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An Energy Systems Engineering Approach to Polygeneration and Hydrogen Infrastructure Systems Analysis & Design

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Energy systems engineering provides a methodological scientific framework to arrive at realistic integrated solutions to complex energy problems, by adopting a holistic, systems-based approach. Such an integrated approach features:

- A superstructure representation — where alternatives in terms of energy technologies, raw materials and possible routes towards electricity & hydrogen, amongst others, are captured
- A mixed-integer optimization model — which allows for the development of a single mathematical model to represent all possible energy system alternatives within the superstructure, along with appropriate solution algorithms (MILP, MINLP, etc.)
- A multi-objective optimization approach — to simultaneously address and quantify the trade-offs amongst competing objectives, such as profitability, environmental impacts, energy consumption, and system operability
- An optimization under uncertainty strategy — to analyze the impact of technological uncertainties over a long-term horizon on the profit/energy consumption/environmental impacts of an energy system

In this paper, we will demonstrate the potential of energy systems engineering to systematically quantify different options at different levels of complexity (technology, plant, mega-system) through two real-life applications: (i) polygeneration energy systems, where a variety of fuel stocks, such as coal, natural gas and biomass, can be converted into a variety of products, such as electricity, transport fuels and chemicals, and (ii) hydrogen infrastructure planning problems, where the potential for using hydrogen as a clean sustainable fuel is assessed in some detail.

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1. Introduction

Energy is one of the most critical international issues at the moment and most likely to be so for the years to come. As part of the energy debate, it is becoming gradually accepted that current energy systems, networks encompassing everything from primary energy sources to final energy services, are becoming unsustainable. Driven primarily by concerns over urban air quality, global warming caused by greenhouse gas emissions and dependence on depleting fossil fuel reserves, a transition to alternative energy systems is receiving serious attention. Such a tradition will certainly involve meeting the growing energy demand of the future with greater efficiency as well as using more renewable energy sources (such as wind, solar, biomass, etc). While many technical options exist for developing a future sustainable and less environmentally damaging energy supply, they are often treated separately driven by their own technical communities and political groups.

Energy systems engineering provides a methodological scientific framework to arrive at realistic integrated solutions to the complex energy problems, by adopting a holistic, systems-based approach. Such an approach starts from a superstructure based representation of an energy system, where all possible primary energy feedstocks, conversion technologies, energy carriers, and potential combinations amongst them are captured. A mixed-integer optimization model is then built up to mathematically formulate the superstructure representation. Depending on the nature of the model, different algorithms are employed to obtain a optimum solution, for instance, mixed-integer linear programming (MILP) and mixed-integer nonlinear programming (MINLP). Based on the mixed-integer optimization model, a multi-objective optimization scheme can be set up, where system design or control can be optimized according to more than one objective, allowing simultaneously optimizing an energy system towards profitability, environmental impacts, and energy consumption rate. Moreover, impacts of inevitable uncertainties on system design and operation at the planning stage can be represented by applying an optimization under uncertainty strategy.

In this paper, we will discuss these methodologies and illustrate their applications in energy systems engineering through two real-life applications: polygeneration energy systems designing problems and hydrogen infrastructure designing problems.

2. Planning and Design of Polygeneration Energy Systems

Polygeneration is a potential cost-effective and environmentally friendly energy conversion technology to tackle serious energy and environmental problems faced by all human-beings in the 21^{st} century and to release the currently huge pressure on oil oriented liquid fuel consumption.

A polygeneration plant is a multi-in multi-out energy system that produces electricity, chemicals, and synthetic fuels. A generic polygeneration process, as can be seen in Figure 1, starts from gasification of coal, biomass, petroleum coke, or other feedstocks, and produces electricity and synthesis fuels via integrated power generation and chemical synthesis processes.

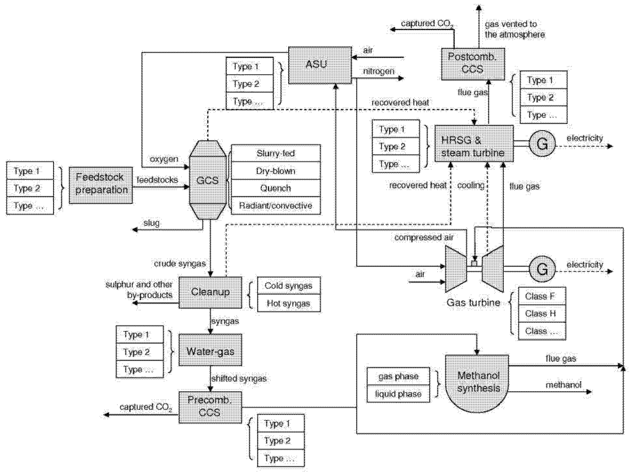

Figure 1. A superstructure representation of a polygeneration process

Despite of the benefits of a polygeneration process, for instance, high energy conversion efficiency and low/zero emissions (Ni et al., 2000; Liu et al., 2006), designing such a complicated and highly-integrated system over its long-term operating horizon considering both economic and environmental performances remains a challenging problem, with the following scientific issues to be solved:

- Many technical alternatives for each functional unit.
- High degree of integration among functional units.
- Trade-off between profitability and environmental impacts.
- Unpredictable behavior of the chemical synthesis unit due to different composition of inlet gas.

These problems have been tackled from both strategic level and process level. At strategic level, a polygeneration process is taken as a whole, and more focus is put on selection of feedstocks, products, technologies, investment planning and process capacity expansion (Liu et al., 2007a; Liu et al., 2007b). At the process level, a polygeneration plant is divided into several functional blocks, and mass and energy balances are established for each block. First principle formulations of chemical kinetics are also introduced for chemical blocks. Modelling and optimization at this level focuses on the selection of types of equipment and technologies and their combinations, process profitability and life-cycle assessment (LCA) based environmental impacts (Liu and Pistikopoulos, 2008; Liu et al., 2008).

2.1 Modelling and Optimization at the Strategic Level

Energy policy is of great significance to energy systems, especially to the development of renewable or sustainable energy. Policymakers usually need to establish policies based on detailed assessment of competing technologies and huge amounts of scenario analyses. However, this procedure could be greatly facilitated by superstructure based modelling and optimization.

At the strategic level, the operating horizon of a polygeneration plant is divided into several time intervals. Over a time interval, each alternative feedstock, conversion technologies, and product is denoted by a binary variable, representing their adoption in the plant. Other decision variables, for instance, production rate and process capacity, are represented by continuous variables. Process capacity expansion is also considered via changes of process capacity between time intervals.

This model is formulated as a MILP problem and implemented in GAMS (GAMS Development Corporation, 2008). A case study for the investment planning of polygeneration energy systems between 2010 and 2035 has been conducted. A technology roadmap with the capacity of each technology over the whole operating horizon is presented in Figure 2a. It shows that coal based polygeneration processes should be constructed in the first half of the horizon, whilst in the second half biomass based processes will replace the coal based ones as a result of technology improvement and decreasing price of biomass.

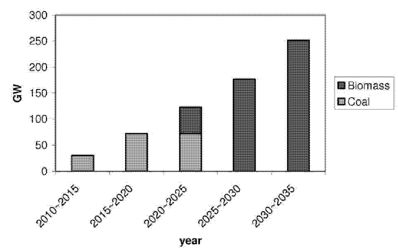

Figure 2a. Technology roadmap of polygeneration energy systems between 2010 and 2035

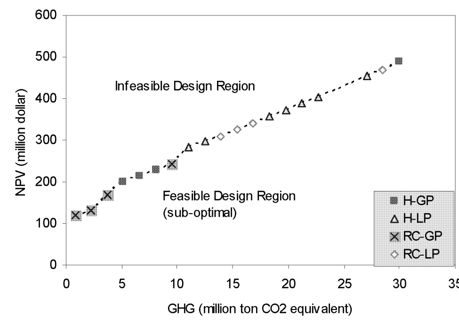

Figure 2b. Optimal design points of a polygeneration plant according to economic and environmental objectives

2.2 Modelling and Optimization at the Process Level

At the process level, a polygeneration plant is divided into several functional blocks, each having its own candidate technologies and types of equipment, shown in Figure 1. A plant represented by such a superstructure will be in operation over a long-term horizon. The whole operating horizon is divided into several time intervals. Time-variant parameters are denoted as piecewise functions over these intervals.

Mass and energy balances of input and output streams of each functional block are established. For the chemical synthesis block, chemical kinetics and phase equilibrium are formulated to handle the different mole compositions of inlet syngas resulted from different technologies implemented in upstream blocks.

Net present value (NPV) of the plant over its whole operating horizon is selected as an economic objective, whilst a cradle-to-gate life cycle assessment based GHG emission indicator behaves as an environmental objective.

A case study has been performed using the proposed methodology on a methanol/electricity polygeneration plant over a 15-year horizon. The mathematical model involves two objective functions, 9 binary variables, 1642 continuous variables, and 1781 equality and inequality constraints. It is solved in GAMS using BARON

solver to obtain a feasible starting point and DICOPT to continue. It takes 183 seconds of CPU time on a Pentium 4 platform to produce 20 pairs of optimal solutions.
The optimal solutions, as shown in Figure 2b, form a frontier that separates the feasible, or sub-optimal, design region and infeasible design region. A decision-maker can pick up any point from the Pareto curve as the process design, according to his specific requirements and interest.

3. Hydrogen Infrastructure Planning

Hydrogen is being promoted as an alternative energy carrier for a sustainable future. Its use as a transportation fuel in fuel cell vehicles could offer a number of attractive advantages over existing energy sources, especially in terms of well-to-wheel greenhouse emissions. However, the challenge of developing a future commercial hydrogen economy still remains as to establish energy efficient, environmentally benign and cost effective pathways to deliver hydrogen to consumers. This task is not trivial, given that a large number of technological options exist and are still in development for hydrogen manufacturing, storage, distribution and dispensing. Cost, operability, reliability, environmental impacts, safety and social implications are all performance measures that should be considered when assessing the different pathways.
This is another group of problems where superstructure based modelling and optimization methodologies could be of great help. A generic multi-objective MILP model for the strategic long-range investment planning and design of future hydrogen supply chains has been presented in (Hugo et al., 2005). This model can be readily applied to different scenarios, geographical regions and cases studies, and provide optimal technology roadmaps according to both economic and environmental objectives.
A superstructure, as shown in Figure 3a, forms the basis of the hydrogen infrastructure planning model, capturing existing infrastructure, large-scale centralized and small-scale distributed/on-site/forecourt production technologies, gas and liquid distribution technologies, and geographical site allocation.

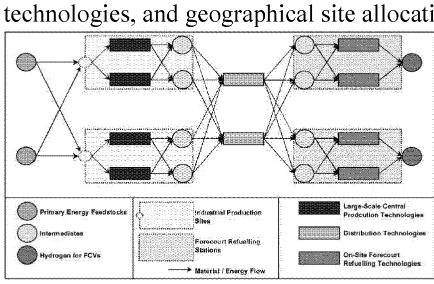

Figure 3a. Superstructure representation for hydrogen infrastructure planning

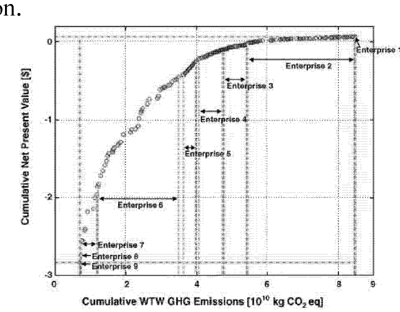

Figure 3b. Optimal trade-off results for hydrogen infrastructure planning

A case study has been performed for six potential production sites and six potential markets between 2004 and 2038. The optimal solutions are shown in Figure 3b. Each point on the frontier corresponds to a specific infrastructure design. A decision maker can pick up any point from the frontier according to their specific economic and environmental requirements. The optimal trade-off front can also be broken into critical enterprises based upon the different feedstock, production, distribution and refueling components of the supply chain.

4. Conclusions

Superstructure based modelling strategy, along with MILP and MINLP solution algorithms, are efficient and effective in solving energy systems engineering problems, especially at decision making and planning stage. Based on this, multi-objective optimization and optimization under uncertainty produces further in-depth analyses and allows a decision maker to make the final decision from many aspects of view. Applications of this methodology to polygeneration energy systems and hydrogen infrastructure planning problems prove its superior ability to solve large-scale real industrial problems and its great potential to be more widely applied in energy systems engineering field.

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