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Modelling, Investment Planning and Optimisation for the Design of a Polygeneration Energy System

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Abstract

The forecasted shortage of fossil fuels and the ever-increasing effect of greenhouse gas (GHG) emissions on global warming and environmental stability are two international problems with major technical, economic and political implications in the 21st century. Therefore, it is urgent to restructure present energy production and utilization systems in order to ensure that fossil fuels are used with high efficiency and low to zero emissions. Polygeneration energy systems combine power generation and chemical fuel synthesis in a single plant (producing both electricity and fuels) and thus provide a promising alternative pathway towards achieving sustainable and flexible economic development. Mixed-integer programming (MIP) is useful in constructing long-term decision models that are suitable for investment planning and design of polygeneration infrastructure systems. This paper presents a model for the investment planning of a polygeneration energy system, and uses this model for a case study addressing a system for production of methanol and electricity.

Keywords: polygeneration, energy, mixed-integer programming, optimisation.

1. Introduction and Motivation

Global energy consumption has been constantly rising since 1970: according to the U.S. Department of Energy (DOE) projections, this trend will persist in the future. Nevertheless, the global GHG emissions must be rapidly and significantly reduced: in fact, most countries (excluding the U.S.A.) had ratified the Kyoto Protocol by 2005. The latter requires that all participating nations take appropriate action to reduce GHG emissions below the respective 1990 levels, during the period 2008-2012 (DOE, 2006). This ambitious objective is obviously to be satisfied without impeding the quintessential economic growth.

A severe and lasting global energy problem is the shortage of liquid fuels. Worldwide proved oil reserves amount to 1293 billion barrels by 2006, and the daily consumption in 2003 was 80 million barrels (DOE, 2006): even if this consumption rate were not to increase, all global oil reserves would be depleted in about 44 years. Moreover, 57% of the oil reserves are found in the Middle East, the most politically unstable region around the world: thus, countries that depend heavily on oil importation need to seek diversification of liquid fuel suppliers to increase options and enhance national energy security.

A possible solution to these acute problems is to utilize efficient technologies. Power generation is the largest primary energy consumer, accounting for ca. 40% of the primary energy and using all energy resources (including coal, natural gas and oil). Consequently, it is a colossal source of GHG emissions, being the cause for the release of more than 7.7 billion tons of carbon dioxide (CO₂) annually; thus, power generation accounts for 37.5% of the total annual carbon dioxide emissions (Sims et al., 2003). Innovation in power generation technologies for higher efficiency and lower emissions has never ceased over the decades: the Integrated Gasification Combined Cycle (IGCC) combines a gasifier, a gas turbine cycle and a steam turbine cycle for power generation, delivering reliable performance but also increased efficiency.

Fortunately, oil is not the only energy source for the production of liquid fuels: they can also be synthesized from other fossil fuels (coal, natural gas, petroleum coke), as well as renewable energy sources (biomass). The resulting synthetic liquid fuels have the potential to substitute conventional, oil-based liquid fuels: for example, methanol (MeOH) and dimethyl ether (DME) can be successfully used in automobiles as gasoline and diesel oil, respectively.

Liquid fuel synthesis processes have similarities with combined cycle power generation: e.g., both processes require syngas (CO+H₂) as an intermediate product. These similarities indicate a possibility to co-produce electricity, synthetic liquid fuels, but also hydrogen, heat and chemicals in one process, with higher conversion efficiency that will result in lower polluting emission levels: this is the concept of *polygeneration*. A polygeneration energy system can improve profit margins and market penetration, decrease capital investment, reduce GHG emissions and increase feedstock flexibility crucially. A polygeneration energy system for production of MeOH and electricity (Figure 1) relies on coal or carbon-based fuels fed to a gasifier, where they react with oxygen to produce syngas; part of it is fed to a chemical synthesis plant to produce methanol, which can be sold, stored or transported to other plants for additional peak-time power generation. The flue gas from the

chemical synthesis plant, together with the other part of the fresh syngas flow, undergoes combustion in a combined cycle power plant to generate electricity.



Figure 1: A polygeneration energy system for producing methanol and electricity (NETL, 2003).

Polygeneration energy systems have many advantages over conventional standalone power or chemical plants: for example, the production cost for methanol can be reduced by 40% in a polygeneration plant co-producing methanol, heat and electricity. For a quad-generation plant co-producing syngas, methanol, heat and power, the reduction over conventional plants is 46% for syngas production cost, 38% for capital investment, 31% for operating cost per energy unit, and 22.6% for CO_2 emission (Ni et al., 2000). For a polygeneration plant coproducing DME and electricity, the DME production cost will be 6 - 6.5 \$/GJ, a figure that is comparable with conventional fuel prices (Cocco et al., 2006).

2. Previous Work and Current Challenges

A number of scientific publications address the mathematical modelling and simulation of polygeneration energy systems. However, they either focus on the evaluation of existing plants and technologies (Strickland and Tsang, 2003), on the configuration design of processes (Carapellucci et al., 2001; Ma et al., 2004; Cocco et al., 2006), or on the performance and operation of these plants (Yamashita et al., 2005; Liu et al., 2006). Research in large-scale investment planning for polygeneration energy systems has been limited, albeit clearly crucial for strategic policy-making in regions and countries. Systematic decision-making is an essential step in for any energy infrastructure project as it is a basis for determining whether a project should be initiated, which feedstock and technology must be utilized, and the total potential profit over the project life time. The goal is to select the best plan among many possible alternatives, according to explicit economic objectives, and subject to quantified technical and environmental constraints that vary by region. The research

procedure entails data compilation, process design and simulation, multiperiod investment and operation evaluation, and mixed-integer process optimisation.

3. Problem Definition and Mathematical Model Formulation

Mixed-Integer Programming (MIP) methods are suitable for modelling and analyzing polygeneration energy systems towards design, investment planning and optimisation: this algorithmic framework considers a superstructure of process alternatives (Figure 2), representing all possible process design choices for a system by binary (0-1) variables, while all the physical and economic quantities are expressed as continuous variables. All logical and physical relations are translated into equality or inequality constraints. The best plan can then be derived by conducting an optimisation for a specific objective function.



Figure 2: Mathematical model superstructure for the design of polygeneration energy systems.

A generic MIP mathematical model has been constructed and implemented in GAMS[®]. The objective function is the project's Net Present Value (NPV) over a fixed horizon. Firstly, the model divides the complete planning horizon into several time intervals: in each, it considers the set of available feedstocks, the set of available technologies, and the set of attainable products (the latter of course vary by process and are pre-specified). The model relies on exhaustive enumeration of possible energy production alternatives, connecting the elements of each set to the permissible elements of the next set and then activating the eligible groups of pertinent equality and inequality constraints; for every combination, it then calculates economic quantities within the time interval considered. Then, it summarizes the economic results in all time intervals and gets a NPV value. The procedure is continued for the next combination and its NPV (the largest is stored). When all possibilities have been evaluated, the optimal result (max. NPV) is obtained. The detailed discussion and a complete model description have been published (Liu, 2006). Table 1 presents the most important model equations for the present case study.

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Table 1: Model equations for polygeneration energy system design and optimisation (Liu, 2006).

$$\begin{array}{l}
\text{NPV}\\
\text{(Objective}\\
\text{function)}
\end{array}
\qquad \max_{t} NPV = \sum_{t} \frac{NetCashFlow(t) * Years(t)}{(1 + DiscountRate)^{n(t)}} \tag{1}$$

Capacity
$$\begin{array}{c} F(a,t) = FE(a,t), \quad t = t_{1} \\ F(a,t) = F(a,t-1) + FE(a,t) - FD(a,t), \quad t > t_{1} \end{array}$$
(2)

$$\begin{array}{l} \text{Capacity} \\ \text{expansion} \end{array} \quad 0 \le FE(a,t) \le Y(a,t)^* UpperLimit \tag{3}$$

Capacity $0 \le FD(a,t) \le (1 - Y(a,t)) * UpperLimit$ (4)decrease

Energy
onversion
$$\sum_{f} Fuel(a, f, t)^* Conversion Rate(a, p) = Product(a, p, t)$$
(5)

$$\frac{Product}{demand} \qquad \sum_{a} Product(a, p, t) \le Demand(p, t) \tag{6}$$

$$\frac{Fuel}{constraint} \sum_{f} Fuel(a, f, t) \le F(a, t)^* Operating TimePerYear$$
(7)

Fuel
supply
$$\sum_{f} Fuel(a, f, t) \leq FuelSupply(f, t)$$
 (8)

ment
$$Invest(a,t) = \left(\frac{Ref Invest(a)}{Years(t)}\right) \left(\frac{FE(a,t)}{Ref Capacity}\right)^{SizeFactor(a)}$$
 (9)

Fixed
cost
$$FixedCost(a,t) = \left(\frac{RefFixedCost(a)}{Years(t)}\right) \left(\frac{F(a,t)}{RefCapacity}\right)^{SizeFactor(a)}$$
(10)

 $VarCost(a,t) = \sum_{f} FuelPrice(f,t) * Fuel(a,f,t)$ Operating (11)

$$Income(a,t) = \sum_{p} ProductPrice(p,t)*Product(a,p,t)$$
(12)

$$\sum_{a}^{Net} NetCashFlow(t) = \sum_{a} \left(\frac{Income(a,t) - Invest(a,t)}{-FixedCost(a,t) - VarCost(a,t)} \right)$$
(13)

4. Case Study and Results Discussion

conv

Invest

cost

Incom

The case study using the model focuses on investment planning of polygeneration energy systems co-producing methanol and electricity in China between 2010-2035. Available feedstocks (4) include coal, domestic and imported natural gas, and biomass. A set of technologies (12) has been selected, and it consists of all possible alternative paths for transforming these primary energy feedstocks into final products (Liu, 2006). A subset of the selected technologies (6) are novel polygeneration flowsheet pathways, while the remaining (6) are conventional, stand-alone methanol synthesis technologies.

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Table 2: Technologies (unique flowsheet combinations) and abbreviations used in the study.

#	Technology			
1	COAL-LPMEOHe-CC-P			
2	COAL-LPMEOHm-CC-M			
3	COAL-GPMEOH-CC-M			
4	NG-SMRRMS-NONE-M			
5	NG-ATROTMS-NONE-M			
6	NG-ATRRMS-NONE-M			
7	BIO-LPMEOHm-CC-P			
8	BIO-LPMEOHe-CC-P			
9	BIO-LPMEOHhg-CC-P			
10	BIO-LPMEOH-SC-M			
11	BIO-GPMEOH-SC-M			
12	BIO-GPMEOHhg-SC-M			
Abbreviation	Explanation			
COAL	Coal			
COAL NG	Coal Natural gas			
COAL NG BIO	Coal Natural gas Biomass			
COAL NG BIO LPMEOHe	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity			
COAL NG BIO LPMEOHe LPMEOHm	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol			
COAL NG BIO LPMEOHe LPMEOHm LPMEOHhg	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol Liquid phase methanol synthesis with hot gas cleaning			
COAL NG BIO LPMEOHe LPMEOHm LPMEOHhg GPMEOH	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol Liquid phase methanol synthesis with hot gas cleaning Conventional gas phase methanol synthesis			
COAL NG BIO LPMEOHe LPMEOHm LPMEOHhg GPMEOH GPMEOHhg	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol Liquid phase methanol synthesis with hot gas cleaning Conventional gas phase methanol synthesis Conventional gas phase methanol synthesis with hot gas cleaning			
COAL NG BIO LPMEOHe LPMEOHm LPMEOHhg GPMEOH GPMEOHhg SMRRMS	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol Liquid phase methanol synthesis with hot gas cleaning Conventional gas phase methanol synthesis Conventional gas phase methanol synthesis with hot gas cleaning Steam methane reforming and recycle methane synthesis			
COAL NG BIO LPMEOHe LPMEOHm LPMEOHhg GPMEOH GPMEOHhg SMRRMS ATROTMS	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol Liquid phase methanol synthesis with hot gas cleaning Conventional gas phase methanol synthesis Conventional gas phase methanol synthesis with hot gas cleaning Steam methane reforming and recycle methane synthesis Auto-thermal reforming and once-through methane synthesis			
COAL NG BIO LPMEOHe LPMEOHm LPMEOHhg GPMEOH GPMEOHhg SMRRMS ATROTMS ATRRMS	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol Liquid phase methanol synthesis with hot gas cleaning Conventional gas phase methanol synthesis Conventional gas phase methanol synthesis with hot gas cleaning Steam methane reforming and recycle methane synthesis Auto-thermal reforming and recycle methane synthesis Auto-thermal reforming and recycle methane synthesis			
COAL NG BIO LPMEOHe LPMEOHm LPMEOHhg GPMEOH GPMEOHhg SMRRMS ATROTMS ATRRMS CC	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol Liquid phase methanol synthesis with hot gas cleaning Conventional gas phase methanol synthesis Conventional gas phase methanol synthesis with hot gas cleaning Steam methane reforming and recycle methane synthesis Auto-thermal reforming and recycle methane synthesis Auto-thermal reforming and recycle methane synthesis Combined cycle of gas turbine and steam turbine			
COAL NG BIO LPMEOHe LPMEOHm LPMEOHhg GPMEOH GPMEOHhg SMRRMS ATROTMS ATROTMS ATRRMS CC NONE	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol Liquid phase methanol synthesis with hot gas cleaning Conventional gas phase methanol synthesis Conventional gas phase methanol synthesis with hot gas cleaning Steam methane reforming and recycle methane synthesis Auto-thermal reforming and nec-through methane synthesis Auto-thermal reforming and recycle methane synthesis Combined cycle of gas turbine and steam turbine No electricity generation			
COAL NG BIO LPMEOHe LPMEOHm LPMEOHhg GPMEOH GPMEOHhg SMRRMS ATROTMS ATROTMS ATRRMS CC NONE P	Coal Natural gas Biomass Liquid phase methanol synthesis, suitable to produce more electricity Liquid phase methanol synthesis, suitable to produce more methanol Liquid phase methanol synthesis with hot gas cleaning Conventional gas phase methanol synthesis Conventional gas phase methanol synthesis Conventional gas phase methanol synthesis with hot gas cleaning Steam methane reforming and recycle methane synthesis Auto-thermal reforming and recycle methane synthesis Auto-thermal reforming and recycle methane synthesis Combined cycle of gas turbine and steam turbine No electricity generation Polygeneration of methanol and electricity			

Table 3: Key parameters of reference plants for all types of technologies considered in the study.

Technology	Capacity	Investment	Fixed cost
(abbreviation)	(GW)	(million \$)	(million \$/year)
COAL-LPMEOHe-CC-P	1.29	628	35.3
COAL-LPMEOHm-CC-M	1.29	594	39.9
COAL-GPMEOH-CC-M	1.29	496	31.9
NG-SMRRMS-NONE-M	0.744	429	23.6
NG-ATROTMS-NONE-M	0.705	369	20.3
NG-ATRRMS-NONE-M	0.716	326	17.9
BIO-LPMEOHm-CC-P	0.428	279	11.2
BIO-LPMEOHe-CC-P	0.428	288	11.5
BIO-LPMEOHhg-CC-P	0.428	323	12.9
BIO-LPMEOH-SC-M	0.432	256	10.3
BIO-GPMEOH-SC-M	0.428	322	12.9
BIO-GPMEOHhg-SC-M	0.432	271	10.8



Figure 3: Installed capacity of polygeneration technologies over the complete planning horizon.

The total installed power generation capacity in each time interval is shown in Figure 3. Two (2) technologies emerge as optimal throughout the planning horizon considered. The first technology, the coal-based Liquid Phase Methanol Synthesis (LPMeOH) integrated with a Combined Cycle (CC), is optimal in the beginning (denoted as *Coal*). The second technology, the biomass-based LPMeOH that is again integrated with a CC, is found to be optimal well into the first decade and thereafter (denoted as *Biomass*). Clearly, both these polygeneration technologies have overwhelming advantages over stand-alone technologies, since no conventional process flowsheets have been obtained. Results show that coal-based technologies appear superior during the first half, while biomass-based pathways emerge as optimal in the second half of the planning horizon. The advanced efficiency of biomass-based technologies is a possible underlying reason, but another (optimistic yet plausible) assumption made is that the price of biomass will gradually drop to a competitive level and reach carbon alternative in the near future. Both technologies tend to favour the production of more electricity than methanol, due to the relatively higher price of electricity than methanol (per unit energy produced). Another remarkable observation is that none of the natural gas-based technologies are selected, because of the stand-alone nature and the high price of natural gas considered. Clearly, the choice of polygeneration over conventional energy production is in principle influenced by a multitude of factors, and by the accuracy of price forecasting. Yet, a sensitivity analysis of model results with respect to several model parameters shows that the influence of each of the latter on optima are of quite different magnitude. For example, one parameter set found to have a significant impact on decisions is that of economic characteristics of products, such as the ratio of methanol to electricity price. The case study and our sensitivity analysis has found that stand-alone technologies are only favourable when electricity price drops to below 10 % of the methanol price. Another parameter set that has been found to be less important here is that of economic

characteristics of production technologies (e.g. capital investment and operating

cost). For the large-scale investment planning case study considered, the impact of these costs on investment decisions is negligible compared with the income generated by product sales, and thus have little influence on the optimal choices required for project and investment planning.

5. Conclusions and Future Goals

Polygeneration is a promising technology that can provide alternatives for solving the pressing global problems of fossil fuel shortage and greenhouse gas (GHG) emissions; it can enhance energy conversion and use many conventional and renewable resources. Attainable products include various liquid fuels that can replace gasoline and diesel oil, thus reducing oil requirements and enhancing energy security, especially in oil-importing countries. Furthermore, polygeneration schemes can generate many flowsheet configurations and thus allow for design flexibility that accommodates specific regional conditions.

Model simulation and Mixed-Integer Programming (MIP) optimisation show that polygeneration technologies are superior to conventional stand-alone technologies. Biomass-based polygeneration technology is the most preferable if biomass prices drop to levels similar to coal; moreover, in the current economic climate, polygeneration technologies that produce more electricity are more preferable due to high power prices. Natural gas-based technologies do not show any advantages because of their stand-alone nature and the high price of natural gas: using these technologies is advantageous only after simultaneous decreases of the natural gas price as well as the electricity to MeOH price ratio.

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