

# Modeling and optimization of polygeneration energy systems

Pei Liu, Dimitrios I. Gerogiorgis<sup>\*</sup>, Efstratios N. Pistikopoulos

*Centre for Process Systems Engineering (CPSE), Imperial College, London SW7 2AZ, UK*

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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 a case study addressing a system for production of methanol and electricity in China during the period from 2010 to 2035. It contains five different feedstocks and twelve polygeneration technologies.

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## 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 [1]. Nevertheless, the global greenhouse gas (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 [2,3].

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 [2,3]: 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 enhance national energy security.

One possible solution to the current acute energy and environmental problems is to utilize advanced, innovative – above all, efficient – primary energy 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 (CO<sub>2</sub>) annually; thus, power generation accounts for 37.5% of the total annual carbon dioxide emissions [4]. Innovations and improvements of power generation technologies for higher efficiency and lower emissions have never ceased to emerge and be licensed over the decades [5]. The integrated gasification combined cycle (IGCC), which combines a gasifier with a gas turbine cycle and a steam turbine cycle, is one of the most promising alternatives [6].

Fortunately, oil is not the only energy source for the production of liquid fuels [7]: they can also be synthesized from other fossil fuels (coal, natural gas and petroleum coke) as well as renewable energy sources (biomass) [8–12]. The resulting synthetic liquid fuels have the potential to substitute conventional, oil-based liquid fuels: for example, methanol (MeOH) and

<sup>\*</sup> Corresponding author. Tel.: +44 20 7594 6659; fax: +44 20 7594 6606.

E-mail address: [D.Gerogiorgis@imperial.ac.uk](mailto:D.Gerogiorgis@imperial.ac.uk) (D.I. Gerogiorgis).

dimethyl ether (DME) can be used as gasoline and diesel oil, respectively.

Liquid fuel synthesis processes have similarities with combined cycle power generation: e.g., both processes require syngas ( $\text{CO} + \text{H}_2$ ) 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 the overall capital investment cost, reduce GHG emissions, increase feedstock flexibility and alleviate the current grave dependence on crude oil and all refinery fuels. An exemplary polygeneration energy system for integrated production of methanol and electricity is shown in Fig. 1: coal or other carbon-based fuels are 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 [13], which can be either sold, stored in the plant for peak-time power generation, or transported to other power plants for 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 power generation plant to generate electricity [14].

Polygeneration energy systems have many advantages over conventional stand-alone 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  $\text{CO}_2$  emission [15]. In a polygeneration plant co-producing DME and electricity, the DME production cost will be 6–6.5/GJ, thus comparable with conventional fuel prices [16].

A number of scientific publications address the mathematical modeling and simulation of polygeneration energy systems. However, they either focus on the evaluation of existing plants and process technologies [17], on the configuration design of processes [18–20,16], or on the performance and operation of these plants [21,22]. 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 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 [23–27]. The goal is to select the best plan among many possible alternatives, e.g. alternative feedstocks and production technologies, according to economic objectives, and subject to quantified technical and environmental constraints. The research procedure comprises data compilation, process design and simulation, multiperiod investment and operation evaluation, and then mixed-integer optimization. Accordingly, a suitably detailed mathematical model is always needed for the analysis.

Mixed-Integer Programming (MIP) methods [28] are suitable for modeling and analyzing polygeneration energy systems towards design, investment planning and optimization: this established algorithmic framework fulfills the requirements and captures the complexities of an investment planning procedure, by considering the superstructure of all alternatives, representing all possible 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 is derived by conducting an optimization for a specific objective function.

A general model for facilitating strategic decisions in the development progress of polygeneration energy systems was built using Mixed-Integer Programming methodology. The purpose of this model is to help make plans for the future development of polygeneration energy systems in specific regions or countries. It includes all alternative technologies, feedstocks and products and selects the most profitable combination by maximizing the net present value (NPV) over a future planning time horizon.

## 2. Mathematical model structure

A general model for strategic decisions in the development progress of polygeneration energy systems was built using Mixed-Integer Programming methodology. It included all alternative technologies, feedstocks and products and selected the most profitable combination by maximizing the net present value over a future planning time horizon. The model is presented in this chapter by first presenting its main assumptions and features, then listing definitions of variables together with their physical meanings, followed by the mathematical equations, and last, linearization of non-linear equations. The model is thus linear and includes binary and continuous variables. A global optimum can be achieved directly and more easily, compared with a non-linear one. General Algebraic Modelling System (GAMS<sup>®</sup>) is a reliable and efficient mathematical tool to solve this MILP problem.

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

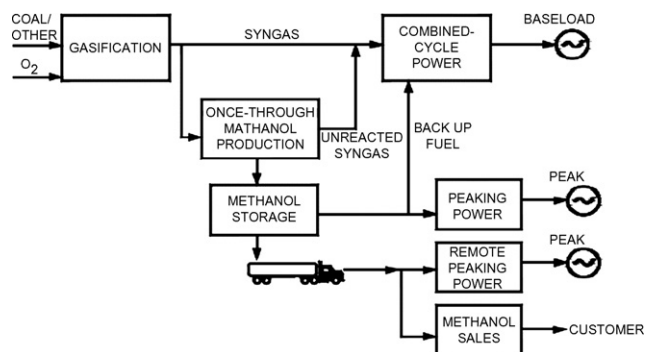


Fig. 1. A polygeneration energy system for methanol and electricity [37].

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). Then another round of iteration begins until all the element combinations are checked. When all possibilities have been evaluated, the optimal result (maximum NPV) is obtained. The MIP mathematical model also contains a number of simplifying assumptions and also forecasting models not shown, and it has been implemented in GAMS<sup>®</sup> (CPLEX).

Some unique features of polygeneration energy systems were explicitly considered before applying MILP algorithm to model the strategic investment decisions associated with their development. More specifically, the model must be able to accommodate:

- A medium-term or long-term future planning horizon.
- Construction periods of polygeneration energy systems are around 5 years, while operation time can be as long as 30 years (DOE) [29]. Thus, it is quite obvious that the model should focus on a medium-term or long-time horizon.
- Multiple and diverse primary energy feedstocks and production technologies.
- Diversity of feedstocks and alternative technologies is a key property of polygeneration energy systems. The model has collected large sets of economic and technical data of feedstocks and alternative technologies.
- Transition from one production technology to another and capacity expansions over time. As more advanced technologies, cheaper and more environmental friendly feedstocks may become available in the future, transitions of technologies may lead to more profit.
- Economics of scale of large-scale production technologies or so called size effect. Capacity expansions are essential to the capital investment of polygeneration energy systems in the progress of development. Capital investment and installation fees decrease while plants get more engineering experience and maturer technologies.

The superstructure of the model is shown in Fig. 2. It acts as the overriding model, capturing all the possible alternatives and

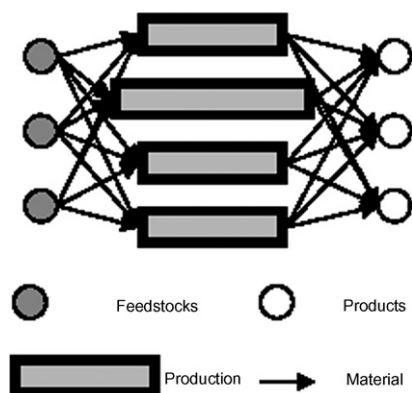


Fig. 2. Mathematical model superstructure for the design of a polygeneration system.

interactions between the various production components. From this superstructure, the optimization algorithm then searches for the best combinations by eliminating the existence of units and links between them. The superstructure construction starts with a set of primary energy sources:

$$F = \{\text{Fuel 1, Fuel 2, Fuel 3, } \dots\} \quad (1)$$

which can be used as feedstocks for polygeneration energy systems using any technologies in set A:

$$A = \{\text{Technology1, Technology2, Technology3, } \dots\} \quad (2)$$

Each of these production technologies are defined such that they can perform conversion of primary energy feedstocks into final products:

$$P = \{\text{Product1, Product2, Product3, } \dots\} \quad (3)$$

The primary objective of the model is to support the optimal strategic investment planning over a long-term future horizon,  $t$  in  $T$ . The model achieves this by making optimal decisions in terms of four levels:

- *Level 1: Strategic process design*
  - Selection of primary feedstocks.
  - Selection of conversion technologies.
  - Assignment of feedstocks to technologies.
- *Level 2: Capacity expansion planning*
  - Estimation of when to expand which technologies and how much should the exact quantity be.
- *Level 3: Production planning*
  - Estimation of how much of each primary energy feedstocks the selected technologies require and what the rates of products production are.
- *Level 4: Performance index assessment*
  - Computation of financial objective such as net present value.

Using MILP modeling techniques, constrains can be formulated representing these various decisions. In addition to constrains describing the physical phenomena, an objective function also has to be formulated for the financial performance criteria. This objective function drives the optimization in search of the best investment strategy. Since a long-term future investment horizon is of interest, the net present value is chosen as the financial performance measure, thereby capturing both the capital expenditure and operating cost requirements of processes as well as the time value of the investment over the future horizon.

There are several assumptions behind this model, listed below:

- Existing capacity of all technologies before the planning time horizon is not considered, such that capacity of all technologies is 0 at the beginning of the planning horizon.
- Capacity expansion and decrease cannot exist in the same time interval.
- Production of chemical products cannot exceed market demands, while production of electricity and other possible

products and by-products does not have such a constraint and all these products are sold to the market regardless of quantity.

- Variable operating cost of polygeneration plants includes only purchase of feedstocks, which overwhelm other components in real operations.

The model for the optimal planning and design of polygeneration energy systems is then formulated as a MILP problem, which is summarized as follows (the variables are explained in Table 1).

The objective function is the net present value, which is a summation of discounted net cash flows over all time intervals:

$$\max^{\text{NPV}} = \sum_t \frac{\text{NetCashFlow}(t) * \text{Years}(t)}{(1 + \text{DiscountRate})^{n(t)}} \quad (4)$$

Table 1

Nomenclature list of variables and parameters for the MILP mathematical model

Continuous variables	
$F(a,t)$	Capacity of technology $a$ during time interval $t$
$FE(a,t)$	Amount of capacity expansion of technology $a$ during time interval $t$
$FD(a,t)$	Amount of capacity decrease of technology $a$ during time interval $t$
$\text{Fuel}(a,f,t)$	Consumption of feedstock $f$ through technology $a$ during time interval $t$
$\text{Product}(a,p,t)$	Production of product $p$ through technology $a$ during time interval $t$
$\text{Invest}(a,t)$	Capital investment in technology $a$ during time interval $t$
$\text{FixedCost}(a,t)$	Fixed operating cost of technology $a$ during time interval $t$
$\text{VarCost}(a,t)$	Variable operating cost of technology $a$ during time interval $t$
$\text{Income}(a,t)$	Income of technology $a$ during time interval $t$
$\text{NetCashFlow}(t)$	Net cash flow before tax during time interval $t$
NPV	Net present value over the whole planning horizon
Discrete variable	
$Y(a,t)$	1 if the capacity of technology $a$ expands or remains unchanged during time interval $t$ , 0 if it decreases
Parameters	
DiscountRate	Discount rate throughout the planning horizon
OperatingTimePerYear	Operating time per year for all technologies
Years( $t$ )	Number of years within time interval $t$
$\text{FuelSupply}(f,t)$	Maximum supply of fuel $f$ during time interval $t$
$\text{Demand}(p,t)$	Market demand for product $p$ during time interval $t$
$\text{FuelPrice}(f,t)$	Price of feedstock $f$ during time interval $t$
$\text{ProductPrice}(p,t)$	Price of product $p$ during time interval $t$
$\text{RefCapacity}(a)$	Capacity of the reference plant for technology $a$
$\text{RefInvest}(a)$	Capital investment of the reference plant for technology $a$
$\text{RefFixedCost}(a)$	Fixed cost of the reference plant for technology $a$
$\text{SizeFactor}(a)$	Size factor of technology $a$
$\text{ConversionRate}(a,p)$	Conversion rate of feedstocks to product $p$ through technology $a$ , on a HHV (higher heating value) basis
$\text{FuelTechnology}(a,f)$	Binary, 1 if technology $a$ can utilize feedstock $f$ , 0 otherwise
$n(t)$	Number of years from beginning of the planning horizon to the beginning of time interval $t$
$\text{Size\_factor}(a)$	An indicator of size effect of technology $a$

Production and economic constraints consist of both equalities and inequalities. The total installed capacity for a specific technology is an accumulation of capacity expansions:

$$F(a,t) = FE(a,t), \quad t = t_1 \quad (5)$$

$$F(a,t) = F(a,t-1) + FE(a,t) - FD(a,t), \quad t > t_1 \quad (6)$$

The time of capacity expansion is defined as its finishing time, thus  $FE(a,t)$  means there is “FE” amount of installation of technology  $a$  finished in period  $t$  rather than started in it. Its starting time can be calculated using the finishing time minus its construction time. Capacity expansion of a technology during a time interval cannot exceed its proper upper limit:

$$0 \leq FE(a,t) \leq Y(a,t) * \text{UpperLimit} \quad (7)$$

Capacity decrease of a technology during a time interval cannot exceed its proper upper limit:

$$0 \leq FD(a,t) \leq (1 - Y(a,t)) * \text{UpperLimit} \quad (8)$$

Conversion from feedstocks to products can occur through a series of different technologies:

$$\sum_f \text{Fuel}(a,f,t) * \text{ConversionRate}(a,p) = \text{Product}(a,p,t) \quad (9)$$

Production of chemical products cannot exceed the demand of the respective products:

$$\sum_a \text{Product}(a,p,t) \leq \text{Demand}(p,t), \quad p \text{ in } P(\text{chemical products}) \quad (10)$$

Consumption of feedstocks through a technology should also not exceed its installed capacity:

$$\sum_f \text{Fuel}(a,f,t) \leq F(a,t) * \text{OperatingTimePerYear} \quad (11)$$

Furthermore, the consumption of feedstocks should not exceed available supplies:

$$\sum_f \text{Fuel}(a,f,t) \leq \text{FuelSupply}(f,t) \quad (12)$$

Capital investment and fixed cost of each technology can be calculated on an annual basis, considering the size effect with respect to a reference plant:

$$\text{Invest}(a,t) = \left( \frac{\text{RefInvest}(a)}{\text{Years}(t)} \right) \left( \frac{FE(a,t)}{\text{RefCapacity}(a)} \right)^{\text{size factor}(a)} \quad (13)$$

$$\begin{aligned} \text{FixedCost}(a,t) &= \left( \frac{\text{RefFixedCost}(a)}{\text{Years}(t)} \right) \left( \frac{F(a,t)}{\text{RefCapacity}(a)} \right)^{\text{size factor}(a)} \end{aligned} \quad (14)$$

The variable operating cost is a summation of the cost of feedstocks:

$$\text{VarCost}(a, t) = \sum_f \text{Fuel Price}(f, t) * \text{Fuel}(a, f, t) \quad (15)$$

The income of a technology occurs as a result of the sale of its products:

$$\text{Income}(a, t) = \sum_p \text{Product Price}(p, t) * \text{Product}(a, p, t) \quad (16)$$

The Net cash flow during a time interval is the algebraic summation of capital investment, fixed cost, variable cost and income:

$$\begin{aligned} \text{NetCashFlow}(t) \\ = \sum_a (\text{Income}(a, t) - \text{Invest}(a, t) - \text{FixedCost}(a, t) \\ - \text{VarCost}(a, t)) \end{aligned} \quad (17)$$

We can use this general model for any specific polygeneration energy system if we have enough information and data about this system. Once the model gets all data it needs, it generates the most profitable strategy based on these data hence a sensitivity analysis can also be conducted.

### 3. Mathematical model linearization

The model is non-linear because of Eqs. (13) and (14). However, modern algorithms and scientific computation softwares (like GAMS<sup>®</sup>) usually only guarantee a local optimum for a non-linear problem. More complicated work, such as a demonstration of the convexity, is required to get a global optimum. Another problem for non-linear models is the computation time, which is several orders longer than that of linear models with similar scales. Since most equations in the model are linear except Eqs. (13) and (14), it is desirable to linearize this model. Linearization of non-linear equations can be realized using a mathematical technique [30]. Although this method requires introduction of extra discrete and continuous variables to the model, we believe it still brings more benefits to the model considering the much higher calculation efficiency of MIP algorithm than non-linear programming (NLP) or mixed-integer non-linear programming (MINLP).

The linearization algorithm is stated below. Assume that  $y$  is a non-linear function of variable  $x$ :

$$y = f(x) \quad (18)$$

Our aim is to linearize the non-linear Eq. (18). We first introduce a set of discrete points, expressed as  $\{x_1, x_2, \dots, x_n\}$ , of which  $x_1$  and  $x_n$  are the lower and upper bound of  $x$ , respectively. These discrete points are usually evenly distributed within the range of  $x$ . Then calculate from Eq. (18) the corresponding values of  $y$  at each point, thus we get another set

of discrete points, expressed as  $\{y_1, y_2, \dots, y_n\}$ , where

$$y_i = f(x_i), \quad i = 1, 2, \dots, n \quad (19)$$

Secondly, we introduce another set of variables,  $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$ , which relate  $y$  to  $x$  by the following relationships:

$$x = \sum_{i=1}^n \lambda_i x_i \quad (20)$$

$$y = \sum_{i=1}^n \lambda_i y_i \quad (21)$$

These variables ( $\lambda_i$ ) are subject to the following equality and inequality constraints:

$$\sum_{i=1}^n \lambda_i = 1 \quad (22)$$

$$\lambda_i \geq 0, \quad i = 1, 2, \dots, n \quad (23)$$

Another constraint for  $\lambda_i$  is that at most two adjacent  $\lambda_i$  can be non-zero. This constraint is realized by introducing a new set of binary variables,  $\{\delta_1, \delta_2, \dots, \delta_n\}$ , which satisfy the following constraints:

$$\sum_{i=1}^{n-1} \delta_i = 1 \quad (24)$$

$$\lambda_1 - \delta_1 \leq 0 \quad (25)$$

$$\lambda_i - \delta_{i-1} - \delta_i \leq 0, \quad i = 2, 3, \dots, n-1 \quad (26)$$

$$\lambda_n - \delta_{n-1} \leq 0 \quad (27)$$

Using this technique, we linearize Eqs. (13) and (14) by first introducing discrete points  $\text{FE}_i(a, t)$ ,  $\text{Invest}_i(a, t)$ ,  $F_i(a, t)$  and  $\text{FixedCost}_i(a, t)$ , continuous variables  $\lambda_i^{\text{Invest}}(a, t)$  and  $\lambda_i^{\text{FixedCost}}(a, t)$ , and binary variables  $\delta_i^{\text{Invest}}(a, t)$  and  $\delta_i^{\text{FixedCost}}(a, t)$ , subject to:

$$\text{Invest}(a, t) = \left( \frac{\text{Ref Invest}(a)}{\text{Years}(t)} \right) \left( \frac{\text{FE}(a, t)}{\text{Ref Capacity}(a)} \right)^{\text{size factor}(a)} \quad (28)$$

$$\text{FE}(a, t) = \sum_{i=1}^n \lambda_i^{\text{Invest}}(a, t) \cdot \text{FE}_i(a, t) \quad (29)$$

$$\text{Invest}(a, t) = \sum_{i=1}^n \lambda_i^{\text{Invest}}(a, t) \cdot \text{Invest}_i(a, t) \quad (30)$$

$$\sum_{i=1}^n \lambda_i^{\text{Invest}} = 1 \quad (31)$$

$$\lambda_i^{\text{Invest}} \geq 0, \quad i = 1, 2, \dots, n \quad (32)$$

$$\sum_{i=1}^{n-1} \delta_i^{\text{Invest}} = 1 \quad (33)$$

$$\lambda_1^{\text{Invest}} - \delta_1^{\text{Invest}} \leq 0 \quad (34)$$



$$\lambda_i^{\text{Invest}} - \delta_{i-1}^{\text{Invest}} - \delta_i^{\text{Invest}} \leq 0, \quad i = 2, 3, \dots, n-1 \quad (35)$$

$$\lambda_n^{\text{Invest}} - \delta_{n-1}^{\text{Invest}} \leq 0 \quad (36)$$

$$\begin{aligned} \text{FixedCost}_i(a, t) \\ = \left( \frac{\text{Ref Fixed Cost}(a)}{\text{Years}(t)} \right) \left( \frac{F_i(a, t)}{\text{Ref Capacity}(a)} \right)^{\text{size factor}(a)} \end{aligned} \quad (37)$$

$$F(a, t) = \sum_{i=1}^n \lambda_i^{\text{FixedCost}}(a, t) \cdot F_i(a, t) \quad (38)$$

$$\text{FixedCost}(a, t) = \sum_{i=1}^n \lambda_i^{\text{FixedCost}}(a, t) \cdot \text{FixedCost}_i(a, t) \quad (39)$$

$$\sum_{i=1}^n \lambda_i^{\text{FixedCost}} = 1 \quad (40)$$

$$\lambda_i^{\text{FixedCost}} \geq 0, \quad i = 1, 2, \dots, n \quad (41)$$

$$\sum_{i=1}^{n-1} \delta_i^{\text{FixedCost}} = 1 \quad (42)$$

$$\lambda_1^{\text{FixedCost}} - \delta_1^{\text{FixedCost}} \leq 0 \quad (43)$$

$$\lambda_i^{\text{FixedCost}} - \delta_{i-1}^{\text{FixedCost}} - \delta_i^{\text{FixedCost}} \leq 0, \quad i = 2, 3, \dots, n-1 \quad (44)$$

$$\lambda_n^{\text{FixedCost}} - \delta_{n-1}^{\text{FixedCost}} \leq 0 \quad (45)$$

After substituting Eqs. (13) and (14) by Eqs. (28)–(45), the whole model is linear and a global optimum can be achieved directly. The foregoing deterministic Mixed-Integer Linear Programming (MILP) model is implemented in GAMS<sup>®</sup>.

#### 4. Case study and analysis

The case study using the model focuses on investment planning of polygeneration energy systems co-producing methanol and electricity in China between 2010 and 2035. Available four feedstocks include coal, domestic and imported natural gas and biomass. A set of 12 technologies has been selected, and it consists of all possible alternative paths for transforming these primary energy feedstocks into final products [22]. Out of the selected technologies, six are polygeneration flowsheet pathways, while the remaining six are conventional, stand-alone methanol synthesis technologies. Eleven discrete points have been used for the linearization of each non-linear equation.

We used this model in a case study for the development planning of a polygeneration energy system in China that co-produces methanol and electricity, from 2010 to 2035 with 5-year intervals, represented as *t1*–*t5*.

#### 4.1. Model inputs

Feedstocks in this system include coal, natural gas (both domestic and imported) and biomass. The detailed classification of these primary energy feedstocks is not under consideration, instead we use average values of their key physical and economical parameters, shown in Table 2. Imported natural gas and biomass have no supply limits. Since exact price of mass biomass was not available, we made an optimistic assumption that it would be 500%, 400%, 300%, 200% and 100%, respectively, of that of coal during each time interval.

Products of this system include methanol and electricity. Since the demand for methanol is relatively quite small compared with the demand for electricity and their production rate depends on each other, the electricity can be absorbed by the market easily with little impact. Thus, we assume that methanol production throughout the time horizon should never exceed its market demand, while all electricity is sold to the market. Since there are few forecasts of methanol demand in China and it will be used as a substitution of gasoline, we estimate the market demand of methanol by making an assumption that in each time interval, methanol, as a kind of clean liquid fuel, would substitute 1–5% of the projected oil consumption in China, respectively. Table 3 shows prices of both products and estimated market demand for methanol.

A set of 12 technologies consists of all alternative paths to transform these primary energy feedstocks to final products. These technologies were different in their main feedstocks, chemical synthesis and electricity generation modules, and their representations are given in Table 4.

Terms in these names refer to main feedstocks, chemical synthesis technologies, electricity generation technologies and main products. Table 5 shows the details.

Each technology used a reference plant as its calculation basis. All capacity expansions and their costs were based on

Table 2  
Key parameters of feedstocks over the complete planning horizon [38,2,3,39]

	t1	t2	t3	t4	t5
Price (million \$/EJ) <sup>a</sup>					
Coal	1038	1038	1038	1038	1038
Natural gas					
Domestic	2999	3152	3313	3482	3659
Imported	5805	6102	6413	6740	7084
Biomass	5188	4151	3113	2075	1038
Supply (EJ/year)					
Coal	38	42	45	49	53
Natural gas					
Domestic	2.0	2.8	4.0	5.6	7.8
Imported Biomass					
HHV (MJ/kg)					
Coal	34.1				
Natural gas					
Domestic	42.5				
Imported	42.5				
Biomass	16.8				

<sup>a</sup> All prices are in real 2006 US dollars.

Table 3

Key parameters of products over the complete planning horizon [17,2,3,40]

	<i>t</i> 1	<i>t</i> 2	<i>t</i> 3	<i>t</i> 4	<i>t</i> 5
Price of methanol (million \$/EJ)	15,114	15,217	15,320	15,423	15,526
Price of electricity (million \$/EJ)	21,689	21,011	21,011	21,011	21,011
Demand for methanol (EJ/year)	0.19	0.45	0.79	1.18	1.68

Table 4

Abbreviations of technologies (unique flowsheet combinations) in the technology set

#	Technology
1	COAL-LPMEOH <sub>He</sub> -CC-P
2	COAL-LPMEOH <sub>m</sub> -CC-P
3	COAL-GPMEOH-CC-P
4	NG-SMRRMS-NONE-M
5	NG-ATROTMS-NONE-M
6	NG-ATRRMS-NONE-M
7	BIO-LPMEOH <sub>m</sub> -CC-P
8	BIO-LPMEOH <sub>He</sub> -CC-P
9	BIO-LPMEOH <sub>hg</sub> -CC-P
10	BIO-LPMEOH-SC-M
11	BIO-GPMEOH-SC-M
12	BIO-GPMEOH <sub>hg</sub> -SC-M

these reference plants. Table 6 shows the capacity, capital investment and fixed operation cost of these reference plants.

Conversion rate was used to represent the efficiency of energy conversion from feedstocks to final products. It was defined as the ratio of the HHV of a specific product to the summation of HHV of all feedstocks. Table 7 shows these conversion rates.

## 5. Results and discussion

The total installed power generation capacity in each time interval is shown in Fig. 3. Two technologies emerge as optimal throughout the planning horizon considered. The first

Table 5

Meanings of symbols and abbreviations in the technology set

Symbol	Explanation
COAL	Coal
NG	Natural gas
BIO	Biomass
LPMEOH <sub>He</sub>	Liquid phase methanol synthesis, suitable to produce more electricity
LPMEOH <sub>m</sub>	Liquid phase methanol synthesis, suitable to produce more methanol
LPMEOH <sub>hg</sub>	Liquid phase methanol synthesis with hot gas cleaning
GPMEOH	Conventional gas phase methanol synthesis
GPMEOH <sub>hg</sub>	Conventional gas phase methanol synthesis with hot gas cleaning
SMRRMS	Steam methane reforming and recycle methane synthesis
ATROTMS	Auto-thermal reforming and once-through methane synthesis
ATRRMS	Auto-thermal reforming and recycle methane synthesis
CC	Combined cycle of gas turbine and steam turbine
NONE	No electricity generation
P	Polygeneration of methanol and electricity
M	Stand-alone methanol production

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 favor 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 have found that stand-alone technologies are only favorable when electricity price drops to below 10% of the

Table 6

Key parameters of reference plants [17,41,42]

	Capacity (GW)	Investment (million \$)	Fixed cost (million \$/year)
COAL-LPMEOH-CC-P	1.29	628	35.3
COAL-LPMEOH-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-LPMEOH <sub>m</sub> -CC-P	0.428	279	11.2
BIO-LPMEOH <sub>He</sub> -CC-P	0.428	288	11.5
BIO-LPMEOH <sub>hg</sub> -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-GPMEOH <sub>hg</sub> -SC-M	0.432	271	10.8

Table 7  
Conversion rates of technologies [17,41,42]

Conversion rate	Methanol	Electricity
COAL-LPMEOH-CC-P	0.156	0.247
COAL-LPMEOH-CC-M	−0.002	0.482
COAL-GPMEOH-CC-M	−0.066	0.517
NG-SMRMS-NONE-M	−0.007	0.635
NG-ATROTMS-NONE-M	−0.007	0.670
NG-ATRRMS-NONE-M	−0.007	0.660
BIO-LPMEOHm-CC-P	0.124	0.376
BIO-LPMEOHc-CC-P	0.244	0.265
BIO-LPMEOHhg-CC-P	0.144	0.403
BIO-LPMEOH-SC-M	0.000	0.570
BIO-GPMEOH-SC-M	0.035	0.515
BIO-GPMEOHhg-SC-M	−0.040	0.589

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 are negligible compared with the income generated by product sales, and thus have little influence on the optimal choices required for project planning.

### 5.1. Temporal and technological evolution of installed capacity

The mathematical model has been used (after assigning the designated parameters, found in Tables 2–7) in order to conduct a future development planning study, by maximizing the net present value of the polygeneration system over the time horizon from 2010 to 2035. The optimized result showed a net present value of \$89,991 million, with the technology development roadmap shown in Fig. 3.

Coal-based technology developed in the first two time intervals remains unchanged during the third one and shut down in the fourth one. Conversely, biomass-based technology did not have any capacity installed during the first two time intervals, but kept on developing thereafter and soon overwhelmed the coal-based one. There are two main reasons for this development. One is the high conversion rate of the biomass-based technology.

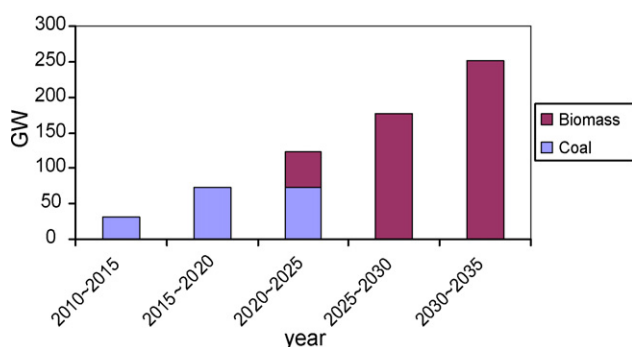


Fig. 3. Installed capacity of polygeneration technologies over the complete planning horizon: first case.

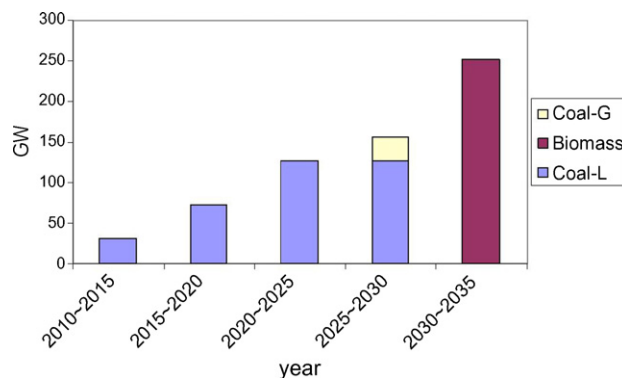


Fig. 4. Installed capacity of polygeneration technologies over the complete planning horizon: second case.

From Table 7, we can find that the conversion rate for methanol in technology BIO-LPMEOHc-CC-P is 56% higher than that in COAL-LPMEOHc-CC-P, which for electricity is 7% higher, and the overall conversion rate is 26% higher. This means that the BIO-LPMEOHc-CC-P technology is more efficient than COAL-LPMEOHc-CC-P technology. The other reason is the price of biomass. Based on our assumption, the price of biomass was much higher than that of coal at the beginning, thus no technology could afford it. However, as the price of biomass decreases dramatically in the following time intervals, the advantage of high efficiency appears gradually in the results. Consequently, the comparison of biomass and coal prices is instrumental towards determining whether biomass-based technology will prevail over coal-based technology.

Fig. 4 illustrates the installed capacity of polygeneration technologies under a slightly different scenario, which allows for the coexistence of two different coal-based technologies (Coal-G and Coal-L, respectively). While the breakdown of implemented technologies is obviously different in the different time periods, the overall installed capacity as a function of time, over the complete planning horizon, exhibits a trend which is very similar to that illustrated in Fig. 3.

We can also find observe that both technologies are polygeneration based and favor the production of electricity. This is because of the high price of electricity compared with that of methanol. From Table 3, the price of electricity is at least

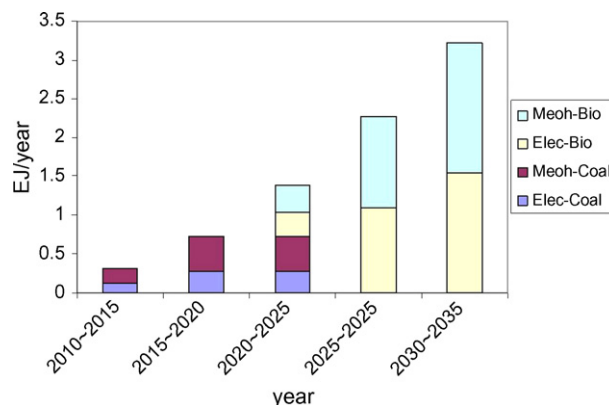


Fig. 5. Methanol and electricity production as a function of time over the complete planning horizon.



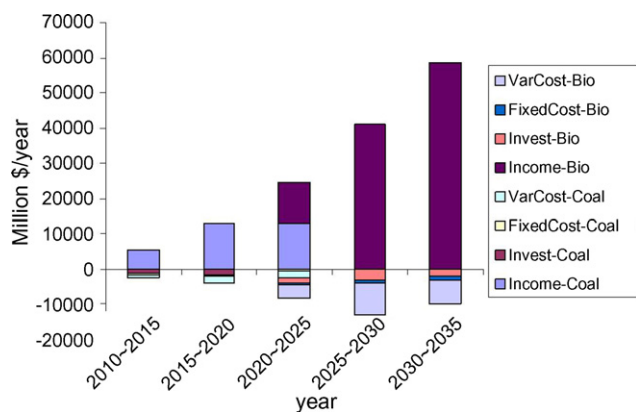


Fig. 6. Cash flow as a function of time over the complete planning horizon.

35% higher than that of methanol during all time intervals. Thus, it is more profitable to produce electricity than methanol.

None of the natural gas-based technologies has been selected as a result of using the MILP model. This observation can be explained by the above analysis. One aspect is that those technologies are stand-alone, producing little electricity. Another is that the price of natural gas, both domestic and imported, is much higher than that of coal. These two aspects imply that it is impossible for natural gas-based technologies to be employed, although they had very high conversion rates.

Products by each technology are shown in Fig. 5. Methanol and electricity are presented as Meoh and Elec, respectively, while Bio and Coal have the same meaning as in Figs. 3 and 4. Methanol and electricity production was nearly equal to each other throughout the time horizon. During the period from 2020 to 2025, the production of BIO-LPMEOH-CC-P technology grows to a similar extent as that of COAL-LPMEOH-CC-P technology.

Fig. 6 shows the cash flow of technologies in each time interval. The terms VarCost, FixedCost, Invest and Income represent variable operating cost, fixed operating cost, capital investment and income, respectively. The total income keeps on increasing over the time horizon because of the increasing market demand for methanol and due to the continuous expansions of production capacity. The total expenditure reaches its maximum in the time interval from 2025 to 2030, and drops thereafter, due to the decreasing price of biomass.

The variable operating cost holds a larger fraction in the total expenditure than the summation of capital investment and fixed operating cost. From Eq. (15), we can see that it is the product of the fuel price and quantity. Moreover, the quantity of feeding fuel is decided by the conversion rate of specific technologies to produce the same quantity of products. Thus, a conclusion can be drawn that, for all technologies, the conversion rate and price of feeding fuel have stronger influence than the economic parameters such as capital investment and fixed operating cost on the development planning.

## 5.2. Threshold analysis

It has been shown in Section 5.1 that the model selects two main technologies out of 12 alternatives. The purpose of this

section is to conduct a threshold analysis to find out the conditions in which those unfavored technologies could have a chance of implementation.

### 5.2.1. Utilization of natural gas

None of the natural gas-based technologies seemed competitive because of the high price of natural gas and the *methanol only* production strategy, as analyzed in Section 5.1. It is thus desirable to examine to what extent the price of natural gas or electricity should decrease to make natural gas-based technologies more attractive.

First, we decreased the price of natural gas while keeping the price of electricity and all the other parameters in the model. However, the model result remained unchanged although the price of natural gas had dropped dramatically to 10% of that of coal.

We then changed the price of natural gas back to its original value and decreased the price of electricity. However, natural gas-based technologies still had no advantage at all even though the price of electricity had been as low as 10% of that of methanol.

Thus, the utilization of natural gas-based technologies requires both the prices of natural gas and electricity to decrease. The critical point for the utilization of natural gas is shown in Fig. 7. The *x*-axis is the ratio of price of natural gas to coal. The *y*-axis is the ratio of price of electricity to methanol. Natural gas-based technologies can only appear in the region below this critical line. We can conclude that the following conditions are required for natural gas-based technologies to be utilized:

- the price of natural gas must be lower than 155% of that of coal.
- At any given ratio of price of natural gas to coal, the corresponding ratio of electricity price to methanol price must be lower than the critical point.

### 5.3. Polygeneration versus stand-alone production

The choice of polygeneration or stand-alone production is influenced by three groups of factors. One factor is the economic properties of products, such as the ratio of prices. Another factor is the economic properties of technologies, such

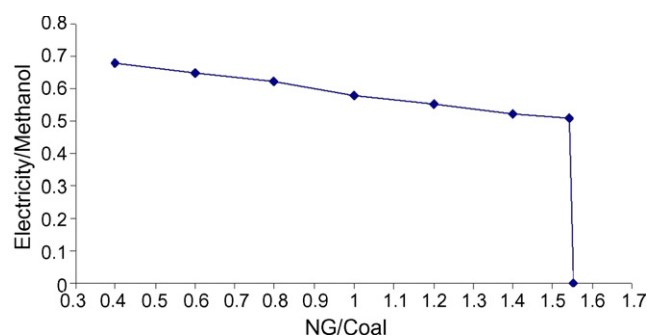


Fig. 7. Critical points for the utilization of natural gas-based energy carrier production technologies.

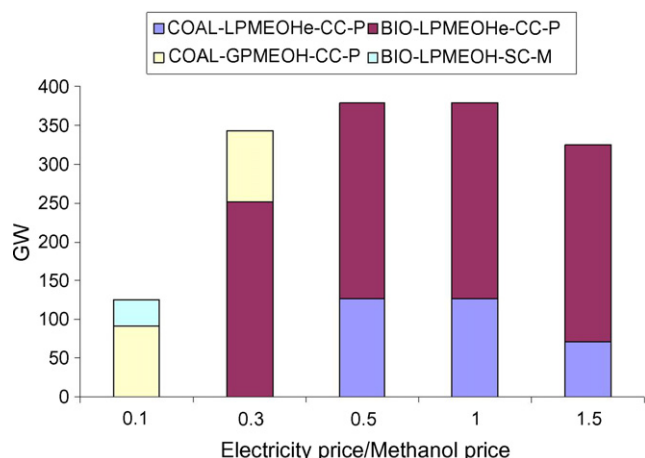


Fig. 8. Installed capacity of polygeneration technologies over the complete planning horizon as a function of electricity to methanol price ratio.

as the capital investment and operating cost. The third one is the technical properties of technologies, such as the conversion rate. Next, we will analyze the influence of these factors one by one.

Polygeneration technologies have two products, methanol and electricity, while stand-alone technologies produce only methanol. Thus, polygeneration technologies are more preferable at a high ratio of price of electricity to methanol. It is shown in Fig. 8 that a stand-alone technology, {BIO-LPMEOH-SC-M}, only appears at a 10% ratio of price of electricity to methanol. So polygeneration technologies have advantages over stand-alone in a vast region of price ratios.

We then decreased the capital investment cost and fixed operating cost by 50% and increased the conversion rate by 50% simultaneously, but the model result remained the same. This can be explained on the basis of Fig. 6. The profit from products is much higher than capital investment, fixed operation cost and variable operation cost, which consists mainly of the purchase of feedstocks. Changes of these costs are negligible to the huge profit that can be realized, and thus cannot influence the selection of technologies.

## 6. Sensitivity analysis

We will analyze the influence of perturbations of model parameters and inputs to the model result using sensitivity analysis (SA) methodology. A brief introduction to this methodology comes first, then its realization to our model.

### 6.1. Methodology

Sensitivity analysis is the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variation, and of how the given model depends upon the information fed into it [31]. According to SA, its function is to help modellers to determine:

- if a model resembles the system or processes under study;
- the factors that mostly contribute to the output variability and that require additional research to strengthen the knowledge base;
- the model parameters (or parts of the model itself) that are insignificant, and that can be eliminated from the final model;
- if there is some region in the space of input factors for which the model variation is maximum;
- the optimal regions within the space of the factors for use in a subsequent calibration study;
- if and which (group of) factors interact with each other.

There are mainly three classes of sensitivity analysis methods: screening methods, local SA methods and global SA methods. These methods have their own advantages in different field. Screening methods are suitable to deal with models that are computationally expensive to evaluate and have a large number of input parameters. Local SA methods concentrate on the local impact of the factors on the model and are usually carried out by computing partial derivatives of the output functions with respect to the input variables. Global SA methods focus on the impact of the uncertainty in the input factors on the output uncertainty.

Local SA methods are suitable for analyzing our model result, thus we will only make a brief introduction to the methodology of this class. Suppose a time-independent system can be expressed by the following algebraic equations:

$$f(y, k) = 0 \quad (46)$$

where  $y$  is the  $n$ -vector of variables and  $k$  is the  $m$ -vector of parameters. The solution of Eq. (46) changes when the values of parameter  $k$  are changed. The simplest way to calculate local sensitivities is by slightly changing one parameter at a time and rerunning the model. The sensitivity matrix can be approximated by:

$$\frac{\partial y}{\partial k_j} \approx \frac{y(k_j + \Delta k_j) - y(k_j)}{\Delta k_j}, \quad j = 1, 2, \dots, m. \quad (47)$$

The accuracies of the sensitivities calculated depend on the parameter change  $\Delta k_j$ . Parameter changes that are too large (e.g. >5%) would damage the assumption of linearity. However, if the changes are too small, the difference between the original and perturbed solutions is too small and the round-off error is too high. In most cases, a 1% perturbation is a good practical choice.

The sensitivity coefficient  $\partial y_i / \partial k_j$  is a linear estimate of the number of units change in the variable  $y_i$  as a result of a unit change in the parameter  $j$ . This means that the sensitivity result depends on the physical units of variables and parameters. In the general case, the variables and the parameters each have different physical units, and therefore the sensitivity coefficients are not comparable with each other and do not have any physical meaning at all.

To make the sensitivity results independent of the units of the model, normalization of sensitivity coefficients is necessary.

The normalized local sensitivity matrix is denoted by  $\tilde{S}$  and defined as

$$\tilde{S} = \left[ \frac{k_j}{y_i} \frac{\partial y_i}{\partial k_j} \right] \quad (48)$$

These sensitivity coefficients represent a linear estimate of the percentage change in the variable  $y_i$  caused by the percentage change in the parameter  $k_i$ .

## 6.2. Application

Using Eq. (48), we apply the methodology of local sensitivity analysis to our model to find out the relationship between our optimized variable, the net present value, and all model parameters and inputs. All non-zero sensitivity coefficients are shown in Table 8.

Sensitivity coefficients in Table 8 are classified into two groups, parameters and inputs. Parameters are based on model assumptions. Inputs are economic and technical data of feedstocks, products and technologies. In the parameters group, the discount rate has the largest influence on the model objective, and it is also the only sensitivity coefficient greater

than 1. The influences of size factors for both operating technologies are comparable. The least influence comes from the annual operating time. Overall, sensitivity coefficients of all parameters have large values, thus all these parameters are significant to the model.

In the inputs group, the largest influences come from the conversion rates to electricity. This again proves our conclusion in Section 5, that the electricity production is more profitable than methanol. Moreover, the sensitivity coefficients of the conversion rates to methanol are negative, which means the profit will drop if the conversion rates to methanol increase. This can be explained from our model constraints, that the methanol production should never exceed its market demand. Mathematically, this means the methanol production has an upper limit. In this condition, increasing the conversion rate to methanol decreases the production ratio of electricity to methanol. Thus, it has two opposite effects to increase the conversion rate to methanol. The advantage is from the saving of feedstocks, while the disadvantage is that the electricity production suffers. Since the saving of feedstocks cannot compensate the decrease of production, the overall effect is negative.

Market demand for methanol has the second largest influence on the model result. It is not only because of the increased production of methanol, but also the more co-produced electricity. Prices of electricity and methanol have almost the same influence, which is much larger than the price of feedstocks. The least influences are from the price of feedstocks, the capital investment and fixed operating cost.

Table 8  
Sensitivity coefficients calculated from the sensitivity analysis

Parameters and inputs	Sensitivity coefficients
DiscountRate	−1.49
SizeFactor(BIO-LPMEOH-CC-P)	−0.28
SizeFactor(COAL-LPMEOH-CC-P)	−0.25
OperatingTimePerYear	0.12
RefInvest(COAL-LPMEOH-CC-P)	−0.07
RefInvest(BIO-LPMEOH-CC-P)	−0.06
RefFixedCost(COAL-LPMEOH-CC-P)	−0.03
RefFixedCost(BIO-LPMEOH-CC-P)	−0.02
ConversionRate(COAL-LPMEOH-CC-P,ELECTRICITY)	0.30
ConversionRate(COAL-LPMEOH-CC-P,MEOH)	−0.13
ConversionRate(BIO-LPMEOH-CC-P,ELECTRICITY)	0.44
ConversionRate(BIO-LPMEOH-CC-P,MEOH)	−0.23
MeohDemand( <i>t</i> 1)	0.14
MeohDemand( <i>t</i> 2)	0.20
MeohDemand( <i>t</i> 3)	0.22
MeohDemand( <i>t</i> 4)	0.25
MeohDemand( <i>t</i> 5)	0.24
ProductPrice(ELECTRICITY, <i>t</i> 1)	0.09
ProductPrice(ELECTRICITY, <i>t</i> 2)	0.13
ProductPrice(ELECTRICITY, <i>t</i> 3)	0.17
ProductPrice(ELECTRICITY, <i>t</i> 4)	0.19
ProductPrice(ELECTRICITY, <i>t</i> 5)	0.17
ProductPrice(MEOH, <i>t</i> 1)	0.10
ProductPrice(MEOH, <i>t</i> 2)	0.15
ProductPrice(MEOH, <i>t</i> 3)	0.16
ProductPrice(MEOH, <i>t</i> 4)	0.15
ProductPrice(MEOH, <i>t</i> 5)	0.13
FuelPrice(COAL, <i>t</i> 1)	−0.03
FuelPrice(COAL, <i>t</i> 2)	−0.04
FuelPrice(COAL, <i>t</i> 3)	−0.03
FuelPrice(BIO, <i>t</i> 3)	−0.05
FuelPrice(BIO, <i>t</i> 4)	−0.08
FuelPrice(BIO, <i>t</i> 5)	−0.03

## 7. Conclusions

Polygeneration is a promising technology that can provide alternatives for solving the pressing global problems of fossil fuel shortage [32] and greenhouse gas 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 in oil-importing countries [33]. Furthermore, polygeneration schemes can generate many flowsheet configurations and thus allow for ample design flexibility that accommodates specific regional conditions. Thus, it can reduce the dependence on oil and enhance energy security for oil-importing countries. Many countries have enacted plans or policies to develop poly-generation energy systems. The Vision 21 plan of U.S. has been put into practice, including many scientific research endeavors and industrial operation practices [29]. China also plans to develop polygeneration energy systems based on coal gasification to solve its increasing demand for electricity and oil [34].

Model simulation and Mixed-Integer Programming optimization 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 [35] do not show any advantages because of their stand-alone nature and the high price of natural gas. The implementation of natural gas technologies requires simultaneous decrease in the price of natural gas and the price ratio of electricity to MeOH.

A generic Mixed-Integer Programming mathematical model has been constructed and implemented in GAMS<sup>®</sup> with the purpose of facilitating planning and strategic decision-making towards the current and future development of polygeneration energy systems [36]. It includes all alternative technologies, feedstocks and products and selects the most profitable combination by maximizing the objective function (the project's net present value) over a fixed future planning time 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 varies by process and is prespecified).

A specific case study was conducted on a polygeneration energy system that co-produces electricity and methanol, using coal, natural gas and biomass as feedstocks. The case study and the ensuing model result analysis, threshold analysis and sensitivity analysis lead to a number of significant conclusions regarding the design, investment planning and optimization of polygeneration energy systems addressing the combined production of electricity and methanol:

- Polygeneration technologies have more advantages than stand-alone technologies.
- Biomass-based polygeneration technology is the most preferable if the price of biomass can drop to the same level as that of coal.
- Polygeneration technologies that produce more electricity are more preferable because of the high price of electricity.
- Natural gas-based technologies do not show any advantages because of their inherent stand-alone property and the high price of natural gas. The utilization of these technologies requires simultaneous decreases of the price of natural gas and the price ratio of electricity to methanol.
- The price of feedstocks has a much stronger influence on the net present value than the capital investment and the fixed operating cost.
- Model parameters have strong influences on model results. The discount rate has the largest influence among them.
- The conversion rate of technologies has the strongest influence on the model result among all model inputs, while the price of feedstocks, the capital investment and the fixed operating cost have the least influence.

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