THERMODYNAMICS AND THE OPTIMISATION OF ENERGY SYSTEMS: STRENGTHS AND LIMITS

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ABSTRACT

The Second Law of thermodynamics is known to be an essential guide for the improvement of energy conversion systems. Throughout the years it has been applied to various engineering methods in particular in methods based on exergy [1] including the 2nd Law, thermoeconomics and exergoeconomics. It has also been used in graphically attractive energy integration techniques such as pinch technology and its derivatives. Apart from economic considerations, the emissions and the overall life cycle impacts have become of growing importance, exceeding the scope of pure thermodynamics. The latter point is related to the fact that there is no direct link between the entropy of local pollutants and their impacts on health. An appropriate combination between thermodynamics and advanced optimisation techniques allows to overcome the inherent limits of thermodynamic approaches and provides meaningful results on real systems. Examples of thermoeconomic, extended exergy analysis and environomic optimisation problems including Life cycle considerations are also considered. Drying processes, power plants, fuel cell systems and storage systems are dealt with.

INTRODUCTION

Energy systems play a crucial role in the development of our societies, by providing some of the essential services, going from electricity generation to comfort conditioning and transport. Gradual awareness of the global environmental impacts, and concerns for resources with the fast growing world population reinforce the need for increased efficiency and cleaner systems. This can be achieved not only by improving individual processes but also by an increased use of systems integrating several complementary technologies and simultaneously providing several different services. Combined cycles, energy integration as well as co- or tri-generation or post-treatment have become fairly common terms. Furthermore the optimisation of these complex systems during the operation is often not sufficient anymore and life cycle analysis, including the fabrication and the dismantling or the recycling of components, is more and more requested. The increased number of parameters and constraints exceed the human capabilities if the significant potential of modern information technology is not better exploited. Thermodynamics as the key engineering science, in this highly technological energy era, is to account for this development in order to contribute to more sustainable energy solutions.

ENTROPY AND EXERGY IN A LIFE CYCLE PERSPECTIVE

Basic approaches

From the early major contributions of the 19th century key players like Carnot, Clausius and later Gouy, the quest to reduce the entropy creation in energy conversion systems has been a constant concern. Accounting for the physical environment in which these systems are embedded has been further acknowledged by the development of the exergy theory in its various forms. Bejan [1] and Reistad et al. [2] emphasized the need for a trade-off between the irreversibilities of heat transfer, friction and, for the latter, of the embedded energy of components like heat exchangers in particular. This was later illustrated by Staine [3] for the case of shell-in-tube heat exchangers as can be seen in Fig 1. In this case the designer is faced with the option of increasing the heat exchange area and to distribute the heat exchange area so as to reduce the pressure drop for a given duty.

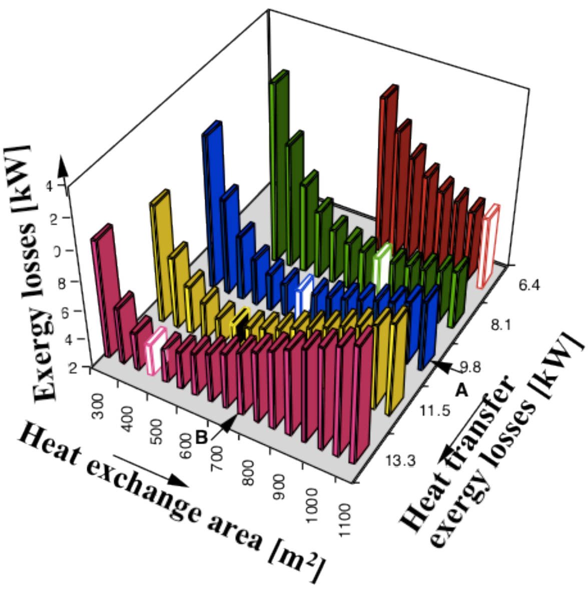

Fig.1 Extended exergy optimisation of a heat exchanger

The black block of the second raw of Fig. 1 corresponds with the minimum of the overall exergy losses. This can then be applied to all heat exchangers of an integrated energy system.

Linnhof et al. [4] simplified the 2nd Law practical application to account for economic factors by developing clever graphical representations and systematic rules for the energy targeting and design of integrated industrial processes. The so-called pinch technology, often wrongly opposed to exergy or mathematical programming approaches, did bring efficient tools to the engineers. An example of composites applied to a plaster panel drying process is shown in Fig. 2.

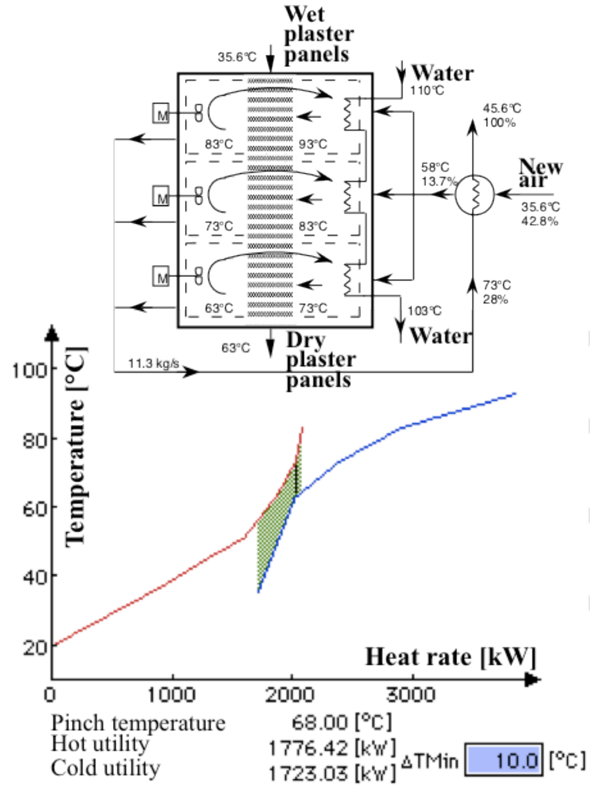

Fig. 2 Composites of a plaster drying process [3, 5]

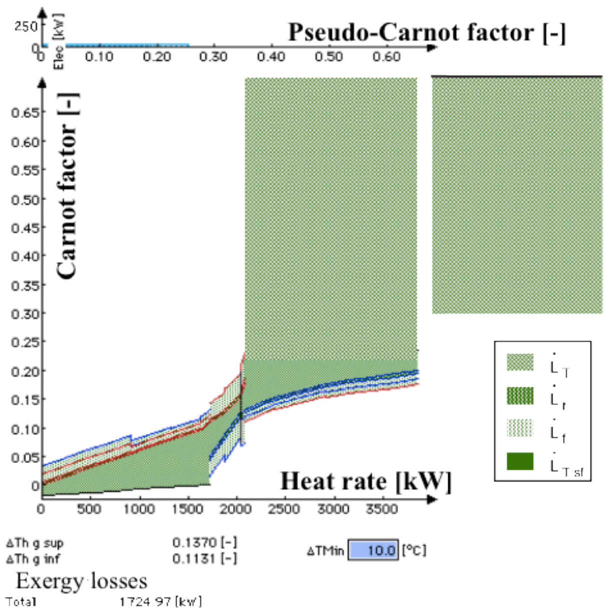

Fig. 3 Extended composite representation including the 3 main exergy losses (heat transfer T, friction r, fabrication f and heat transfer to the cold utility T_{sf})

Staine [3, 6] proposed an extension of the latter to simultaneously consider the three main irreversibilities (heat transfer, friction and fabrication losses) as shown in Fig. 3.

He also introduced a formalism and a graphical representation highlighting the electrical balance of the process or site considered. Fabrication losses can be expressed in terms of power (Watts) by using the ratio of the total embedded energy divided by the expected lifetime of the equipment. This method allows to approach the thermodynamic optimum. In this representation the total area of the coloured zones is proportional to the exergy losses.

Fig. 2 and Fig. 3 show the composites corresponding to the present situation with a gas boiler satisfying the heating energy needs for drying. As can be observed there is little overlap of the curves, so the potential for energy recovery within the process is minimal. In Fig. 3 the coloured areas are increased compared to Fig. 2 since they include the exergy losses of the gas boiler that were not shown in Fig. 2. Moreover the topping diagram illustrates the electricity consumption of the auxiliaries (fan, pump) and the corresponding exergy losses. In this representation the pseudo Carnot factor is adapted so that the coloured areas represent those losses.

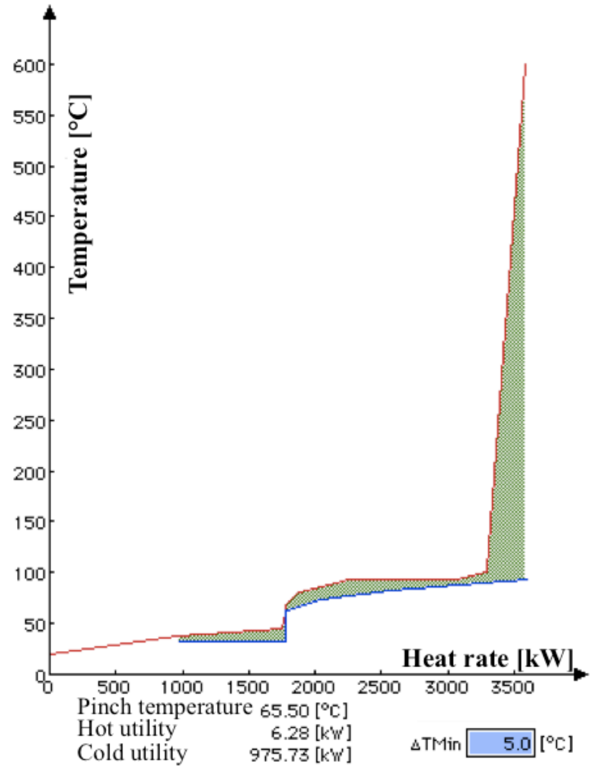

Fig. 4 Composites of the plaster drying process retrofitted with a heat pump and a gas cogeneration engine.

Fig. 4 and Fig. 5 show the result of the proposed retrofit consisting of replacing the boiler by a cogeneration gas engine and an industrial heat pump. As shown by the coloured areas of Fig. 5, the exergy losses of the retrofitted system could be reduced by 40%. The topping diagram of Fig. 5 shows the increased electricity consumption of the electrical heat pump with its corresponding area of exergy losses. The right part beyond a pseudo-Carnot factor of 1 represents the exergy losses of the gas engine. The empty box on the left of a pseudo-Carnot of 1 indicates the power supplied by the engine, which balances the electrical needs of the plant.

The power of this thermodynamic approach, which accounts for the exergy of fabrication, is its capability to identify a meaningful lower bound of the optimum pinch. This lower bound is more realistic than the bound, which would result from an ideal reversible approach. Taking into account the embedded exergy is not entirely sufficient and the economic optimised solution accounting for all factors such as transport, marketing cost and so on, will be different. However, the thermodynamic optimum, including the embedded exergy, is more robust in function of time, since it does not depend on the variable economic conditions. With that approach the decision maker has a narrower range of optima. He knows that, in case of an increase of energy costs, the real optimum will move closer to the thermodynamic one.

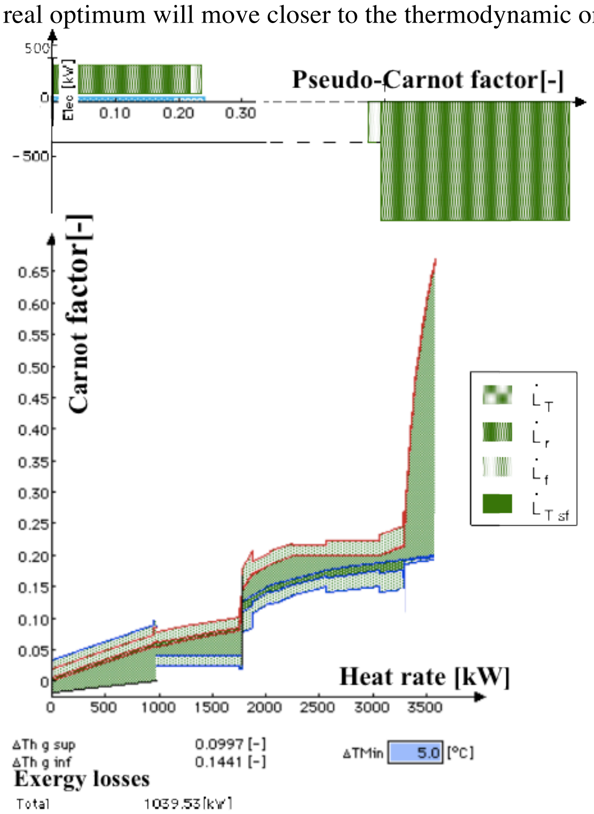

Fig. 5 Extended composite view of the drying process retrofitted with a heat pump and a cogeneration engine

The embedded exergy is becoming more important when analysing the true potential of many concepts proposed recently to recover the exergy of waste heat. Some of these concepts claim the possibility to recover energy from streams with temperature differences as low as a few tens of °C. This remark is related in particular to thermoelectric devices, or to osmotic concepts not based on natural fluids.

The power of thermodynamics should also be used to clearly rank future energy conversion paths, as shown by Agrawal and Singh [7] for the conversion from solar energy to biofuels.

Emissions and their impacts are more difficult to account for by thermodynamics alone. While there usually is a direct link between efficiency and global warming emissions for fossil based systems, it is less obvious for local pollutants. This is due to the fact that there is no direct link between the entropy of a substance, like NOx, and the effects that these pollutants have on health. Moreover the existing level of the local pollution at a given implementation site has a role to play on the conditions imposed on the implementation of new energy systems. This can be accounted for by pollution factors as proposed by Curti [8]. However, such local pollution factors cannot be visualized in a thermodynamic diagram such as the extended composite diagram. Therefore optimisation tools have to come into play.

Many attempts have been made to apply gradient based linear mixed integer algorithm to complex integrated energy systems, including economic and environmental factors as shown, for example, in the papers of von Spakovsky [9] and Valero et al. [10]. For solution spaces highly non linear and potentially non contiguous, such approaches had difficulties to identify and distinguish the global optimum from the local optima. Fortunately progress made in the late 90ies in the so-called non deterministic approaches, like those based on genetic algorithms, did provide a significant step forward to deal with these problems. Moreover, the gradual availability of cheap clusters of processors reinforced the possibilities of treating large integrated system problems. It became possible to do it without having to rely on the decomposition in sub-problems, with the associated difficulties of energy or exergy costing in order to keep the coherence of the system. Thermodynamics had reached limits, which progresses in information technology helped to bypass. The results from superstructure based mono-objective optimisation like used by Curti et al.[8], or Pelster et al. [11] demonstrated the power of these combined approaches for district heating as well as for power plants with or without CO_2 separation. Olsommer et al. [12] extended the scope by also including reliability factors with the passive and/or active redundancy that often have to be accounted for in real projects. For these studies, thermodynamics, including pinch analysis, was still a vital tool. But it was used, at first to build a coherent superstructure, and lateron for the interpretation of the results. Some genetic algorithms proved to be so powerful that no complex decomposition was needed anymore. Cost functions, which could also deal with the step functions of a library of real component of different scale could be used.

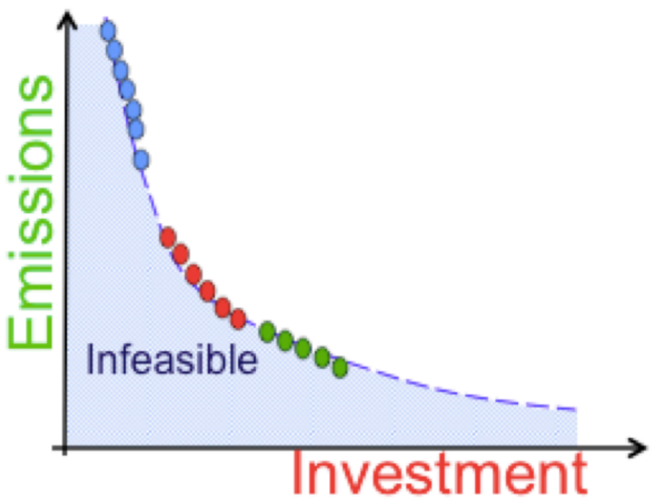

Fig. 6 Concept of Pareto curves applied to energy systems (the dotted points correspond to optimal solutions

Mono-objective optimisation with genetic algorithm was a lengthy and inefficient process. This was corrected by the emergence of multi-objective algorithm of practical relevance for the engineering of energy systems, such as the algorithm QMOO briefly described in Molyneaux et al. [13]. Knowledge gained during the computer search is kept and the results can be expressed by the optima distributed along a

Pareto curve in function of two main decision parameters, like efficiency and costs. The thermodynamicist is then better equipped to discuss the relevant trade-offs with the stakeholders.

Another way to structure the information, essentially for a faster numerical treatment, is to work with pre-optimised functions of technologies by using the concept of performance typification of those technologies that can be considered in a superstructure. This was illustrated by Li et al. [14,15] in examples of power plants, with or without cogeneration. Thus the knowledge of the purely thermodynamic performances that do not depend on economics, could be saved without repeating the calculation for each change of economic conditions.

Multi-objective optimisation was also applied by Pelet et al. [16] and coupled with a LCA data basis to optimize the retrofit of the energy system of a remote community. Here again thermodynamics was used to better define the superstructure of the integrated system including Diesel generators, Organic Rankine Cycles with thermal storage, solar thermal or Photovoltaic panels.

Accounting for reactive phenomena

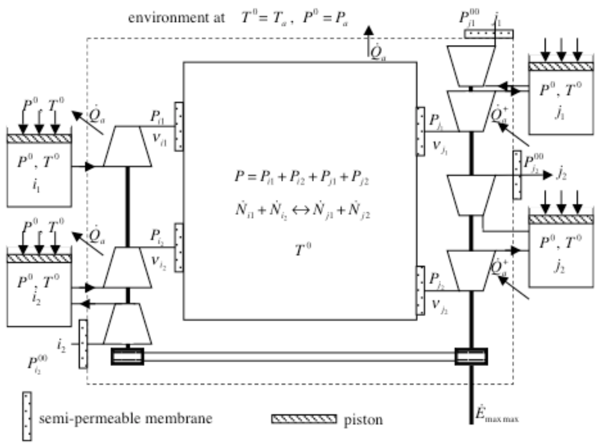

Fig. 7 Representation of the irreversible oxidation using a van't Hoff box and a mechanistic model [17]

Present energy conversion from fuel is mainly done through reactive phenomena with quasi-complete oxidation, like in the boilers or combustion chambers of power plants or of engines, without CO_2 separation. Among new concepts aiming at efficiency improvement let us cite the partial oxidation (gasification) and/or the electrochemical conversion that take place in fuel cells. CO_2 separation can be reached by either conditioning the combustible mixture directly upstream, or in the system through mass transfer in a membrane, or downstream in the tail pipe through sorption techniques. In such cases, a proper account of the exergy terms is essential to be able to define appropriate performance factors.

The representation of the reversible combustion using the van't Hoff box and turbomachines, as shown in Borel and Favrat [17], is useful (Fig. 7). Thanks to the specific semi-permeable membranes, both the components of the reactive mixture and of the oxidation products can be separated. Small changes on one side of the box could induce the change of direction of the flows, hence the reversible feature of this setup made for one fuel and one oxidizer and resulting in two products.

One additional compressor illustrates the diffusion exergy involved in the uptake of oxygen diluted in the atmosphere. Two additional turbines (or expanders), one for each oxidation product, illustrate the diffusion exergy, which could be recovered by expanding the gases to the same partial pressure they have in the atmosphere.

The cartoon representation of Fig. 8 illustrates the exergy pit showing the specific coenergy ($j= u+P_a v-T_a s$) of substances. The thermo-mechanical equilibrium dead state relative to the environment (P_a,T_a) is shown at the bottom of the pit. The physico-chemical equilibrium with the environment is represented by the lower sub-pits (physico-chemical dead states) corresponding to each of the oxidation products (here CO_2 and H_2O). Some of the different technologies for house heating are represented as well and the small characters represent the units of mass. The significant drop of exergy level of the direct electrical heating or of the simple boiler heating are clearly shown. Cogeneration and electrical heat pumps are also represented. These various representations are useful, in particular for the education of students, but also as a reminder for engineers in the practice, who too often consider exergy with scepticism.

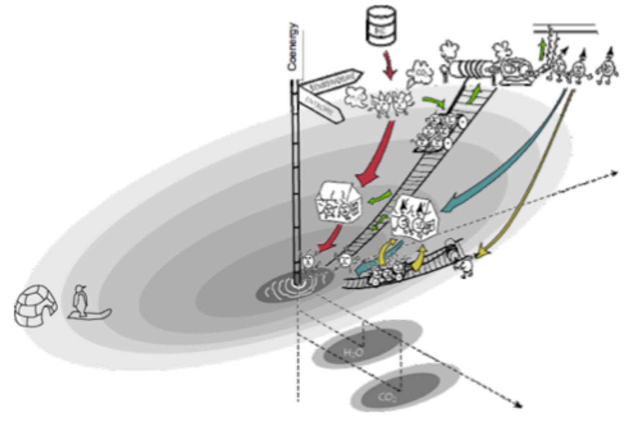

Fig. 8 Schematic representation of the exergy pit with the illustration of some technologies for heating

ANALYSIS OF ADVANCED ENERGY CONVERSION SYSTEMS

Trying to stay in the upper part of the exergy pit is partly made possible by direct electricity conversion using electrochemical phenomena. The solid oxide fuel cell (SOFC) is a good example since the solid electrolyte is also inherently a separator of the oxygen and nitrogen from the air. This feature is fully exploited in the concept developed by Facchinetti et al. [18] in which CO_2 is finally separated without exergy penalty.

The so-called SOFC-GT hybrid cycle used couples an atmospheric pressure SOFC with a sub-atmospheric Brayton cycle in which the water vapor is condensed at the lower pressure level (Fig. 9). This allows not only a lower compressor power for the compressor of the Brayton cycle, but also an easy separation of the CO_2. In such a concept, energy integration with optimized heat exchangers is a key to reaching electrical efficiencies in decentralized plants higher than 70%, which is higher than those of centralized power plants. In such a case the definition of the effectiveness (First Law efficiency) is not obvious when pure O_2 is supplied to the burner to facilitate CO_2 separation. In Equation (1) we propose a hybrid approach where the exergy of diffusion of oxygen in air is added to the denominator instead of trying to introduce an effectiveness of separation in the sense of the First Law.

$$\varepsilon = \frac{\dot{E}^{-}_{FC} + \dot{E}^{-}_{GT}}{\dot{M}^{+}_{F}\underline{\Delta} h^{0}_{i} + \dot{M}^{+}_{O2} e^{0}_{dO2}} \qquad (1)$$

The definition of the exergy efficiency is more straightforward as follows:

$$\eta = \frac{\dot{E}^{-}_{FC} + \dot{E}^{-}_{GT} + \dot{M}^{-}_{CO2} e^{0}_{dCO2}}{\dot{M}^{+}_{F}\underline{\Delta} h^{0}_{i} + \dot{M}^{+}_{O2} e^{0}_{dO2}} \qquad (2)$$

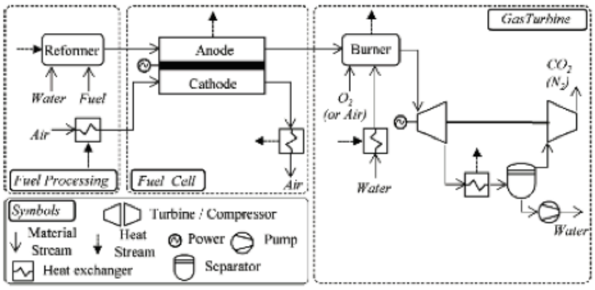

Fig.9 Concept of hybrid SOFC-GT with CO_2 separation [18]

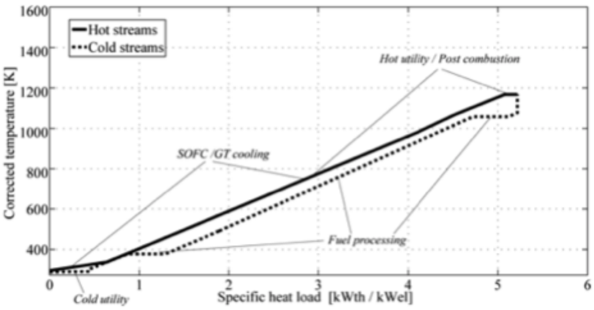

Fig.10 Composite curves corresponding to the integration of a hybrid SOF-GT unit

Energy storage

Thermodynamics is important for evaluating and optimising energy storage systems. Powertrains of vehicles concepts, including compressed air or liquid nitrogen, have been explored in recent years. Often, thermodynamics, and in particular exergy analysis, allows to quickly evaluate the potential from these forms of storage, independently from the details of the mechanical device or thermodynamic cycles used. The difference between the coenergy of the fluid contained in the tanks and the coenergy of the environment (atmosphere) gives an indication of the maximum work, which can be extracted by the drivetrains. Using this criterion Iglesisas et al. [20] compare, on an exergy basis, different drive trains and storage systems. They show how difficult and challenging it is to meet some of the claims of autonomy of compressed air or liquid nitrogen cars. However, the global picture, when comparing with standard gasoline or Diesel vehicles, should include the emissions. Then, the so-called environomic optimisation for given duties should be made using advanced algorithm.

Stationary electricity storage systems are more and more needed with the growth of wind and solar power. This application is less demanding in terms of power density and weight. Compressed air storage, often coupled with thermal storage or fossil fuel use, can be considered and have been analysed by Kim et al. [21]. The same paper also compares these concepts with concepts using thermodynamic cycles that can be operated in power mode when electricity is needed and in heat pump mode when cheap or excess electricity needs to be stored. Once again, detailed thermoeconomic optimisation for superstructure defined by thermodynamics, allows the identification of better designs as shown by Morandin et al. [22].

CONCLUSION

Thermodynamics is essential for the design and the operation of more sustainable systems. However, it is important to realize its limitations. The recent advent of powerful MINLP optimisation algorithms based on evolutionary algorithm provides the necessary complement to tackle the more holistic considerations needed for modern energy systems. The main challenge is to combine detailed thermodynamic models of processes with full system integration.

NOMENCLATURE

Symbol	Quantity	SI Unit
$\dot{E}^{-}$	Exiting exergy rate (mechanical or electrical power)	W
e	Specific exergy	J/kg
J	Coenergy (exergy of a substance)	J
j	Specific coenergy	J/kg
$\dot{M}^{-}$	Exiting mass flow rate	kg/s
$\dot{M}^{+}$	Entering mass flow rate	kg/s
$\underline{\Delta} h^{0}_{i}$	Lower heating value	J/kg_F
$\underline{\Delta} k^{0}$	Exergy value	J/kg_F
GT	Gas turbine	
SOFC	Solid Oxide Fuel Cell	

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