# A Multiscale and Multiobjective Approach for Environmentally Conscious Process Retrofitting

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*Introduction*

Industrial society is increasingly recognizing the need for shifting to more sustainable activities. Business leaders have begun to realize that such changes are not only essential to prevent adverse social and environmental impacts, but also to assure the long term survival and success of their enterprises (Holliday, 1999). Sustainable practices can benefit a business directly by increasing its tangible financial value through costs and risk reduction, increasing efficiency and capital conservation; or by building up intangible value through reputation, strategic relationships, human capital, and innovation (Bakshi and Fiksel, 2003). This new direction in global thinking demands deep transformations in all organizations of society, including industrial, governmental and civil entities. Among the critical areas that need to change is Process Systems Engineering (PSE). There is a need for modifying the design and operation of existing processes and developing new products and technologies that minimizes environmental impact while still providing stimulating economic value to businesses. As part of these changes, other aspects of the process – such as resource consumption and environmental impact – must be included in the design process. In addition, since sustainability is a property of the entire system, design and assessment of industrial processes can no longer be studied in isolation, meaning that the system boundaries have to be expanded beyond the limits of the plant (Bakshi and Fiksel, 2003).

A formidable challenge lies in the development and adoption of a multiscale and multiobjective strategy, as opposed to the traditional narrowly focused cost-benefit analysis. As in process Life Cycle Assessment (ISO 14040, 1997), defining the system boundaries by including only the relevant processes may result in large truncation errors, while expanding it to include all interactions is computationally intractable. In practice, data and models are available at multiple spatial scales ranging from individual equipments and processes, to the supply and demand chains, to the economy and ecosystem. Nonetheless, indiscriminate combination of such models is prone to unreliable outcomes since data become more aggregated and uncertain at larger scales. This work presents a novel multiscale and multiobjective approach for utilizing available information at all these scales and providing the most comprehensive scenario on which process alternatives can be tested and better decisions at the plant scale be made. The multiscale approach is closely related to existing hybrid (tiered) LCA methods (Suh et al., 2004), but represents inputs and outputs in terms of cumulative exergy consumption (CEC) (Szargut et al., 1988). Contribution of labor and capital are also included in the analysis. Exergetic information at equipment and process scales is available from engineering analysis, while that at economy and ecosystem scales is obtained by combining exergy analysis with economic input-output analysis (Ukidwe and Bakshi, 2004).

The proposed methodology considers two objective functions: economic cost and cumulative exergy consumption of the process life cycle at multiple Scales. Trade-off between these objectives is represented via a series of Pareto optimal surfaces at various scales. These surfaces are obtained via data envelopment analysis. Case studies of a heat exchanger and a cogeneration system compare the proposed approach with existing methods, and highlight the benefits of adopting a multiscale and multiobjective view. Opportunities for retrofitting existing industrial systems are also identified via the proposed approach.

*Background*

Thermodynamic methods provide the means for objectively valuing ecosystem products and services. In particular, Exergy has been successfully used to describe many ecological systems (Jorgensen, 2002; Odum, 1996). *Exergy* or *Available energy* is the maximum amount of *work* that can be extracted when a system is brought to equilibrium with its surroundings, that is by means of reversible processes (Szargut et al., 1988). For instance, the exergy of a heat stream is the work that can be extracted in a reversibly-operated thermal engine, i.e. the fraction of the stream's heat content determined by the *Carnot efficiency factor*. As opposed to mass and energy, exergy is not conserved in real processes. On the contrary, exergy is lost in any process that involves frictional forces, heat conduction, mixing, chemical reactions, and other irreversibilities. Consequently, it is the ultimate limiting resource for the functioning of all processes.

Accounting for exergy losses provides powerful means of identifying and improving sources of imperfection. *Cumulative Exergy Consumption* (CEC) accounts for the exergy of all the natural resources consumed in all steps of the process and processes in the supply chain (Szargut et al., 1988). *Cumulative Degree of Perfection* (CDP) is defined as the ratio of the exergy of the final product(s) to the cumulative exergy consumed to make the product(s).

CEC faces similar challenges as Life Cycle Assessment; defining the system boundaries by including only the relevant processes may result in large truncation errors, while expanding it to include all interactions is computationally intractable. In practice, data and models are available at multiple spatial scales ranging from individual equipments and processes, to the supply chains, to the economy and ecosystem. The data and models used in this work are summarized below.

*Equipment Scale* – System boundaries include only the process of interest. Traditional process design methodologies (Turton et al., 1998; Douglas, 1988) and process simulation software provide most thermodynamic and cost data for this scale. Information at this scale is high with details available at each piece of equipment.

*Life Cycle Scale* – System boundaries include the process of interest and relevant processes in the supply chain. Thermodynamic data and models for a wide variety of common processes are available in the literature (see for example, Jimenez-Gonzalez et al., 2000; Jimenez-Gonzalez and Overcash, 2000) and as part of the library of most process simulation software, such as Aspen Plus. CEC data for common processes can be found in Szargut et al. (1988). Information at this scale is lower than at the equipment scale and is generally present for the entire process or clustered in sub-modules, but is rarely present for each piece of equipment.

*Economy Scale* – System boundaries include the whole U.S. economy. Economic and Physical data is typically available by regions or economic sectors. Ukidwe and Bakshi (2004) have calculated the values of CEC for the entire U.S. economy by using economic input-output data.

*Ecosystem Scale* – Ecological goods and services constitute the productive base that is essential for all industrial and economic activity. Accounting for nature's contribution is also important for determining the impact and sustainability of industrial activity. These contribution can drastically change the outcome of a decision, specially in comparative analyses, because many natural resources that are easier to harness have already undergone transformations in which nature has taken a low quality raw material into a high quality product (Hau and Bakshi, 2004b). Data at this scale is typically available as case studies (see for example, Brown and Bardi, 2001). Ukidwe and Bakshi (2004) have also calculated the values of CEC for the U.S. economy, in which nature's contribution is accounted for.

*Methodology*

The purpose of this approach is to identify the optimal values, from a sustainability standpoint, of the decision variables in a process design. Consequently, this paper considers two objective functions: Total Rate of Return (TRR) of the process and CDP. The optimization problem is solved at various levels of analysis: Equipment, Life Cycle, Economy and Ecosystem. The equipment level of analysis considers only the process of interest. The following levels consider broader system boundaries and incorporate data from the corresponding scales. At each level, CDP is the ratio of the sum of the exergy of the products to the sum of the exergy of the inputs to that particular system determined by the system boundaries. Trade-off between these objectives is represented via a series of Pareto optimal surfaces at various levels, thus avoiding arbitrary combinations until the final stages of decision making. This approach is described in detail by Hau and Bakshi (2004a).

The technique used to solve the multiobjective optimization problem in this approach is known as *Data Envelopment Analysis* (DEA) (Charnes et al., 1993). DEA compares the relative efficiency of different alternatives from a discrete set of the feasible region. By identifying the most efficient alternatives, DEA determines the optimal Pareto surface or set of non-dominated solutions.

*Case Study: The CGAM Problem*

The CGAM problem is a predefined problem of optimization used to compare thermodynamic-economic methodologies (Valero et al., 1994). The problem is a cogeneration system that delivers 30 MW of electricity and 14 kg/s of saturated steam at 20 bar. The system operates at steady state. Air is passed through a compressor and a preheater to achieve high pressure and temperature. The compressed air reacts with Natural gas in a combustion chamber. The combustion gases drive a turbine that produces energy to generate the 30MW of electricity and to operate the compressor. The combustion gases leaving the turbine are used as heating fluid for the air preheater and to bring 14 kg/s of liquid water to saturated steam at 20 bar. Ideal-gas mixture principles apply for the air and the combustion products. The fuel (natural gas) is taken as methane modeled as an ideal gas. The fuel is provided to the combustion chamber at the required pressure by throttling from a high-pressure source. The combustion in the combustion chamber is complete. Nitrogen is inert. Heat transfer from the combustion chamber is 2% of the fuel lower heating value. All other components operate without heat loss.

The decision variables selected for the optimization are the compressor pressure ratio, the compressor and turbine isentropic efficiencies, the temperatures of the air at the preheater exit and the combustion gases at the exit of the combustion chamber, and the mass flowrate of methane fed to the combustion chamber. Thermodynamic and economic data and models are provided by Valero et al. (1994).

Figure 1 shows the feasible region of the optimization problem at the four levels of analysis. Notice that the overall CDP decreases at higher levels of analysis. This is because the amount of exergy losses increase as the system boundaries expand. The sharp decrease in CDP from the Life Cycle level to the Economy level denotes the large amount of exergy consumed that is not capture at the life cycle level. Similarly, there is a sharp decrease in CDP from the Economy level to the Ecosystem level that indicates the large contribution from ecosystem services.

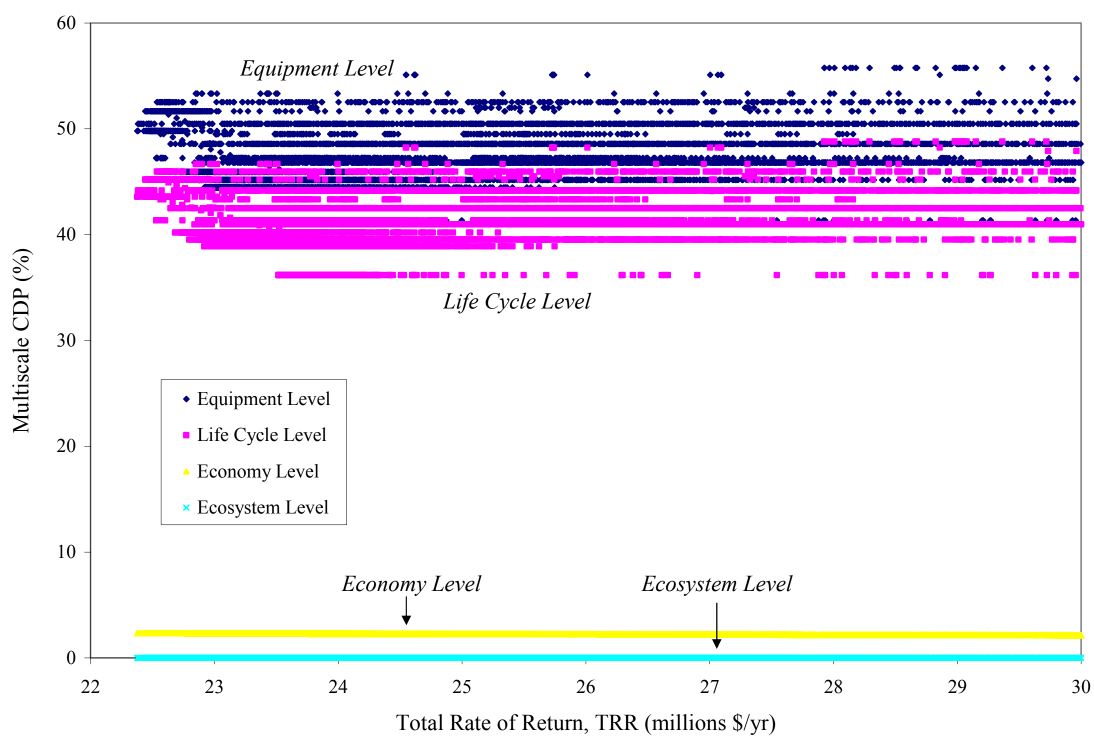


Figure 1: CDP vs. Total Rate of Return for the set of feasible solutions at all levels of analysis.

Figure 2 shows the results of the optimization problem for each level of analysis. There are not significant differences between the equipment and life cycle level. The set of solutions is identical in both levels, mostly because at these levels, CEC of capital investment and labor inputs are not considered and CEC of water and air is negligible when compared to methane. The economic optimal is located at the left extreme of the optimal surface. From the economic optimal value, it can be observed that higher efficiencies are achievable at higher costs. This increase is consequence of getting more efficient equipment that reduces exergy losses. At the economy level, the optimal surface is reduced to a smaller set of solutions, thus reducing the gap between the economic and exergetic optima. Notice that the feasible solutions are increasingly shifted down as the TRR increases in the figure. This is because CEC of capital investment and labor is included at this level. Consequently, the fact that more efficient equipment results in larger exergy consumption is reflected at this level. The optimal surface at the ecosystem level is also shown in Figure 2. The wide gap between economic and exergetic optima suggests that both objectives value different the inputs to the process and it makes clear that including the nature's contribution can greatly affect the outcome of current designs.

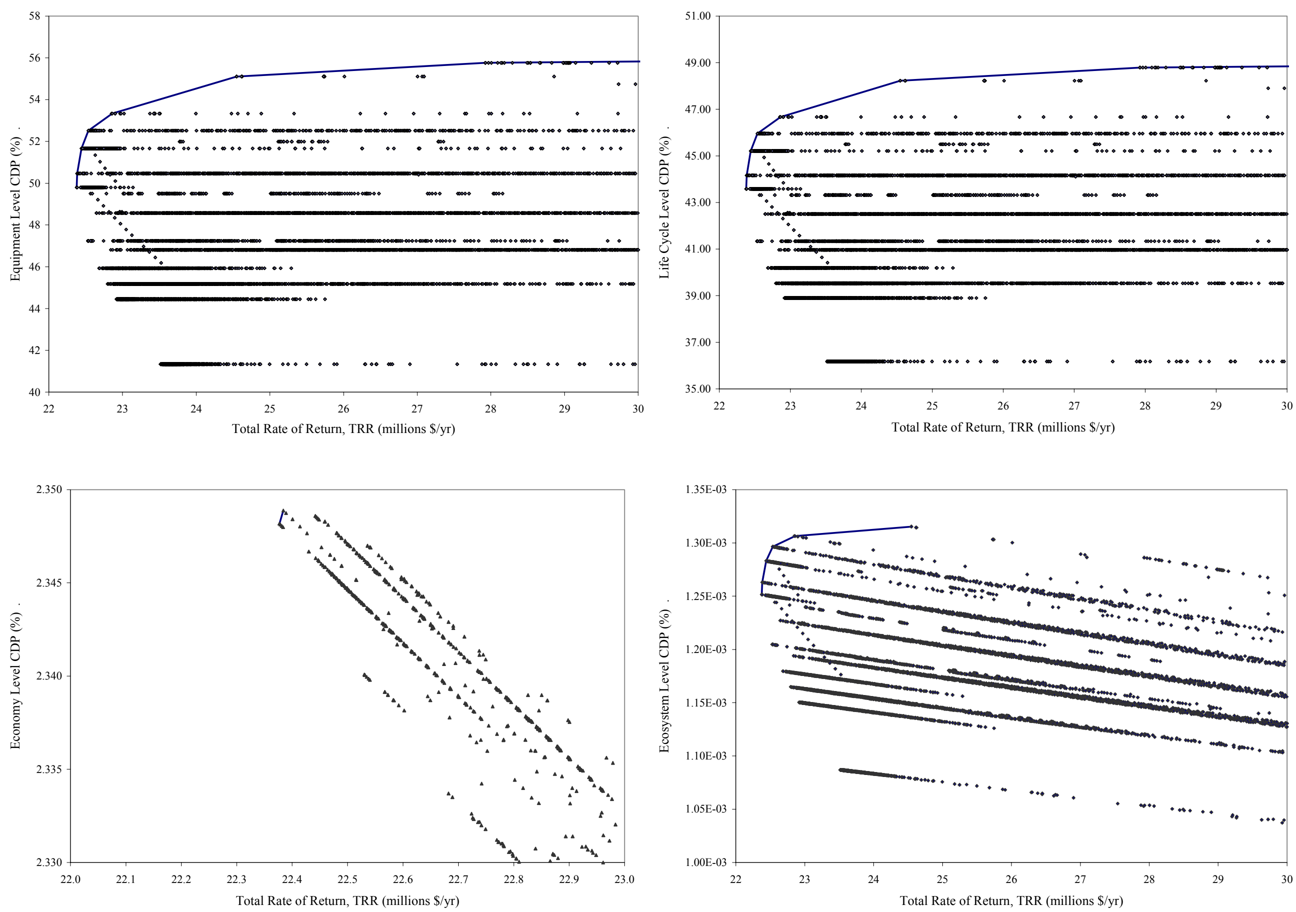


Figure 2: CDP-TRR Pareto Optimal Surface at the equipment level (top left), life cycle level (top right), economy level (left bottom) and ecosystem level (right bottom).

Summarizing, optimization of single objectives only shows extreme points. The proposed approach identifies the tradeoff between ecological and economic objectives as opposed to the traditional design methods. Arbitrary selection of system boundaries may result in large truncation errors. Benefits of the multiscale approach presented in this paper is that it is thermodynamically rigorous, it utilizes information at all scales and avoids arbitrary selection of system boundaries. Future work includes incorporating uncertainty analysis and LCA objectives at each level of analysis.

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