Analysis of optimal application for exhaust gas in thermal oxidizers with case studies

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Abstract: There is potential for optimizing thermal oxidizer plants to increase industrial energy efficiency results in environmental and economic dimension of sustainability. In the present work, genetic algorithm is implemented for three thermal oxidizer cases in three different petrochemical plants to optimize the fuel cost for the three Heat Recovery Steam Generators (HRSG's) which are going to be used for the recovery of the heat from the outlet of the thermal oxidizer units. Generally, thermal oxidizers are used in petrochemical plants to burn waste gases in the plant to reduce the environmental impact of the off-gases of plant and normally the waste heat are released to the atmosphere via a stack. The optimization results have been compared for three cases. Five decision variables have been selected and the objective function was optimized. By increasing the fuel price, the values of thermo-economical decision variables tend to those thermodynamically optimal designs.

Keywords: *Heat Recovery Steam Generator (HRSG), thermo-economics, Optimization, Thermal Oxidizer, Genetic Algorithm, Low Density Polyethylene (LDPE) Plant.*

Nomenclatures

c	*Cost per exergy unit…………..* $\$.MJ^{-1}$
c	*Cost of fuel per energy unit…* $\$.MJ^{-1}$
$\dot{c}$	*Cost flow rate………………..* $\$.sec^{-1}$
c_p	*Specific heat at constant Pressure……………* $KJ.Kg^{-1}.K^{-1}$
CRF	*Capital recovery factor*
h	*Enthalpy……………………* $KJ.Kg^{-1}$
LHV	*Lower heating value…………* $KJ.Kg^{-1}$
$\dot{m}$	*Mass flow rate…………………* $Kg.s^{-1}$
r_c	*Compressor pressure ratio*
T	*Temperature…………………………...K*
Z	*Capital cost of a component…………..$*
$\dot{Z}$	*Capital cost rate……………* $\$.sec^{-1}$
ΔP	*Pressure loss*
η_{ac}	*Compressor isentropic efficiency*
η_{cc}	*Combustion chamber first law efficiency*
γ	*Specific heat ratio*
φ	*Maintenance factor*
EA	*Evolutionary algorithm*
GA	*Genetic algorithm*
P,/Pr,	*pressure ratio of compressor*
r_{ih}	*Inlet humidity percent*
η_{to}	Thermal efficiency of thermal oxidizer
$\dot{W}$	Work……………………KW

Subscripts

ac	*Air compressor*
a	*Air*
cc	*Combustion chamber*
ev	*Evaporator*
ec	*Economizer*
f	*Fuel*
F	*Fuel for a component*
g	*Combustion gasses*
j	*Stream*
k	*Component*
s	*Steam*
P	*Product of a component*
Pinch	*Pinch point*

1. Introduction

One of the important ways to reduce the effects of environmental impacts of industrial plants is increasing energy efficiency of the plants. Developing techniques for designing efficient and cost-effective energy systems is one of the foremost challenges of energy engineering face. In a world with finite natural resources and increasing energy demand by developing countries, it becomes increasingly important to understand the mechanisms which degrade energy and resources and to develop systematic approaches for improving the design of energy systems and reducing the impact on t he environment. The second law of thermodynamics combined with economics represents a very powerful tool for the systematic study and optimization of energy systems. This combination forms the basis of the relatively new field of thermo-economics.

Ethylene is the main feed of LDPE (Low density polyethylene) plant to produce LDPE product(s) in high pressure. By using a compressor system, excess ethylene in different units of the plant, some traced gases like Methane and Propane, small quantity of water and air are forced to a multi channel combustion chamber of thermal oxidizer unit to burn and diminish the concentration of pollutant, as consequences of imposed environmental limitations that exist for the petrochemical off-gases. After burning the off-gases in the combustion chamber, the considerable medium quality waste gas is released to atmosphere via vent stack. In practise, in most of the petrochemical plants the thermal oxidizer units work continuously as a matter of excess amount of ethylene and other mentioned substances.

For a medium LDPE plant, maximum volume off gases reaches 55000 kg/h with constant steady state pressure. This flow produces an average thermal caloric value of 45000 KJ/kg with average 300 °C flue gas.

The structure of a common thermal oxidizer is illustrated in figure 1. The installation consists of two compressor systems, multi channel combustion chambers, fuel supply and burner systems. In current models for the environmental condition the following are considered (T = 298.15 K and P = 1.013 bar). The operating fuel for the total plant is natural gas (taken as methane) with a lower heating value (LHV) equal to 50000 kJ/kg.

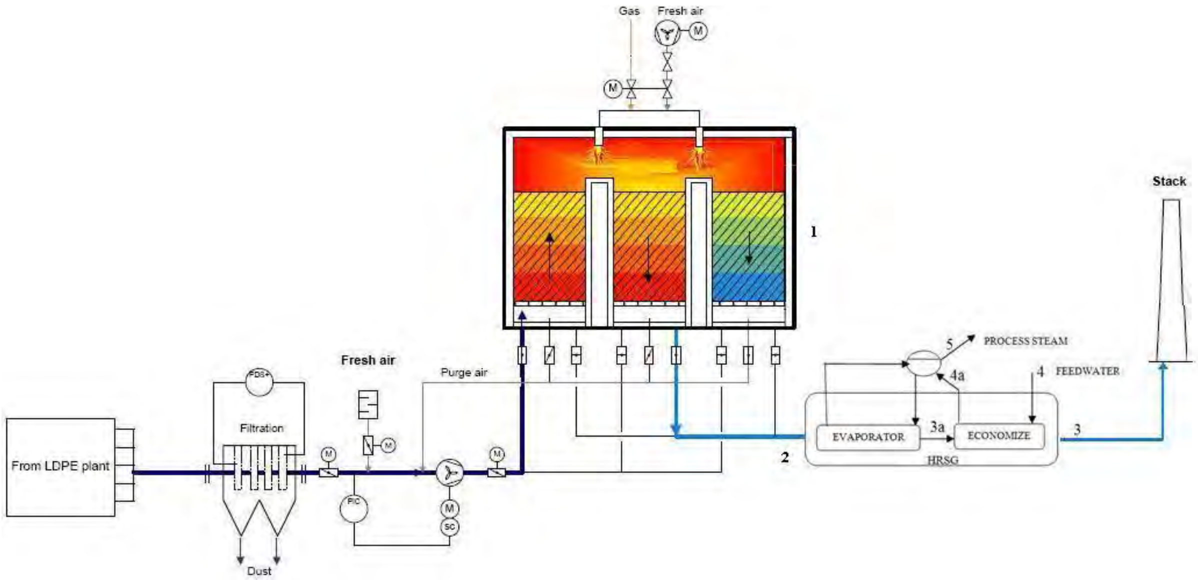

Fig. 1. Schematic sketch of thermal oxidizer with HRSG

In the current research, a part of waste heat energy system (thermal oxidizer) in LDPE (Low Density Polyethylene) plant is optimized according to some decision variables. The hot gases from the combustion chamber are conducted to a HRSG (Heat Recovery Steam Generator) to be utilized for producing steam and hot water. This steam and/or hot water can be used in different ways in this plant (LDPE Plant) or other adjacent industrial plants. Moreover, in this investigation three different thermal oxidizers units were studied and data obtained are analysed for research validation. The models used in this paper are realistic but incomplete from an engineering point of view since the object of this study is to present distinct models of thermoeconomic optimization. Therefore, it would be unreasonable to use an excessively complicated mathematical model to describe the performance of the plant.

2. Methodology

For modelling the system three categories of equations have been considered, the equations which describe the behaviour of the system (physical model), the equations for calculating the capital costs of the components (economic model) and the equations which has been used to calculate the thermodynamic properties (thermodynamic model) [1,2]. The decision variables selected for the optimization are the compressor pressure ratio P,/Pr, the isentropic efficiencies of the compressor (η_c), inlet humidity percent (r_{ih}), the temperature of the combustion gas at the HRSG inlet (T_2) and thermal efficiency of thermal oxidizer (η_{to}).

The following models are formulated as a function of these decision variables. To simplify these models without loss of methodological generality, the following assumptions are made: (1) The air and the combustion gases behave as ideal gases with constant specific heats. (2) For combustion calculations, the fuel is taken to be methane CH4 (3) All components, except the combustion chamber, are adiabatic. (4) Reasonable values are chosen for the pressure loss of the air and gas flows in the combustion chamber and recuperate boiler.

Our optimization program that is based on evolutionary algorithm has good convergence and better results due to using three input category data from three different petrochemical plants. As we know the optimization procedure is so crucial in engineering fields, especially mechanical engineering. Among the various techniques evolutionary algorithms (EAs) are of the greatest importance because of their convergence rate. Among EA algorithms, the Genetic Algorithm is the best option due to its less time consuming for iteration time as well as satisfying the several constraints. Besides, at the end of this study the influence of alteration in the demanded steam on the design parameters has been also studied.

In this paper, after thermodynamic modelling of the system and formation of the objective function, a cogeneration unit with thermal characteristics of well known problem [1,3,4,5] are simulated, optimized, and its results are compared to the results of other cases; in order to ensure the validity of our physical modelling and optimization procedure. Subsequently, parameters of problem are modified to match the conditions and requirements of the present work.

2.1. Thermodynamic modeling of thermal oxidizer with HRSG

Having known the values of decision variables (r_c, η_c, η_{to}, T2 and r_{ih}) for a set of fixed demands of process steam, the values of temperature and pressure in all lines of system was computed. Consequently, the value of fuel mass flow rate $\dot{m}_f$, which should be expressed in terms of decision variables, is determined. The relations of thermodynamic modelling are as follows:

Air compressor

$$T_{out} = T_{in}\left\{1+\frac{1}{\eta_{AC}}\left[r_c^{\frac{\gamma_a-1}{\gamma_a}}-1\right]\right\}, \tag{1}$$

$$\dot{W}_{ac} = \dot{m}_a.c_{p,a}(T_{out}-T_{in}) \tag{2}$$

Combustion chamber

$$\dot{m}_a h_1 + \dot{m}_f\, LHV = \dot{m}_g h_2 + (1-\eta_{cc})\,\dot{m}_f\, LHV \qquad (3)$$

$$\frac{P_2}{P_1} = (1-\Delta P_{cc}) \qquad (4)$$

Heat recovery steam generator

$$\dot{m}_s(h_5 - h_4) = \dot{m}_g(h_2 - h_3) \qquad (5)$$

$$\dot{m}_s(h_5 - h_{4a}) = \dot{m}_g(h_2 - h_{3a}) \qquad (6)$$

2.2. Objective function

The objective function is defined as the sum of two parts; the operational cost rate, which is related to the fuel expense, the rate of capital cost which stands for the capital investment and maintenance expenses. Therefore, the objective function represents total cost rate of the plant in terms of dollar per unit of time.

$$Obj.Func. = c_f \dot{m}_f LHV + \sum \dot{Z}_k \qquad (7)$$

Since the amounts of ultimate products (process steam) are fixed, the objective function is to be minimized so that the values of optimal design parameters would be obtained. For calculating the rate of operating cost equation, we have:

$$\dot{c}_f = c_f \dot{m}_f LHV \qquad (8)$$

In which c_f = 0.003 \$/MJ is the regional cost of fuel per unit of energy,$\dot{m}_f$ is the fuel mass flow rate, and LHV = 50000 kJ/kg is the lower heating value of Methane.

For expressing the purchase cost of equipment in terms of design parameters, several method have been suggested [2, 7-11]. In this paper, we used the cost functions mentioned in ref [2]. However, some modifications were made to tailor these results to the regional conditions in Iran and taking into account the inflammation rate. For converting the capital investment into cost per time unit:

$$\dot{Z}_k = Z_k.CRF.\,\varphi/(N \times 3600) \qquad (9)$$

Where, Z_k is the purchase cost of component in dollar, CRF (18%) is the capital recovery factor, N is the annual number of the operation hours of the unit (7500 hr), and φ (1.06) is the maintenance factor.

2.3. Optimization Procedure

Minimizing the objective function Eq.7 is a nonlinear optimization problem. In order to achieve feasible design parameters some physical constraints should be considered seriously. The list of these constraints and their reasons are briefed in table 1. Moreover, the following inequality constraints should be satisfied in heat exchangers (air pre-heater and heat recovery steam generator).

$$T_2 > T_1, \quad T_2 > T_5, \quad T_{3a} > T_5 + \Delta T_{pinch,\, min} \qquad (10)$$

In the present work a genetic algorithm code is developed in Matlab Software Programming.

Table1. The list of constraints

Constraints	Reason
$T_2 \le 1600^\circ K$	Material limitation
$r_c \le 16$	Commercial availability
$\eta_{ac} \le 0.9$	Commercial availability
$\eta_{to} \le 0.96$	Commercial availability
$T_3 \ge 400^\circ K$	To avoid formation of sulfuric acid in exhaust gases
$T_{4a} = T_5 - 15^\circ K$	To avoid evaporation of water in HRSG economizer

2.4. Evolutionary algorithm (Genetic Algorithm)

Such algorithms simulate an evolutionary process where the goal is to evolve solutions by means of cross over, mutation, and selection based on their quality (fitness) with respect to the optimization problem at hand. Evolutionary algorithms (EAs) are highly relevant for industrial applications, because they are capable of handling problems with non-linear constraints, multiple objectives and dynamic components properties that frequently appear in real-world problems. Moreover the input and output values for Genetic Algorithm method used in this study are shown in tables 2, 3.

Table 2. Genetic algorithm input

Tuning Parameters	Value
Population size	500
Maximum number of generation	1000
PC(Probability of Crossover) %	70
Pm (Probability of mutation) %	1
Number of crossover	2
Selection in process	Tournament
Tournament size	2

3. Discussion and result

The numerical values of the optimum design parameters of the thermal oxidizer with HRSG are listed in table 3. Moreover, the constraints of the problem are listed in table 1. These results are compared with other case's results. Figure 2 depicts the changes in the objective function versus generation in the developed genetic algorithm code.

Table 3. The comparison of simulation and optimization numerical output for three mentioned cases.

Decision variable	Optimum design	Optimum design	Optimum design
r_c	8.597	8.523	8.504
η_C	0.8465	0.8468	0.83292
η_{to}	94.5	95	95.4
T_2 (K)	504	573	642.3
r_{ih} (K)	80	70	65
Objective Function	0.362 (\$/s)	0.3617 (\$/s)	0.3294 (\$/s)

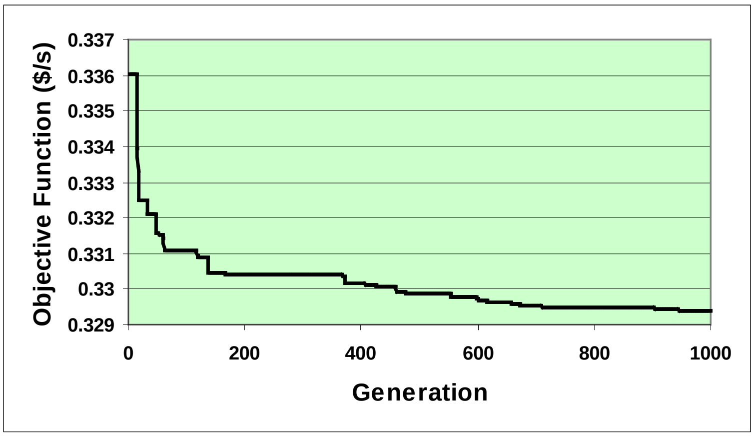

Fig. 2. Variation of Objective Function of the system with Generation (CE=.003\$/MJ).

Study of the variation of the optimal decision variables versus fuel unit cost reveals that by increasing the fuel cost optimal decision variables generally shift to thermodynamically more efficient design. As it can be clearly seen the values of decision variables r_p, η_{ac}, and HRSG inlet temperature (T_2) increase with increasing fuel unit cost. It is worthy to mention that while increasing combustion inlet temperature (T_1) reduces the exergy destruction in combustion chamber and heat exchangers (HRSG), due to the exhaust gases constraint (T_3 > 400K); it decreases with increasing the fuel unit cost. It should be noted that for each T_2 there exists a T_1 in which the best thermodynamical efficiency may be achieved. Moreover, an increase in HRSG inlet temperature reduces the exergy destruction in combustion chamber; and since increasing T_2 results in higher exhaust temperature of exhaust gases, the constraint T_3 > 400K does not cause any limitation for rising T_2. Due the fact that any increase in T_2 will dramatically affects the HRSG investment cost, figures 3-5 show the influence of the unit cost of fuel on the values of some the optimal decision variables. Figure 5 shows that when the fuel price increased the combustion chamber fuel mass flow rate decrease for minimizing the objective function. Due to uncertainty of capital investment data, it is imperative to study the results of capital expense variation on the optimal values of decision variables.

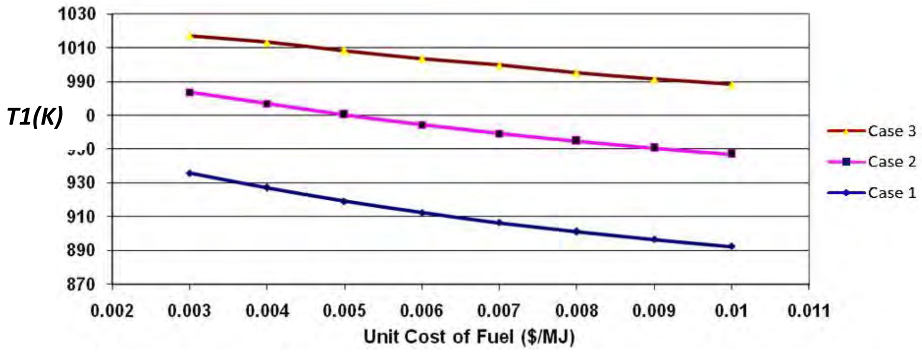

Fig. 3. The effects of fuel unit cost on the optimal value of combustion chamber inlet temperature, T1

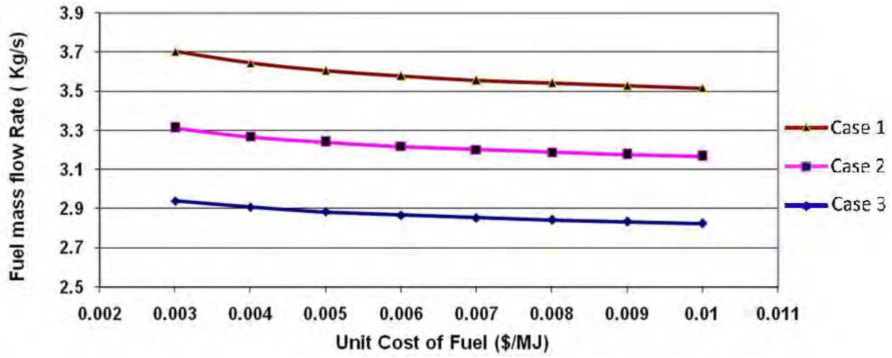

Fig. 4. The effects of fuel unit cost on the optimal value of Fuel Mass Flow Rate, mf

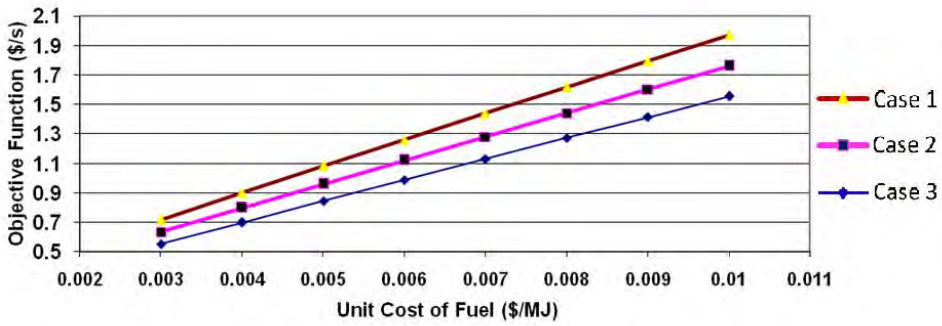

Fig. 5. The effects of fuel unit cost on the optimal value of Objective Function ($/s)

4. Conclusion

The determined optimum design parameters for thermal oxidizer with HRSG apparently show a trade-off between thermodynamically and economically optimal designs. For example, from thermodynamic point of view, the decision variable η_c should be selected as high as possible while this leads to an increase in capital cost. It should be noted that any change in the numerical values of a decision variable not only affects the performance of the related equipment but also all the performance of other equipments as well. It can be deduced from the figures 3-5 that by increasing the fuel price the values of decision variable in thermo-economically optimal design tend to those of thermodynamically optimal design.

Using heat recovery, thermal oxidizers cause more energy efficiency and decrease the level of green house gases accordingly. In spite of the fact that utilizing these types of technologies categorized as an end-of-pipe solution, nevertheless according to the three pillars of sustainability it contribute to both environmental dimension and economic dimension of sustainability.

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