methodology

The integrated methodology contains three main steps, model construction, solution and decision-making for the optimum solution.

2.1. Model construction – Step 1

In this step, the process system model and environmental impact assessment model will be constructed and illustrated.

2.1.1. Process system model

All the potential separation techniques, such as distillation, membrane, extraction distillation, crystallization and so on, suitable for separation of the specific mixtures are collected in database, the separation models were developed (Douglas, 1988) Based on the feasible separation methods, the superstructure is established, in which we can use the value 1 or 0 to decide selection. The detail explanation is shown in the cases.

2.1.1.1. Economic function. The objective of any industrial process is obviously, profit maximization, as outlined by Cutler and Perry (1983). Hence, the profit function is a natural choice as an objective function, such as fixed capital investment, net present value, operating cost, and pay back period. Details of the study are given below.

Profit function: the profit function ϕ is calculated as follows:

$$\phi = P_1 - P_2 - \text{Operation cost} - \text{Depreciation cost} \quad (1)$$

(A) P_1 = Income of the products ($/year)

$$= \sum_i \text{Prod}_i \times \text{Price}_i; \quad i = 1, 2, \ldots, n$$

Prod_i: draw rate of product i (kg/year)
Price_i: price of product i ($/kg)