

TaesLab: An advanced software tool for circular thermoeconomics

C. Torres^a, A. Valero^b and A. Valero-Delgado^c

^a CIRCE Institute, University of Zaragoza, Spain, ctorresc@unizar.es, CA

^b CIRCE Institute, University of Zaragoza, Spain, valero@unizar.es

^c CIRCE Institute, University of Zaragoza, Spain, avdelgado@unizar.es

Abstract:

Circular thermoeconomics encompasses the physical principles of the circular economy (strictly spiral economy), industrial symbiosis, and second law costing and diagnosis of complex energy systems. This article describes a new software tool for circular thermoeconomics distributed as a MATLAB package. The software implements the algorithms described in the latest revisions of the exergy cost theory. In addition to production cost calculation and diagnostics functions, TaesLab incorporates new ones for determining energy savings due to waste recovery and process integration. The production structure model makes it possible to analyse different plant configurations, integrating other processes for waste recovery or energy storage. For demonstration purposes, the article presents a short example of a cogeneration plant with waste recovery and describes its data model and the functionality of this software tool.

Keywords:

thermoeconomics, waste cost allocation, circular economy, software tools.

1. Introduction

Thermoeconomics, an energy analysis methodology combining thermodynamics and economics, support energy systems' design, synthesis, and operation with higher efficiency and lower production costs. Thermoeconomics methods are usually applied to assess the energy and monetary cost of energy systems' internal flows and final products. These methods detect inefficiencies and evaluate their economic effects using thermoeconomic diagnosis [1]. Environmental issues have been incorporated into the analysis [2] to consider waste treatment and emission cost allocation. Classic exergy cost theory [3] has been recently revisited to include general waste cost allocation methods [4].

This methodology, called Circular Thermoeconomics [5], is based on the theory of exergy cost and its generalisation, the *structural theory*, which allows the accounting of physical or thermodynamic costs, both of functional products and waste generated in parallel. It makes it possible to identify which part of these costs are due to internal irreversibilities and which are due to the waste produced or external irreversibilities. Each of these irreversibilities can be reduced to certain limits: Internal irreversibilities by improving the efficiency of the processes or changing the technology, but always up to a specific limit; External irreversibilities by recycling waste. Internal irreversibilities are, at the same time, also the cause of waste and their transfer and disposal increment costs.

The word "recycling" is used interchangeably by Thermoeconomics, Circular Economy and Industrial Symbiosis. One may wonder if it means the same thing in all three fields of activity. Recycling means efficient use of resources. What is different is the type of systems it studies. In general, the objective of the circular economy is the recovery of any solid waste, while the system analysed is the recovery plant. Industrial symbiosis deals with reusing waste or by-products from one plant by other plants. In this case, the system under study is the set of interacting plants. Thermoeconomics cover the general use, no matter how complex the subsystems and flow interconnections are.

If a waste leaves the boundaries of a plant, it is dissipated into the environment, but its formation and disposal costs must be accounted for by identifying its origin. Some of this waste could be reused in other processes or plants. This theory allows for calculating its formation costs and providing a target cost as a basis for discussion with other plants interested in using it.

There is a wide range of software for the modelling, process integration, simulation, and optimisation of energy systems, such as EES [6], HSC Chemistry [7], or ASPEN PLUS [8]. Still, in general, they do not include thermoeconomic analysis. Torres et al. [9] provide the guidelines for developing thermoeconomic

analysis software and present an Excel-based application [10] that implements these ideas. These ideas are applied in some specific tools for energy analysis software [11].

This paper describes a new software tool, called TaesLab, that implements the algorithms described in [4], including waste cost allocation and recycling analysis. The software is presented as a MATLAB package or as a stand-alone application. TaesLab provides a set of functions and tools that allow a complete thermoeconomic analysis of an energy system, starting from the definition of its thermoeconomic model, a collection of plant states defined by the exergies of its mass and energy flows, and the costs of its external resources. The main functions are:

- Read and Check the Thermoeconomic Data Model.
- Compute Exergy Balances and Fuel Product table.
- Compute Exergy Cost.
- Analyse the Cost Formation Process of Products and Waste.
- Recycling Analysis.
- Thermoeconomic Diagnosis.

The results are presented in the form of graphs and tables. These can be saved in Excel sheets or text files for further analysis.

An Organic Rankine Cycle (ORC) is used as an example to illustrate the application's functionality. It uses waste heat to produce electricity. Part of the heat dissipated in the condenser could be recycled and used to produce air conditioning in another plant process, for example, an ejector refrigeration cycle [12].

2. Thermoeconomic Data Model

To make a thermoeconomic analysis of an energy system, a set of information that constitutes the thermoeconomic data model is needed.

2.1. Physical structure

For a given level of aggregation, an energy system can be represented by a directed graph, whose nodes are the thermodynamic processes and edges are the flows of matter and energy exchanged. Figure 1 depicts the physical structure of the plant used as example.

2.2 Thermodynamic model

To perform the thermoeconomic analysis of an energy system, it is necessary to define the exergy of each flow specified in the physical structure. The thermodynamic model of the plant is described by a set of equations (including mass, energy and entropy balances) that allow the determination of each mass, heat and work stream involved in the physical structure of the plant from a set of input variables, which define a thermodynamic state of the plant. In this example, an EES model obtains the exergy flows. The main parameters of the plant are also shown in Figure 1.

2.3 Productive structure

Each component or process of the system has a productive purpose established by its exergy efficiency, defined as the amount of exergy produced per unit of exergy of resources used, and which measures the quality of the process. Thus, for each process of the system, it is necessary to identify which flows constitute the product or products of the process and which resources or fuels are used to produce them. In this definition, it is also necessary to indicate which flows are waste and which processes are used to eliminate them, called dissipative processes [13]

2.4 Waste Cost Allocation

How the waste cost is allocated to the production processes of a system depends on the type and nature of the waste. There is no general criterion for assigning the cost of system waste. For example, in the case of heat dissipated in the condenser of a Rankine cycle, we can distribute the cost proportionally to the entropy generated by each process. On the other hand, the flue gases removed by the stack of the combined cycle are allocated to the combustion process. Therefore, the allocation of the residual costs should be based on the following criteria:

- The waste cost must be allocated to the production units that have generated it. Here, it is essential to establish a conceptual difference between the exergy of waste and its cost. Costs also encompass exergy consumption to be involved in eliminating the system waste. Therefore, the cost, not its exergy, is of actual interest. It raises a need that is expressed in the second premise.
- It is needed to identify the process of cost formation of waste. It parallels the production cost formation process because the residues are removed in the dissipative components but are formed together with the production processes. The responsibility of a productive component for waste generation lies in its contribution to the formation cost of waste.

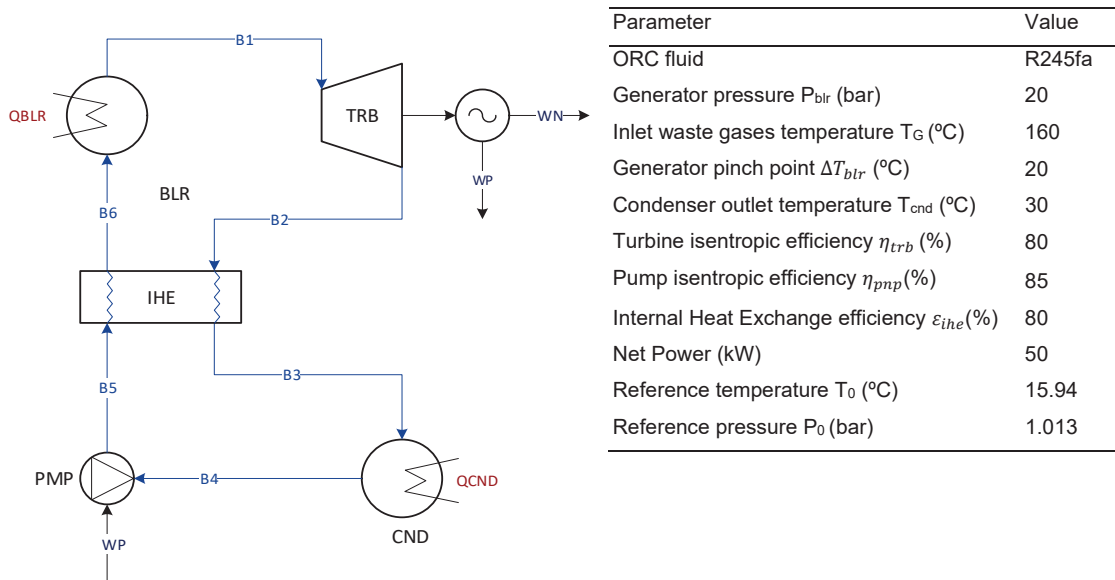


Figure 1. Thermodynamic diagram of the ORC plant and main operational parameters,

To identify waste flows at the process level, relating each flow with the physical and chemical processes in dissipative units is necessary. We must define as many dissipative units as waste flows. Dissipative units are defined in such a way that the output product stream is a waste flow, and input fuel streams are these flows that one wants to be eliminated and the resources required to do that. The irreversibility carriers allow one to identify the waste stream's origin, path, and end. The Fuel-Product and the Irreversibility-Cost tables can help to determine the cost formation process of products and wastes.

TaesLab uses the following methods, described in detail in reference [4]

- **EXERGY:** This method looks for the immediate cause and distributes the waste's costs to the components that have produced it directly and in proportion to their exergy.
- **COST:** This allocation method is like the previous one but distributes the cost proportionately to its exergy cost instead of its exergy. It should be noted that, in many cases, a waste's exergy is irrelevant, but its cost is relevant.
- **RESOURCES:** This method is based on the definition of cost, i.e. the cost of a waste is the amount of external resources expended to produce it. The method internalises the waste cost to the external resources proportionally to the amount used to make it. This is the DEFAULT method used by TaesLab if no waste definition is provided.
- **IRREVERSIBILITY:** This method identifies the waste cost formation process from the cost-irreversibility table and distributes the cost according to the irreversibility carriers of waste streams.
- **HYBRID:** This method combines the IRREVERSIBILITY and EXERGY methods. The method considers the full path of the waste cost formation. See reference [14]

2.5. Economic and environmental model

The exergy cost is relative to the limits of the system. Therefore, we must define the thermodynamic system's boundaries that constitute the installation and its environment. The exergy cost, also called direct exergy cost, only considers the irreversibility of the processes (both internal and external) within the system boundaries.

From the viewpoint of natural resource management, the system boundaries should be set at the level of extraction of non-renewable resources from nature [15]. The exergy cost of natural gas processed in a gas turbine will be higher than its exergy due to the extraction, storage and transportation processes required to use it. Moreover, the direct exergy cost does not consider that the installation processes have their own exergy cost because additional exergy will be needed to keep them in operation. On the other hand, when considering the economic aspects, the perspective is broadened by the introduction of two additional factors: the market prices of fuels ($\text{€}/\text{MWh}$) that are not linked to the exergy of the resources processed and the cost of investment, maintenance and operation of the facility necessary for the production process ($\text{€}/\text{h}$) For these

reasons, the concept *generalised exergy cost* is presented as a broader view of the exergy cost, in which the costs of the system flows take into account the interactions with the physical and economic environment. Therefore, the external valuation of resources could be measured in mass, energy or monetary units per unit of time; and the costs of the plant processes, measured in terms of mass, energy or monetary units and levelized per unit of time, must be considered.

Some examples of generalised exergy costs are the thermo-ecological cost [16] or the exergoeconomic cost [17], which assesses the monetary cost of internal flows and outputs of complex plants.

2.6 Thermoeconomic Data Model

Defining this thermoeconomic model requires a collection of structured data or tables that provide the information needed to analyse a system using TaesLab. The data model can be saved in an XLSX spreadsheet workbook, but other formats, such as CSV, JSON or XML, can also be used. The required tables, defined for the ORC plant in Appendix A, are:

- *Flows*: Enumerate the flows of the system. See Table A1 (a). The *type* field indicates if the flow connects to the plant process (INTERNAL), is an external resource (RESOURCE), is a final product (OUTPUT) or a waste leaving the system (WASTE).
- *Processes*: Enumerate the process of the system. See Table A1 (b). The *type* field indicates if the process is PRODUCTIVE or DISSIPATIVE. The productive structure is defined in the fields: *fuel* and *product*. We show which flows, described in the previous table, constitute the fuel and which flows are the product. For example, in the case of the Steam Generator (BLR), the fuel is the waste heat (QBLR), and the product is (B1-B6), the exergy difference between flows B1 and B6.

These two tables define the productive structure of the plant.

- *Format*: The numerical format used for the results tables and the units in which the different quantities appear are indicated. For example, exergy values (EXERGY) are expressed in (kW) and are shown with up to ten significant digits and three decimal places. See Table A4
- *Exergy*: It contains the values of the flow exergies for different plant states or simulations. See Table A2. Each column represents a plant state. The first column of values is used as the reference state, and the column name serves as a key to identify that state. TCND45 use $T_{\text{cond}}=45^{\circ}\text{C}$, ETAT75 simulates the plant with $\eta_{\text{tr,b}}=75\%$, PBLR15 use $P_{\text{blr}}=15$ bar, nolHE bypasses the internal heat interchange, and n-Butane uses that fluid instead R234fa.

The rest of the tables described below are optional:

- *WasteDefinition*: Defines how the waste cost is allocated; see table A3. The different types of waste cost allocation have been described in section 2.5
- *WasteAllocation*: It manually defines the ratios for allocating waste costs to production processes. See also Table A.5
- *ResourcesCost*: Values of external resource costs, both flow costs (FLOW) and process costs (PROCESS). The units must be those indicated in the Format table for GENERALIZED_UNIT_COST and GENERALIZED_COST, respectively. Table A5 shows the economic costs of the processes in c€/kWh, according to the reference [18]. In the case of waste gases, they are considered amortised in the plant that produces them. Therefore the unit cost of the external resource flow QBLR is zero.

3. The TaesLab Application

TaesLab is a MATLAB package compatible with Octave, which provides a set of functions to perform the thermoeconomic analysis of a plant interactively from the MATLAB console. It also provides an application with a graphical user interface, see Figure 2, where the essential functions can be performed. See reference [10] for complete information on the use of the package, the user guide and its download.

TaesLab GUI has three panels. In the left panel, select the status to be calculated and the rest of the parameters. In the right panel, select the tables and graphs of the current state to be displayed in the central panel.

TaesLab has three groups of functions.

- Read and check the thermoeconomic model files.
- Cost analysis and thermoeconomic diagnosis.
- Show and save the results.

There are five blocks of results:

- Productive Structure.
- Thermoeconomic State.

- Thermo-economic Analysis
- Thermo-economic Diagnosis
- Summary Results

For each of these blocks, we can show the tables obtained, graph representations, and see internal information of the calculations using the workspace inspector. All the results could be saved into text files or XLSX spreadsheet workbooks for further analysis. The complete list of tables and graphs that could be obtained is explained in the user manual [10] mentioned above.

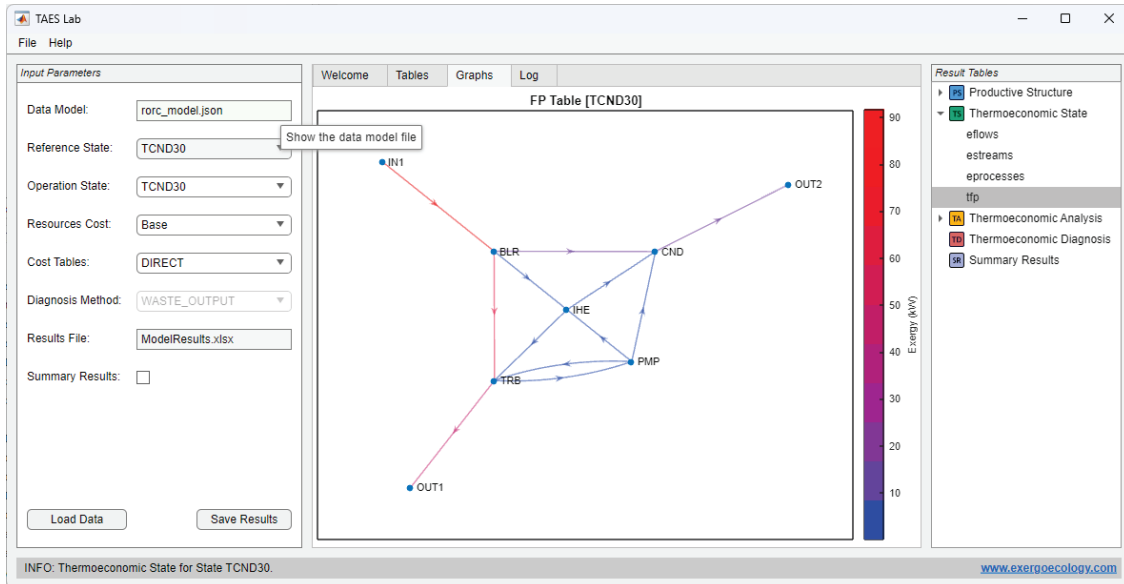


Fig.2 Screenshot of the GUI Application of TaesLab

3.1. Input Parameters

The application has several parameters that can be modified interactively.

- *State*: Indicates the state where we want to perform the analysis.
- *CostTables*: Indicates which types of tables we want to generate.
 - DIRECT: Only direct exergy costs are calculated
 - GENERALIZED: If external resources data are available, obtain generalised exergy costs
 - ALL: Both cost types are selected.
- *ResourcesCost*: Allows selecting the data to calculate the generalised costs.
- *ReferenceState*: Indicates which state will be used as the reference when running the thermo-economic diagnosis.
- *DiagnosisMethod*: Indicates the method used to make the thermo-economic diagnosis.
 - NONE: The thermo-economic diagnosis calculations are deactivated.
 - WASTE_OUTPUT: Waste is considered as plant output flows.
 - WASTE_INTERNAL: The cost of waste is assessed according to the chosen waste cost allocation.
- Summary Results: Activate Summary Results tables and graphs.

Appendix B shows the Live Script used to obtain the tables and figures obtained below.

3.2. Productive Structure

In this block of results, the information on the production structure graph, including the production groups, also called streams, is shown. The construction of the adjacency matrix of the production structure graph is explained in detail in reference [4]. Figure 3 shows the production structure of the example plant. It has been drawn with yEd graph software [19] from a file obtained by the app function SaveProductiveDiagram.

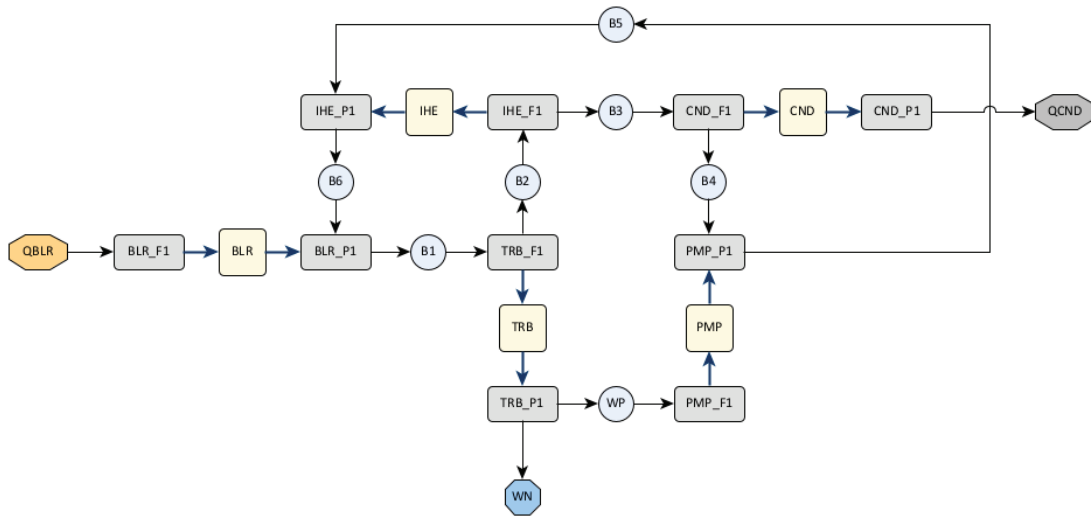


Figure 3. Productive structure graph of the ORC plant,

In this graph, the yellow squares represent the processes, the grey rectangles the productive groups, and the blue circles the flows. Resources are drawn as an orange octagon, waste as a grey octagon, and Final products as a blue octagon. Each Internal flow connects two productive groups, and each process connects to one or several fuel and product groups.

3.3 Thermo-economic State

This results block shows the plant's exergy balances and its Fuel-Product table. Table 1 shows the exergy balance of the example ORC plant.

Table 1. Process Exergy Balance of ORC plant

| Key | F(kW) | P(kW) | I(kW) | k(J/J) | η (%) |
|-----|-------|-------|-------|--------|------------|
| BLR | 99.53 | 73.70 | 25.84 | 1.3506 | 74.04 |
| TRB | 65.67 | 52.43 | 13.24 | 1.2525 | 79.84 |
| IHE | 2.07 | 1.51 | 0.57 | 1.3754 | 72.71 |
| PMP | 2.43 | 2.08 | 0.35 | 1.1698 | 85.49 |
| CND | 9.54 | 9.54 | 0.00 | 1.0000 | 100.00 |
| ENV | 99.53 | 50.00 | 49.53 | 1.9906 | 50.24 |

The application checks if fuel (F), product (P) and irreversibility (I) are non-negative values. If both fuel and product are zero, the component is bypassed and not considered in the calculation. It permits to analyse of several plant configurations in the same data model.

Table 2. Fuel-Product Exergy Table (kW)

| Key | BLR | TRB | IHE | PMP | CND | ENV | Total |
|-------|-------|-------|------|------|------|-------|--------|
| BLR | 0.00 | 62.62 | 1.97 | 0.00 | 9.10 | 0.00 | 73.70 |
| TRB | 0.00 | 0.00 | 0.00 | 2.43 | 0.00 | 50.00 | 52.43 |
| IHE | 0.00 | 1.28 | 0.04 | 0.00 | 0.19 | 0.00 | 1.51 |
| PMP | 0.00 | 1.77 | 0.06 | 0.00 | 0.26 | 0.00 | 2.08 |
| CND | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 9.54 | 9.54 |
| ENV | 99.53 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 99.53 |
| Total | 99.53 | 65.67 | 2.07 | 2.43 | 9.54 | 59.54 | 238.78 |

Table 2 shows the Fuel-Product table of the plant. This table shows the role of each plant's processes. The most important ones are the steam generator (BLR) and the turbine (TRB), while the IHE and the pump (PMP) recover a small part of the exergy.

3.4. Thermo-economic analysis

This section presents the results of calculating a plant state's direct and generalised energy costs. There are several types of tables:

- Summary tables of costs for flows and processes.
- Fuel-Product Cost Tables
- Irreversibility Cost Tables

The values of direct exergy costs are decomposed between the part due to internal irreversibilities B_{IN}^* and the costs due to waste B_{EX}^* , applying the selected criterion for waste cost allocation.

$$B^* = B_{IN}^* + B_{EX}^* \quad (1)$$

In the case of generalised exergy costs, they are broken down into the part due to the cost of external resources C_e , the costs associated with processes, C_z , and the cost due to waste, C_r , see Table 3.

$$C = C_e + C_z + C_r \quad (2)$$

Table 3. Generalised (exergoeconomic) cost of ORC flows.

| Key | B(kW) | C(c€/h) | C _e (c€/h) | C _z (c€/h) | C _r (c€/h) | c(c€/kWh) | c _e (c€/kWh) | c _z (c€/kWh) |
|------|-------|---------|-----------------------|-----------------------|-----------------------|-----------|-------------------------|-------------------------|
| B1 | 82.99 | 37.96 | 0.00 | 20.96 | 17.01 | 0.4574 | 0.0000 | 0.2525 |
| B2 | 17.32 | 7.92 | 0.00 | 4.37 | 3.55 | 0.4574 | 0.0000 | 0.2525 |
| B3 | 15.25 | 6.98 | 0.00 | 3.85 | 3.12 | 0.4574 | 0.0000 | 0.2525 |
| B4 | 5.71 | 2.61 | 0.00 | 1.44 | 1.17 | 0.4574 | 0.0000 | 0.2525 |
| B5 | 7.79 | 13.37 | 0.00 | 11.36 | 2.01 | 1.7163 | 0.0000 | 1.4589 |
| B6 | 9.30 | 17.19 | 0.00 | 14.45 | 2.74 | 1.8491 | 0.0000 | 1.5542 |
| QBLR | 99.53 | 0.00 | 0.00 | 0.00 | 0.00 | 0.0000 | 0.0000 | 0.0000 |
| WP | 2.43 | 8.45 | 0.00 | 7.81 | 0.64 | 3.4736 | 0.0000 | 3.2105 |
| WN | 50.00 | 173.68 | 0.00 | 160.52 | 13.16 | 3.4736 | 0.0000 | 3.2105 |
| QCND | 9.54 | 15.11 | 0.00 | 13.16 | 1.95 | 1.5841 | 0.0000 | 1.3791 |

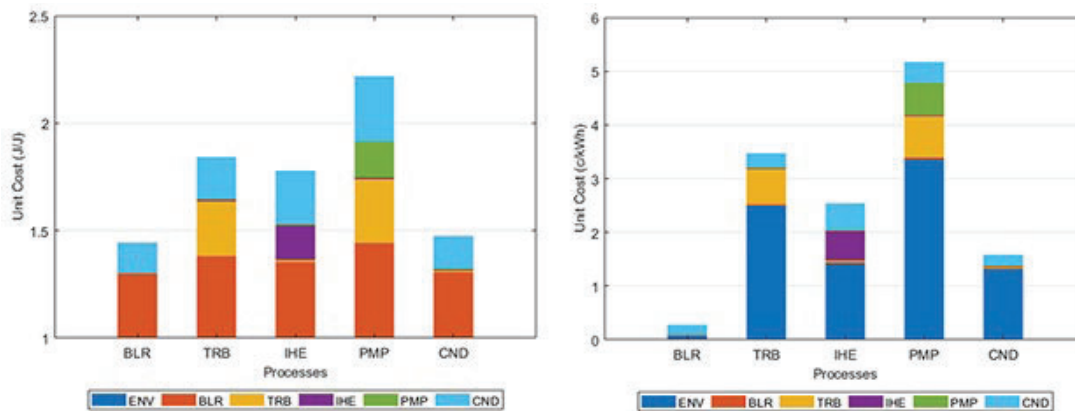


Fig. 4 Direct and Generalized irreversibility cost graphs

Table 3 shows the generalised cost of flows. The main contribution is the investment and maintenance costs of the equipment. Here the cost of waste does not reach 10%, and it is assumed that the heat used in the steam generator has no cost. Then the electricity cost is 34.73 €/MWh and the heat 15.84 €/MWh.

The irreversibility cost charts analyse the cost formation process, considering the effect of each process's internal and external irreversibilities. In the case of generalised cost, the impact of the cost of external resources associated with flows and processes is also considered. See Fig. 4.

In the case of direct cost, the main contribution to the cost of each component is the steam generator, as it is the least efficient component located at the beginning of the production chain, also noting that waste costs have a significant weight. In the case of exogenous economic costs, an essential part, as already mentioned, is the equipment costs, together with the irreversibilities of the turbine, due to its high cost.

The application provides an additional function (Summary of Results) that allows the generation of comparative tables and graphs for the different states of the plant.

3.5. Waste Recycling Analysis

As long as residual streams have exergy, they can be retrieved in *recovery units*; the condenser/heat exchange is in the ORC example. These recovery units are integrated into the plant and constitute productive units. Instead of expending exergy to dispose of waste, their exergy is recovered to produce another by-product. In the case of the ORC plant, the recovery unit could produce steam for an ejector refrigeration system. The potential savings from waste recycling can be estimated if one knows the production costs due to external irreversibilities. The production cost due to waste k_{EX}^* indicates the maximum amount of resources that could be saved if waste were recycled.

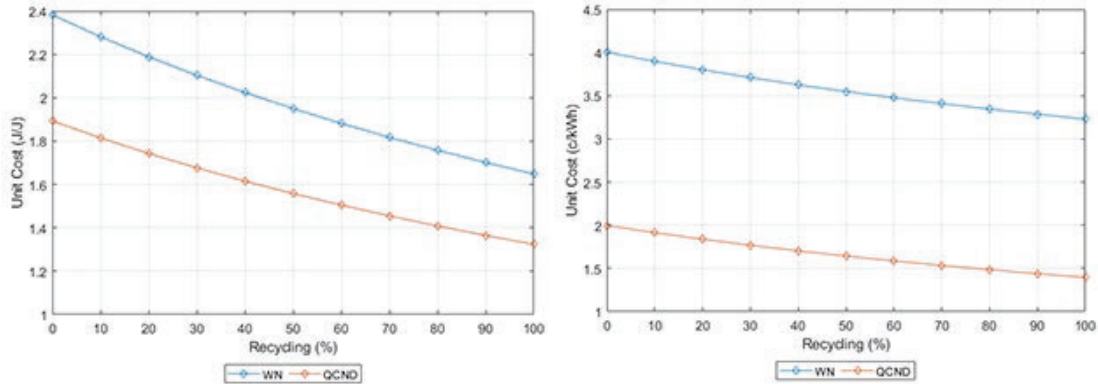


Fig. 5 Direct and Generalized cost of output flows as a function of waste QCND recycled for TCND45 state.

It is well known that not all waste can be saved for technical and economic reasons. But, using process integration and Industrial Symbiosis[21], other systems may convert this waste into resources. The exergy cost theory allows for evaluating the waste cost, accounting for resource savings, and providing fair prices to waste becoming by-products.

TaesLab allows computing the production costs if a part of the waste stream is recycled. Figure 6 shows the plots of the output system flows as a function of the portion of waste recycled for the TCND45 state. In the case of recycling up to 66% of the heat, the cost of electricity is 34.35 €/MWh, which is lower than operating the plant under reference conditions.

3.6 Thermo-economic Diagnosis

The thermo-economic diagnosis allows for comparing two states of the plant, identifying the causes of the increase in resource consumption between a reference state and another state (operating state). It also allows for evaluating the cost of production increase and the increase of the waste cost.

Diagnosis results are generated when *DiagnosisMethod* is active, and the *ReferenceState* and *State* parameters have different values. The application provides two methods for the analysis of waste cost variation. The first one, *WASTE_OUTPUT*, is the standard method of thermo-economic diagnosis, in which the impact on fuel is the sum of the cost of malfunctions caused by the variation of internal irreversibilities MF_i^* , plus the cost of the variation of external outputs, including final products and wastes. The increase in the waste cost implies a useless consumption of resources but not an increase in the final product.

$$\Delta F_T = \sum_i MF_i^* + \sum_j k_{P,N}^* \Delta \omega_s \quad (3)$$

The second method, *WASTE_INTERNAL*, addresses this limitation. It is a new implementation of the fuel impact calculation. The cost of waste variation is reallocated to the plant's production processes and final products, according to the defined waste cost allocation criteria.

$$\sum_j k_{N,j}^* \Delta \omega_{R,j} = \sum_i MR_i^* + \sum_j k_{EX,j}^* \Delta \omega_{T,j}, \quad (4)$$

where MR_i^* is the cost of process malfunctions due to the external irreversibility increase, and $\Delta \omega_T$ is the variation of the final products. In such a case, the fuel impact formula is rewritten as follows:

$$\Delta F_T = \sum_i MF_i^* + \sum_j MR_j^* + \sum_j k_{P,j}^* \Delta \omega_{T,j} \quad (5)$$

If we compare the waste heat consumption of the plant in the reference state with that used in the TCND45 (66% recycling) state condition, we can see a fuel impact of 19.47 kW. However, in Table 4 and Figure 8, it can be seen that there is also an extra production of 18.17 kW and a real exergy saving of 7.398 kW.

Table 4. Diagnosis table comparison between Reference and TCND45 (%66 Recycling) states

| Key | MF (kW) | ΔI (kW) | ΔP_s (kW) | MF* (kW) | MR* (kW) | ΔP_T^* (kW) |
|-----|---------|-----------------|-------------------|----------|----------|---------------------|
| BLR | -3.679 | 1.695 | 0.000 | -3.679 | -2.712 | 0.000 |
| TRB | -0.385 | -0.240 | 0.000 | -0.368 | 0.041 | 0.000 |
| IHE | -0.330 | -0.125 | 0.000 | -0.433 | -0.226 | 0.000 |
| PMP | -0.016 | 0.068 | 0.000 | -0.027 | -0.024 | 0.000 |
| CND | 0.000 | 0.000 | 18.172 | 0.021 | 0.010 | 26.968 |
| ENV | -4.410 | 1.398 | 18.172 | -4.486 | -2.912 | 26.968 |

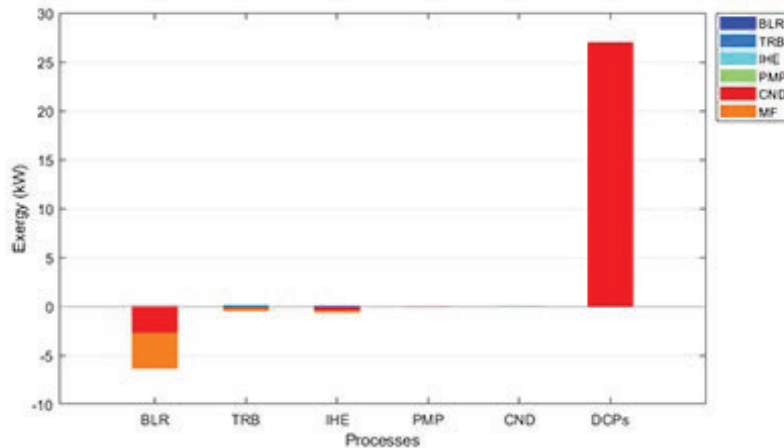


Fig. 6. Malfunction Cost graph comparison between Reference and TCND45 (%66 recycling) states

4. Conclusions

This paper presents a new software application for the thermoeconomic analysis of energy systems. The application follows the methodology described in [9]. It is an evolution of the TAESS application [web], which implements the new algorithms for circular thermoeconomics described in [4], with particular emphasis on analysing the waste cost formation process and its effect on production costs.

The application is presented as a MATLAB package, which includes both applications with a graphical user interface (GUI) and interactive functions that can be used in the MATLAB environment. The fact that it is written in MATLAB language facilitates the calculations of mathematical structures and provides an efficient environment for visualising the results obtained. Through notebooks or Live Scripts, it is possible to use TaesLab for educational purposes and applications adapted to users' needs. In addition, a library of classes is available, allowing new applications and functions to be developed by reusing the source code already generated. Most of the functionality of this software is also compatible with Octave, the open-source alternative to MATLAB.

TaesLab allows focusing on obtaining results without defining the cost equations as in other methodologies. The paper describes the data model, including its physical and productive structure and thermodynamic, economic and environmental data, and shows with an example its capabilities.

As future perspectives for TaesLab, besides adding new functionalities such as aggregation and integration of systems and models with energy storage..., is to integrate it with other simulation packages of energy systems such as Simulink [22], ASPEN or HSC.

Acknowledgements

This paper has been funded by the Spanish Ministry of Science and Technology under project RESET PID-116851RB-100, and project G/5423/740121/32444 funded by the Aragon Government under the Renewable Energy and Hydrogen program within the framework of the complementary plans foreseen in the plan for recovery, transformation and resilience-MRR

Appendix A

This appendix shows the data model tables of the ORC plant example.

Table A1. Physical and Productive Structure definition.

| (a) Flows definition | | (b) Process definition | | | | |
|----------------------|----------|------------------------|-------|---------|-------------|-------------------------|
| key | type | key | fuel | product | type | description |
| B1 | INTERNAL | BLR | QBLR | B1-B6 | PRODUCTIVE | Steam Generator |
| B2 | INTERNAL | TRB | B1-B2 | WN+WP | PRODUCTIVE | Turbine |
| B3 | INTERNAL | IHE | B2-B3 | B6-B5 | PRODUCTIVE | Internal Heat Exchanger |
| B4 | INTERNAL | PMP | WP | B5-B4 | PRODUCTIVE | Pump |
| B5 | INTERNAL | CND | B3-B4 | QCND | DISSIPATIVE | Condenser |
| B6 | INTERNAL | | | | | |
| QBLR | RESOURCE | | | | | |
| WP | INTERNAL | | | | | |
| WN | OUTPUT | | | | | |
| QCND | WASTE | | | | | |

Table A2. Exergy States values (kW)

| Key | Reference | TCND45 | ETAT75 | PBLR15 | NoIHE | N-Butane |
|------|-----------|--------|--------|--------|--------|----------|
| B1 | 82.99 | 106.70 | 88.81 | 84.14 | 82.99 | 103.5 |
| B2 | 17.32 | 40.68 | 18.92 | 18.96 | 17.32 | 37.2 |
| B3 | 15.25 | 37.42 | 16.36 | 17.02 | 17.32 | 35.03 |
| B4 | 5.71 | 9.71 | 6.11 | 6.39 | 5.711 | 24.87 |
| B5 | 7.79 | 12.31 | 8.34 | 8.09 | 7.79 | 27.41 |
| B6 | 9.30 | 15.13 | 10.17 | 9.51 | 7.79 | 29.02 |
| QBLR | 99.53 | 119.10 | 105.80 | 102.80 | 106.4 | 100.8 |
| WP | 2.43 | 3.02 | 2.60 | 1.98 | 2.432 | 2.967 |
| WN | 50.00 | 50.00 | 50.00 | 50.00 | 50 | 50 |
| QCND | 9.54 | 27.71 | 10.25 | 10.63 | 11.609 | 10.16 |

Table A3. Waste Definition and allocation (values in %)

| key | type | recycle | key | QCND |
|------|-----------------|---------|-----|-------|
| QCND | IRREVERSIBILITY | 0.00 | BLR | 94.40 |
| | | | TRB | 2.24 |
| | | | IHE | 2.06 |
| | | | PMP | 1.29 |

Table A4. Format definition

| key | width | precision | unit |
|-----------------------|-------|-----------|----------|
| EXERGY | 10 | 3 | (kW) |
| EXERGY_COST | 10 | 3 | (kW) |
| EXERGY_UNIT_COST | 10 | 4 | (J/J) |
| GENERALIZED_COST | 10 | 3 | (c€/h) |
| GENERALIZED_UNIT_COST | 10 | 4 | (c€/kWh) |
| DIAGNOSIS | 10 | 4 | (kW) |

Table A5. Resources Cost Values (The units of the values are as defined in the format table)

| key | type | Base |
|------|---------|--------|
| QBLR | FLOW | 0.00 |
| BLR | PROCESS | 6.51 |
| TRB | PROCESS | 151.75 |
| IHE | PROCESS | 2.56 |
| PMP | PROCESS | 2.11 |
| CND | PROCESS | 10.75 |

Appendix B

This appendix shows the LiveScript commands of the TaesLab application used to generate the figures and tables of the paper.

Read and check the Data Model file.

Read the data model `rorc_model.xlsx`, select all tables and deactivate diagnosis

```
model=ThermoeconomicTool('rorc_model.xlsx', 'CostTables', 'ALL',...
'DiagnosisMethod', 'NONE', 'Debug',false);
```

Get tables and graphs for the reference state TCND30.

Save results tables in an Excel workbook. Tables 1-3 and Figure 3

```
SaveResults(model,'rorc_results.xlsx');
model.saveProductiveDiagram('rorc_ps.xlsx');
```

Generate Irreversibility Cost Graph. Figure 4

```
model.graphCost(cType.Tables.PROCESS_EXERGY_COST);
model.graphCost(cType.Tables.PROCESS_GENERAL_COST);
```

Recycling Analysis

Get the recycling graphs for state **TCND45**. Figure 5

```
model.State='TCND45';
res=recyclingAnalysis(model);
res.graphRecycling(cType.Tables.WASTE_RECYCLING_DIRECT);
res.graphRecycling(cType.Tables.WASTE_RECYCLING_GENERAL);
```

Thermoeconomic Diagnosis

Compare **TCND30** (reference state) with **TCND45**, recycling 66% of the condenser heat.

```
mode.setRecycledRatio('QCND',0.66)
model.DiagnosisMethod='TCND45';
```

Save the thermoeconomic diagnosis results, table 4, and show the malfunction cost graph, figure 6.

```
SaveResults(model, 'rorc_TCND45.xlsx');  
model.graphDiagnosis(cType.Tables.MALFUNCTION_COST);
```

References

- [1] Torres C., Valero A., Serra L., Royo J., Structural theory and thermoeconomic diagnosis: Part I. On malfunction and dysfunction analysis. *Energy Conver Manag.* 2002; 43(9-12): 1503-1518.
- [2] Stanek W., *Thermodynamics for Sustainable Management of Natural Resources*; Springer: Cham, Switzerland, 2017.
- [3] Lozano, M.; Valero, A. Theory of the exergetic cost. *Energy* 1993, 18, 939–960.
- [4] Torres C., Valero A., The Exergy Cost Theory Revisited. *Energies*, 2021, 14, 1594.
- [5] Valero A., Torres C., Thermoeconomics as a cost accounting methodology for Spiral Economy and Industrial Symbiosis. ECOS 2021, 34th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, June 27-July 2, Taormina, Italy: 656-666.
- [6] EES: Engineering Equation Solver. Available at <https://fchartsoftware.com/ees/> [accessed 20.3.2023]
- [7] HSC Chemistry Software for Process Simulation. Available at: <http://www.hsc-chemistry.net/> [accessed 20.3.2023]
- [8] Aspen PLUS. Available at: <https://www.aspentech.com/en/products/engineering/aspen-plus> [accessed 20.3.2023]
- [9] Torres, C., Valero, A., Perez, E., Guidelines to developing software for thermoeconomic analysis of energy systems, ECOS 2007, 20th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, June 24-28, Padova Italy, vol. 1:435–490.
- [10] TAESS. Thermoeconomic Analysis of Energy Systems Software. The Exergoecology Portal. Available online: <https://www.exergoecology.com/> [accessed 10/3/2023].
- [11] Picallo A., Sala J.M., Portillo L., Development of a tool based on thermoeconomics for control and diagnosis build thermal facilities, *Energy*, 2022, 239, 122304.
- [12] Rostamzadeh H., Ebadollahi M., Ghaebi H., Amidpour M., Kheiri R. Energy and exergy analysis of novel combined cooling and power Cycles. *Applied Thermal Engineering*, 2017, 124, 152–169
- [13] Torres C., Valero A., Rangel V., Zaleta A. On the cost formation process of the residues. *Energy* 2008, 33, 144–152.
- [14] Agudelo, A.; Valero, A.; Torres, C. Allocation of waste cost in thermoeconomic analysis. *Energy* 2012, 45, 634–643.
- [15] Usón, S.; Kostowski, W.J.; Stanek, W.; Gazda, W. Thermoeconomic cost of electricity, heat and cold generated in a trigeneration module fuelled with selected fossil and renewable fuels. *Energy* 2015, 92, 308–319.
- [16] Szargut, J. *Exergy Method: Technical and Ecological Applications*; WIT Press: Southampton, UK, 2005.
- [17] Tsatsaronis, G., Winhold, M. Exergoeconomic analysis and evaluation of energy-conversion plants-I. A new general methodology. *Energy* 1985, 10, 69–80.
- [18] Ghaebi H., Parikhani T., Rostamzadeh H., Farhang B., Thermodynamic and thermoeconomic analysis and optimization of a novel combined cooling and power (CCP) cycle by integrating of ejector refrigeration and Kalina cycles. *Energy* 2017, 139, 262-276
- [19] yWorks. yEd Graph Editor. Available online: <https://www.yworks.com/products/yed> [accessed on 10.3.2023].
- [20] e!Sankey – Show the Flow. Available online: <https://www.ifu.com/e-sankey/> [accessed on 10.3.2023].
- [21] Valero, A.; Uson, S.; Torres, C.; Valero, A.; Agudelo, A.; Costa, J. Thermoeconomic tools for the analysis of eco-industrial parks. *Energy* 2013, 62, 62–72.
- [22] Simulink, Available at: <https://www.mathworks.com/products/simulink.html> [accessed on 10.3.2023]