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Optimization of a gas turbine in the methanol process, using the NLP model

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Abstract

Heat and power integration can reduce fuel usage, CO_2 and SO_2 emissions and, thereby, pollution. In the simultaneous heat and power integration approach and including additional production, the optimization problem is formulated using a simplified process superstructure. Nonlinear programming (NLP) contains equations which enable structural heat and power integration and parametric optimization. In the present work, the NLP model is formulated as an optimum energy target of process integration and electricity generation using a gas turbine with a separator. The reactor acts as a combustion chamber of the gas turbine plant, producing high temperature. The simultaneous NLP approach can account for capital cost, integration of combined heat and power, process modification, and additional production trade-offs accurately, and can thus yield a better solution. It gives better results than non-simultaneous methods. The NLP model does not guarantee a global cost optimum, but it does lead to good, perhaps near optimum designs.

This approach is illustrated by an existing, complex methanol production process. The objective function generates a possible increase in annual profit of 1.7 MEUR/a.

Keywords: Simultaneous optimisation; NLP; Model; Cogeneration; Gas turbine

1. Introduction

Heat and power integration can be performed using pinch analysis or mathematical programming methods, for example, nonlinear programming, NLP.

Pinch analysis is guiding heat and power integration using an extended grand-composite curve [5]. Thermodynamic analysis does not guarantee a global optimum solution because it cannot be used simultaneously with the material balance, but it quickly proposes good ideas for the heat and power integration of complex processes. Combined heat and power design adds degrees of freedom to the optimisation method [12]. Pinch analysis helps us to better understand integration using graphical representation of a gas turbine [11]. A step-wise methodology for gas turbine integration, combined with heat and power cogeneration, as developed by Axelsson et al. [2] is based on pinch analysis.

Lucas [10] has analysed a cogeneration system on the basis of thermodynamic laws. Thermodynamic criteria, such as plant efficiency and power to heat ratio, have been defined. Kalitventzeff and co-authors [7] have described this application in an ammonia production plant, revisiting the major rules of energy integration from the perspective of overall energy efficiency, including the combined production of heat and mechanical power for an existing process.

The NLP algorithm [3], which is based on mathematical programming, can be used for rigorous process and power integration. Although simultaneous, it is difficult to converge for complex and energy intensive processes because the number of variables increases with the number of combinations.

In this paper, we are concerned with simultaneous mathematical optimization techniques using NLP, including combined heat and power, as well as increased production.

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Nomenclature

NLP	nonlinear programming
Parameters	
A	area of heat exchanger (m^2)
C_{37}	cost of 37 bar steam (EUR/(kW a))
C_{el}	cost of electricity (EUR/(kW a))
C_M	price of methanol (EUR/t)
C_m	molar heat capacity (J/(mol K))
F	amount flow rate (mol/s)
P	power (W)
r	payback multiplier (1)
s	massic entropy (J/(K kg))
T	temperature (K)
V_{max}	maximum additional annual profit (EUR/a)
η_{tur}	thermodynamic efficiency of the medium pressure turbine (1)
η_{gen}	mechanical efficiency of the generator (1)
Φ	heat flow rate (W)

2. Heat and power integration

First, in this study, heat integration and generation of electricity was applied, using a gas turbine. Then, the simultaneous mathematical optimization method was applied, including combined heat and power, and increased production. The NLP model contained equations of structural and parametric optimization, with process operating constraints [4]. NLP can simultaneously optimize process integration and electric power production. The parameters for this process operation are left unchanged.

2.1. Gas turbine system

The gas turbine has rendered increasing service in the petrochemical industry. In industry, open-cycle gas turbine power plants are widely applied. A conventional power plant uses fuel energy to produce work and reject heat.

Usually, a gas turbine operates by internal combustion. Air and fuel pass through a compressor into a combustion chamber. The combustion products are expanded in a turbine, which drives an electric generator.

Many chemicals are produced under high pressure and at a high temperature. The reactor acts as the combustion chamber of the gas turbine plant. Then, separation at lower pressure and temperature follows and this pressure change can be used to drive a turbine, coupled to an electricity generator. The turbine uses process gas as a working fluid [6]. The power cycle is described as the ‘‘Brayton cycle’’.

The high operating pressure of the reactor outlet can be exploited to produce electricity using an open gas turbine. The open gas turbine is the basic gas turbine unit. The working fluid comes from the reactor and cycles through the following units (Fig. 1):

- gas turbine,
- heat exchanger,

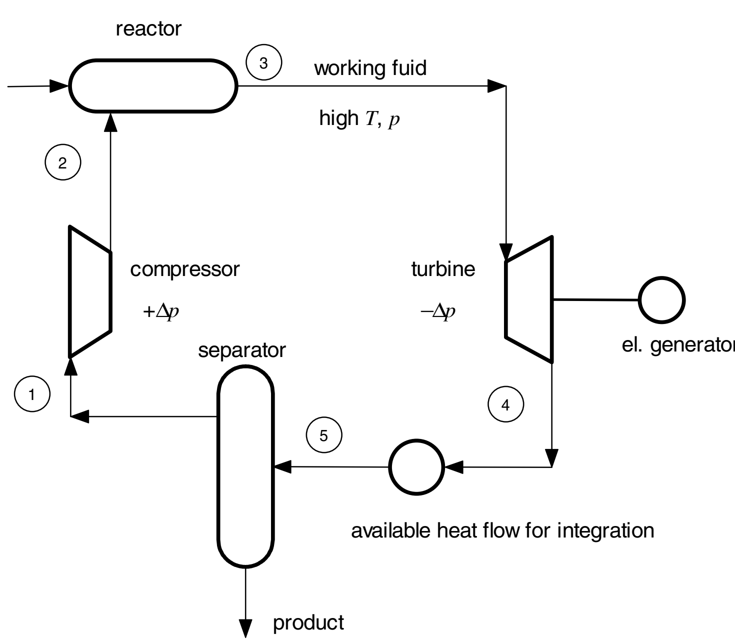

Fig. 1. Open circuit gas turbine with separator.

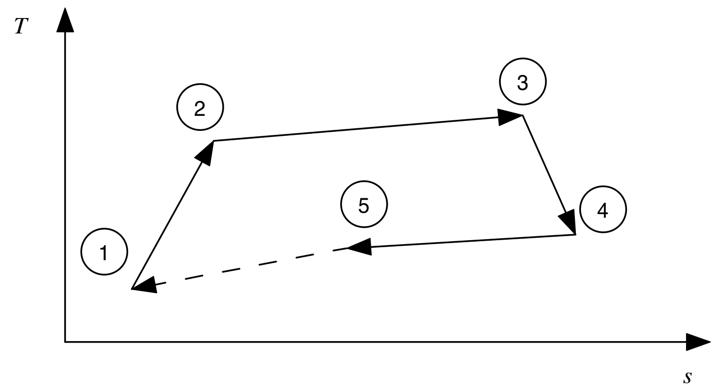

Fig. 2. The simplified temperature/massic entropy (T/s) diagram.

- separator, where the liquid product separates off and
- compressor.

The working fluid undergoes the following process steps, as shown in a simplified T/s (temperature/massic entropy) diagram (Fig. 2):

- 1-2 adiabatic compression,
- 2-3 reaction,
- 3-4 adiabatic expansion of reaction outlet stream in a turbine,
- 4-5 cooling or/and available heat flow for heat integration,
- 5 separation.

The power of the gas turbine depends on the primary variables: inlet temperature and compressing pressure ratio. The inlet temperature is restricted by the metallurgical limit of the turbine blades to about 800 °C.

The medium pressure of the designed turbine can be varied. Its power (P_{tur}) is a function of the outlet temperature ($T_{tur,out}$), molar heat capacity (C_m) and amount flow rate (F; Eq. (1)):

$$P_{tur} = C_m \cdot (T_{tur,\,in} - T_{tur,\,out}) \cdot F \qquad (1)$$

The inlet temperature ($T_{tur,\,in}$) is kept constant.

3. Case study

The suggested superstructural approach for a gas turbine has been tested in an existing complex, low-pressure Lurgi methanol plant producing crude methanol. The process is composed of three subsystems (Fig. 3):

- production of synthesis gas,
- production of crude methanol and
- purification of methanol.

In the first subsystem, natural gas is desulphurized (D101) and synthesis gas is produced from the natural gas and steam, in a steam reformer (REA-1). The purge gas and expansion gas are burnt in the reformer. The hot stream of the synthesis gas is cooled in a boiler E107, in heat exchangers E109, E110, E111, in an air cooler EA101 and in water coolers E112, E201. In the second subsystem, methanol is produced by the catalytic hydrogenation of carbon monoxide and/or carbon dioxide in the reactor REA. The outlet stream of the crude methanol is cooled with its inlet stream in the heat exchanger HEPR, in the air cooler HEA, and in the water cooler HEW. The methanol is flashed in SEP. In the third subsystem crude methanol is refined to pure methanol by distillation in the purification section of the process (D301–D304), to remove water and a variety of other impurities.

The present work [9] focuses on an efficient NLP model formulation including all the process units of crude methanol production over the cycle (Fig. 4). The methanol reactor (REA) is operated under high pressure, and the unconverted gas is recycled. The reactor's high recycle ratio and operating pressure are exploited to produce electricity in the open gas turbine (TUR). In conventional processes, the outlet stream of heat flow rate downstream the reactor is heat integrated with its inlet equivalent, without cogeneration. The exothermic reactor (REA) is operated within the existing parameters. The inlet stream of the reactor is heated by a process stream (HEPR) or by high pressure steam (HEST) or a combination of both. The gas turbine is placed downstream of the reactor. Its outlet stream is cooled using air (HEA) and water (HEW) heat exchangers before entering the flash (SEP). The liquid stream of the separation contains the product, whilst the recycled gas stream is compressed to 51 bar in a two-stage compressor (COMP1, 2), having an intermediate water cooling (HEW1). The exhaust flow rate of the purge gas is optimised.

The methanol production plan can be optimised by using the NLP model, which contains the same amount and enthalpy balances as all the above-mentioned process units (Fig. 4; case streams are presented in Table 2). The NLP model includes [8]:

- amount and enthalpy balances of process units,
- equations of reaction conversion,
- process constraints (flow rate, temperature and pressure),

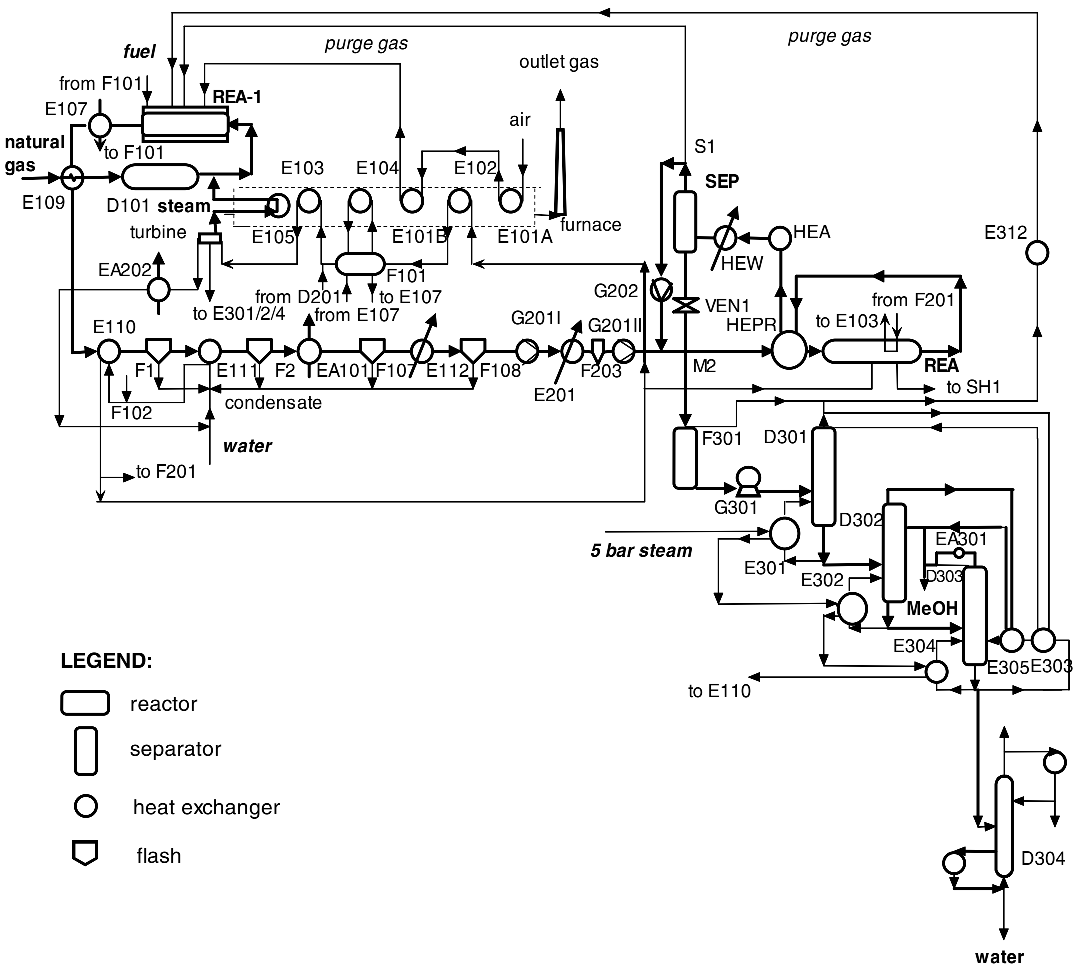

Fig. 3. Process flow diagram of a low-pressure Lurgi methanol plant.

- retrofit equations for reusing existing process units (heat exchangers) and
- an objective function.

Using the NLP model, the simultaneous mathematical optimization method presents the effects of the:

- increased methanol production depending on reaction conversions, and the degree of separation (SEP)
- electricity cogeneration,
- integration of heat flows in the heat exchangers and
- optimized exhaust flow rate (purge gas).

The goal of optimization is to maximize additional annual income, and minimize the additional annual depreciation (Eq. (4)). The additional annual income sums up:

- the additional cogeneration of electricity ($P_{\text{tur}} \cdot \eta_{\text{tur}} \cdot \eta_{\text{gen}}$) and
- the additional production of methanol (ΔF_{M}).

High reactant flow rate favours reactions with higher conversion and optimisation of raw material composition and can increase production; therefore, the flow rate of reaction, separator and exhaust are optimised.

The additional production of methanol, ΔF_{M}, can be calculated by the equation:

$$\Delta F_{\text{M}} = F_{\text{M}} - 138.97 \tag{2}$$

F_{M} being the optimized amount flow rate for methanol, 138.97 mol/s being the existing one.

The thermodynamic efficiency of the medium pressure turbine (η_{tur}) and the mechanical efficiency of the generator (η_{gen}) is supposed to be 85% for each.

The annual depreciation of the medium pressure turbine ($C_{\text{d, tur}}$ in EUR/a) is a function of the power (P_{tur}; [3]):

$$C_{\text{d, tur}} = (22{,}946 + 13.5 \cdot P_{\text{tur}}) \cdot 4 \tag{3}$$

The published cost equations for the equipment are not usually adjusted to the real, higher industrial costs; therefore, the costs are multiplied by a factor, determined by experience [15].

The additional annual depreciation cost sums up (Table 1):

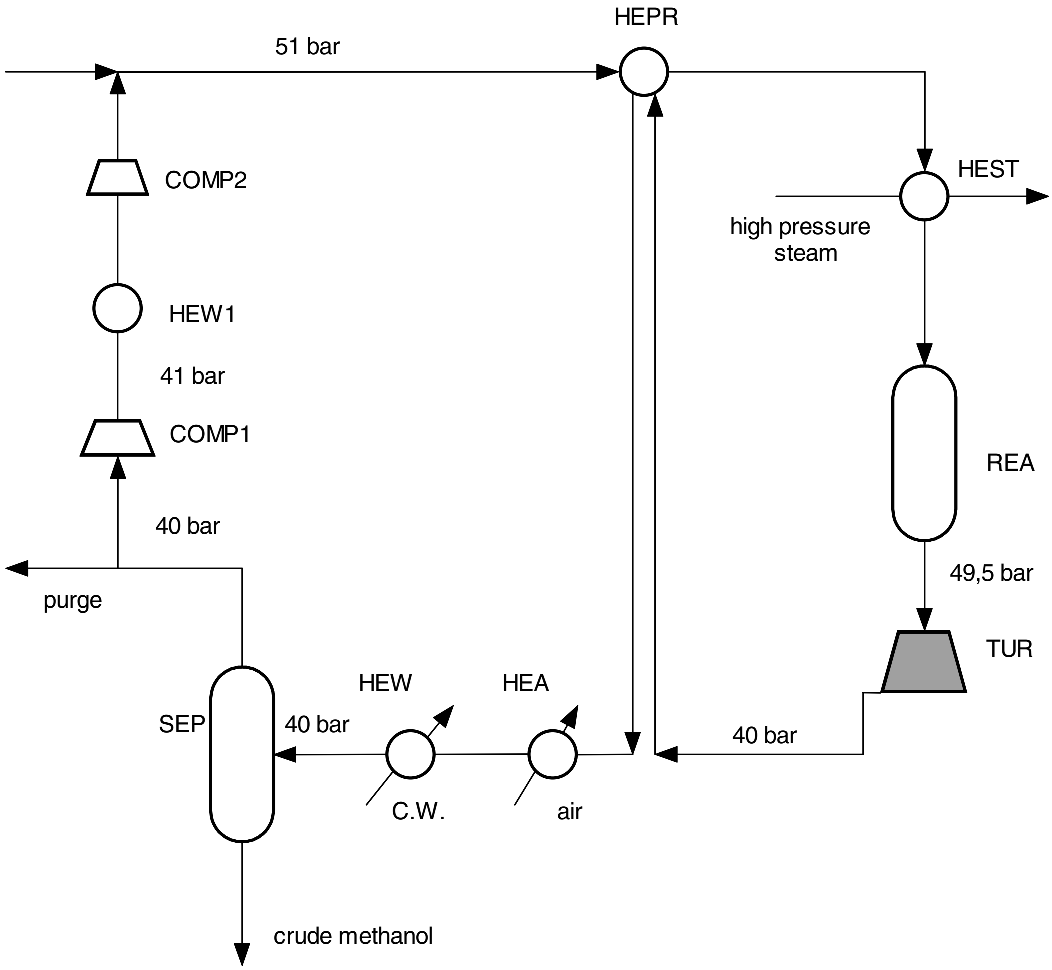

Fig. 4. Flow sheet of crude methanol production with a gas turbine.

Table 1
Cost items for example process

Installed cost of heat exchanger[a]/EUR: $(8600 + 670\ A^{0.83}) \cdot 3.5 \cdot 2$[e]
Installed cost of compressor, C_{com}[c]/EUR: $2605 \cdot P^{0.82}$
Installed cost of gas turbine, C_{tur}[c]/(EUR/a): $(22{,}946 + 13.5\ P_{tur}) \cdot 4$[e]
Price of methanol (C_M)[d]/(EUR/t): 115.0
Price of electricity (C_{el})[b]/(EUR/(kW · a)): 435.4
Cost of 37 bar steam (C_{37})[b]/(EUR/(kW · a)): 106.3
Cost of cooling water (C_{CW})[b]/(EUR/(kW · a)): 6.2

[a] Ref. [14]; A = area in m^2.
[b] Ref. [13].
[c] Ref. [3]; P = power in kW.
[d] Ten years average.
[e] The published cost equations for the equipment are adjusted to the real, higher industrial costs using multipliers (2 or 4).

- the gas turbine producing power P_{tur},
- the compressors COMP1 and COMP2 which are substituting the existing one, but they do not increase the existing instrumentation, maintenance and other costs,
- the enlarged and new areas of heat exchanger (A_{HE}).

The objective function includes the cost of high pressure steam in the heat exchanger HEST.

In the model, the existing areas can be used ($A_{HE,\ ex}$), enlarging them with additional ones ($\Delta A_{HE,\ add}$), if necessary. The additional annual depreciation of the

Table 2
Comparisons between case and optimized streams

Component	Case mass flow rate (q/(kg/h))	Optimized mass flow rate (q/(kg/h))
After reactor REA-1		
CO	10,846	10,846
CO_2	6986	6986
H_2	3606	3606
CH_4	1616	1616
Reactor REA outlet		
CO	8169	9295
CO_2	13,447	12,093
H_2	22,874	21,751
CH_4	30,526	24,195
CH_3OH	18,330	18,422
Crude methanol after separator SEP		
CO	20	15
CO_2	318	253
H_2	4	3
CH_4	140	93
CH_3OH	16,031	16,117

enlarged and new areas ($A_{\mathrm{HE,new}}$) of the heat exchangers (Table 1) is multiplied by the payback multiplier ($r = 0.216$ [1]) to obtain the maximum annual profit in heat and power integration.

Maximum additional annual profit for retrofit:

$$\begin{aligned} V_{\max} = {} & C_{\mathrm{el}} \cdot P_{\mathrm{tur}} \cdot \eta_{\mathrm{tur}} \cdot \eta_{\mathrm{gen}} + C_{\mathrm{M}} \cdot \Delta F_{\mathrm{M}} \\ & - C_{37} \cdot \Phi_{\mathrm{HEST}} - (22,946 + 13.5 \cdot P_{\mathrm{tur}}) \cdot 4 \\ & - [2605 \cdot P^{0.82}_{\mathrm{COMP1}} - 2605 \cdot P^{0.82}_{\mathrm{COMP2}} \\ & - \Sigma_{\mathrm{new}}(8600 + 670 \cdot A^{0.83}_{\mathrm{HE,\,new}}) \cdot 3.5 \cdot 2 \\ & - \Sigma_{\mathrm{add}} 670 \cdot \Delta A^{0.83}_{\mathrm{HE,\,add}} \cdot 3.5 \cdot 2] \cdot r \end{aligned} \tag{4}$$

new = HEST, HEW1
add = HEW, HEA, HEPR

The simultaneous NLP of heat and power integration, and the optimization selected for electricity generation is using the gas turbine pressure drop from 49.7 bar to 35 bar with an outlet temperature of $T_{\mathrm{tur,out}} = 110\ ^\circ\mathrm{C}$ (Fig. 5). The structure enables the generation of 12.7 MW of electricity. The steam exchanger (HEST) needs 16.5 MW of heat flow rate. The integrated process streams in HEPR, exchange 3.6 MW of heat flow rate. The power of the first and the second compressors are 2.0 MW and 2.8 MW, respectively. The HEW1 exchanges 2.0 MW. In the heat exchangers HEW and HEA, 7.1 MW and 4.7 MW of heat flow rate are exchanged with the existing areas respectively, when cooling. The additional annual methanol production is 0.75 mol/s, purge gas outlet flow rate is decreased from 210 mol/s to 190 mol/s.

The additional annual depreciation of the gas turbine, new heat exchangers (HEST, HEW1, having areas of 527 m^2 and 324 m^2), and the new two-stage compressor is 2040 kEUR/a. The cost of the high pressure steam used in HEST is 1750 kEUR/a. In the depreciation account for retrofit we included additional costs to the new units only: 30 kEUR/a for the instrumentation cost (which is estimated to be 15% of the additional plant direct cost [15]), 10 kEUR/a for the contingency (estimated at 5% of the additional plant direct cost [15]), 4 kEUR/a for the maintenance cost (estimated as 2% of the additional plant direct cost) and 15 kEUR/a for the turbine down time (estimated as 5% of the additional plant direct cost). The additional annual income of the electricity produced is 5530 kEUR/a. The additional annual income of the methanol produced is 79 kEUR/a. The additional profit from

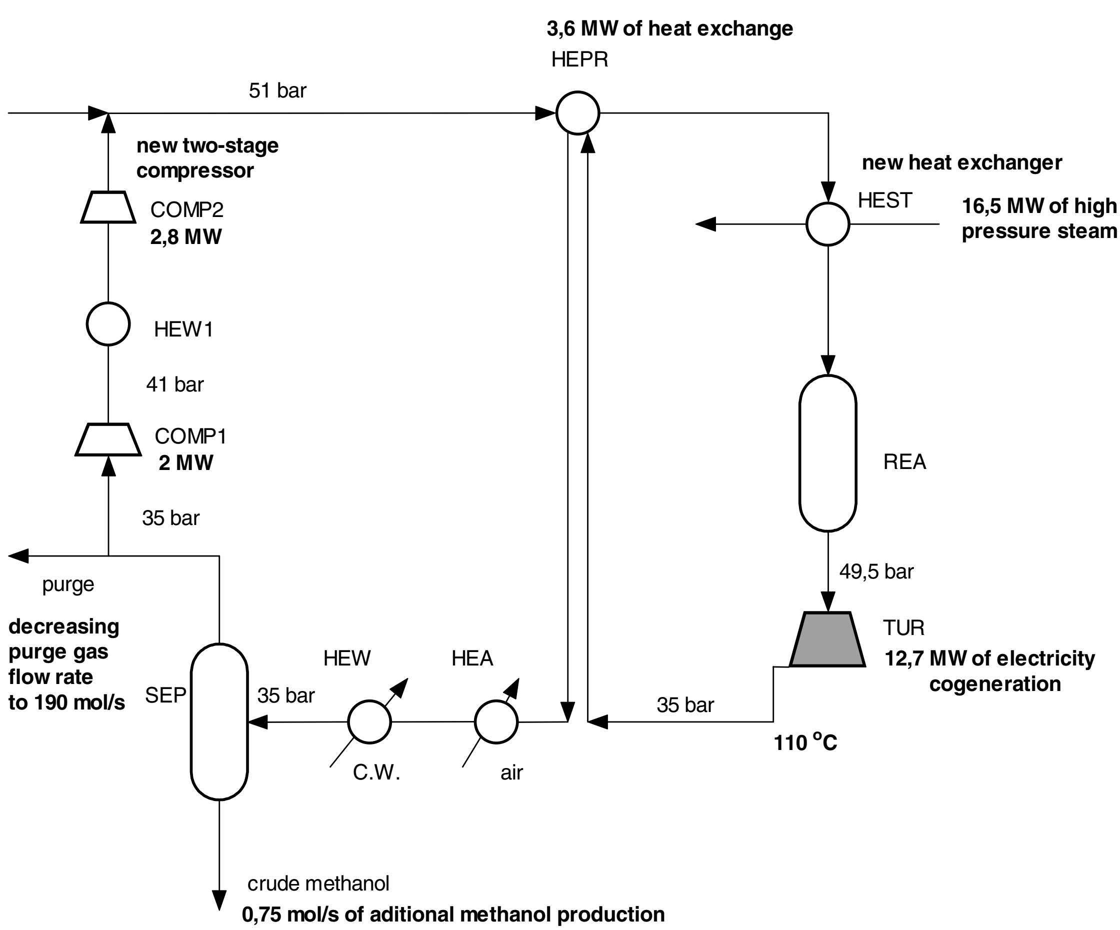

Fig. 5. Optimised flow sheet for crude methanol production, using a gas turbine.

process and power integration is estimated to be 1760 kEUR/a for the modified process. Table 2 compares the stream data of the case and the optimized process.

The NLP program included 111 equations and 120 variables with a computation time of 13.46 s on the VAX-3100 using the GAMS program [4].

Operability and control issues have not been dealt with so far.

4. Conclusions

The paper presents an efficient NLP model formulation for the simultaneous cogeneration of electricity using an open gas turbine with a separator, and process heat integration. The simultaneous mathematical optimization method which includes combined heat and power and increased production can add same degrees of freedom to the optimisation method. The gas turbine with its pressure and temperature drop is included in the process cycle. The working fluid comes from the reactor and cycles through the process units: gas turbine, heat exchanger, separator (where the liquid product separates), and the compressor. The higher equilibrium conversion in the reactor can increase the conversion of methanol by 0.54%, producing 690 t/a of additional methanol. Simultaneous heat and power optimization is promising an additional profit of 1.7 MEUR/a.

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