

111Equation Chapter 1 Section 1Stochastic optimization-based sustainable retrofit of petrochemical energy systems under multiple uncertainty

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Abstract

We report a multi-objective stochastic mixed-integer non-linear programming (MINLP) framework for sustainable retrofit and capability expansion of traditional energy systems in petrochemical complexes. Multiple uncertainties including energy demands, solar radiations and wind speeds are considered in the optimization framework, which are characterized by normal distributions of historical data or normal distributions pre-defined with assumed mean values and standard variations. A stochastic reduced order model sampling technique is introduced to describe the uncertainties by a small number of scenarios and their individual probabilities. The optimization framework further accounts for system configuration selection and sizing of the candidate energy conversion equipment, such as thermal storage units, gas turbines, boilers, steam turbines, as well as their operating capacities in each time period. A case study is investigated to demonstrate the performance of the proposed strategy and the optimization results under three modes (deterministic, stochastic and semi-stochastic programs) are compared.

Keywords:

Sustainable energy system; Retrofit; Mixed-integer non-linear programming; Stochastic reduced order model; Multiple uncertainty.

Highlights

- A multi-objective stochastic MINLP model framework is presented for the sustainable retrofit of energy systems in petrochemical complexes.
- Multiple uncertainties including energy demands and renewable energy loads are considered.
- SROM sampling technique is introduced to describe the uncertain space with less samples.
- Retrofit under deterministic assumptions can lead to almost a 10% underestimation of TAC.

1. Introduction

Current energy reformation is forcing petrochemical complexes to transform from producing common gasoline and diesel oils to producing more fine chemicals or basic chemical materials. This leads to the new processes and units being installed in petrochemical complexes. As a result, energy and utility requirements in petrochemical complexes are increasing¹. Petrochemical complexes consume a lot of energy to produce steam at different pressure levels and power to meet the process requirements. Fossil fuels, including coal, oils and natural gas, are the main energy resources of utility systems. For higher energy efficiency and lower economic cost², combined heating, cooling and power (CCHP) generation in energy systems has gained considerable interest during recent decades^{3,4,5}. How to expand such existing energy systems, while considering the sustainability and uncertainty, is very challenging for the economic and environmental benefits of petrochemical complexes.

The methodologies of synthesizing energy systems can be classified as deterministic methods and design under uncertainty. For the deterministic methodology, parameters related to the systems are all considered unchanged while in the method of design under uncertainty, the uncertainty of some parameters is taken into account^{6,7,8}. Research on deterministic synthesis of CCHP systems has paid attention to synthesis with new processes or technologies, including organic ranking cycle⁹, CO₂ capture and LNG cold energy utilization¹⁰, wastewater treatment plant¹¹, high-temperature heat pumps¹² and biomass gasification¹³. For petrochemical complexes, Ponce-Ortega et al.¹⁴ presented a novel superstructure-based approach to synthesize sustainable tri-generation systems integrated with heat exchanger networks. A steam Rankine cycle driven by multiple primary energy sources (i.e. solar, biofuels, and fossil fuels) is considered. Luo et al.³ investigated a retrofitted natural gas-based cogeneration system. Compared to the original cogeneration system waste heat recovery is a new addition. Parameters are all treated deterministically in

these studies, however over the long lifetime of the plant, some parameters are uncertain, including but not limited to energy demands, fuel and electricity prices, as well as available loads of energy^{15,16}. Disregarding uncertainty on the system design and operation could lead to sub-optimal solutions, where the objectives would not keep longstanding optimal values or reduce financial and environmental risks.

Methods for optimization under uncertainty have been proposed to handle the uncertainty in process optimization, the main techniques include robust optimization^{17,18,19}, parametric programming^{20,21,22} and stochastic programming^{23,24,25}. For parametric programming, uncertain space is given by ranges of uncertain parameters (usually their upper and lower bounds) and the solution is given by parametric profiles, while for the other two methods, some forms of data are required to characterize the uncertain space, such as probability distributions or uncertainty sets. These methods are mature enough to be used in practical applications²⁶. According to the literature²⁷, robust programming is more favorable for short-term problems, whereas stochastic programming is more favorable for long-term production planning and strategic design problems. Onishi et al.¹⁵ introduced a new time-independent scenario-based modelling approach for the synthesis and optimization of CCHP systems under long-term uncertainty in energy load demands and prices. They assume that all uncertain parameters can follow normal correlated and/or uncorrelated distributions without considering their historical data. The new scenario-based modelling approach can individually reduce the data scale, but the physical meaning deserves further consideration. Fuentes-Cortés et al.²⁸ investigated the optimal design of residential co-generation systems in an hourly seasonal period of a typical day under uncertainty, while taking economic and environmental objectives into consideration at the same time. Uncertain ambient temperature, energy demands and prices of the local energy market are incorporated, and their normal distributions based on the historical data were used to generate the uncertain scenarios. Mavromatidis et al.²⁹ presented

a two-stage stochastic programming approach for design of distributed energy systems. Energy carrier prices and emission factors, building heating and electricity demands, and incoming solar radiation patterns are considered as uncertain parameters. In this literature scenario reduction techniques are introduced for development of probabilistic uncertainty scenarios.

To the best of our knowledge, very little work has been attempted for sustainable retrofit of energy systems under multiple uncertainty for petrochemical industries whilst considering enough possible mature energy conversion equipment in the market. Especially, the synthesis of energy systems in past research usually considered heating demands as a virtual stream of heat. In this article, renewable energy and as many mature devices as possible are considered to construct the superstructure of the sustainable energy system to be retrofitted. Heating demand is described as steam at different pressure levels.

For the sampling process, the Monte Carlo sampling technique is widely used in previous studies to generate scenarios^{28,30,31}. However, its main disadvantage is that a large number of samples is needed to accurately reproduce the uncertain space, which could hinder the computation²⁹. Therefore, in this paper, a different scenario generation approach, based on a stochastic reduced order modelling sampling technique is applied to obtain a smaller number of scenarios with different probabilities.

The rest of the paper is structured as follows: in section 2 the problem statement of optimal sustainable retrofit design and operation of petrochemical energy systems under multiple uncertainty is introduced. The proposed methodology regarding the superstructure construction and scenarios generation framework is then proposed in section 3, and the stochastic multi-period mathematical model is formulated in section 4. In section 5 we focus on the application of the proposed framework of the case study. Finally, some important conclusions are drawn.

2. Description of the sustainable retrofit problem

2.1 Superstructure of sustainable retrofit

Figure 1 displays the general superstructure for the sustainable synthesis, retrofit and operation of an energy system in petrochemical complexes, where the grey part is the existing steam system to be retrofitted, composed of coal/gas fired boilers, steam turbines and pressure reducing valves. The green part is the new device introduced to the energy system for sustainable retrofit. During the retrofit process, the existing devices are kept in place but their operational states are determined by the optimization results. The equipment with the same model and capacity as the old one can be introduced, the number of which is denoted by n . Renewable energy (i.e. solar and wind) and other energy conversion devices are introduced to achieve the environmental and economic goals. For the variation of solar radiation, thermal energy storage tanks are considered to store solar energy in the daytime and release it at night. Extraction steam turbines can be installed between the pressure levels of 9.5 and 3.5 MPa, where middle and low-pressure steams can be extracted, while back-pressure turbines are considered between 3.5 and 1.0 MPa pressure levels. Heating and cooling demand should be satisfied while a bi-directional grid connection is considered to allow electricity purchase or sale. Electric and absorption chillers can both be used to produce cold water. Except for the heat storage, refrigeration and solar heat collector units, maximum and minimum capacity limits are considered for boilers, steam turbines and gas turbines.

2.2 Given conditions

The problem of sustainable retrofit of energy systems in petrochemical complexes under multiple uncertainty can be stated as follows:

- (1) Given is an existing refinery energy system with periodic heating, cooling and power demand. The heating demand is described as steams under different pressure levels.

For example, steam of four pressure levels, 9.5 MPa, 3.5 MPa, 1.0 MPa and 0.4 MPa, is often used in refineries.

- (2) Taking account of the capacity expansion of process units in refineries, the demand increases of heating and power is involved in the sustainable retrofit. In this study, 35% increase of heating load and 25% increase of power demand are considered.
- (3) A set of available fuels or renewable energy to the system, including natural gas, coal, solar, etc. Their specific cost and carbon dioxide emissions (GHGE) are considered.
- (4) The existing energy conversion equipment with their hardware capacities, including coal-fired boilers (CFB), gas-fired boilers (GB), extraction condensing steam turbines (ST) and back-pressure turbines (BT).
- (5) For sustainable retrofit, new possible energy conversion and storage units are considered for heating, cooling, power generation and thermal storage, including natural gas-fired gas turbines (GT), wind turbines (WT), solar heat collectors (SHC), heat recovery steam generators (HRSG), electric compression chiller (EC), absorption chiller (AC), and thermal energy storage tank (TES).
- (6) All devices are provided with known technological characteristics (i.e. maximum or minimum capacities in commercial and nominal efficiencies) and their capital costs.
- (7) For the thermal energy storage unit, also given are the minimum approach temperature for heat exchange and heat storage efficiency.

2.3 Assumptions

For this large-scale optimization problem of sustainable retrofit of energy systems, several assumptions are proposed as follows:

- (1) Land cost is negligible in economic analysis for this retrofit problem.
- (2) The operation status of equipment is treated as a continuous variable.

(3) The air and flue gas are treated as ideal gas.

3. Solution framework of sustainable retrofit problem under uncertainty

3.1 Solution framework

Due to the long-term operational horizon, uncertainty is almost inevitable at the sustainable retrofit design stage. Uncertain energy carrier prices, energy demands, and incoming solar radiation patterns have been studied in the literature^{15,28,29}. Onishi et al.¹⁵ assumes that uncertain energy demands and prices can follow normal correlated and/or uncorrelated distributions without considering their historical data. In this way, the uncertain parameters can be mathematically modelled through multi-variate normal probability distributions^{16,32}. In addition, Fuentes-Cortés et al.³³ generate scenarios of uncertain ambient temperature with the probability density function based on historical data. In this paper, we consider energy demands (i.e. heating and cooling demands) along with random wind speeds and solar radiation as uncertain parameters. For the reason that production planning and scheduling in refineries are significantly affected by the petrochemical product market, heating and cooling demands are assumed as random variables following the given normal distributions with corresponding mean values and standard variances^{15,16}. For the characterization of uncertain wind speed and solar radiation, normal distribution based on historical data is adopted.

In terms of stochastic programming, the description of random variables defines a set of different scenarios. By incorporating the uncertainty into the deterministic design problem, Liu et al.³⁴ presented the two-stage stochastic programming problem, which is then reformed into a multi-period problem, as illustrated in Eq. (1):

$$\begin{aligned}
& \min_{y, d, x_{t, sen}} f_d(y, d) + \sum_{sen=1}^N B_{sen} f_o(y, d, x_{t, sen}, \theta_{sen}) \\
& \text{s.t.} \quad h^{dc}(y, d) = 0 \\
& \quad g^{dc}(y, d) \leq 0 \\
& \quad h^{oc, sen}(y, d, x_{t, sen}, \theta_{sen}) = 0 \\
& \quad g^{oc, sen}(y, d, x_{t, sen}, \theta_{sen}) \leq 0 \\
& \quad d \in R^l, y \in \{0, 1\}^m, x_{t, sen} \in R^n, sen = 1, \dots, N
\end{aligned} \tag{1}$$

where B_{sen} can approximately be the probability of scenario sen , and N is the number of scenarios. The deterministic term f_d represents decisions at the design stage and the expectation of a stochastic term f_o depends on the realization of uncertain parameter θ at the operation stage. Discrete variables y and continuous variable d are “here-and now” (design) variables which should be decided at the first-stage problem before the realization of uncertain parameter θ occurs, and x_t is a vector of “wait and see” (operational) variables which can be decided at the time interval t of the second-stage problem where all uncertain parameters have been observed³⁴. In the context of sustainable retrofit design of an energy system in this article, y are often binary variables determining whether a device should be installed/operated or not, continuous variable d often represents the designed capacities of equipment while “wait and see” variables x_t often refer to operating variables, such as molar flowrates, power generated and actual loads of equipment.

Then, the problem consists of determining the optimal retrofit configuration and operation scheme of the energy system under multiple uncertainties. Factors such as sizing and selection of the equipment and the scheme of purchase-sale of power to the grid are also considered, while accounting for the simultaneous assessment of the financial risk through the values of the total annual cost and the analysis of the environmental risk using carbon dioxide emissions.

3.2 Samples generation for uncertainty

We treat the available renewable energy loads along with heating and cooling demands as uncertain parameters. To generate samples, Monte Carlo sampling technique has been used in the previous CCHP system studies^{15,29,31}. However, the main disadvantage of the Monte Carlo sampling technology is that typically a large number of samples is needed, which leads to high computational costs.

In this paper random values of uncertain parameters are generated via a different approach which is characterized as the stochastic reduced order modelling (SROM) sampling technique^{36,37,38}. Unlike the Monte Carlo sampling technique which generates many scenarios with equal probability, the SROM sampling technique generates a small number of scenarios with unequal probability based on optimization theory. The defining SROM parameters (scenarios and probabilities) are chosen through the following optimization problem and more details can be found in the literature³⁸:

$$\begin{aligned} \hat{\mathbf{X}} &\equiv \arg \min_{\{\hat{\mathbf{x}}, p\}} \left(\sum_{i=1}^3 \alpha_i e_i(\{\hat{\mathbf{x}}\}, p) \right) \\ \text{s.t. } \sum_{j=1}^n p^{(j)} &= 1 \quad \text{and} \quad p^{(j)} \geq 0, \quad j = 1, \dots, n \end{aligned} \quad (2)$$

where SROM $\hat{\mathbf{X}}$, a finite collection of samples $\{\hat{\mathbf{X}}^{(1)}, \dots, \hat{\mathbf{X}}^{(n)}\}$ and corresponding

probabilities $\{p^{(1)}, \dots, p^{(n)}\}$, is an optimal representation of d -dimensional vector \mathbf{X} in a statistical sense; e_1 , e_2 , and e_3 quantify the error between the SROM and target cumulative distribution functions (CDFs), moments and correlation matrix of \mathbf{X} , respectively. α_i are weighting factors and n is referred to as the SROM size.

4. Detailed stochastic multiperiod model of sustainable retrofit

In this section, formulation of the stochastic multi-period model for the task of optimal retrofit and operation of a sustainable energy system under multiple uncertainties is presented. The proposed model formulation, a mixed-integer non-linear programming problem (MINLP), is based on the superstructure illustrated in Fig 1. In the model, the indexes representing coal-fired boilers, gas-fired boilers, steam turbines, back-pressure turbines, gas turbines, wind turbines are cb , gb , st , bt , gt , nw , respectively. The index p represents seasons (Summer and Winter) and h represents day and night. Heating demand and cold water are represented by index s for HP (high pressure steam), MP (middle pressure steam), LP (low pressure steam), LLP (very low-pressure steam) and CW (cold water). The index used to denote samples is sen .

4.1 Modelling of existing steam system

Coal-Fired Boilers (CFB). The energy released by the coal burning in the CFB boilers Q^b is used for water heating in three stages: before vaporizing Q^{wp} , water vaporizing (Q^{wv}), and steam overheating (Q^{oh}). Heat loss is considered in three parts: heat loss from boiler blowdown (Q^{bd}), heat loss from the wall (Q^{wl}), and heat loss from flue gas (Q^{sk}). This energy balance is expressed in Eq. (3). The heat released by the coal is calculated in Eq. (4), where H^{lc} is the lower calorific value of standard coal, mc is the mass flowrate of coal burned in CFBs. The detailed expressions of Q^{wp} , Q^{wv} , Q^{oh} , Q^{bd} and Q^{wl} are given as Eqs. (A1) - (A5) in Appendix A of the supplementary information. Q^{sk} can be calculated with the composition of the flue gas after burning of coal, given as Eqs. (A6) - (A10) in Appendix A of the supplementary information.

$$Q_{cb,p,h,sen}^b = Q_{cb,p,h,sen}^{wp} + Q_{cb,p,h,sen}^{wv} + Q_{cb,p,h,sen}^{oh} + Q_{cb,p,h,sen}^{bd} + Q_{cb,p,h,sen}^{wl} + Q_{cb,p,h,sen}^{sk} \quad (3)$$

$$Q_{ch,p,h,sen}^b = m_{ch,p,h,sen}^{coal} H^{lcv} \quad (4)$$

Pressure Relief Valve (Vl). Pressure relief valves are designed between steams of different pressure levels. Energy balance for this pressure reducing process is described in Eq. (5), where $Fv_{s,p,h,sen}$ is the molar flowrate of higher-pressure steam s to lower-pressure steam $s-1$. $Deth^{wt}$ and $Deth_s$ are molar enthalpy values for 25°C water and steam s , respectively.

$$Fv_{s,p,h,sen} Deth_s + Fw_{s,p,h,sen} Deth^{wt} = \left(Fv_{s,p,h,sen} + Fw_{s,p,h,sen} \right) Deth_{s-1} \quad (5)$$

Condensing/Back-Pressure steam turbines (ST/BST). As shown in Figure 1, it is supposed that *MP* and *LP* steams can be extracted from the *HP* steam turbines. The real power generated by *HP* steam turbines $W_{st,p,h,sen}^{rST}$ can be calculated using Eq. (6). $W_{s=HP,st,p,h,sen}^{vST}$, $W_{s=MP,st,p,h,sen}^{vST}$ and $W_{s=LP,st,p,h,sen}^{vST}$ are the power produced by the virtual *HP*, *MP* and *LP* steam condensing turbines without extraction, respectively.

$$W_{st,p,h,sen}^{rST} = W_{s=HP,st,p,h,sen}^{vST} - W_{s=MP,st,p,h,sen}^{vST} - W_{s=LP,st,p,h,sen}^{vST} \quad (6)$$

Relationship³ between power generation and steam consumption of turbines is described in Eq. (7). Continuous variables $W_{s,st,p,h,sen}^{rST}$ and $F_{s,st,p,h,sen}$ denote the power produced by turbine st with the input steam s and the molar flowrate of steam s , respectively. F_{st}^{max} denotes the steam consumed by turbine st . Parameter G_s is the specific isentropic enthalpy change of steam s . Binary variable $Z_{st,s}$ is introduced to denote the presence of the turbine. Eq. (8) denotes that only when the high-pressure steam turbines are in operation ($Z_{st,HP}=1$) can the medium and low-pressure steam can be extracted. Eq. (9) indicates that molar flowrate of the inlet steam must be larger than, or equal to, that of the total extracted steam. Eq. (10) is used to constrain the hardware capacity of condensing turbines st . The mathematical models of back pressure turbines are given as Eqs. (A11) - (A12) in Appendix A of the supplementary information.

$$3.6W_{s,st,p,h,sen}^{vST} = \frac{6}{5} \frac{1}{\theta^{ST}} \left(G_s - \frac{\epsilon^{ST}}{F_{st}^{max}} \right) \left(F_{s,st,p,h,sen} - \frac{1}{6} F_{st}^{max} Z_{st,s} \right), \quad s = HP, MP, LP \quad (7)$$

$$Z_{st,s=MP} \leq Z_{st,s=HP}, \quad Z_{st,s=LP} \leq Z_{st,s=HP} \quad (8)$$

$$F_{s=HP,st,p,h,sen} \quad F_{s=MP,st,p,h,sen} + F_{s=LP,st,p,h,sen} \quad (9)$$

$$F_{st}^{min} Z_{s,st} \leq F_{s,st,p,h,sen} \leq F_{st}^{max} Z_{s,st} \quad (10)$$

4.2 New possible equipment and energy sources

Renewable energy solar and wind are considered in the superstructure. As shown in Figure 1, the solar is designed to generated *LLP* steam through the solar heat collectors and the wind is used for power generation. The Hottel-Whillier equation³⁹ describing the relationship between collector heat gain rate and area, considering heat losses from the collector is used here. A is the surface area of the collector, Fr is the heat removal factor, ief is the optical efficiency, rad is the solar radiation and U^{SHC} is the overall collector loss coefficient⁴⁰. The molar flowrate of water heated up by the collector F^{sw} can be calculated in Eqs. (11) and (12). Z_h^{SHC} is equal to 1 when index h indicates the day and 0 when h indicates the night.

$$Q_{p,h,sen}^{SHC} \times 10^9 = A \times Fr \times \left(ief \times rad_{p,h,sen} - U^{SHC} (T^{sin} - T^0) Z_h^{SHC} \right) \times 3600 \quad (11)$$

$$Q_{p,h,sen}^{SHC} = F_{p,h,sen}^{sw} \times \left[Cp^{SHC} (T^{ss} - T^{sin}) + Dw^{SHC} + Cp^{SHC} (T^{sout} - T^{ss}) \right] \quad (12)$$

The amount of power generated by a wind turbine is estimated using the power curve equation⁴¹, denoted by Eq. (13). W_{er} is the rated electrical power, V is the wind speed, V_c is the cut-in wind speed; V_r is the rated wind speed and V_f is the cut-out wind speed. According to the literature⁴¹, exponents m and n are often set to 2 and 3. The total amount of power generated by nw wind turbines is calculated by Eq. (14). Z_{mw} is a binary variable.

$$W_{p,h,sen}^{max} = \begin{cases} 0 & \text{if } V_{p,h,sen}^n < V_c \\ W_{cr} \left(\frac{V_{p,h,sen}^n - V_c^n}{V_\tau^m - V_c^m} \right) & \text{if } V_c < V_{p,h,sen}^n < V_\tau \\ W_{cr} & \text{if } V_\tau < V_{p,h,sen}^n < V_f \end{cases} \quad (13)$$

$$W_{p,h,sen}^{win} = \sum_{nw} (Z_{nw} W_{p,h,sen}^{max}) \quad (14)$$

A gas turbine cycle (as shown in Figure A1 available in supplementary information) is mainly used to convert chemical energy of fossil fuels into power and heat, while the latter is often in the form of flue gas. The gas turbine cycle can be divided into three parts: air compressor (ACm), combustion chamber (CC) and gas turbine (GT). Energy balance⁴⁰ of ACm, CC and GT are given as Eqs. (A13) - (A25) in Appendix A of the supplementary information.

Heat Recovery Steam Generator (HRSG). Flue gas out of the gas turbine is of high temperature and worthy of heat recovery. Therefore, a waste heat boiler is installed after the gas turbine to recover the waste heat. The heat recovery steam generator works like a boiler, and the energy balance can be expressed in Eq. (15), where T_f is the temperature of flue gas out of the HRSG, and η_R is the efficiency. Parameters $Cp^{R,wt}$, $Cp^{R,mps}$ and $\Delta H^{R,mps}$ are the specific heat capacities of water and middle-pressure steam, and the latent heat of water, respectively. Variable $F_{p,h,sen}^{R,mps}$ denotes the molar flowrate of *MP* steams generated by the HRSG.

$$\sum_{gt} [F_{pt,gt,p,h,sen} Cp_p (T_{4,gt} - T_f)] \cdot \eta_R = Cp^{R,wt} F_{p,h,sen}^{R,mps} (T_{p,h,sen}^{R,mps} - T_{p,h,sen}^{R,in}) + F_{p,h,sen}^{R,mps} \Delta H^{R,mps} + Cp^{R,mps} F_{p,h,sen}^{R,mps} (T_{p,h,sen}^{R,mps} - T_{p,h,sen}^{R,mps}) \quad (15)$$

Refrigeration Devices. An electric compression chiller and an absorption chiller are compared in this paper with different energy conversion coefficients COP^{ec} and COP^{ac} , as described by Eqs. (16) and (17). $Deth_{LLP}$ is the molar enthalpy value of *LLP* steam.

$$Q_{p,h,sen}^{ac} = Deth_{LLP} F_{p,h,sen}^{ac,LLP} COP^{ac} \quad (16)$$

$$\underline{Q}_{p,h,sen}^{ec} = W_{p,h,sen}^{ec} COP^{ec} \quad (17)$$

4.3 Demand constraints of energy sink

The net production of *MP* steams can be calculated by Eq. (18):

$$\begin{aligned} \underline{Q}_{p,s,p,h,sen} = & Deth_s \sum_{gb,sl,ht} \left(F_{s,sl,p,h,sen} + F_{gb,p,h,sen}^{mps} - F_{v,s,p,h,sen} - F_{ht,p,h,sen} \right) \\ & + Deth_s \sum_{s=HP} \left(F_{v,s,p,h,sen} + F_{w,s,p,h,sen} + F_{p,h,sen}^{R,mps} \right), \quad s = MP \end{aligned} \quad (18)$$

where $Deth_s$ denotes molar enthalpy value of steam s , $F_{gb,p,h,sen}^{mps}$ denotes molar flowrate of steam generated by gas-fired boilers. According to Eq. (18), *MP* steams are produced by the extraction condensing turbines, gas boilers, HRSG and the valves between *HP* and *MP* steams. However, the back-pressure turbines and valves between *MP* and *LP* steams consume some of the *MP* steams. Similarly, the net production of *LP*, *LLP*, *CW* and power is given as Eqs. (A26) - (A29) in Appendix A of the supplementary information.

The net output of heating and cooling energy should satisfy the needs of the refinery. Parameter $Dmd_{s,p}$ denotes demand of steam s in season p , as illustrated in Eq. (19). For the existing thermal storage tanks, the energy balance of *LLP* steams is different from the other steams. As presented in Eq. (20), $\underline{Q}_{p,h,sen}^{tkin}$ and $\underline{Q}_{p,h,sen}^{tkout}$ are the amounts of thermal input and output of the storage tanks, respectively. η^{tk} is the heat exchange efficiency.

$$\underline{Q}_{p,s,p,h,sen} = Dmd_{s,p}, \quad s = MP, LP, CW \quad (19)$$

$$Dmd_{s,p} + \underline{Q}_{p,h,sen}^{tkin} / \eta^{tk} + \underline{Q}_{p,h,sen}^{ws} = \eta^{tk} \underline{Q}_{p,h,sen}^{tkout} + \underline{Q}_{p,s,p,h,sen}, \quad s = LLP \quad (20)$$

On the other hand, net power output $W_{p,h,sen}^{outp}$ is not asked to satisfy the electricity demand, for the reason that the system can purchase (or sell) the lack (or excess) electricity from the grid, expressed by Eq. (21). W_p^{pd} denotes the demand for electricity. $W_{p,h,sen}^{in}$ and $W_{p,h,sen}^{out}$ refers to the amount of electricity purchased from the grid and sold to the grid respectively, as follows:

$$W_{p,h,sen}^{outp} + W_{p,h,sen}^{in} = W_{p,h,sen}^{out} + W_p^{pd} + W_{p,h,sen}^{ec} \quad (21)$$

The tri-generation system is not allowed to purchase and sell electricity in the same period, which means that one of the two variables $W_{p,h,sen}^{in}$ and $W_{p,h,sen}^{out}$ must be 0. This relationship is described by binary variables $Z_{p,h,sen}^{in}$ and $Z_{p,h,sen}^{out}$, as illustrated in Equation set (22).

$$\begin{aligned} W_{p,h,sen}^{in} &\leq Z_{p,h,sen}^{in} BM \\ W_{p,h,sen}^{out} &\leq Z_{p,h,sen}^{out} BM \\ Z_{p,h,sen}^{in} + Z_{p,h,sen}^{out} &= 1 \end{aligned} \quad (22)$$

4.4 Thermal energy storage (TES)

In this paper, a year is divided into two upper-level time intervals according to Summer and Winter, denoted by set p . In order to express the great change of solar radiation in a day, the lower-level time interval is a typical day divided into day and night, denoted by set h . For the variation of solar radiation in a day, a thermal storage unit is designed. Supposing that the heat storage process can be approximated as the heat transfer process, thus, the amount of thermal energy stored in the TES tank $Q_{p,h,sen}^{tk}$ is given by Eqs. (23) and (24), where η^k is the heat storage efficiency, DH refers to the length of a period h in hour and Q_0^{tk} is the amount of thermal energy stored at the beginning of a day.

$$Q_{p,h,sen}^{tk} = \eta^k Q_{p,h-1,sen}^{tk} + Q_{p,h,sen}^{tkin} - Q_{p,h,sen}^{tkout}, \quad h > 1 \quad (23)$$

$$Q_{p,h,sen}^{tk} = \eta^k Q_0^{tk} / DH + Q_{p,h,sen}^{tkin} - Q_{p,h,sen}^{tkout}, \quad h = 1 \quad (24)$$

The logical relation between thermal energy put in TES $Q_{p,h,sen}^{tkin}$ and out of TES $Q_{p,h,sen}^{tkout}$ is given as Eqs. (A30) - (A32) in Appendix A of the supplementary information. Only when the temperature of the thermal stream is higher than that of the heat storage medium, the heat can be transferred into the tank. Conversely, only when the temperature of the heat storage medium is higher than the heat flow temperature, can the heat be output to satisfy the heating

demand. These logical constraints are expressed in Eqs. (25) and (26).

$$Q_{p,h,sen}^{tikin} \left(T^{steam} - Dt^{min} - T_{p,h-1,sen}^{fk} \right) \leq 0, \quad h > 1 \quad (25)$$

$$Q_{p,h,sen}^{tikout} \left(T_{p,h-1,sen}^{fk} - T^{steam} - Dt^{min} \right) \leq 0, \quad h > 1 \quad (26)$$

where T^{steam} and Dt^{min} are temperatures of heat streams and the minimum heat transfer temperature approach, respectively.

Many devices depend on periods and scenarios, but the sizing of equipment is period and scenario independent. For example, dimensioning of a gas turbine mW_{gt}^{GT} is determined by its highest capacity available in the market W^{GT-Tec} and the largest load required for operation during all time periods and for all scenarios. The sizing of GT is defined in Eq. (27):

$$W_{gt,p,h,sen}^{GT} \leq mW_{gt}^{GT} \leq W^{GT-Tec} \quad (27)$$

4.5 Objective functions

Total annual cost (TAC). The total annual cost for each scenario TAC_{sen} is determined by the sum of the fixed costs CAP and the operating expenditures OP_{sen} , stated in Eq. (28):

$$TAC_{sen} = CAP + OP_{sen} \quad (28)$$

where CAP and OP_{sen} can be calculated using Eqs. (29) and (30). fr is the fractional interest rate per year during the operation year n . FI is the overall installation factor for the retrofit project while DP represents the number of days in Summer or Winter. fg_{sen} , fc_{sen} , fw_{sen} , p_{sen}^{cost} and p_{sen}^{sell} are the unit prices for natural gas, coal, water, electricity purchase cost and unit selling price, respectively. Furthermore, BC is the purchasing cost^{9,40,42,43,44} for each equipment, given in Table A1 in Appendix A of the supplementary information.

$$CAP = \frac{fr(fr+1)^n}{(fr+1)^n - 1} \times FI \times \left[\begin{aligned} &\sum_{cb, cb \geq 2} BC_{cb}^{CFB} + \sum_{gb, gb \geq 3} BC_{gb}^{GB} + \sum_{st, st \geq 2} BC_{st}^{ST} \\ &+ \sum_{bt, bt \geq 1} BC_{bt}^{BST} + \sum_{gt} (BC_{gt}^{GT} + BC_{gt}^{ACm} + BC_{gt}^{CC}) \\ &+ BC^{WT} + BC^{SBC} + BC^{HRSG} \\ &+ BC^{AC} + BC^{EC} + BC^{TES} \end{aligned} \right] \quad (29)$$

$$OP_{sen} = DH \times DP \times \left[\begin{aligned} &\left(fg_{sen} Q_{sen}^{ng} + fc_{sen} Q_{sen}^{coal} \right)^{fuel} + \left(fwt \times M_{sen}^{water} \right)^{water} \\ &+ \left(3.6 p_{sen}^{cost} W_{p,h,sen}^{in} + 3.6 p_{sen}^{sell} W_{p,h,sen}^{out} \right)^{electricity} \end{aligned} \right] \quad (30)$$

Then, the expected value of TAC is stated in Eq. (31), where $prob_{sen}$ stands for the occurrence probability of scenario sen .

$$TAC = \sum_{sen}^{N_s} prob_{sen} \cdot TAC_{sen} \quad (31)$$

Green House Gas Emissions (GHGE). The greenhouse gas emissions of renewable energy are assumed to be zero, however, when fossil fuels are burned, they release carbon dioxide and make an adverse effect on the environment. Furthermore, the purchased electricity also has greenhouse gas emissions in the generation progress. For sustainable retrofit and design, the effect on the environment should be considered at the design stage. The greenhouse gas emissions for each scenario $GHGE_{sen}$ is calculated in Eq. (32), as follows:

$$GHGE_{sen} = DH \times DP \left(Q_{sen}^{ng} Gng + Q_{sen}^{coal} Gcl + 3.6 W_{p,h,sen}^{in} Ge \right) \quad (32)$$

where Gng , Gcl and Ge are greenhouse gas emissions of natural gas, coal and purchased electricity, given in units of metric tons (t) of CO₂ equivalent reduction per kilojoule (kJ) provided¹⁴.

Then, the expected greenhouse gas emissions of all the analyzed scenarios can be written as Eq. (33):

$$GHGE = \sum_{sen}^{N_s} prob_{sen} \cdot GHGE_{sen} \quad (33)$$

The proposed stochastic MINLP model involves the sustainable retrofit and operation of energy systems under uncertain environmental and economic parameters. The model is denoted as SMP and presented below:

$$\begin{aligned}
 \text{(SMP)} \quad & \min \quad TAC \ \& \ GHGE \\
 & s.t. \quad \text{Eqs. (3)-(10) (A1)-(A12) Superstructure of the Existing Steam System} \\
 & \quad \text{Eqs. (11)-(17) (23)-(27) (A13)-(A25) New Possible Equipment} \\
 & \quad \text{Eqs. (18)-(22) (A26)-(A29) Heating, Cooling and Power Demand} \\
 & \quad \text{Constraints} \\
 & \quad \text{Eqs. (28)-(31) Economic Constraints} \\
 & \quad \text{Eqs. (32)-(33) Environmental Constraints}
 \end{aligned}$$

4.6 Optimization strategy

The proposed formulation is a stochastic multi-period MINLP problem accounting for the economic and environmental objectives sustainability. The first economic objective is to minimize the expected *TAC*, while the next target is minimizing the mean *GHGE*. These two objectives usually contradict each other. The constraint method is used to carry out the multi-objectives task and the strategy of multi-objective optimization is illustrated in Figure C1 (available in Appendix C of the supplementary information), which can be stated as follows:

$$\begin{aligned}
 \min \quad & TAC \\
 s.t \quad & GHGE \leq \beta_i \\
 & \text{model relationships}
 \end{aligned} \tag{36}$$

The optimization framework is shown in Figure 2. Three parallel strategies are presented to deal with the supposed uncertain space θ^R . They are deterministic multi-period and - objectives program (DMP), stochastic multi-period program (SMP) and semi-stochastic multi-period program (SSMP). First, the uncertain space is described by the supposed normal

distributions or historical data set. Then the SRM sampling technique is used to generate the reduced scenarios and corresponding probabilities for the SMP, and mean values are individually assigned to uncertain parameters to formulate the DMP. A detailed multi-objective analysis is conducted in DMP to obtain the pareto optimal *GHGE*, with which SMP and SSMP are then transformed into a single objective problem. Furthermore, solutions of design variables d' and binary variables y' in DMP are assigned to SMP and then SMP is changed into SSMP, which is a semi-stochastic problem with fixed design variables d' and binary variables y' while only the operating variables x_t^* need to be optimized.

SMP is a problem composed of massive variables and some non-linear expressions. To solve the problem, the non-linearity of the equipment's economic model is reduced by quadratic fitting and the MINLP program is firstly solved with the solver DICOPT⁴⁵ in conjunction with the solvers CONOPT⁴⁶ and CPLEX⁴⁷ to get the initial guess. Finally, the solver ANTIGONE⁴⁸ is implemented for further solution.

5. Results and discussion

To illustrate the proposed stochastic MINLP model for optimal retrofit design and operation of the energy system under multiple uncertainty, a case study is presented. Figure 1 depicts the superstructure considered for the case study, which is based on a real retrofit project in South China. The essential data is listed in Tables B1-B3 ((available in Appendix C of the supplementary information)). In this sense, the solver ANTIGONE implemented in the General Algebraic Modelling System (GAMS, version 24.4.6) was used. A computer with Intel Core™ i5-4210U CPU @ 1.70 GHz 2.40 GHz processor and 4 GB RAM running with Windows 8 is used.

5.1 Generated samples

As stated in section 3.1, uncertain energy demands are assumed to follow normal correlated (demands in each season) and uncorrelated (demands between two seasons) distributions. The mean values and standard deviations for the eight uncertain parameters are given in Table 1. Coupled with historical data of solar radiations⁴⁹ and wind speeds⁵⁰, the reducing sampling technology SROM is used to generate 19 samples and their corresponding probabilities, illustrated in Figure 3. The goal of sample generation is to identify the set of samples and their associated probabilities which could represent the uncertain space accurately. Therefore, it is necessary to consider whether the generated samples can satisfy the above requirements. For this purpose, cumulative distribution functions (CDFs) of the original normal distributions and the generated samples are compared. As illustrated in Figure 4, taking the uncertain energy demands in summer as example, the blue line and the black ladder line are the CDFs of original Normal distributions and the samples, respectively. The samples are all near the original CDF curve which indicates that the generated samples can effectively reflect the characteristics of the original uncertain space.

5.2 Pareto-optimal designs and solution analysis (DMP)

DMP problem, considering the trade-off between two objectives of minimizing *TAC* and *GHGE*, is firstly investigated. The Pareto curve for the two objectives is shown in Figure 5, where the vertical co-ordinate is the *TAC* in 10^5 \$/year, and the horizontal co-ordinate is the carbon dioxide emissions *GHGE* in 10^4 ton CO₂-eq/year. This curve shows the trade-off between economic performance and environmental conservancy for DMP. The graph is divided into three parts, the infeasible region below the curve, sub-optimal region above the curve and the Pareto-optimal points on the curve indicating that the *TAC* is minimized with respect to the specified *GHGE* limit. Point A on the upper left corner has the maximum *TAC*

and the minimum *GHGE* while on the contrast point B has the maximum *GHGE* and the minimum *TAC* among all feasible solutions. Furthermore, note that from point A to point C, *TAC* is significantly reduced, while there is a smaller decrease after the turning point C. According to this curve trend, point C is recognized as the Pareto trade-off solution. Table 2 presents the detailed calculated results for the solutions A, C and B. The high *TAC* of solution A can be explained by the high electricity purchase cost and the high *GHGE* of the solution is mainly caused by the high coal consumption.

Optimal configuration of solution A, B and C are illustrated in Figure C2, Figure C3 and Figure C4 respectively (available in Appendix C of the supplementary information). In solution C, a combination of fossil fuels and renewable energy is used to supply the required energy to the refining process. Furthermore, the variety of equipment for energy exchange is the most complex, including a 50000 m² solar heat collector which collects 6.47 MW, 30 wind turbines producing 7.97 MW. In this *GHGE* limit, solution C shares the same loads of renewable energy with solution A, which are also the maximum capacities of renewable energy collectors. An electric chiller and an absorption chiller are both installed in this solution, especially, the absorption chiller operates in Summer to produce cold water from LLP steams and electric chiller operates during the whole year.

5.3 Stochastic optimization results (SMP vs DMP)

The problem can be changed into a single objective problem (min *TAC*) in stochastic optimization, with an upper bound for the maximum of *GHGE_{sen}* obtained in solution C. Different from the deterministic retrofit case, uncertain renewable energy loads and energy demands (i.e. demands of MP, LP, LLP, CW) are considered in SMP. Figure 6 illustrates the optimal configuration for the stochastic retrofit case under 19 scenarios. The configuration for SMP is very similar to that of solution C in DMP. For further analysis, Figure 7 depicts the

distribution of the TAC and the operating expense distribution throughout the 19 scenarios sampled. The result of the deterministic case (solution C) is listed on the right side of the graph for comparison.

In Figure 7 the green blocks stand for the electricity purchasing cost where the blocks below the zero line indicate that electricity is delivered to the grid. The expected TAC obtained in the stochastic program is 10.03% higher than the deterministic case, among which, the electricity selling income and fixed cost for the stochastic case contribute 79.43% and 20.31% of this gap, respectively. As illustrated in Figure 8, a negative value means the sales of electricity, while a positive value represents purchasing electricity. For most scenarios of SMP, electricity is purchased from the grid to satisfy the power demand. These differences suggest that TAC of the new sustainable energy system may be underestimated by the conventional deterministic method, which is mainly caused by the overestimation of the amount of electricity generated.

The financial risk associated with the uncertain search space is assessed through the cumulative probability curve, as displayed in Figure 9. To construct the probability curve, the scenarios are sorted in ascending order of their economic performance values. The vertical axis shows the probability of reaching an economic performance (TAC) lesser not greater than a target limit indicated in the horizontal axis. Take the expected TAC of $906.63 \times 10^5 \$ \text{ year}^{-1}$ in SMP program for example, Figure 9 indicates that in this uncertain space, the system has a probability of about 38% to obtain a TAC exceeding $906.63 \times 10^5 \$/\text{year}$. The occurrence probability of TAC exceeding the Pareto optimal point C is more than 90%, which indicates that design under deterministic assumptions can lead to underestimation of TAC . Similarly, Figure 10 shows the environmental risk curve for the stochastic case and the vertical line reveals that all the estimated scenarios share the same carbon dioxide emissions value, which is also the upper bound for the maximum of $GHGE_{sen}$ in the model.

To verify whether the configuration obtained by the DMP is applicable in the uncertain environment described by the seven normal distributions of uncertain parameters, design variables (capacities of equipment) of solution C is delivered to SMP. The results and comparative analysis between SMP, DMP and SSMP are listed in Table 3. We can see that design under the deterministic environment without considering the uncertainties can lead to infeasible operation.

6. Conclusion

Stochastic optimization-based retrofit of traditional energy systems under multiple uncertainties in renewable energy loads and energy demands is presented for petrochemical complexes. To accurately describe the uncertain space, a reduced sampling technique SROM which can obtain a limited number of scenarios and their associated probabilities is adopted. With this sampling technique, the stochastic two-stage problem can be solved within a reasonable computer time. For the sustainable retrofit of the existing petrochemical energy system, a superstructure including renewable energy and thermal storage units is constructed. Two seasons in conjunction with a typical day divided into day and night in each season are considered as four periods. The operation strategies in each period are optimized simultaneously with the optimal configuration. Based on the stochastic program, a deterministic program with mean values as input for 10 uncertain parameters and semi-stochastic program with fixed design variables obtained in the deterministic program are also formulated for comparison.

The framework is implemented to a retrofit case. Results show that combining renewable energy with natural gas as the energy source leads to the minimum *GHGE* while wide use of coal brings profit to the system but also has the worst effect on the environment. The comparison results between SMP, DMP and SSMP problems reveal that ignoring the long-

term uncertainty can result in nearly 10% underestimation of TAC in this case. However, even though the SROM sampling technique is introduced to reduce the number of scenarios and then reduce the computer load, the calculation time of SMP takes still more than 400 times longer than DMP. A new efficient method is expected to balance the computer time and accuracy of the optimization results.

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Nomenclature

Sets and indices

CB	set of coal-fired boilers indexed by cb
GB	set of gas-fired boilers indexed by gb
ST	set of steam turbines indexed by st
BT	set of back-pressure steam turbines indexed by bt
GT	set of back-pressure steam turbines indexed by gt
W	set of wind turbines indexed by nw
P	set of seasons (summer and winter) indexed by p
H	set of day and night indexed by h
SN	scenarios of uncertain parameters indexed by sen
S	five stages of steams: HP , MP , LP , LLP and CW
I	energy technologies indexed by i

Deterministic parameters

H^{lc_v}	lower calorific value [GJ/Mmol]
η_{ACm}	compressor isentropic efficiency
r_{ACm}	pressure ratio of compressor
γ_a	specific heat capacity ratio
V_c	cut-in wind speed [m/s]
η_{CC}	efficiency of combustion chamber
A	surface area of the solar heat collector [m ²]
Fr	heat removal factor
r	fuel to air ratio
COP	energy conversion coefficient
$Deth$	molar enthalpy value [GJ/Mmol]
ief	optical efficiency
V_f	cut-out wind speed [m/s]
C_p	specific heat capacity [GJ/Mmol/K]
ΔH	enthalpy change [GJ/Mmol]
φ	ratio of boiler blowdown
DH	hours in day or night [12 hours]
DP	days in each season [182 days]

Uncertain parameters

$rad_{p,h,sen}$	solar radiation [W/m ²]
$V_{p,h,sen}$	wind speed [m/s]
$Dmd_{s,p}$	demand of steam s in period p [GJ/h]

First stage variables

$Z_{st,s}$	1 if the virtual steam turbine st of steam s exits
Z_{bt}	1 if the back-pressure steam turbine exits
Z_{gt}	1 if the gas turbine exits
Z_{nw}	1 if the wind turbine nw exits
mW_i	the maximum capacity of equipment i

Second stage variables

$Q_{cb,p,h,sen}$	heat released by CFB boiler cb [GJ/h]
$F_{cb,p,h,sen}^{hps}$	steam generated by the boiler cb [Mmol/h]
$mC_{cb,p,h,sen}$	mass flowrate of coal [t/h]
$W_{st,p,h,sen}$	power produced by st [MW]
$tin_{p,h,sen}$	1 if store thermal into the tank
$tout_{p,h,sen}$	1 if release thermal out of the tank
$W_{p,h,sen}^{mx}$	power generated by a wind turbine [MW]
$F_{p,h,sen}^{sw}$	molar flowrate of steam generated by the SHC [Mmol/h]
$Fv_{s,p,h,sen}$	molar flowrate of steam s to the valve [Mmol/h]

Superscript

wv	water vaporizing in boiler
wt	boiler water
wp	water preheating in boiler
bd	blowdown of boiler
sk	flue gas from boiler
wl	wall loss of boiler
oh	steam overheating in boiler

<i>hpss</i>	saturated high-pressure steam
<i>hpso</i>	overheated high-pressure steam
<i>tk/k</i>	thermal storage tank
<i>GB</i>	gas boiler
<i>ST</i>	steam turbine
<i>CFB</i>	coal-fired boiler
<i>BST</i>	back pressure turbine
<i>CC</i>	combustion chamber
<i>WT</i>	wind turbine
<i>SHC</i>	solar heat collector
<i>EC</i>	electric chiller
<i>HRSG</i>	heat recovery steam generator
<i>AC</i>	absorption chiller
<i>ACm</i>	air compressor
<i>GT</i>	gas turbine

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