PROCESS ENERGY SYSTEMS: CONTROL, ECONOMIC, AND SUSTAINABILITY OBJECTIVES

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Abstract

Economic, energy, and sustainability metrics are key performance indicators for process operations. The relative importance of these metrics varies from plant to plant, and often some metrics are in conflict with each other (sustainability vs. profitability). In this paper we discuss the current plant environment and how various metrics can be aligned by focusing on energy efficiency. Power-steam systems are the major energy drivers for most plants, and we discuss possible operational changes that might improve energy efficiency, as well as the role of process control. Managing the interplay of real-time optimization and regulatory control is a challenge for the future, as well as interfacing with the implementation of smart power grids by the utility industry. Combined heat and power along with energy storage presents interesting control and optimization opportunities to maximize energy efficiency.

Keywords

Sustainability, energy efficiency, cogeneration, carbon dioxide, process operations, process control, smart grids

Introduction

The transition of the U.S. economy from a manufacturing-based economy to a service-based economy has been an accepted fact for the past 20 years, largely due to the lower cost of labor overseas, especially in Asia and South and Central America. However, given the slow recovery of the U.S. economy with lower than expected impact on reducing unemployment, the U.S. government is now making the revitalization of the U.S. manufacturing high priority. Reversing the trend of manufacturing decline in the U.S. may be aided by a number of new developments that will make manufacturing a strong component of the U.S. economy in the future (National Science and Technology Council, 2008; European Commission, 2009; Smart Manufacturing Leadership Coalition, 2011; National Association of Manufacturing, 2010; National Economic Council, 2011; Science and Technology Policy Institute, 2010). This resurgence in manufacturing also has implications for the process systems engineering (PSE) area.

- The United States is the world's largest market, and dynamic changes in customer preference happen with increasing frequency. Manufacturers who sell to end consumers are finding increased value in locating facilities close to their end customer so as to be able to react more quickly to changes in customer preference.
- The tsunami and nuclear incident in Japan, overall political volatility throughout the world, and weakness in emerging economy intellectual property and contract law are forcing companies to rethink the risks within their global supply chain.
- There is narrowing of the labor-related cost benefits of locating in East Asia compared with Western developed economies. China is experiencing cost increases of 15% to 30% for skilled labor, leading to shortages in skilled labor.
- We are leaving an era in which labor costs were the primary driver to determining the location of a manufacturing facility to an era in which proximity to a reliable energy source begins to take equal precedence. The United States is projected to have one of the largest national gas supplies in the world, which has positive implications for greenhouse gas emissions. According to the study, "Shale and U.S. National Security," from the Baker Institute for Public Policy at Rice University, the surge of drilling in shale formations will have an impact on global supply for years to come and limit the need for the U.S. to import liquefied natural gas, or LNG, for at least 20 to 30 years. Domestic production of shale gas will more than quadruple by 2040, from 2010 levels, and account for more than half of all U.S. gas production by the 2030s. The increased natural gas supplies will be used mostly in power production, but will keep feedstock costs low relative to other countries, thus giving U.S.

manufacturing a competitive advantage and allowing some reduction in greenhouse gas (GHG) production by the chemical sector.

- The implementation of smart (advanced) manufacturing, a topic covered in another paper at this conference by Davis and Sarli (2012), will help companies gain a competitive advantage. This implies a significant increase in the industrial use of computationally-enabled models to integrate data and knowledge in order to make dynamic decisions.

In this paper we examine the interplay of economic, energy, and sustainability objectives in the context of operations and control. We do not address the many design options to meet energy and sustainability objectives, but focus on the already built plant facility. We also do not address biofuel substitutions for commercial fuels or biorefineries in depth but mainly focus on the fossil fuel energy infrastructure that will dominate the process industries over the next 25 years. The next section covers the regulatory environment for carbon emissions followed by a discussion of maximizing energy efficiency of power/steam systems. The role of process control (sensor and control methodologies) in minimizing energy use is examined next. Then the emerging role of energy storage and smart grids is described, which provides an opportunity to access renewable energy sources such as solar or wind. Finally we address general sustainability considerations in operations.

Regulatory Environment for Carbon Dioxide

Increased levels of CO_2 have the potential to disrupt the climate and environment on earth. Already, increasing global temperatures have resulted in the melting of the ice caps and the destruction of habitat on the ice. While the actual impact of a changing climate is uncertain, it is the consensus of many nations that something must be done to reduce the amount of carbon dioxide emitted into the atmosphere. In the United States, there are three proposed policies that can reduce the amount of emitted carbon dioxide: an outright emission limit, cap-and-trade system, or a carbon tax (Hepburn, 2006; Stavins and Jaffe, 2008). Since 2009, the makeup of the U.S. Congress has changed considerably while economic recovery remains feeble. Due to the projected costs of carbon dioxide removal, there is little sentiment to penalize the U.S. economy with costly CO_2 regulations at the present time. Whether this will change in the future is unclear. However, even in the absence of such regulation, industry still will have incentives to save energy and reduce CO_2 emissions, because increased efficiency is a supportable goal both economically and environmentally. In addition, future regulations need to be anticipated.

As a first step to regulation of greenhouse gases (GHGs), EPA issued in 2009 new rules on “Mandatory Reporting of Greenhouse Gases” (to CFR part 98). Comprehensive nationwide emissions data will provide a better understanding of where GHGs are being produced, so that better policies to reduce emissions can be developed. Comparison of emissions from similar facilities can be made from these data. Businesses below 25,000 metric tons/year of CO_2 emissions will not be required to report emissions.

Although the process industries are energy-intensive, their contribution to total U.S. CO_2 emissions is relatively small (less than ten percent). Transportation currently contributes half, power generation about a third, and distributed heating by fossil fuels about a sixth (industry altogether is smaller than the building sector). Nevertheless, to meet proposed stringent greenhouse gas goals, the emissions from all of these sectors must be virtually eliminated (or offset). There would be some shifting among sectors (for example, increased electrification of transportation and distributed heating with that electricity made from nuclear, renewables, or fossil fuels with centralized carbon capture). Compared to existing chemical industry emissions, the chemical technology role in energy sector centralized carbon capture is far greater. The analysis of this entire undertaking cannot be done piecemeal, but requires a systems approach.

With federal legislation stalled for the foreseeable future, a number of companies have de-emphasized their plant sustainability efforts and replaced it with the normal profitability goals. On the other hand, some companies have continued to view sustainable manufacturing as a socially responsible action despite the lack of legislation. Reducing the carbon footprint of a manufacturing facility is still a credible goal, since it focuses on maximizing energy efficiency. Under the Kerry-Boxer bill, the U.S. levels of CO_2 emissions would drop to one-third of the 1990s levels, a very aggressive goal. This corresponds to less than one-sixth of present emission levels by 2050 and effectively implies a requirement to attack ALL emissions, notwithstanding the fact that global economic growth is projected to cause energy use to more than double in the same time period.

Most CO_2 emissions result from the combustion of carbonaceous fuels, with only a few percent coming from industrial chemical processes, primarily the production of lime and cement and to a lesser degree from unselective nature of partial oxidations (for example, ethylene oxide production). While most CO_2 results from the combustion of fossil fuels, the practice of clearing land and burning the removed accumulated biomass also adds significantly to current CO_2 emissions. The combustion of sustainably-grown biomass, e.g., annual crops or woody plantations, produces CO_2 emissions, but is generally considered to be carbon neutral and might avoid a requirement for mitigation; however, only a minuscule amount of energy is currently produced this way. The debate over crop competition aside, there is not enough renewable biomass growing in the entire country (wild plus cultivated) to meet our total current energy needs. This does not mean that sustainable carbon-neutral biomass cannot meet some energy needs in some specific locations, but cannot meet all of them.

Reducing the carbon footprint of chemical plants could involve two strategies: reduce the energy requirement of the chemical plant and reduce the carbon emissions associated with what remaining energy is required. Reducing chemical plant energy requirements generally involves three approaches: changing the processes to one involving less energy-intensive chemistry routes or less energy-intensive unit operations; changing the process to enable greater reuse of rejected energy (greater use of heat integration and co-generation) and changing the process to alter the relative requirement for thermal and electrical-mechanical energy. Furthermore, altering the lifecycle carbon footprint associated with energy production involves consideration of the efficiency of energy production (electricity or steam) itself.

On average, it is unlikely that energy conservation measures (process change, heat integration, etc.) will reduce chemical plant energy consumption more than an order of 10-20%. This implies that significant effort will be required to control CO_2 emissions from the utility system itself. Currently, virtually all chemical plant thermal energy comes from the combustion of fossil fuels, as does most of its electrical energy. Reducing CO_2 from utility systems is not now significantly practiced. Thus systems approaches will be essential to attack the problem.

Energy Efficiency and Power/Steam Systems

Manufacturing addresses the need to minimize energy usage while also providing tools for energy production, which itself is a process that is often co-located with the plant. Natural gas and biomass-based energy to make power and steam will play a dominant role in the process industries in the future. Advanced combustion systems using natural gas such as combined cycle can competitively produce low-cost electricity at efficiencies higher than those of current power plants. Additional carbon management strategies could include (1) fuel swapping (for example, substitution of less carbon intensive natural gas for more carbon-intensive coal with some derating of the boiler); (2) converting to non-fossil sources of energy (especially electrical energy) which now include hydroelectric and nuclear power and could also include wind, photovoltaic, or geothermal; (3) developing nuclear thermal process energy (assuming reliability issues can be resolved); and (4) capturing and disposing of CO_2 from fossil-fired energy systems. This includes using post-combustion flue gas treatment, oxy-fuel systems, or pre-combustion de-carbonization (gasification/shift or reforming/shift) and burning of the resulting hydrogen. The CO_2 would be stored underground, neutralized and stored in the ocean, or converted to industrially useful products. Each of these alternatives is extremely complicated and may have interactions, impacts, and implications from entities far outside the chemical plant, and all require very large scale systems analysis to understand ultimate benefits.

Current estimated costs for carbon capture and storage for coal power plants are several times greater than the cost of the fuel itself for a plant without capture. The U.S. has lived through discontinuities of this magnitude before (as when natural gas was decontrolled in the U.S. in the late 70s and early 80s), but in a globally competitive marketplace, carbon management requirements not applied to all parties will have immediate survival implications for companies in the international marketplace.

One promising conversion technology from a sustainability point of view is biomass gasification. Biomass is gasified with oxygen and steam to produce a medium Btu gas followed by catalytic water gas shift to convert all carbon monoxide to carbon dioxide, making more hydrogen. The gas is then cleaned to remove sulfur and nitrogen-bearing compounds and particulates prior to use as a chemical feedstock or for power production. This clean gas can be burned in a gas turbine followed by extraction of heat in a steam turbine (combined cycle) to produce electricity. Because the combined cycle approach can, theoretically, yield higher thermal efficiencies (biomass to electricity) than conventional combustion, there is much interest in this kind of fuel cycle. Another power alternative is medium Btu gasification of coal with combined cycle (Integrated Gasification Combines Cycle), which can also achieve overall fuel to electric efficiencies over 40%. However, in this technology the carbon dioxide would be sequestered underground after removal because the overall lifecycle is not carbon neutral (Adams and Barton, 2010).

The use of natural gas and biomass gasification for power production, cogeneration, or chemical production will grow significantly during the next 20 years. The incentive to use this new technology will undoubtedly hinge on its being cost-competitive, although changes in environmental regulations on emissions of sulfur, nitrogen, particulates, and ultimately carbon dioxide will affect bottom-line costs of all energy sources. For each emission type, natural gas and biomass-based gas are superior to coal. Sustainable energy solutions will be necessary to achieve the goal of zero emissions, which will in turn cause significant changes in how plants are designed and operated. Development and application of Process Systems Engineering (PSE) tools will be crucial to making such a transition, especially in the areas of real-time optimization, high fidelity models, improved sensors, and model-based controls.

With an existing energy base of coal-fired power plants in utilities and industry, it is important to examine the costs and efficiencies of removing CO_2 from flue gas. While the CO_2 emission rate of each individual coal-fired power plant is highly dependent on plant technology and type of coal, an emission rate of approximately 10,000 ton CO_2/day is typical for a 500 MW_e plant (Fisher et al., 2005). Coal is the largest electricity producer in the United States, accounting for nearly 50% of the total production (EIA, 2006). For this reason, coal-fired power plants have been recognized as the most important target for reducing point source emissions of CO_2.

Absorption/stripping using alkanolamine solvents is the benchmark technology for removing CO_2 from the flue gas of coal-fired power plants. It is a post-combustion technology, and a flowsheet describing its expected integration with a power plant is shown in Figure 1. This tail-end process could be installed with new plants, but it could also be retrofitted to current plants with few changes to the existing power plant. Most coal-fired power plants already use an electrostatic precipitator (ESP) to remove fly ash and flue gas desulfurization unit (FGD) to remove SOx. The absorption/stripping unit would treat the flue gas after exiting the FGD. After CO_2 removal, the cleaned flue gas travels to the stack, and the removed CO_2 is compressed for underground storage. The absorption/stripping unit uses low pressure steam taken from steam turbines in the coal plant. Electricity is used to run the CO_2 compressor and solvent circulation pumps.

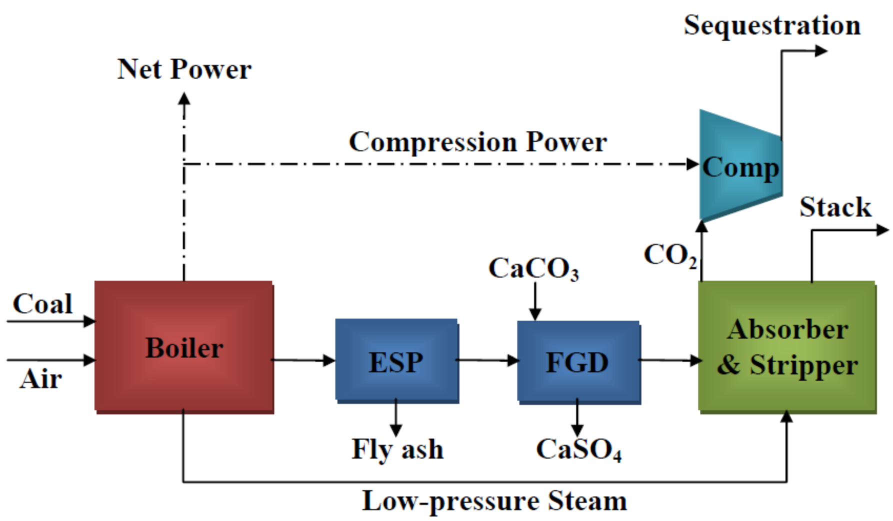

Figure 1. Absorption/Stripping as a post-combustion process for CO_2 capture from coal-fired power plants

In Figure 1, flue gas enters the absorber with approximately 12 mol% CO_2 and is counter-currently contacted by the amine solvent, which absorbs 90% of the CO_2 by a reversible chemical reaction. The treated gas is then sent to the stack. The rich solvent exits the bottom of the absorber and is heated by hot lean solvent in a cross heat exchanger, and then enters the top of the stripper. Steam strips the CO_2 from the solvent as it travels up the column. The lean solvent exits from the reboiler and is recycled to the top of the absorber after being cooled. Aqueous monoethanolamine (MEA) is the current standard solvent for CO_2 removal; removing 90% of CO_2 using MEA is possible with this technology, but the capital cost and energy requirement of current systems are currently prohibitive (Ziaii et al., 2009). The parasitic steam and electricity used for operating the pumps, compressors, and stripper-reboiler typically account for 30% of the total power plant output using current technology, a significant penalty. In order to be a practical solution for industrial CO_2 production, the total energy penalty must be reduced closer to the theoretical minimum based on Gibbs free energy calculations of about 12% (Rochelle, 2009), thus it is unlikely the flue gas treatment option is economically viable for the near future.

As a way to increase energy efficiency, combined heat and power (CHP), also known as cogeneration, concurrently produces electricity or mechanical power and thermal energy. In a conventional (e.g., non-CHP) system, electricity is generated at a power plant (usually operated by the local utility) and the waste heat from the system is vented via cooling towers or ponds. Facilities that get their power from the utilities then must use additional energy to provide their heating or cooling. CHP is one type of distributed power generation which has a major advantage over the traditional systems because it can utilize the waste heat to meet the heating and cooling loads of the facility (see Figure 2 for a comparison of the two alternatives). CHP therefore increases thermal efficiency and reduces greenhouse gas emissions. Currently only about one-fourth of the U.S. chemical plants use cogeneration with local power production.

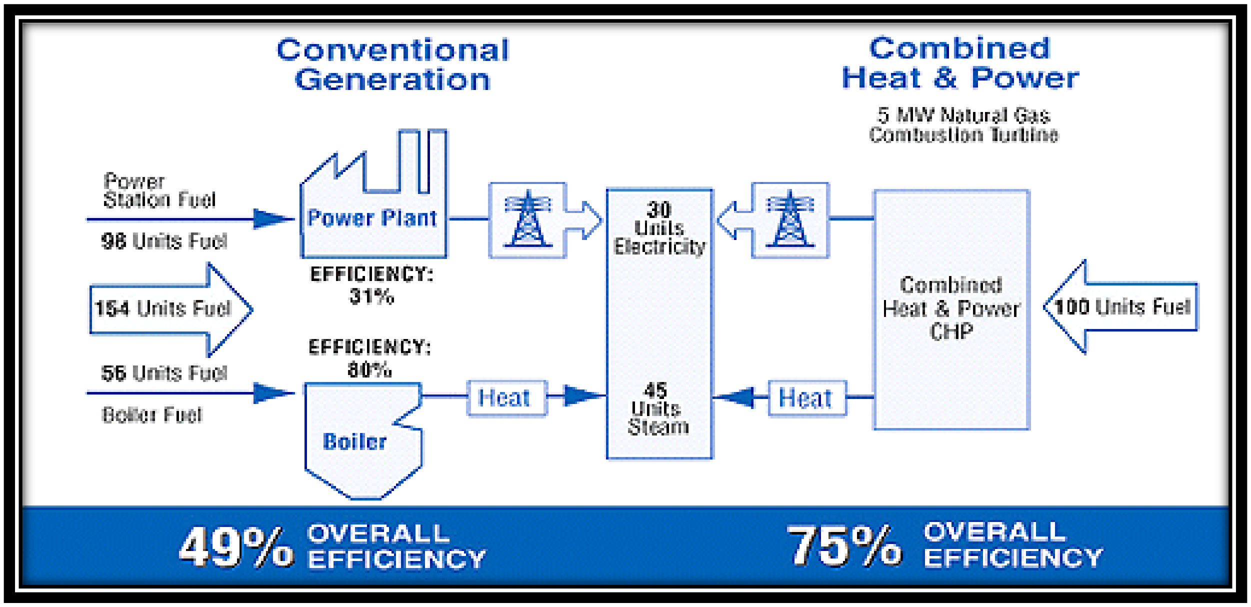

Figure 2 Comparison of energy flows for conventional generation vs. combined heat and power (cogeneration), Source: EPA.

CHP can come in a variety of configurations and use nearly any fuel. Because of the waste heat utilization, overall CHP efficiencies can be as high as 95%, though 70-85% is more typical. Conventional electricity generations systems (such as coal power plants) have efficiencies of 30-40%, and combined cycle power plants yield efficiencies of 45-50%. The size of CHP systems can range anywhere from 5 kW (the average demand of a single-family home) to hundreds of MW (typical of a major process facility).

An alternative combined heat and power system could use solid oxide fuel cells (SOFC) combined with a reformer and gas turbine (GT). The SOFC system can achieve high efficiencies over a wide power range (1kW – 100MW) e.g., 40-50% for SOFC, 60-70% for GT-SOFC, 80-90% for GT-SOFC + cogeneration. Fuel flexibility includes all fossil fuels, with natural gas being a preferred feed. It has low noise and emission levels. SOFCs are not in widespread use yet due to cost operability concerns. Reported lifetimes have yet to reach goals of 40,000 h, causing cost of electricity to be high. Tube microcracking, sulfur catalyst poisoning, carbon deposition, and air and fuel starvation decrease the lifetime of the SOFC system.

CHP is used in building complexes as well as in chemical plants and refineries. The University of Texas at Austin built its CHP plant in 1928 (Ontiveros, 2007). The plant has expanded over the years, and today provides 100% of the electrical, heating, and cooling loads for over 150 buildings totaling more than 16 million square feet. The power plant, which uses natural gas as its fuel, has 137 MW of CHP and can produce 1.2 million lb of steam per hour. The system also includes four chilling stations with a 46,000 ton capacity and over six miles of distribution lines. A 4 million gallon/10,000 ton-hour thermal energy storage system (TES) has been installed, which increases the plant's overall efficiency through more efficient chiller operation. The CHP system has been 99.9998% reliable over the past 35 years (Ontiveros, 2010). In 2009 the entire UT CHP system exceeded 90% efficiency. Virtually no electricity is required to cool the buildings. During the summer the cooling load is sometimes more than the waste heat can meet on its own, and when that happens additional boilers are operated to provide the extra steam to drive the absorption chillers.

The integration of steam and power systems offers additional means to reduce the costs of power and increase thermal efficiency. In some plants power is supplied both internally and from an external provider, which may have variable time-of-day pricing of its power. So it is desirable to optimize the production of power from within the plant and sell it back to the utility when it is cost-effective to do so. Figure 3 shows a schematic of such a steam-power system (Edgar, et al., 2001).

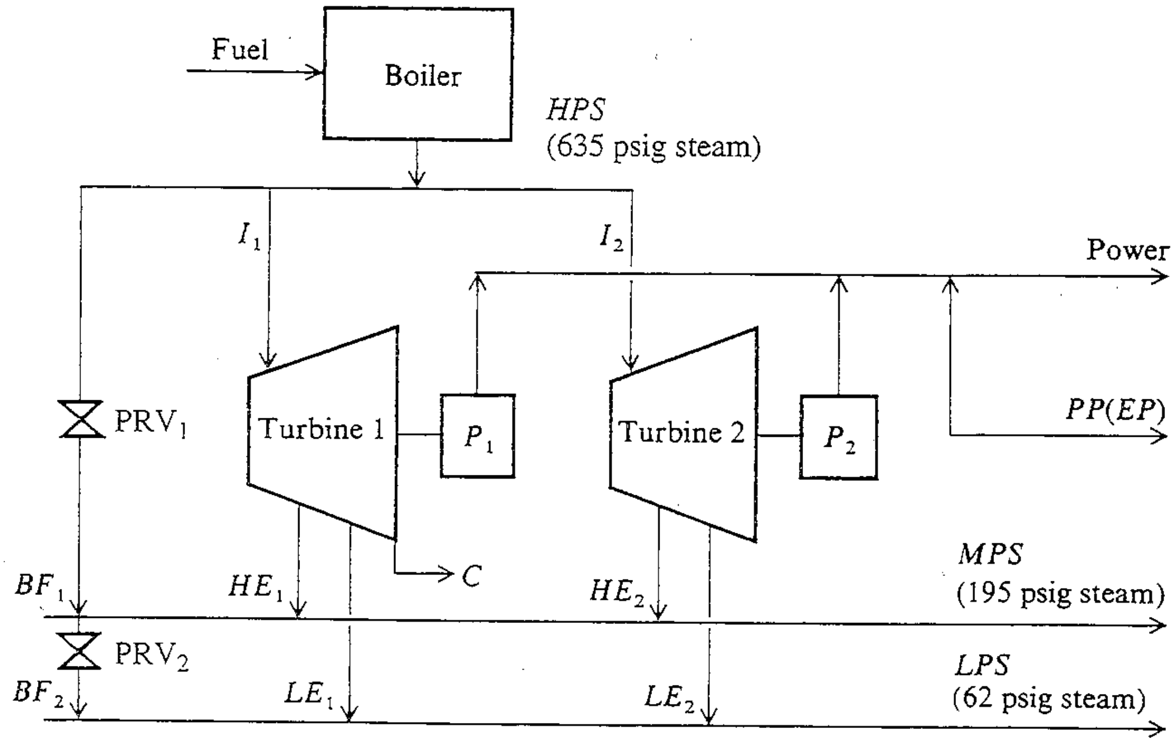

Figure 3. Steam-power system with power generation and/or purchase (Edgar et al., 2001).

To produce electric power, this system contains two turbo-generators. Turbine 1 is a double-extraction turbine with two intermediate streams leaving at 195 and 62 psi; the final stage produces condensate that is used as a boiler feed water. Turbine 2 is a single-extraction turbine with one intermediate stream at 195 psi and an exit stream leaving at 62 psi with no condensate being formed. The first turbine is more efficient due to the energy released from the condensation of steam, but it cannot produce as much power as the second turbine. Excess steam may bypass the turbines to the two levels of steam through pressure-reducing valves. To meet the electric power demand, electric power may be purchased from another producer with a minimum base of 12,000 kW. If the electric power required to meet the system demand is less than this base, the power that is not used will be charged at a penalty cost.

The system shown in Figure 3 may be modeled as linear equality and inequality constraints and combined with a linear objective function. The objective is to minimize the operating costs of the system by choice of steam flow rates and power generated or purchased, subject to the demands and restrictions on the system. The objective function is the cost to operate the system per hour, namely, the sum of steam produced *HPS*, purchased power required *PP*, and excess power *EP*. Therefore, this steam-power system is quite amenable to real-time optimization.

Nuclear power is an attractive option for electricity generation with a negligible carbon footprint, in spite of the recent accident at the Fukushima plant. Nuclear electricity is widely available (backed up by the grid) whereas nuclear-based process heat using multiple redundant small units have not yet been licensed. Some chemical processes could shift electrical energy from fossil energy to nuclear (or hydro or geothermal or solar/wind if storage technology were developed). This might increase the role for electricity-driven electrochemical reactions, vapor recompression distillation and other heat pump applications, and membrane and similar pressure gradient separations.

Minimization of Energy Costs via Process Control

Profitability is the criterion by which most if not all decisions are made in the chemical industry. It is necessary to quantify profitability mathematically in order to apply modern tools used in process design, operations, and control. However, when process control strategies are to be developed or changed, the key economic considerations, or business drivers, are not easily formulated by a single objective function.

Table 1 lists six business drivers used today for process control (Edgar, 2004). Different drivers have been emphasized at different times during the past 50 years. In the 1960s, a plant was considered successful if the products met customer specifications and could be manufactured reliably and more or less consistently (BD1). Automation systems in the 1970s utilized supervisory control based on rudimentary optimization tools to maximize profits, thus justifying the investment in computing equipment (BD2), but process dynamics and feedback control played no explicit role in determining economic feasibility. In the 1980s the statistical quality control movement focused on minimizing product variability in order to achieve profitability (BD3). The goal was meeting product quality specifications the first time, which eliminates the negative effects on profitability of waste, rework, blending, or off-spec products. Feedback control became a principal tool for achieving BD1. Meeting safety and regulatory requirements via process control became much more important during the 1980s as well. In the 1990s additional imperatives on manufacturing were added, namely that process equipment should be used fully (maximized asset utilization) and that the plant should be operated as flexibly as possible, in order to adapt to market, raw materials, and energy considerations (BD5). Improving the efficiency of information and control systems and workforce productivity became as added driving force in the late 1990s (BD6).

Table 1. 21st Century Business Drivers for Process Control (Edgar, 2004)

BD1.	Deliver a product that meets customer specifications consistently.
BD2.	Maximize the cost benefits of implementing and supporting control and information systems.
BD3.	Minimize product variability.
BD4.	Meet safety and regulatory (environmental) requirements.
BD5.	Maximize asset utilization and operate the plant flexibly.
BD6.	Improve the operating range and reliability of control and information systems and increase the operator's pan of control.

Recently there have been some additions to the list of business drivers. Sustainability (under the rubric of the triple bottom line) involves economics, environment, and social responsibility. In the context of chemical processes, these categories have been additionally refined to include such things as health and safety, raw material minimization, energy efficiency, waste minimization, environmental protection, water management, supply chain management, climate change mitigation, and biological feedstocks and/or processing. However, if these sustainability aspects are important, it appears that plants do not explicitly control for them.

Currently most plants do not control for energy minimization on a unit operation basis. Engineers may design for it, but there are no provisions to control for energy except in some plant-wide optimization studies. Design decisions are made for one chemical route over another, for type of separation technology over another, to enable heat integration, vapor recompression, or multi-effect operation. Engineers design for energy efficiency, but then do not control for it. Instead, utilities are the preferred method to reject disturbances. Plants control for plant production rate, and control for fitness for use characteristics (purity, molecular weight, color, component mass balances, etc., but generally adjust utilities to achieve these goals. Rarely are any of the available degrees of freedom consumed to control/minimize energy utilization. This is so prevalent that in most cases, individual users of utilities (steam to individual reboilers/heaters, cooling water to individual condensers/coolers, etc.) are not even measured or recorded although valve positions in energy flows are known. All too often, only the total plant utility use is measured (at the plant boundary) and that is generally for accounting purposes. Utility systems often are optimized separately from the plant because they have faster time constants than the process, and they may have integer variables (starting or stopping a boiler or a chiller), thus requiring mixed-integer programming.

Clearly, systems analysis approaches are critical in considering strategies to minimize energy. Energy conservation impacts plant performance or product fitness for use. Energy reuse (heat and power integration) may create unit and control loop interactions or decrease degrees of freedom that previously existed. Swapping thermal and electrical forms of energy can have unexpected utilities systems impacts. Attempting to control carbon emissions from energy production involves an entirely new set of technologies and processes that have very little existing experience base within the chemical industries. Beneficial impacts from this retrofitting are more likely to come from the design step than from operations.

For example, multieffecting a distillation column may halve the energy requirement, but one of the column temperatures (and pressures) will be much higher than the original design, possibly requiring a higher quality energy source or exposing the process to higher temperatures (and greater decomposition). In addition, the original single column is rarely suitable for either of the new multieffect columns. Similarly, adding instances of heat integration not only consumes degrees of freedom but also alters the path by which disturbances get rejected to ultimate utilities.

What if all individual uses of utilities could be easily measured? What could be done with this information? Are there additional degrees of freedom that exist or could be made to exist so that some of these other sustainability metrics (energy efficiency in this case) could be "improved" (assuming all other traditional production and fitness-for-use objectives were met)? How would such a control strategy be implemented? What kinds of computational tools/assets would be required? These observations hold for other aspects of sustainability. It is curious that we screen design alternatives for such things as lower energy consumption, lower waste generation, lower greenhouse gas generation, and similar objectives, but we rarely directly control or in real time optimize these factors during the process operation.

Figure 4 shows there are five levels of control activities in a manufacturing process where various optimization, control, monitoring, and data acquisition activities are employed (Seborg et al., 2010). Data from the plant (flows, levels, temperatures, pressures, compositions) as well as so-called enterprise data, consisting of commercial and financial information, are used to make decisions in a timely fashion. The highest level (level 5) deals with planning and scheduling, sets production goals to meet supply and logistic constraints, and addresses time-varying capacity and manpower utilization decisions. This is called enterprise resource planning (ERP). In a refinery the planning and scheduling model can be optimized to obtain target levels and prices for inter-refinery transfers, crude and product allocations to each refinery, production targets, inventory targets, optimal operating conditions, stream allocations, and blends for each refinery (Shobrys and White, 2002).

Regulatory control is carried out in level 3 (e.g., model predictive control or single-loop or multi-loop control). Level 2 (safety, environment, and equipment protection) includes activities such as alarm management and emergency shutdowns. Level 1 (process measurement and actuation) provides data acquisition and on-line analysis and actuation functions, including some sensor validation. The time scale for decision-making at the highest level (planning and scheduling) may be of the order of months, while at lower levels (e.g., process control), decisions affecting the process can be made frequently, e.g., in fractions of a second.

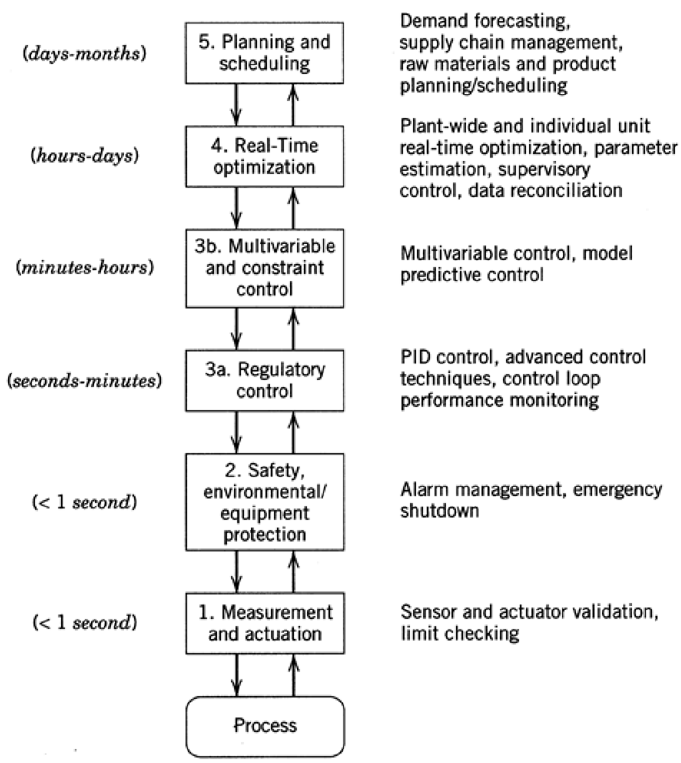

Figure 4. The five levels of process control and optimization in manufacturing. Time scales are shown for each level (Seborg et al., 2010)

For regulatory control the quadratic loss objective function used so frequently in optimal control could mislead researchers into thinking it is a meaningful economic measure of control. Unfortunately, the cost of deviation of a state variable (e.g., concentration) about a desired set point is usually different for positive deviations and negative deviations (profit reduction vs. off-spec product). The cost of control (*u*) can be zero or can correspond to the cost of utilities, which may be significant. When only positive control changes incur a significant cost (and negative control changes reduce costs), a quadratic objective function is not appropriate except in some fortuitous cases where the control effort is positive for all time, thus giving economic meaning to a quadratic term. In general this will not happen, because a well-tuned output response will yield overshoot and some oscillations in both state and control variables. Figure 5 (Downs and Doss, 1991) shows how the utility stream exchanges temperature variations in the reactor feed stream to reduce variability in the ultimate product. Explicit control weighting in the objective function for optimal control can be eliminated by adding a quadratic term involving *du/dt*. Thus control effort is ignored but changes in the input are penalized. This approach affectively incorporates integral control into the overall feedback control law, a desirable attribute leading to no offset from the target. Penalizing the rate of change of the control induces more inertia into the controller, causing it to change position less often, which is desirable because constant adjustment of a control valve causes faster valve wear (a hidden cost).

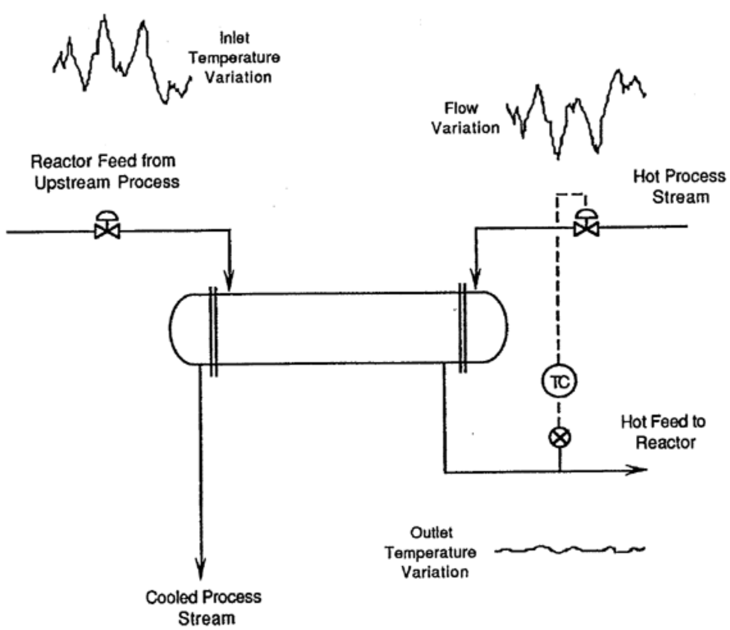

Figure 5. Transformation of variation from the temperature to flow for a reactor feed preheater (Downs et al., 1991)

Significant potential benefits can be realized by using a combination of MPC and RTO. At the present time, most commercial MPC packages integrate the two methodologies together in a hierarchical manner (see Fig. 4). The MPC calculations are imbedded in the prediction and controller blocks and are carried out quite often (e.g., every 1-10 min). A prediction block predicts the future trajectory of all controlled variables, and the controller achieves the desired response while keeping the process within limits. The targets for the MPC calculations are generated by solving a steady-state optimization problem (LP or NLP) based on a linear process model, which also finds the best path to achieve the new targets (Backx, 2002). These calculations may be performed as often as the MPC calculations. More recent contributions to the idea of "economic" control have been made by Kadam and Marquardt (2007) and Angeli et al. (2011).

Linear model predictive control based on a quadratic performance index has been successfully applied to many continuous plants, which has encouraged the consideration of control strategies based on nonlinear fundamental models. Backx (2002) has stated that the performance and robustness of the control systems are directly related to the quality and accuracy of the prediction models in the control scheme. It is important that the models describe all relevant process dynamics and cover the full operating range, consisting of operating points as well as transition states or trajectories, which may not be possible with linear models. To generalize further, one can define objective functions that include profits earned along a trajectory plus a capital inventory term. For continuous processes this permits computing an optimal transition between operating conditions (e.g., grade changes) or the optimal path to recover from disturbances to the normal operating point. The control strategies based on an explicit economic objective function can change depending on different prices for product quality and on market conditions.

Earlier the fact that energy is not monitored loop by loop was noted. In many cases of steam or cooling water flow as the manipulated variable, often the valve position is known but there is no meter on the specific flow rate. Of course it would be valuable to be able to monitor these individual energy flows and determine when they are different than what is expected day-to-day. The addition of sensors or manipulated variables would allow one to optimize energy use in a real-time fashion. One example could be the monitoring of flooding conditions in a column. As is well known, flooding conditions need to be avoided, but if one could operate near the flooding point by manipulating reflux flow, then separation yield (tray efficiency) could be maximized, with the optimum balanced between composition improvement and energy usage. This approach is different than cases where RTO is applied (typically by optimizing steady state conditions).

This idea could be extended to individual tray efficiency if additional MV's could be added (multiple feed points, bypasses, etc.). But of course this extra cost needs to be justified based on possible energy savings. The Dzyacky flooding predictor is a soft sensor approach to keep column throughput at a maximum and has been demonstrated to achieve 6 to 7% increase in throughput. The Dzyacky flooding predictor evaluates time derivatives of typical process variables such as pressure drop, bottom temperature, level, and flow rates to predict when the column will flood, and then keeps operations just below the flood point. The predictor is based on tracking of patterns of column variables which are highly repeatable prior to a flooding event and in testing showed a 6% increase in feed rate over the conventional approach.

Smart Grids and Energy Storage

In a previous section we focused on the case where the plant generates power and steam locally by cogeneration. However, most plants rely on power generated by a utility. Today's electric grid was designed using technologies that were state of the art more than a century ago. While these technologies have been largely able to meet 20th century needs, today's aging infrastructure and antiquated technologies need significant investment for upgrades and improvements. Most utilities plan to invest in updating the grid using modern technologies (including advanced automation), innovative market structures, and a smart grid design that has the potential to improve system reliability, reduce environmental impacts, and enable end-users to affordably reduce energy consumption.

A smart grid has the following attributes:

1) Electric power is delivered using two-way digital technology and automation with a goal to save energy, reduce cost, and increase reliability.
2) Power is generated and distributed optimally for a wide range of conditions either centrally or at the customer site, with variable energy pricing based on time of day and power supply/demand.
3) Increased use of intermittent renewable power sources such as solar or wind energy along with energy storage capability requires improved automation to manage the complex, dynamic system.

In a sense, the scheme shown in Fig. 3 was a precursor to the current interest in smart grids. The amount of electricity provided in a large utility service region varies throughout the day and season. The minimum amount of electricity that is used at any given instant in time is called the base load. The maximum amount of electricity used is called the peak load. The daily peak load generally occurs in the late afternoon or early evening. In order to satisfy the variability of demand, electricity generators use power plant technologies that are geared to satisfy peak load versus base load. Coal, nuclear, and natural gas power plants are largely used to supply base load electricity demand. These plants are built to run 24-hours-per-day, for most days of the year. They are generally taken down only for system maintenance and require a significant amount of time to re-start. Hydroelectric and other renewable technologies are also used to supply some base load power needs (often replacing coal and natural gas generation), however, the intermittent availability of these resources can make them undesirable as base load providers because they are not considered "firm" or "dispatchable" power.

Peaking plants are designed to quickly meet sudden spikes in power demand throughout the day. These plants can start-up quickly, providing flexibility in the overall system. Most peaking plants burn natural gas. Some of these plants are referred to as "spinning reserve", because they are paid to stay on (spin), without generating electricity, in order to ensure that demand can be met without a lag period. In the absence of some energy storage innovation, temporally irregular renewable energy sources such as solar and wind will not contribute more than a few percent (perhaps five) of energy requirements before the distribution grid becomes unstable. This contribution might be increased through an advanced systems dispatch/consumption control approach to be developed in the future.

In order to deal with the higher expense of peaking power, three types of utility pricing can be instituted (IEEE, 2010):

1) Time-of-use (TOU) – fixed pricing for set periods of time, such as peak period, off peak, and shoulder
2) Critical peak pricing (CPP) – TOU amended to include especially high rates during peak hours on a small number of critical days; alternatively, peak time rebates (PTR) give customers rebates for reducing peak usage on critical days
3) Real time pricing (RTP) – retail energy price tied to the wholesale rate, varying throughout the day

Similar to the real-time optimization of steam/power systems discussed earlier in Figure 3, smart grids will mostly impact process plants that do not generate their own power. The variable prices of electricity will cause operating strategies to vary during the day to deal with the variable price of energy in changing set points. According to several companies contacted, they would change operating strategies to take advantage of time of day prices, i.e., generating excess power during the afternoon when prices are higher.

Combined Heat and Power plus Thermal Energy Storage

Thermal energy storage (TES) systems heat or cool a storage medium and then use that hot or cold medium for heat transfer at a later point in time. Using thermal storage can reduce the size and initial cost of heating/cooling systems, lower energy costs, and reduce maintenance costs. If electricity costs more during the day than at night, thermal storage systems can reduce utility bills further. Two forms of TES systems are currently used. The first system used a material that changes phase (latent heat), most commonly steam, water or ice. The second type only changes the temperature of a material (sensible heat), most commonly water.

TES economics are attractive for high utility demand costs, utility time-of-use rates (some utilities charge more for energy use during peak periods of day and less during off-peak periods), high daily load variations, and short duration or infrequent loads. When ice or chilled water are produced at night for use during the day, this shifts cooling demands to off-peak times (less expensive in areas with real-time energy pricing), which may be used take advantage of “free” energy produced at night (like wind energy). TES can store solar energy in thermal fluid to use when sunlight is not available. The combination of control systems with TES allows solar concentrating power plants to maintain a constant output over a 24 hour period (Powell and Edgar, 2011), so they are an important tool to deal with intermittent energy sources.

Thermal energy storage can be coupled with CHP (CHP-TES) to provide economic and energy savings, system flexibility, and system feasibility (see Figure 6) (San Man Lai and Hui, 2009). Thermal and electrical loads can be decoupled to some extent by adding TES to a CHP system. This has grown increasingly important as peak loads have grown, increasing the gap and variation in on-peak and off-peak electricity market prices. Proper design and control is necessary to realize the maximum value of a CHP system.

As one example of CHP-TES, a small system for a hospital located in Austin, TX includes a 4.3 MW combustion turbine, a natural gas compressor package, and a 13,500 lb/hr heat recovery steam generator (24,500 lb/hr with duct firing). In this case, the CHP system is owned and operated by the utility, which sells the electricity directly to the user and uses the waste heat to run chillers that provide chilled water. The CHP system produces 100% of the hospital’s power and hot and chilled water needs. The system also includes an 8,000 ton/hour thermal energy storage (TES) tank. When there is more waste heat than is needed to meet the heating and cooling loads, the extra waste heat is used to run chillers that cool the water in the TES tank. Then during peak times (e.g., the afternoon on a very hot day) this chilled water is used to meet the cooling load demanded by the user. Thus, the daily energy demand is leveled out and the combustion turbine can run 24 hours a day without wasting its process heat.

Both the hospital and the utility benefit from CHP-TES system in a number of ways. The hospital has more reliable power to support its power intensive systems, and rather than needing large battery systems to provide backup power, the hospital relies on the grid for its backup power. Also, since the hospital does not rely on the grid for power, it becomes an “island” from the grid. In the case of power outages due to hazardous weather or other conditions the hospital will be able to continue to function normally. The CHP system reduces the hospital’s carbon footprint by an estimated 10,900 tons per year and provides the hospital with $250,000 per year in energy savings. The utility also benefits because it was cheaper for them to build the onsite CHP facility that it was to expand its existing infrastructure. That is in part due to the fact that the CHP system has an efficiency of 75%, which is far better that nearly all of the utility’s producing facilities.

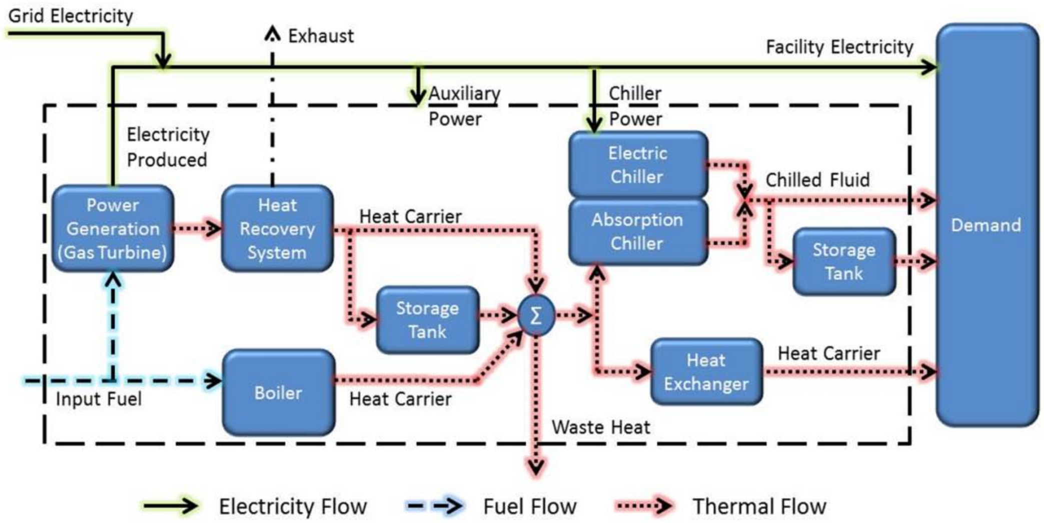

Figure 6. Schematic of CHP-TES system. The demand can be a heating and cooling network (Wang,et al., 2010)

Ristic et al. (2008) described the following conventional strategies for CHP systems with or without TES.

1. Electricity base load: The CHP unit is scaled to only meet the base electrical load. The CHP unit then runs at full capacity all the time. This has the advantage of operating the equipment at its most efficient operating point. However, it cannot take advantage of changing electricity prices.
2. Heat demand following: The CHP system follows the heat demand and electricity is treated as a beneficial by-product. This strategy may reduce auxiliary boiler requirements and ensures that there is never surplus heat that must be wasted. It cannot take advantage of changing electricity prices, and may in fact be negatively impacted by the price variation (of heat production is high when electricity prices are low, it may be more economical to operate a boiler to meet the heat load).
3. Electricity demand following: the CHP system follows the electricity demand and the heat is treated as a beneficial by-product. This strategy is typical when electricity export is not allowed. It also allows the facility to “island,” since all electricity can be produced on-site.

In heating and cooling networks that incorporate CHP, the CHP units produce electricity and use waste heat from the electricity production to meet heating and cooling loads. Typical standalone CHP units are generally operated using the heat demand following strategy. This means that CHP units may be producing large amounts of electricity (because thermal loads are high) during off-peak hours when electricity prices are low, thus reducing revenues. It also means that during on-peak hours, when electricity prices are highest, CHP units may either have to run at partial capacity (because of low thermal loads) or run at full capacity and waste the excess heat. Additionally, because the CHP units are required to follow a changing thermal load, they will not always be operating in their most efficient operating region (i.e., at or near full capacity). Thermal energy storage, almost exclusively in the form of chilled or hot water, has been applied to address these issues. That is in part due to the fact that the CHP system has an efficiency of 75%, which is far better than nearly all of the utility’s producing facilities.

Thermal energy storage has been shown to add significant economic savings to a CHP plant by taking advantage of the electricity rate structure, including the cost of storage. The savings came from maximizing electricity production during peak electrical times (thus garnering the higher electricity market price) and storing the excess heat in the TES. At night with the low electricity prices, the CHP system would shut down and thermal loads would be met by the TES. This results in an overall decrease in annual fuel consumption and electricity production as compared to the CHP only case (Fragaki et al., 2008; Streckiene et al., 2009).

A similar configuration can be installed at a chemical process facility. The CHP and TES units are scaled according to the facility’s thermal and electrical demands, number of operation hours, and the utility prices and pricing structure. Because electrical and thermal loads are not normally matched, deciding how much of each load to meet becomes an economic evaluation whose rules vary from facility to facility. For example, minimizing payback period generally leads to smaller equipment that only meets a portion of the electrical and thermal loads, but maximizing return on investment (ROI) leads to larger equipment that may meet the entire thermal load and a portion of the electrical load. Utility prices and pricing structure are the most significant factors in this economic evaluation. As utility costs increase, CHP-TES systems become more attractive and their economically optimal size increases. For CHP-TES units producing extra electricity, negotiations with the local utility company may be necessary for selling the excess power. The tradeoff between thermal and electrical capacities of CHP-TES also depends on the project goals. For example, if the facility needs to have the ability to island, then the electrical generation capacity must be able to match the electrical load. Efficient operation of a CHP system with TES requires skilled operators with a good understanding of the daily load profiles so that the storage system can be charged and discharged efficiently. There is need for research and development into control and optimization methods that most effectively use TES.

Sustainability Considerations

Sustainability usually refers to economic benefit, resource efficiency, environmental protections, and social development, which engenders a multiple objective function (criteria) perspective that may be difficult to apply in operations. In contrast to process/product design, where life cycle analysis can be applied, process operations are much harder to align with sustainability on an hour to hour basis, especially when some of the objectives may conflict with each other. In the context of RTO, it is possible to apply multiple-objective optimization methods, e.g., You et al. (2011). Metrics for sustainability have been developed by the Institution of Chemical Engineers, Glaxo-Smith-Kline Pharmaceuticals, and AIChE's Institute for Sustainability (IfS). However, the inability to make design modifications in an operations context is a major limitation to an operational focus on sustainability. BASF's eco-efficiency analysis deals with the trade-offs between economics and environment variables, using an environmental "fingerprint" diagram that includes variables such as energy consumption, emissions, toxicity, risk, resource consumption, and land use (Uhlman and Sabry, 2010). The fingerprint makes it easy to compare various alternative strategies, and the variables can span design, operations, and even supply chain, but usually the focus is on sustainable product development. Some subset of these variables could be used for RTO, but we are not aware of a company that has done so. Trade-offs of constraints on environmental variables vs. profitability could be examined easily in the current application of RTO, which can lead to a fingerprint that emphasizes only operations.

Conclusions

Key elements of sustainability including health and safety, energy consumption minimization, yield maximization, and environmental impact and emissions minimization especially of greenhouse gases are not only socially responsible objectives but may be in fact keys to regaining competitive advantage in the chemical manufacturing and allied process industries. Carbon dioxide mitigation in particular may not only be a sustainability objective, but may become the object of new governmental regulation. Current technology for carbon dioxide capture and sequestration, however, is very expensive. Therefore, initial responses to carbon management regulation will likely first concentrate on energy consumption minimization to achieve the corresponding reduction in carbon dioxide generation associated with energy production. Steam-power systems are a major target for increasing overall thermal efficiency.

Although sustainability issues are often a focus in choosing and optimizing among alternatives and conditions in the design phase of chemical process projects, they are rarely direct objectives in the operation and control of the resulting processes. Rather, energy and raw material consumption and emissions and waste disposal are often the independent variables manipulated to reject process disturbances and to maintain production rate, product quality, and other fitness for use attributes.

An increased emphasis on the control and optimization of sustainability issues during process operation is proposed. This emphasis may involve the installation of many additional process sensors, for example to monitor the utility consumption by every individual unit or the internal flows and compositions at every stage within a unit, complex real-time computer algorithms can analyze, interpret, and propose action based on this additional process information, and design modifications may generate additional degrees of freedom to enable operational manipulation to directly optimize sustainability parameters. This includes energy consumption, waste generation, and carbon dioxide emissions in addition to the usual business objectives of product fitness for use and cost. Increased coordination between utility companies and process industry plants will be necessary to realize the benefits of smart grid technology. Thermal energy storage with automation can help process plants take maximum advantage of CHP technology.

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