# STRUCTURAL THEORY OF THERMOECONOMICS

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## Summary

Characteristic equations and average and marginal costs are analyzed in this article. As a consequence the structural theory is a general mathematical formalism either for thermoeconomic cost accounting and/or optimization methods, providing a common basis of comparison among the different thermoeconomic methodologies, which could be considered the standard formalism for thermoeconomics.

The cost calculation method of the structural theory is based on the rules of mathematical derivation applied to a set of characteristic equations that determine the thermoeconomic model. In this way, as more physical and realistic information is contained in the characteristic equations, more physical significance will be contained in the costs obtained.

### **1. Introduction**

During the three decades from 1972 to 2002 various thermoeconomic methodologies have been developed. All of them have in common cost calculated on a rational basis,

which is the Second Law of Thermodynamics. This cost is a very useful tool for solving problems in complex energy systems, such as rational price assessment of the products of a plant based on physical criteria, local optimization, or operation diagnosis. These problems are difficult to solve using conventional energy analysis techniques based on the First Law of Thermodynamics.

As is explained in another article (see *The Thermodynamic Process of Cost Formation*), there are two main groups of thermoeconomic methods: a) cost accounting methods, which use average costs as a basis for a rational price assessment, and b) optimization methods, which employ marginal costs in order to minimize the costs of the products of a system or a component.

When comparing different thermoeconomic methodologies and the underlying ideas of their models, the reader is faced with as many nomenclatures, concepts, and names as there are existing methods. This could be one of the factors that impede a faster development of thermoeconomics. In order to avoid unnecessary confusion and provide a common basis for comparing different thermoeconomic methods, a common mathematical language for thermoeconomics is essential.

Such a common mathematical formulation is provided by the structural theory of thermoeconomics, which can reproduce the results of any thermoeconomic methodology, both cost accounting and optimization, employing a linear thermoeconomic model. The most systematic and widespread thermoeconomic methodologies developed until now use linear models, or models that are easy to linearize. For this reason the structural theory provides a common mathematical formulation for the different thermoeconomic methodologies.

Previous works have already demonstrated that cost accounting methods such as exergy cost theory (ECT), the average cost approach (AVCO), and the last in first out approach (LIFO), as well as the optimization method called thermoeconomic functional analysis (TFA) (see *Functional Analysis*), can be dealt with in the structural theory.

In this article, the concept of cost is analyzed in detail and the mathematical formalism of the structural theory is presented. This theory allows:

- analysis of the process of cost formation, providing a physical and mathematical interpretation to the rules of cost apportioning (see *The Thermodynamic Process* of Cost Formation), and
- unification of the concepts of cost provided by the different cost accounting methodologies and some of the optimization methodologies.

## 2. Marginal Costs

When performing a cost analysis in a system we can distinguish between *average costs*, which are ratios and express the average amount of resources per unit of product, and *marginal costs*, which are partial derivatives and indicate the additional resources required to generate one more unit of the product under specified conditions (see *The Thermodynamic Process of Cost Formation*):

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Unit average 
$$\cot = \frac{E_o}{E_i}$$
 (1)

Unit marginal cost = 
$$\left(\frac{\partial E_0}{\partial E_i}\right)_{conditions}$$

In this section the concept of marginal costs in thermoeconomics is analyzed in detail, and some of its applications are presented. In order to help the reader follow the proposed arguments, the same cogeneration plant presented in other articles within this theme will be used as an example application (see Figures 1 and 2 in the article *The Thermodynamic Process of Cost Formation*).

(2)

### **2.1.** Characteristic Equations

When a thermoeconomic analysis is performed it is very useful to depict a productive structure (for the analyzed cogeneration plant, see Figure 2 in the article *The Thermodynamic Process of Cost Formation*), which represents the productive purpose of the process units: that is, it gives a definition of fuel and product for each device, and the distribution of the resources throughout the plant.

The thermoeconomic model that is the mathematical representation of the productive structure (see *The Thermodynamic Process of Cost Formation*) consists of a set of mathematical functions called *characteristic equations*. They express each inlet flow as a mathematical function of the outlet flows, for all the productive structure process units and a set of internal parameters  $x_i$ :

$$E_i = g_i(x_l, E_j)$$
  $i = 1,...,m-s$  (3)

where the index i refers to the input flows of the process unit l, the index j refers to the output flows of the process unit l, and m and s are respectively the number of flows and the number of system outputs considered in the productive structure. Every flow is an input flow of a process unit, and an output flow of another process unit or to the environment. For the flows interacting with the environment, we define:

$$Em - s + i = \omega i \qquad i = 1, \dots, s \tag{4}$$

where  $\omega_i$  is the total system product, that is, an external variable that determines the total plant product. The characteristic equations for the cogeneration plant of our example (see Figure 2 in the article *The Thermodynamic Process of Cost Formation*) are shown in Table 1.

Nº	Process unit	Entry	Outlet	Characteristic equation
1	Combustor	$\boldsymbol{F}_{I} = \boldsymbol{E}_{I}$	$\boldsymbol{P}_1 = \boldsymbol{E}_3 - \boldsymbol{E}_2$	$F_{I} = g_{FI} \left( \boldsymbol{x}_{I}, \boldsymbol{P}_{I} \right)$
2	Compressor	$\boldsymbol{F_2} = \boldsymbol{E_5} = \boldsymbol{W_{CP}}$	$\boldsymbol{P_2} = \boldsymbol{E_2} - \boldsymbol{E_0}$	$F_2 = g_{F2} (x_2, P_2)$

3	Turbine	$\boldsymbol{F_3} = \boldsymbol{E_3} - \boldsymbol{E_4}$	$\boldsymbol{P_3} = W_{gt} = E_5 + W_{net}$	$F_{3} = g_{F3} \left( \boldsymbol{x}_{3}, P_{3} \right)$
4	H.R.S.G.	$F_4 = E_4$	$P_4 = E_{HEAT} = \omega_4$	$F_4 = g_{F4} (\boldsymbol{x}_4, \boldsymbol{P}_4)$
5	Junction 1	$P_1 = E_3 - E_2$	$P_{j1} = E_3$	$P_{1} = g_{P1}(x_{5}, P_{j1})$
		$\boldsymbol{P_2} = \boldsymbol{E_2} - \boldsymbol{E_0}$		$P_2 = g_{P2} (x_5, P_{j1})$
6	Branching 1	$P_{j1} = E_3$	$\boldsymbol{F}_3 = \boldsymbol{E}_3 - \boldsymbol{E}_4$	$P_{j1} = g_{P_{j1}} (\mathbf{x}_{6}, F_{3}, F_{4})$
			$\boldsymbol{F_4} = \boldsymbol{E_4}$	с у У
7	Branching 2	$P_3 = Wgt = E_5$	$F_2 = W_{CP}$	$P_{3} = g_{P3} (\mathbf{x}_{7}, F_{2}, \omega_{3})$
		$+ W_{net}$	Wnet	

Table 1. Characteristic equations corresponding to the productive structure depicted inFigure 2 of the article The Thermodynamic Process of Cost Formation

The inlet and outlet flows of the productive structure units are of extensive magnitude, and are the product of a quantity (usually mass flow rate) and a quality (specific magnitude). The magnitudes applied by most thermoeconomic methodologies are exergy, negentropy (see *Functional Analysis*), and money. Other magnitudes, like enthalpy or entropy, can also be used.

The internal variables appearing in the thermoeconomic model depend on the behavior of the subsystem, and they are presumably independent of mass flow rates. This implies that relations like efficiencies or pressure and temperature ratios—which are mainly independent of the quantity of the exiting flows—can be used as internal parameters.

Note that the main objective of the productive structure, and hence of the thermoeconomic model, consists of sorting the thermodynamic magnitudes related to the physical mass and energy flow-streams connecting the plant subsystems in a different way from the equations modeling the physical plant behavior, in order to determine explicitly for each subsystem its energy conversion efficiency.

It is important to keep in mind that thermoeconomics connects thermodynamics with economics. That is, by sorting the thermodynamic properties of the physical mass and energy flow-streams of a plant, which in turn provide the energy conversion efficiency of each subsystem, thermoeconomics analyzes the degradation process of energy quality through an installation.

Depending on the scope of the analysis, a subsystem can be identified as a separate piece of equipment, a part of a device, several process units, or even the whole plant. Sometimes the objective consists of analyzing a plant in great detail. In this case it is advisable, if possible, to identify each subsystem with a separate physical process (heat transfer, pressure increase or decrease, and chemical mixture or reaction) in order to locate and quantify, separately if possible, each thermal, mechanical, and chemical irreversible process occurring in the plant. If the objective consists of analyzing a macrosystem composed of several plants, in this case the more convenient approach would probably be to consider each separate plant as a subsystem.

Thus, thermoeconomics always performs a systemic analysis, no matter how complex the system, oriented towards locating and quantifying the energy conversion efficiency and the process of energy quality degradation. It is not within the scope of thermoeconomics to model the behavior of the process units, which is done by the mathematical equations of the physical model.

Even though it is not the objective of thermoeconomics to simulate the behavior of the subsystems, it is very important to build a thermoeconomic model with physical meaning. This is the reason, as already explained, for defining different thermoeconomic models for the same plant. Depending on the aggregation level and the nature of the thermoeconomic equations, the model will contain physical information about the actual system behavior with different degrees of detail. The results obtained from a very rough thermoeconomic model, which is not sensitive to any physical detail related to the actual behavior of the plant, will probably be useless.

## 2.2. General Equation of Marginal Cost

Once the thermoeconomic model has been defined and the characteristic equations corresponding to the productive structure of the system are known, the costs of all flows in the productive structure can easily be calculated.

The thermoeconomic model (characteristic equations) of an energy system contains the mathematical dependence between the resources consumed and plant flows (products and internal flows). Each flow, as a process unit input, is a function (defined by its characteristic equation) of a set of internal variables, x, external variables  $\omega$  and the output flows of the process unit. As a result, the plant resources can be then expressed using Eqs. (3) and (4) as a function of each flow, the set of internal variables of each process unit and the final product of the plant  $E_0 = g_0(E_i, x, \omega)$ .

When the variation of the resources consumed in the plant concerning a flow is calculated, the chain rule can be applied:

$$\frac{\partial E_0}{\partial E_i} = k_{0,i}^* \qquad \mathbf{i} = 1, \dots, \mathbf{e}$$
(5a)

$$\frac{\partial E_0}{\partial E_i} = \sum_{\substack{j=1\\j\neq i}}^m \frac{\partial E_0}{\partial E_j} \frac{\partial g_j}{\partial E_i} \qquad i = e+1,..., m$$
(5b)

The expression  $\frac{\partial E_0}{\partial E_i}$  represents the marginal cost, which evaluates the additional consumption of resources when an additional unit of the flow -i-i is produced, under the conditions that the internal variables, x, do not vary throughout the process. We can denote these marginal costs as  $k_{i}^*$ , and  $\kappa_{ji} = \frac{\partial g_j}{\partial E_i}$  represents the marginal consumption

of flow -j- to produce the flow -i-. With these, we can rewrite the previous expressions as:

$$k_i^* = k_{0,i}^*$$
  $i = 1,..., e$  (6a)

$$k_i^* = \sum_{\substack{j=1\\j\neq i}}^m k_j^* \kappa_{ji}$$
  $i = e + 1, ..., m$  (6b)

Note that when the boundary of the system analyzed coincides with the limits of the plant studied, then the unit exergy cost of each fuel entering the plant is considered equal to 1 because there is no energy quality degradation or exergy destruction at the very beginning of the productive process. Hence, the amount of exergy consumed to obtain each plant's fuel is its own exergy content, and therefore its unit exergy cost is equal to 1.

Then, if the characteristic equations and the marginal consumptions for each process unit are known, the marginal cost  $k^*$  for each flow can be obtained by solving the system of linear Eqs. (6).

For the example of the co-generation plant (see Figure 2 of *The Thermodynamic Process of Cost Formation*), Eqs. (6a) and (6b) can be written as:

$$k_{F_{1}}^{*} = \frac{\partial E_{1}}{\partial F_{1}} \qquad \qquad k_{F_{2}}^{*} = \frac{\partial E_{1}}{\partial F_{2}} = \frac{\partial E_{1}}{\partial F_{2}} \frac{\partial g_{P3}}{\partial F_{2}}$$

$$k_{F_{3}}^{*} = \frac{\partial E_{1}}{\partial F_{3}} = \frac{\partial E_{1}}{\partial P_{j1}} \frac{\partial g_{Pj1}}{\partial F_{3}} \qquad \qquad k_{F_{4}}^{*} = \frac{\partial E_{1}}{\partial F_{4}} = \frac{\partial E_{1}}{\partial P_{j1}} \frac{\partial g_{Pj1}}{\partial F_{4}}$$

$$k_{P_{1}}^{*} = \frac{\partial E_{1}}{\partial P_{1}} = \frac{\partial E_{1}}{\partial F_{1}} \frac{\partial g_{F1}}{\partial P_{1}} \qquad \qquad k_{P_{2}}^{*} = \frac{\partial E_{1}}{\partial P_{2}} = \frac{\partial E_{1}}{\partial F_{2}} \frac{\partial g_{F2}}{\partial P_{2}}$$

$$k_{P_{3}}^{*} = \frac{\partial E_{1}}{\partial P_{3}} = \frac{\partial E_{1}}{\partial F_{3}} \frac{\partial g_{F3}}{\partial P_{3}} \qquad \qquad k_{P_{4}}^{*} = \frac{\partial E_{1}}{\partial P_{4}} = \frac{\partial E_{1}}{\partial F_{4}} \frac{\partial g_{F4}}{\partial P_{4}}$$

$$k_{P_{j1}}^{*} = \frac{\partial E_{1}}{\partial P_{j1}} = \frac{\partial E_{1}}{\partial P_{2}} \frac{\partial g_{P2}}{\partial P_{j1}} + \frac{\partial E_{1}}{\partial P_{1}} \frac{\partial g_{P1}}{\partial P_{j1}} \qquad \qquad k_{W_{net}}^{*} = \frac{\partial E_{1}}{\partial P_{net}} = \frac{\partial E_{1}}{\partial P_{3}} \frac{\partial g_{P3}}{\partial W_{net}}$$

If the unit costs of the inlet plant fuels and the characteristic equations are known, the previous equations are a set of m equations with m unknowns, which are the marginal costs. Note that this set of equations shows the process of cost formation on the productive structure: that is, how the cost is generated through the process units of the plant.

Note that the proposed procedure to calculate the marginal cost of all the flows of a plant is general and valid for any thermoeconomic formulation that uses characteristic equations connecting inlet and outlet flows of each process unit.

The thermoeconomic cost calculation procedure considering monetary units is similar to that explained in the previous paragraphs, but in this case the input plant resources are expressed in monetary units and the process unit capital cost Z must be taken into account. Thus, the capital cost of each process unit Z can be considered an external flow of the plant resources from the environment to the process unit (see Figure 1). This will represent the monetary units per second needed to compensate for the depreciation, maintenance cost, and so on of the process unit.

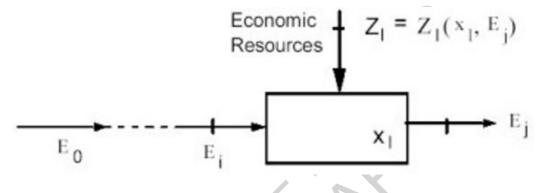


Figure 1. Economic resources scheme

According to marginal cost analysis, Z represents an environmental resource and can be handled in the same mathematical way as energy resources. The amount of resources consumed when manufacturing a device is, in fact, the amount of resources consumed to obtain the plant products. Then the marginal unit cost  $\partial Z/\partial E$  can be considered a marginal consumption  $\kappa_{zj}$ .

For the process unit depicted in Figure 1 the characteristic equations are:

$$E_{\rm i} = f(E_{\rm j}, \boldsymbol{x}_{\rm l}) \tag{7a}$$

$$Z_1 = Z(\mathbf{E}_i, \mathbf{x}_l) \tag{7b}$$

And the cost of the product is, for the case of Figure 1:

$$k_{j}^{*} = \frac{\partial E_{0}}{\partial E_{i}} \frac{\partial g_{i}}{\partial E_{j}} + \frac{\partial Z_{l}}{\partial E_{j}}$$

$$\tag{8}$$

 $k_j^*$  where  $E_0$  represents the resources consumed in the whole plant expressed in terms of exergy (kJ) and  $Z_l$  represents the resources, expressed in terms of exergy (kJ), consumed for manufacturing the device 1. Note that in Eq. (8) the units of cost, are exergy units (kJ/kJ).

In monetary units (\$), Eqs. (5) and (8) can be rewritten as follows:

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$$\frac{\partial C_0}{\partial E_i} = c_{0,i} \quad i = 1, \dots, e$$
(9a)

$$\frac{\partial C_0}{\partial E_i} = \frac{\partial Z_l}{\partial E_i} + \sum_{\substack{j=1\\i\neq i}}^m \frac{\partial C_0}{\partial E_j} \frac{\partial g_j}{\partial E_i} \quad i = e+1..., m$$
(9b)

where  $C_0$  represents the resources consumed in the whole system but in this case expressed in monetary units (\$), and  $Z_i$  is the capital cost of device 1. Note that in this case the unit cost,  $c_i$  is expressed in monetary units per unit of exergy of the flow i, that is, in \$/kJ.

These equations can be written in matrix notation as follows:

$$\left(\mathbf{U}_{\mathrm{D}}-^{\mathrm{t}}\left\langle \mathbf{K}\right\rangle \right)\mathbf{k}^{*}=\mathbf{z}_{\mathrm{e}}$$

where:

U<sub>D</sub> is the identity matrix (*m* dimension)

 $\langle K \rangle$  is a  $m \times m$  matrix containing the Jacobian of the characteristic equations; its elements are the marginal exergy consumptions  $\kappa_{ij}$ 

(10)

 $k^*$  is a vector ( $m \times 1$ ), with the marginal costs of each flow

 $z_e$  is a vector ( $m \times 1$ ), containing the unit costs of plant resources and the capital costs of the devices.

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#### **Biographical Sketches**

Luis Serra graduated in Chemistry from the University of Oviedo in 1988, and obtained a Ph.D. in mechanical engineering from the University of Zaragoza in 1994 with a thesis on *Exergoeconomic Optimization of Complex Energy Systems*. From 1989–1997 he was successively Assistant Professor and Associate Professor at the University of Zaragoza Department of Mechanical Engineering. Since 1993 he has also been Research and Project Manager of the Thermoeconomic Division of CIRCE.

He is an expert in thermoeconomic analysis, participating in and leading several R&D projects on thermoeconomics, including a thermoeconomic diagnosis of the IGCC power plant at Puertollano (Spain), thermoeconomic analysis of the dual-purpose power and desalination plant at Al Taweelah (UAE), and thermoeconomic analysis of the dairy industry. He is participating in and developing various other projects related to sustainable and efficient energy conversion systems applied to conventional coal-fired power plant, such as co-firing in the Escucha power plant, and efficiency monitoring and improvement of the Teruel power plant.

He is author and/or co-author of more than 30 papers and books on thermoeconomics and its applications to complex energy systems, and Secretary of the International Study Group for Water and Energy Systems. He has taught several international courses on thermoeconomics, has been a member of the scientific committee of several international conferences, and is a member of the editorial advisory board of the *International Journal of Energy Environment and Economics*.

**César Torres Cuadra** is a research contributor at the CIRCE foundation (Center of Research for Energy Resources and Consumption), Zaragoza, Spain. He received a Bachelor Diploma in Mathematics from the University of Zaragoza in 1984, worked as researcher in the ITA (Technological Institute of Aragon), and undertook graduate studies in mechanical engineering with a major in energy optimization at the University of Zaragoza, obtaining a Ph.D. in 1991.

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