THERMODYNAMIC APPROACH FOR OPTIMAL DESIGN OF HEAT AND POWER PLANTS. RELATIONSHIPS BETWEEN THERMODYNAMIC AND ECONOMIC SOLUTIONS

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***Abstract*— In this paper, a new procedure for the design and analysis of Heat and Power Plants is presented. In this formulation, thermodynamic solutions obtained by maximizing the plant efficiency are used to find the economic design of the plant. In fact, by applying the Karush-Kuhn-Tucker conditions it is possible to relate thermodynamic and economic solutions. A formal context for the use of thermodynamic models in solving complex optimization problems that arise in the area of synthesis and design of chemical processes is introduced. The proposed methodology has been successfully applied for two plant arrangements. Rigorous models have been used to model the plant equipments. The obtained results are presented in order to illustrate the proposed procedure.**

***Keywords*— Thermodynamic solutions, optimal design of combined power and heat plants, optimization.**

I. INTRODUCTION

To address the problem of design of Combined Heat and Power plants, several methods have been reported in the literature. These methods generally follow two basic approaches: those based on thermodynamic targets and heuristic rules (Thermodynamic and Thermo-economic approach), and those based on optimization techniques (Mathematical Optimization).

The traditional way of designing Combined Heat and Power Plants is to maximize the thermal efficiency of the whole system. For this purpose analysis methods based on both the first and second law of thermodynamics have been extensively discussed in the literature (Linnhoff and Townsend, 1982; Linnhoff et.al, 1982, Colmenares and Seider, 1987). The analysis reveals the thermal inefficiencies of the various subsystems of the plant. Once the inefficiencies have been identified, heuristics rules are applied to improve the performance of the plant. These heuristics form the basis for both parameter and structural modifications to the plant. The capital cost of the plant is assessed after the thermally best design is achieved.

Thermo-economic approach (Valero et.al, 1986, 1989; Frangopoulos C., 1990a, 1990b; Tsatsaronis G. 1990, 1991) is an extension of the thermodynamic approach. The capital cost of the units and the prices of product streams of the units are included in the second law analysis model in the plant. This approach tries to address the trade-off between thermal efficiency and capital expenditure.

Mussati et al. (2001) recently presented a "hybrid methodology" involving thermodynamic solutions as starting points to optimize the Multiple Stage Flash (MSF) desalination system. This equiptment was rigorously modelled and the objective was to find the configuration and operating conditions to minimize the total annual cost of the system which is composed by the investment cost (heat transfer area and flashing chamber area) and operating cost (vapour consumption).

In this paper the "hybrid methodology" presented in Mussati et al. (2001) is extended to the case of cogeneration plants. Precisely, an additional term ìn the objective function which includes investment cost of power production is introduced. New relationships between thermodynamic and economic solutions are derived for power and heat production plants. A formal context for the use of thermodynamic models in solving complex optimization problems that arise in the area of chemical processes design is introduced.

This work is organized as follows. Section II introduces the problem definition. Section III briefly describes the processes to be analyzed. Section IV presents the solution procedure and Section V illustrates a numeric example through a case study. Finally, Section VI presents the conclusions and major challenges for further research.

II. PROBLEM DEFINITION

The problem is stated as follows. Given are the cost data, the process heat demand (or fresh water production and seawater conditions: temperature and composition). The goal of the problem is to determine the optimal operating conditions of a cogeneration plant at minimum cost per unit time. Note that only the process heat demand (or fresh-water demand) is given while the electricity production is a free variable because a benefit of the electricity produced by the systems is considered.

III. PROCESS DESCRIPTION

Figure 1 shows the configuration system to be considered and analyzed in this paper.

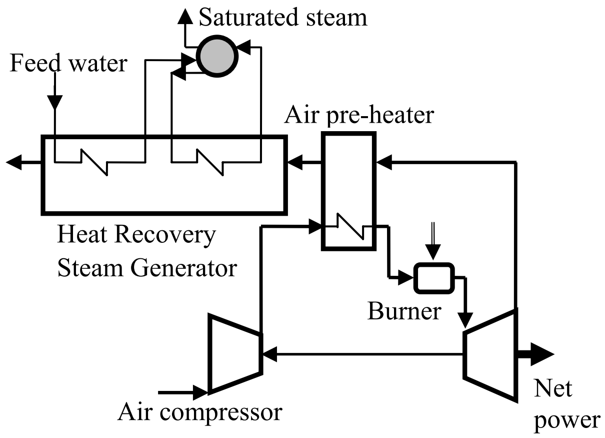

Fig. 1. A simple configuration of a combined power and heat plant

The configuration system to be considered and analyzed in this paper is illustrated in Fig. 1. As is shown, the cogeneration plant consists of a gas turbine followed by an air pre-heater that uses part of the thermal energy of the gases leaving the turbine, and a heat-recovery steam generator system in which the required steam is generated.

IV. HYBRID METHODOLOGY

In this methodology, thermodynamic optimal solutions obtained from problem P2 are used as a starting point to achieve the "economic" optimal solution of problem P1. Both problems are presented in Table 1.1.

Table 1. Economic and Thermodynamic problems.

Economic Model (P1):

Min. TAC = Min. $[C_A K_1 At(x) + C_f K_2 M_f(x) + \ldots$

$\ldots + (C_W K_3 - P_W K_4)\ W(x)]$

subject to: $G_i(x) = 0$

$H_j(x) \leq 0$

$x \in X$ X is an open nonempty set

$G_i(x)$ equality constraint i

$H_j(x)$ inequality constraint j

$G_i(x)$ refer to the mass-energy balances and design equations while inequality constraints $H_j(x)$, for example, are used to avoid overcross of temperature.

Thermodynamic Model (P2):

Maximize $[W(x) / M_f(x)]$

subject to: $At(x) - A_0 \leq 0$ (a)

$G_i(x) = 0$ (b)

$H_j(x) \leq 0$ (c)

$x \in X$ X is an open nonempty set

$G_i(x)$ equality constraint i

$H_j(x)$ inequality constraint j

where C_A, C_f, C_W and P_W are known and refer to the unitary cost of heat transfer area ($\$/m^2$), fuel unitary cost ($/GJ), electricity production cost and sell price of the electricity produced by the system, respectively. W(x), M_f (x) and At(x) refer to the generated power (electricity), fuel consumption and total heat transfer area of the system. A_0 is a model parameter. Finally, the constants K_1, K_2, K_3 and K_4 are unit conversion factors and involve the capital recovery factor, the lower heating value of the fuel and the number of hours of plant operating per year.

Simplified cost functions were assumed to compute capital and operation costs. Both models were implemented in General Algebraic Modeling System GAMS. The generalized reduced gradient algorithm CONOPT 2.041 was used as NLP solver. The mathematical model involves more than 50 variables and 60 constraints (including equality and inequality constraints).

Under certain hypotheses, it is possible to obtain relationships relating the solutions of P1 and P2 problems by applying the classical duality theory and the Karush-Kuhn-Tucker KKT conditions. Refer to Appendix I for the complete derivations.

According to Table 1, the objective of the proposed P2 problem is to find the optimal distribution of the total heat exchange area [At(x)] between the power generation cycle PGC (back-pressure cycle) and the process, in order to obtain the maximum efficiency of the system which is defined as the ratio between W(x) and $M_f(x)$. The objective here is to maximize the efficiency of the system subject to different A_0 values.

Then, a family of thermodynamic solutions can be obtained by solving P2 problem for different At(x) values. Then, these solutions can be efficiently used not only to initialize the "economic" problem P1 but also to predict the range for the optimal values of the main variables of the model (power, total heat transfer area, fuel, among others). The idea is based on the thermodynamic optimization subject to physical size constraints [Mussati et al. (2001), Bejan A. (1999), Aguirre P. and Scenna N. (1991)].

According to Appendix I, the following conditions must hold in order to assure that solutions obtained from problem P1 and problem P2 are identical:

$$C_f K_2 / [C_W K_3 - P_W K_4] = [W(x) / M_f] \quad (1)$$

$$C_A K_1 / [C_W K_3 - P_W K_4] = \mu^* M_f \quad (2)$$

where μ* refers to the lagrange multipliers related to the constraint (a) of the thermodynamic problem P2.

By solving the problem P2 for different total heat transfer area values (parameter A_0) the constitutive parts of the Thermodynamic Costs such as: $\mu^* M_f$ vs. At(x) and $W(x)/ M_f(x)$ vs. At(x) are obtained (Fig. 3a, 3b). Then, the "thermodynamic costs" given by (1) and (2) can be computed and the range of values for the main problem variables can be predicted (e.g. total heat transfer area, fuel consumption, generated power).

Note that the family of "thermodynamic" costs reported in Fig. 3a is universal because it is independent from geographic and contingency factors and they have a general validity.

Given a set of cost parameters (C_A, C_W, P_W, C_f), two situations can occur when the relationships (1) and (2) are computed.

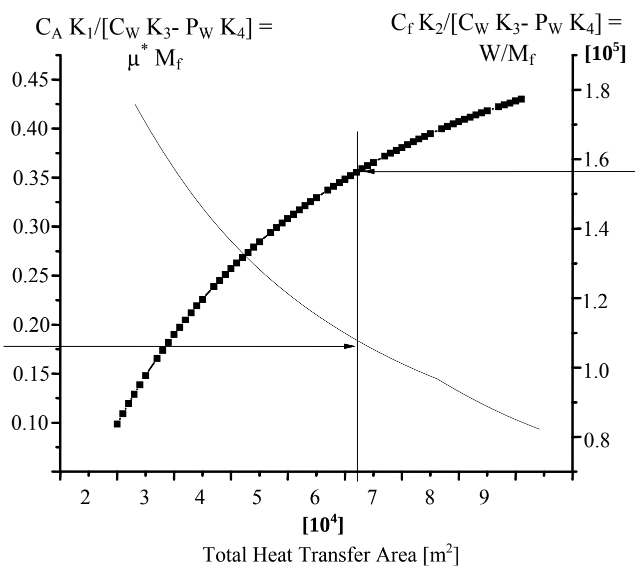

Fig. 3a. Thermodynamic costs vs. total heal transfer area. Case 1

In situation (A), the real cost ratio corresponds to only one point of the "thermodynamic costs" (Fig. 3a). In this case, the starting point determined by eq. (1) and eq. (2) satisfies simultaneously the solution of both P1 and P2 problems. Nevertheless, it should be noted that it is a rare case.

Other situation occurs when eq. (1) and eq. (2) determine two points on the curve of the "thermodynamic costs" defining a range of values as initial conditions (Fig. 3b). In this case the relations (1) and (2) "bound" the optimal values for power production, fuel consumption and total heat transfer area. This case is more frequent (Situation B).

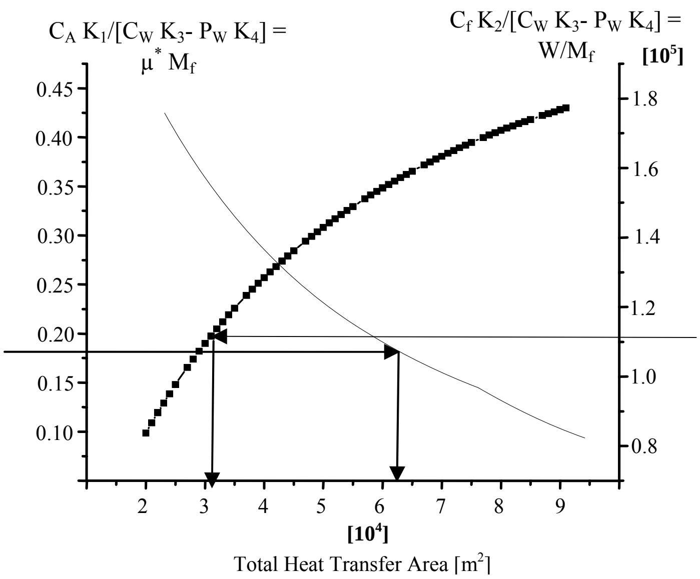

Fig. 3b. Thermodynamic costs vs. total heal transfer area. Case 2

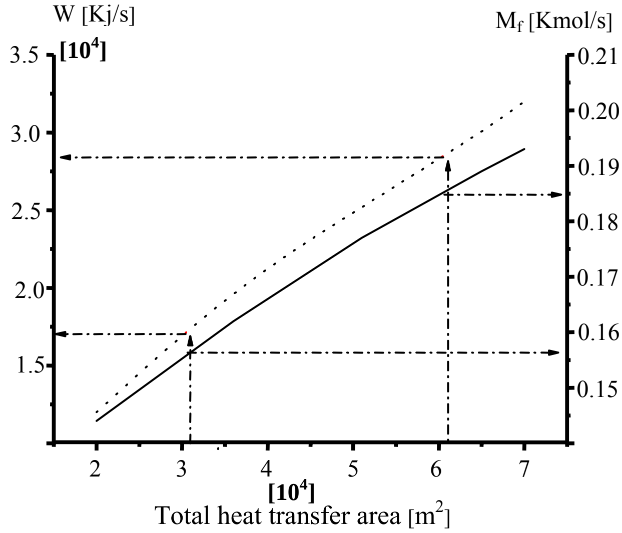

Fig. 3c. W vs At and M_f vs At curves

According to the situations explained above, several ways are possible to be used in order to initialize efficiently the P1 problem. Two alternative initialization procedures are:

a) Continuation method from the "thermodynamic costs" to the "real cost" based solution. From the values corresponding to one point inside on the range predicted by (1) and (2), a simple Continuation Method is used by perturbing the cost parameter from the thermodynamic costs to the real ones used in the actual objective function. This evolution is easy taking as starting point the solution of P2.

b) To adopt a solution in the range given by eq. (1) and eq. (2) as starting point to solve the problem P1.

Both options have been successfully applied to the configuration systems described in Section 3.

Finally, it is important to notice that both problems (P1 and P2) differ only on the objective function (equal constraints) and they are equally complex to solve. Nevertheless, it is possible to find many useful relationships and properties associated to the thermodynamic model which can be used efficiently to facilitate the initialization of economic problems [Mussati (2003), Scenna and Aguirre (1991)].

V. RESULTS AND DISCUSSION

In this section the optimal solution obtained for the system illustrated in Fig. 1 is presented.

Table 2 shows the cost data for the optimization problem.

The following thermodynamic costs are obtained by applying eq. (1) and (2):

$C_A K_1/[C_W K_3 - P_W K_4] = 0.172$

$C_f K_2/[C_W K_3 - P_W K_4] = 110800$

Then, from Fig. 3b and Fig. 3c and by using the thermodynamic costs, lower-upper bounds for the main problem variables are obtained. Therefore, the economic problem was solved by using the "initialization" procedures mentioned previously.

Table 2. Problem Parameters

Cost data	
Capital Recovery Factor	0.182 y^{-1}
Plant operation time	8000 h/y
Heat transfer area cost [C_A]	100 $\$/m^2$
Fuel cost [C_f]	2.68 10^{-3} \$/Kmol
Sell price for the electricity produced [P_W]	8.92 10^{-6} \$/[KJ s]

Table 3 shows the lower-upper bounds and the optimal values for the main variables of the problem.

The initial values reported in Table 3 are average values within the range determined by eq. (1) and eq. (2).

According to the results presented in Table 3, a good prediction of the initialization values for the main optimization variables is performed by the proposed methodology.

On the other hand, problem P1 was also solved for situation (A) described in section IV in order to verify the relationships presented in this paper. For this, we fixed an At value and computed the corresponding set of thermodynamic cost using Fig. (3a) and (3b). Then, the problem P1 is solved for these costs and initialized using the solution corresponding to problem P2 for the given At value. From the obtained result, it is possible to verify that both solutions are equal. We emphasize again that the situtation where the real costs are at the same time the thermodynamic costs is not usual in the real world.

Table 3. Optimal values of the main optimization variables

	Initial value	Lower value	**Optimal value**	Upper value
W [KJ/s]	*23200.00**	17500.00	**27830.56**	28900.00
M_f [Kmol/s]	*1.71 10^{-1}**	1.57 10^{-1}	**1.81 10^{-1}**	1.85 10^{-1}
Atotal [m^2]	*46500.00**	31000.00	**59870.12**	62000.00
Air flow-rate [Kmol/s]	5.144	4.12	**7.148**	9.01
Exit temp. from AC [K]	405.304	380	**449.2**	600
Text_PRE [K]	948.910	612.3	**793.454**	950.2
W_AC [KJ/s]	16133.32	10129.5	**31700.40**	54000.6
W_GT [KJ/s]	*39333.318*	29000.8	**60700.40**	*80152.3*

*values corresponding to initialization way b) described in Section 4.

Finally, given the cost data, the same procedure has been successfully applied to determine the optimal operating conditions for the process illustrated in Fig. 4. As it is shown, the process consists of a back-pressure steam turbine coupled to the MSF deslator system, resulting in fresh water production.

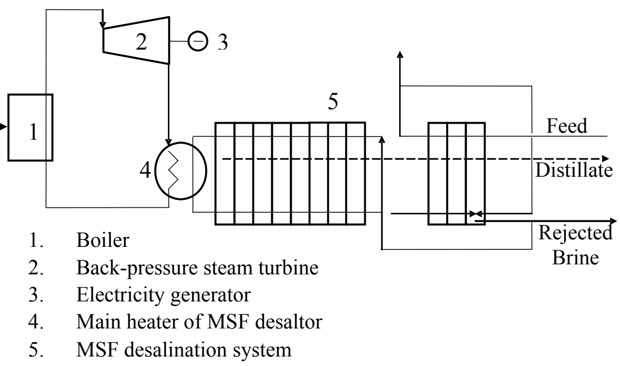

Fig. 4. Back-pressure turbine coupled to MSF desaltor

Again, good lower and upper bounds as well as starting points for the optimization algorithm are determined by applying the developed relationships.

VI. CONCLUSIONS

A new strategy involving and "hybrid" algorithmic procedure for the optimization of combined power and heat plants is presented. The procedure uses optimal solutions obtained from a "thermodynamic method" to find the "economic solution". The proposed hybrid methodology has been successfully applied to determine the optimal design for different sets of costs and for structures illustrated in Fig. (1) and (4).

As is shown in the example presented in this paper, a good prediction of the initial values for the main optimization variables is performed by the proposed methodology. However, it should be mentioned that the drawback of this approach could be the number of problems to be solved in order to construct the optimal curve for the "thermodynamic" costs (Fig. 3a, 3b, 3c). Nevertheless, a set of useful thermodynamic heuristics derived from the universal thermodynamic properties (Scenna and Aguirre, 1991) can be applied to construct these curves relatively easily. For example, one of the "thermodynamic heuristics" previously presented in Mussati (2003) is used to solve the system configuration illustrated in Fig. 4. In fact, the following relationship $(T_j - T_{j-1}) / t_v = K$, (temperature gradient between stages divided by the temperature of the condensing vapor) remain constant for all the stages. So, knowing the K value it is possible to initialize the temperature profiles for the feed, distillate and brine streams. Then, enthalpies of all streams and stages can be initialized taking into account this profile. Using this property, feasible solutions are found in few iterations for problem P2, facilitating the convergence of the optimization algorithm.

Even though the mentioned property is valid for problem P2, it is difficult to prove it from a mathematical point of view. This heuristic is related with several publications discussing the optimal temperature gradient for heat transfer in several processes [Alebrahim and Bejan (1999) Bejan (1999); Tondeur and Kvaalen (1987)]. Also, useful heuristics that could be used for initialization phase for power cycles (electricity generation) can be found in Scenna and Aguirre (1987) and Mussati et al. (1997).

Although the preliminary results obtained by the "thermodynamic" procedure are good it is necessary to extend it to other functionality costs in order to obtain more realistic solutions. For this, re-derivations of the "thermodynamic" costs should be developed and will be considered in future works.

APPENDIX

Table 4. Thermodynamic and Lagrange Problems

Thermodynamic Model (P2):

Maximize $[f(x) = W(x)/M_f(x)]$

subject to:

$At(x) - A_0 \leq 0$ (a)

$G_i(x) = 0$ (b)

$H_j(x) \leq 0$ (c)

$x \in X$ X is an open nonempty set

$G_i(x)$ equality constraint i

$H_j(x)$ inequality constraint j

Lagrange Problem for P2:

$L\_P2(x, g_i, h_j) = [W(x) / M_f(x) - \mu^* (At(x)-A_0) - g_i G_i(x) - h_j H_j(x)]$

where:

μ^* Lagrange multiplier to the total area constraint (a)

g_i Lagrange multiplier to the equality constraint i (b)

h_j Lagrange multiplier to the inequality constraint j (c)

Assuming that:

(a) $f(x)$, G_i, H_j are differentiable,

(b) x^* to be a feasible solution and,

(c) $At(x^*)-A0=0$ (active constraint),

the Karush-Kuhn-Tucker (KKT) conditions for P2 are:

$$- \nabla[W(x^*) / M_f(x^*)] + \mu^* \nabla[At(x^*)-A_0] + g_i \nabla[Gi(x^*)] + h_j \nabla[H_j(x^*)] = 0, \quad \textbf{(A.1)}$$

$G_i(x^*) = 0$ (A.1.1)

$H_j(x^*) \leq 0$ (A.1.2)

$h_j H_j(x^*) = 0$ (A.1.3)

$\mu^* (At(x^*)-A0) = 0;$ (A.1.4)

$\mu^* \geq 0$; $h_j \geq 0$ (A.1.5)

μ^*, g_i and h_j are the Lagrangian multipliers. Constraints (A.1.1) and (A.1.2) are known as feasibilty conditions while constraints (A.1.3) and (A.1.4) are referred to as a complementary slackness conditions. Note that the multipliers μ^* and h_j associated with the inequality constraints are nonnegative, whereas the multipliers associated with the equality constraints are unrestricted in sign.

The first term of the condition (A.1) can be rewritten as follows:

$$[W(x^*)/M_f(x^*)] = [\nabla[W(x^*)/ M_f(x^*)] - W(x^*) / M^2_f(x^*) \nabla M_f(x^*)] \quad \textbf{(A.2)}$$

Substituting (A.2) into (A.1) and multiplying by $M_f(x^*) \neq 0$ the obtained expression, we obtain:

$$-\nabla[W(x^*)] + W(x^*) / M_f(x^*) \nabla[M_f(x^*)] + M_f(x^*) [\mu^*\nabla[At(x^*)-A_0]] + g_i \nabla[Gi(x^*)] + h_j \nabla[H_j(x^*)] =0 \quad \textbf{(A.3)}$$

Table 5. Economic and Lagrange Problems

Economic Model (P1):

$\text{Min.}[C_A K_1 At(x)+C_f K_2 M_f(x^*)+(C_W K_3-P_W K_4)\, W(x)]$

subject to:

$G_i(x) = 0$

$H_j(x) \leq 0$

Lagrange Problem for P1:

$L\_P1(x, g_i, h_j) = [C_A K_1 At(x) + C_f K_2 M_f(x) + (C_W K_3 - P_W K_4)\, W(x) + g_i G_i(x) + h_j H_j(x)]$

The Karush-Kuhn-Tucker conditions for P1 problem is given by:

$$\nabla[L\_P1(x, g_i, h_j)] = 0 \qquad \textbf{(A.4)}$$

Taking into account Lagrange function and eq. (A.4), the following expression is obtained:

$$C_A K_1 \nabla[At(x^*)] + C_f K_2 \nabla[M_f(x^*)] + [C_W K_3 - P_W K_4]\ \nabla[W(x^*)] + gi\, \nabla[Gi(x^*)] + hj\, \nabla[Hj(x^*)] = 0 \qquad \textbf{(A.4.1)}$$

where:

$G_i(x^*) = 0$ (A.4.1.1)

$H_j(x^*) \leq 0$ (A.4.1.2)

$h_j H_j(x^*) = 0$ (A.4.1.3)

$\mu^* \geq 0$; $h_j \geq 0$ (A.4.1.4)

Note that P1 and P2 problems differ between them in the objective function and constraint related to the total heat transfer area (A.1.4).

If eq. (A.4.1) is divided by $[C_W K_3 - P_W K_4]$, the following expression is obtained:

$$-\nabla[W(x^*)] + C_f K_2 / [C_W K_3 - P_W K_4]\ \nabla[M_f(x^*)] + C_A K_1/[C_W K_3 - P_W K_4]\ \nabla[At(x^*)] + gi\, \nabla[Gi(x^*)] + hj \nabla[Hj(x^*)] = 0 \qquad \textbf{(A.5)}$$

By comparing eq. (A.3) and (A.5), problem P1 and P2 have equivalent solutions if the following relationships are satisfied:

$$C_f K_2 / [C_W K_3 - P_W K_4] = [W(x) / M_f] \qquad \textbf{(A.6)}$$

and

$$C_A K_1 / [C_W K_3 - P_W K_4] = \mu^* M_f \qquad \textbf{(A.7)}$$

On the other hand, the Lagrangian Dual for P2 (maximum in this case) provides the following relationship:

$$\nabla[W(x^*) / M_f(x^*)] / \nabla At(x^*) = \mu^* \qquad \textbf{(A.8)}$$

$$[\nabla W(x^*)/M_f(x^*) - W(x^*)/M_f^2(x^*) \nabla M_f(x^*)]/\nabla At(x^*) = \mu^* \qquad \textbf{(A.9)}$$

The following expression is obtained by substituting (A.9) into (A.7):

$$C_A K_1 / [C_W K_3 - P_W K_4] = [\nabla W(x^*) / M_f(x^*) - W(x^*)/M_f^2(x^*)\ \nabla M_f(x^*)] / \nabla At(x^*)\ M_f$$

$$C_A K_1 / [C_W K_3 - P_W K_4] = [\nabla W(x^*) - W(x^*)/M_f(x^*)\ \nabla M_f(x^*)] / \nabla At(x^*) \qquad \textbf{(A.10)}$$

Then, if (A.10) is divided by (A.6), the resulting expression is:

$$C_A K_1 /[C_f K_2] = [M_f / W(x)]\ [\nabla W(x^*)/\nabla At(x^*) - [W(x^*)/M_f(x^*)]\ \nabla M_f(x^*) / \nabla At(x^*)] \qquad \textbf{(A.11)}$$

Equations (A.6) and (A.7) or (A.10) and (A.11) provide the necessary conditions to assure the equivalence between the solutions of P1 and P2 problems. C_A, K_1, C_f, K_2, C_W, K_3, P_W, K_4 are data of the problem.

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