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A disjunctive programming model for superstructure optimization of power and desalting plants

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Abstract

In this paper, a new formulation based on disjunctive programming to model the superstructure of alternative configurations for the synthesis, design and analysis of combined cycle power and desalination plant recently developed in Mussati et al. [Desalination, 182 (2005) 123–129] is presented. In this new formulation, boolean variables model discrete decisions while continuous variables represent the operation conditions of the process, e.g., flow rates, energy demand. Optimal unit configuration and operating conditions are computed by solving the proposed model in order to satisfy electricity generation and freshwater productions demands.

Rigorous, non-convex and highly non-linear constraints are involved in the formulation, therefore, robust and efficient solution algorithms have to be used. The Logic-Based Outer Approximation (LOA) algorithm developed by Turkay and Grossmann [Comp. Chem. Eng., 20 (8) (1996) 959] with the modifications introduced by Yeomans and Grossmann [Ind. Eng. Chem. Res., 39 (6) (2000) 1637] are used as part of the solution procedure.

The model is implemented and solved in the General Algebraic Modeling System (GAMS). Several study cases for different required power to water ratios are presented and analyzed in order to illustrate the robustness and computational performance of the proposed model.

Keywords: Superstructure optimization; Synthesis and design of chemical process; Optimization; Generalized disjunctive programming

1. Introduction

Thermal desalination plants are energy intensive and its coupling with power plants result in appreciable economy compared with separate single purpose power generation and desalination installations. Large dual-purpose power desalination plants are built to reduce the cost of electricity production and freshwater. The dual purpose power desalination plants make use of thermal energy extracted or exhausted from power plants in form of low-pressure steam to provide heat

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input to thermal processes, like multi-stage flash (MSF) or multi-effect (MED) distillation systems.

Different arrangements are possible in order to satisfy electricity and freshwater demands and the selection of the optimal system is a difficult task because it depends strongly on many factors such us the required power to water ratio, cost of fuel energy charged to the desalting process, electricity sales, capital costs and local requirements. Alternative configurations must be considered in order to select the most suitable cogeneration desalting plants. Therefore, the formulation of models for the synthesis and analysis of different design alternatives are very important and useful.

Despite that many contributions dealing with the design of dual purpose desalination plants (DPP) have been published, only few of them focus on the simultaneous optimization of the configuration and operating conditions [1–3]. Commonly, the best configurations are obtained by parametric comparisons of different optimal structures [4–6]. This task is highly time consuming due to the existence of numerous design alternatives which are combinatorial by nature. In addition, there exists an inherent uncertainty whether a better alternative could have been found. For that reason, an efficient and systematic simultaneous optimization procedure is of main importance for the selection of the best design alternative.

Mathematical models including alternative designs involve discrete decisions related to the selection of equipments. There are different formulations to represent problems involving discrete and continuous variables [7].

Mussati et al. [3] presented an optimization mathematical model of a superstructure of alternative configurations of DPP. The superstructure of optional arrangements (optimization problem) is modeled as a Mixed Integer Non-linear Programming (MINLP) Model where binary variables (0–1) are used to select the equipments for the cogeneration plant. The resulting MINLP mathematical model can be used for synthesis as well as for analyzing different design alternatives. The solution obtained by the proposed mathematical model provides the basic design of the DPP.

This paper presents a new mathematical model for the superstructure of alternative configurations of DPP recently proposed by Mussati et al. [3]. The new formulation is based on generalized disjunctive programming (GDP) [8] and can be used for the synthesis as well as for analyzing different design alternatives for this process.

This work is organized as follows. Section II introduces the problem definition while Section III briefly describes the process and the proposed superstructure. Section IV summarizes the formulation assumptions and the mathematical model. Section V presents the solution procedure and Section VI illustrates a numeric example through a case study. Finally, this paper concludes in Section VII with conclusions and major challenges for further research.

2. Problem definition

The problem is stated as follows. Given are the electric power requirement, the freshwater production and the seawater conditions (temperature and composition). The goal of the problem is to determine the optimal configuration and operating conditions of a dual purpose plant at minimum total levelized cost.

3. Superstructure representation

The problem superstructure adopted previously in Mussati et al. [3] is here considered but in this work, the discrete decisions are modeled using disjunctions [8].

Fig. 1 shows the superstructure proposed for the combined power desalination plant, which consists of a gas turbine as a topping cycle and a steam process as a bottoming cycle. Methane is burned in the gas turbine which produces electricity and hot exhaust gases. The exhaust gases

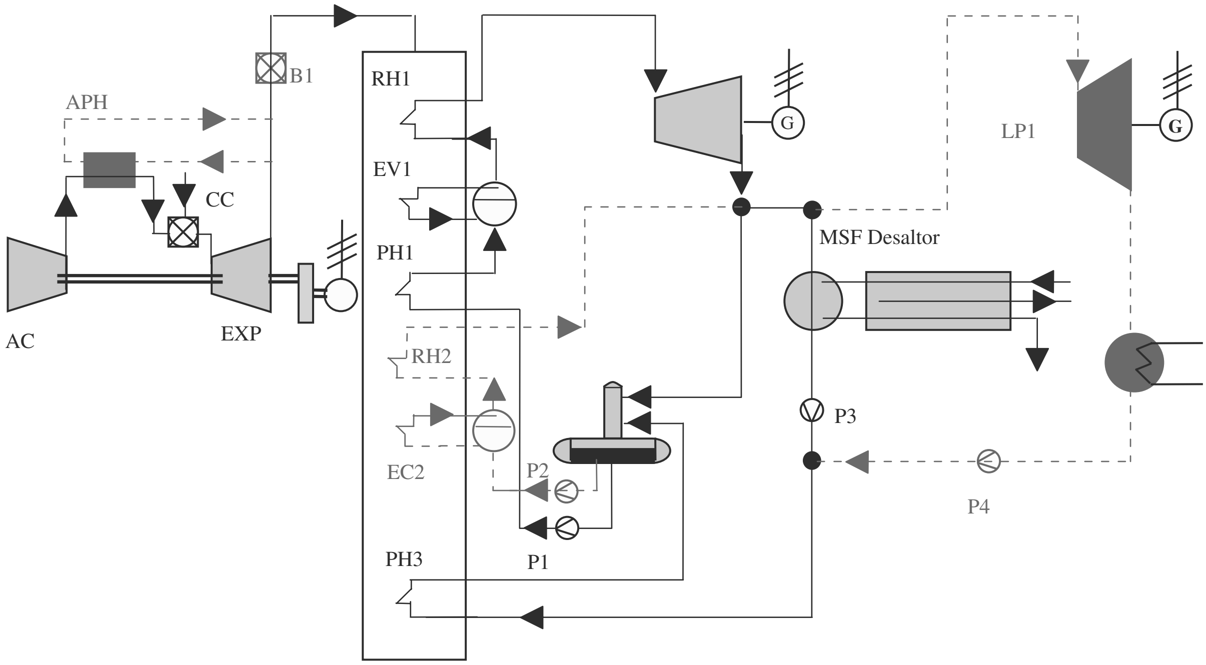

Fig. 1. Combined power cycle coupled to thermal desalination plants.

can be used to pre-heat the incoming air on the optional air pre-heater (APR) and therefore the exhaust gases are used in a heat recovery steam generator (HRSG). The discrete decisions are related with the existence of an APH (Fig. 1), the production of vapor at low pressure (RH2, EV2, DR2, P2) which can be used on the multi-stage flash (MSF) evaporator as hot utility, the existence of an additional combustor (B1) and a condensing steam turbine (LP1).

Finally, the same assumptions for the modeling of the power and desalting plant considered in Mussati et al. [3] are preserved here.

4. Generalized disjunctive formulation

The same assumptions and features considered in the MINLP model recently proposed by Mussati et al. [3] are also considered here for the combined power cycle and desalting plant and are shortly described next.

Water is considered as the working fluid on the HRSG. Rigorous chemical-physical properties (volume, enthalpy and entropy) for all streams are considered assuming ideal gas and liquid behavior. Exact calculation of the logarithmic mean temperature difference is used to compute heat transfer areas. Isentropic and isenthalpic efficiencies are taken into account on the gas turbine and steam turbines, respectively. Regarding the MSF desaltor, temperature and concentration-dependent functionalities for the heat capacity (C_p), boiling point elevation (BPE) and latent heat of evaporation (λ_v) are considered [9]. Specific correlations to compute the overall heat transfer coefficient (U) and the geometric design for the chamber of each stage (length, width and height) are adopted from El-Dessouky et al. [9].

The most important aspects of the mathematical model are presented next. Based on the superstructure illustrated in Fig. 1, the optimization problem is formulated as a GDP problem to minimize the total costs of the plant. The continuous variables are involved on mass, energy and momentum balances of equipments and disjunctions model the selection of equipments.

Consider the following set definition. Let C be the set of components: $C = \{i/i = O_2, N_2, CO_2, H_2O\}$. Let EQ be the set of equipments of the process: EQ{j/j = AC, EXP, RH1, RH2, EC1, EC2, APH, EV1, EV2, HP1, LP1, DR1, DR2, PH1, PH3, B1, CC, P1, P2, P3, P4} where AC is the air compressor, EXP the expander, RH1 and RH2 the re-heaters, EC1 and EC2 economizers, APH the air pre-heater, EV1 and EV2 the evaporators, HP1 and LP1 the steam turbines, DR1 and DR2 the drums, PH1 and PH3 the pre-heaters, B1 and CC the combustors and P1, P2, P3 and P4 the pumps.

Note that due to space limitations, the mathematical model for the MSF desaltor is not presented here. The detailed mathematical formulation can be found in Mussati et al. [10,11].

4.1. Objective function

The objective function involves the minimization of the total levelized costs of the plant. The cost functions for the plant components are taken from the literature [12,13], which are calculated using the total revenue requirement (TRR) method [13].

4.2. Model disjunctions

Boolean variables Y_j are related to the following discrete decisions:

- The existence of an APH (Y_{APH}).
- The production of vapor at low pressure, RH2, EV2, DR2 and P2 (Y_j, j = RH2, EV2, DR2, P2). This vapor can be used on the MSF evaporator as hot utility.
- The existence of an additional combustor B1 (Y_{B1}).
- The existence of a condensing steam turbine LP1 (Y_{LP1}).

The disjunction (1) is formulated to model the existence of the APH, the re-heater (RH2) and the evaporator (EV2):

$$\begin{bmatrix} Y_j \\ A_j = \dfrac{M_j^{gases,inl}(H_j^{gases,inl} - H_j^{gases,out})}{U_j\,\Delta Tml_j} \\ \Delta Tml_j = \dfrac{(T_j^{gases,inl} - T_j^{fluid,out}) - (T_j^{gases,out} - T_j^{fluid,inl})}{\log\dfrac{(T_j^{gases,inl} - T_j^{fluid,out})}{(T_j^{gases,out} - T_j^{fluid,inl})}} \\ T_j^{gases,inl} \geq T_j^{fluid,out} + \Delta T\ \min \\ T_j^{gases,out} \geq T_j^{fluid,inl} + \Delta T\ \min \\ C_j = f(A_j) + \gamma_j \end{bmatrix} \vee \begin{bmatrix} \neg Y_j \\ T_j^{gases,inl} = T_j^{gases,out} \\ C_j = 0 \end{bmatrix} \quad j = \text{APH, RH2, EV2} \qquad (1)$$

The index fluid refers to air for the case of the air compressor and to the working fluid for the re-heater and evaporator. If equipment j is selected, then the area (A_j) is calculated as well as the cost associated with it, which is a function of a fixed cost (γ_j) and of the transference area (A_j).

The disjunction (2) models the selection of an additional combustor (B1):

$$\begin{bmatrix} Y_j \\ C_j = f(M_j^{inl}, T_j^{out}) + \gamma_j \end{bmatrix} \vee \begin{bmatrix} \neg Y_j \\ M_j^{inl} = M_j^{out} \\ X_{j,i}^{inl} = X_{j,i}^{out} \quad \forall i \in C \\ T_j^{inl} = T_j^{out} \\ C_j = 0 \end{bmatrix} \quad j = \text{B1} \qquad (2)$$

Note that if the additional combustor is selected (Y_{B1} = true), a cost (C_j) is related to it whereas if this equipment is not selected, the stream of gases is by passed.

The existence of a condensing steam turbine (LP1) and of the pumps (P2 and P4) is modeled with the disjunction in (3), which imposes a cost (C_j) if the equipment is selected. Otherwise, no pressure and temperature changes take place in the process.

$$\begin{bmatrix} Y_j \\ C_j = f(X) + \gamma_j \end{bmatrix} \vee \begin{bmatrix} \neg Y_j \\ T_j^{inl} = T_j^{out} \\ P_j^{inl} = P_j^{out} \\ C_j = 0 \end{bmatrix}$$
$$j = LP1, P2, P4 \qquad (3)$$

In disjunction (3), the vector $X_j = (W_j, \eta_{isoent})$ for j = LP1, where W_j is the power of the turbine and is η_{isoent} the isentropic efficiency. For j = P2, P4, $X_j = (W_j, P_j^{out})$ where W_j is the power of the pumps and P_j^{out} is the outlet pressure.

4.3. Logic propositions

The logic proposition (4) imposes the condition that if one equipment for the production of low-pressure vapor is selected, all the others are selected too:

$$Y_{RH2} \Rightarrow Y_{EV2} \wedge Y_{DR2} \wedge Y_{P2} \qquad (4)$$

4.4. Global constraints

In Eq. (5), the power ($W_j^{air/gases,inl}$) and isentropic efficiency (η_j) for the air compressor and expander of the gas turbine are formulated. Rigorous correlations are considered to calculate the enthalpy and entropy for the air and gases.

$$\left.\begin{array}{l} W_j^{air/gases,inl} = M_j^{air/gases,inl}(H_j^{air/gases,inl} - H_j^{air/gases,out}) \\ \eta_j = \dfrac{H_j^{air/gases,inl} - H_j^{air/gases,out}}{H_j^{air/gases,inl} - H_j^{air/gases,iso}} \\ S_j^{air/gases,inl} = S_j^{air/gases,iso} \end{array}\right\}$$
$$j = AC, EXP \qquad (5)$$

Regarding to the continuous variables, H, S and M refer to the specific enthalpy, specific entropy and mass flow-rate, respectively.

Energy balances for the equipments of the gas turbine and for the equipments involved in the HRSG are formulated in Eq. (6):

$$M_j^{gases,inl}(H_j^{gases,inl} - H_j^{gases,out}) = M_j^{fluid,inl}(H_j^{fluid,inl} - H_j^{fluid,out})$$
$$j = APH, RH1, RH2, EC1, EC2, PR1, EV1, EV2 \qquad (6)$$

Note that the index fluid is air for the case of the air compressor and expander. In the case of the equipments of the HRSG, the index fluid refers to the working fluid (water).

The area (A_j) for the permanent (fixed) equipments of the HRSG is computed in Eq. (7):

$$\left.\begin{array}{l} A_j = \dfrac{M_j^{gases,inl}(H_j^{gases,inl} - H_j^{gases,out})}{U_j\, \Delta Tml_j} \\ \Delta Tml_j = \dfrac{(T_j^{gases,inl} - T_j^{wf,out}) - (T_j^{gases,out} - T_j^{wf,inl})}{\log\left(\dfrac{T_j^{gases,inl} - T_j^{wf,out}}{T_j^{gases,out} - T_j^{wf,inl}}\right)} \\ T_j^{gases,inl} \geq T_j^{wf,out} + \Delta T_{min} \\ T_j^{gases,out} \geq T_j^{wf,inl} + \Delta T_{min} \end{array}\right\}$$
$$j = RH1, EC1, EC2, PR1, EV1 \qquad (7)$$

The chemical reaction which takes place in the combustors is described by the following equation:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O_{vapor}$$

The mass and energy balances are formulated in Eq. (8), considering that ν_i corresponds to the stechiometric factor of component i in the reaction of combustion and the super index “fuel” refers to CH_4.

$$\left.\begin{aligned} &M_j^{out} = M_j^{inl} + M_j^{fuel} \\ &M_j^{out} H_j^{out} = M_j^{inl} H_j^{inl} + M_j^{fuel} H_j^{fuel} \\ &M_j^{out} x_{j,i}^{out} = M_j^{inl} x_{j,i}^{inl} + v_i M_j^{fuel} \end{aligned}\right\} \; j = CC, B1 \tag{8}$$

Constraints (9) formulate enthalpy and entropy balances for the high- and low-pressure steam turbines, where T_j^* refers to isenthalpic temperature.

$$\left.\begin{aligned} &S_j^{out}(T_j^{out}, P_j^{out}) = (1-\eta_{iso}) \\ &\times\left[S_j^*(T_j^*, P_j^{out}) - S_j^{inl}(T_j^{inl}, P_j^{inl})\right] + \ldots + S_j^{inl}(T_j^{inl}, P_j^{inl}) \\ &H_j^{inl}(T_j^{inl}, P_j^{inl}) = H_j^*(T_j^*, P_j^{out}) \\ &W_j = M_j\left[H_j^{out}(T_j^{out}, P_j^{out}) - H_j^{inl}(T_j^{inl}, P_j^{inl})\right] \end{aligned}\right\} \\ j = HP1, LP1 \tag{9}$$

Eq. (10) formulates the power W_j in the pumps, where sv refers to specific volume:

$$\left.\begin{aligned} &W_j = \frac{M_j \, sv\, (P_j^{out} - P_j^{inl})}{\eta_j} \\ &W_j = M_j\,(H_j^{out} - H_j^{inl}) \end{aligned}\right\} \; j = P1, P2, P3, P4 \tag{10}$$

5. Solution algorithm

The GDP model is solved with the decomposition algorithm proposed by Yeomans and Grossmann [14], which is a modified version of the logic-based outer approximation (LOA) algorithm [15]. This algorithm solves the disjunctive programming problem by iterating between reduced NLP subproblems and MILP master problems. Thus, the GDP model proposed in Section IV is rewritten as a NLP and MILP formulations. A general procedure for making this transformation can be found in Turkay and Grossmann [15].

The model is implemented and solved in the General Algebraic Modeling System (GAMS). The generalized reduced gradient algorithm CONOPT is selected to solve the NLP problems and OSL as the MIP solver.

The decomposition algorithm is initialized by solving an NLP subproblem with all existent equipments (Y_j = true, for all j) which provides linearization for all the non-linear equations in the original model. This problem requires solving the largest possible problem but it is not computationally expensive since a detailed initialization and bounding schemes have been considered.

6. Results and discussion

In this section, two examples are presented to illustrate the performance of the proposed GDP model.

As mentioned in Section II, given a set of demands of electricity and freshwater production, the objective is to design a DPP at minimum total levelized cost by determining the equipment interconnections and its corresponding operating conditions.

Two examples are considered for the illustration of numeric results. Example 1 considers the synthesis of a dual purpose plant to supply 75 MW and 1000 t/h of electricity and freshwater, respectively, while demands of 100 MW and 1000 t/h must be satisfied in Example 2. The problem parameters are given in Table 1.

Example 1

The optimal configuration resulted from the optimization problem is given in Fig. 2 and the main operating conditions to generate the required electricity (75 MW) and freshwater (1000 t/h) requirements are reported in Table 2.

As is shown in Fig. 2, the optimal process configuration has the gas turbine GT, the HRSG2 and the steam turbine HPT coupled to MSF desaltor. The total levelized cost of plant is $5628.23/h.

Table 1
Parameters for the numeric examples

MSF desaltor	
Seawater salinity	45,000 ppm
Seawater temperature	298 K
Maximum operating temperature	390 K
Water production	1000 t/h
Tube diameter	0.030 m
Pitch	1.25 m
Steam turbines	
Turbine efficiency (HPT, LPT)	0.95
Maximum inlet temperature (GT)	1600 K
Maximum inlet temperature (HPT)	870 K
Maximum inlet pressure (HPT)	140 bar

Table 2
Optimal values for example 1

Variable	Value
Objective function value [$/h]	5628.23
Process heat (desaltor) [Gcal/h]	51.43
Process vapor temperature [K]	440.25
Inlet temp. on back pressure steam turbine [K]	700.06
Inlet temperature on condensing turbine [K]	440.25
Total heat transfer area on HRSG [m^2]	9010.12
Total heat transfer area on desaltor [m^2]	67,502.32
Fuel consumption by GT [Kmol/s]	0.22
Fuel consumption by B1 [Kmol/s]	0
Net power produced by GT [MW]	66,290.85
Power produced by back pressure turbine [MW]	7904.98
Power produced by condensing turbine [MW]	804.17
Working fluid flow [kg/s]	30
Steam generation at intermediate pressure [kg/s]	0

Note that since non-convexities are involved in the NLP model due to the non-linearities of the equations, such as for the investments cost and enthalpy balances, a global optimum solution cannot be guaranteed.

Example 2

The same optimization problem is solved but in this example the demand of electricity is 100 MW. The optimal configuration for this example is shown in Fig. 3 and optimal operating conditions are given in Table 3.

As is illustrated, in the final design which involves a total levelized cost of $6235.61/h, vapor at medium pressure is necessary to be produced in order to increase the electricity production in the low-pressure steam turbine to satisfy the required electricity demand. The production of vapor at medium pressure required the selection of the following equipments: the pump P2, the drum DR2 and the re-heater RH2.

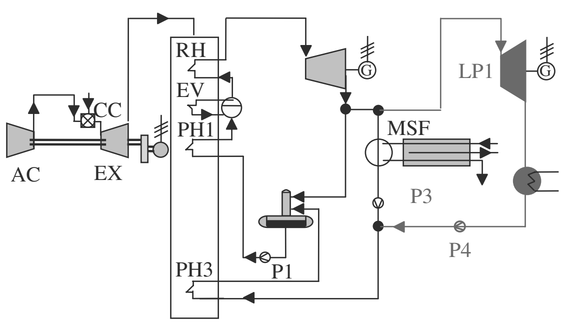

Fig. 2. Optimal configuration for example 1.

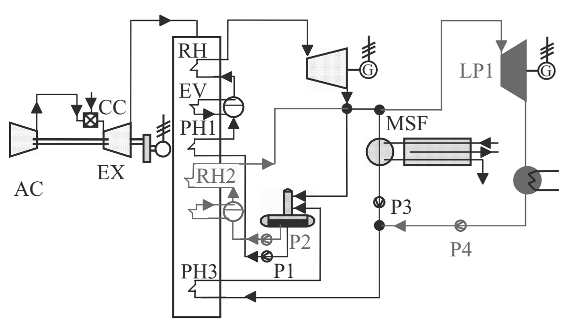

Fig. 3. Optimal configuration for example 3.

Table 3
Optimal values for example 2

Variable	Value
Objective function value [$/h]	6235.61
Process heat (desaltor) [Gcal/h]	55.43
Process vapor temperature [K]	425.62
Inlet temp. on back pressure steam turbine [K]	805.58
Inlet temperature on condensing turbine [K]	425.62
Total heat transfer area on HRSG [m^2]	32,879.12
Total heat transfer area on desaltor [m^2]	66,250.43
Fuel consumption by GT [Kmol/s]	0.260
Fuel consumption by B1 [Kmol/s]	0
Net power produced by GT [MW]	72,333.37
Power produced by back pressure turbine [MW]	22,266.43
Power produced by condensing turbine [MW]	5400.20
Working fluid flow [kg/s]	32.43
Steam generation at intermediate pressure [kg/s]	5.65

7. Conclusions

This paper has presented a Generalized Disjunctive Programming model for the optimal synthesis and design of a DPP. The LOA algorithm developed by Turkay and Grossmann [15] with the modifications introduced by Yeomans and Grossmann [14] has been implemented in the solution procedure. This algorithm solves the disjunctive programming problem by iterating between reduced NLP subproblems and MILP master problems.

Several examples have been successfully solved by applying the algorithm, from which two examples have been presented in this paper to illustrate the robustness and computational performance of the proposed formulation.

Despite that the MINLP formulation presented recently in Mussati et al. [3] has efficiently solved the problem for different demands of freshwater and electricity, the proposed GDP formulation resulted to be more flexible and robust than the MINLP formulation which convergence is strongly dependent on a good initial solution. In fact, the convergence of the NLP subproblems in the GDP solution algorithm is facilitated because the constraints related to selected equipments are only considered in the problem, increasing its robustness and flexibility. In addition, we have observed that the GDP formulation is not as strongly dependent on the initial values as the MINLP formulation.

7.1. Future works

The mathematical model presented in this paper should be extended in order to consider other important aspects related to the operation mode and environment pollution of the plant. Precisely, aspects such as optimal maintenance policy of the main equipments (considering the mean time to failure and repair -MTTF- -MTTR-, maintenance cost, among others) as well as their reliabilities (namely series, parallel, series/parallel and stand-by structures) are necessary to take into account in order to get a real-world solution and to satisfy the freshwater and electricity demands. Regarding to the environment aspects, the treatment of greenhouse gases (namely CO_2) formed during the combustion process should also be focused. In fact, the modeling the chemical absorption of CO_2 with amine (MDEA) in order to remove the CO_2 gas from the fuel gas will be treated. Also mathematical models for the absorber and desorber units by using detailed steady state models will be integrated to the GDP model presented here.

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