Pinch and Exergy Analyses within Process Simulation Software to Enhance Process Energy Efficiency

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Abstract:

Pinch analysis [1] is a well-known methodology, commonly used in the industry to optimize process energy consumption. Specific developments have been done in a commercially-available process simulator, ProSimPlus® Energy [2] to help process engineers in their daily work. Composite curves, characteristics of cold and hot streams of the process are automatically generated and an appropriate heat exchanger network is proposed by the software, depending on several constraints provided by the user. Energy management specific unit operations (heat pumps, ORC, boilers…) were also added in the library of the software to help the user to quickly analyse the impact on energy efficiency for this equipment. To tackle the challenge of process energy management enhancement, exergy analysis has been shown by Kotas [3] to also be a useful tool that exploits the concept of energy quality to quantify the portion of energy that can be practically recovered. Unfortunately, in contrast to enthalpy, this concept is less familiar to chemical engineers and can be rather difficult to handle. In particular, this physical quantity is rarely implemented in process simulators. To make exergy analysis more understandable and to demonstrate its value for the analysis of the energy efficiency of a process and its utilities, a fully-automated exergy analysis tool has been developed and integrated in ProSimPlus® Energy [3], [4]. The software combines these approaches, allowing the user to propose the most efficient process taking into account all of the defined constraints.

Keywords:

Energy efficiency, exergy analysis, ProSimPlus Energy, pinch analysis, simulation software.

1. Introduction

Process energy efficiency typically involves, among other things, an optimization of the utilities production and the process unit operations. Here we focus on the optimization of the process unit operations using two complementary methods: the Pinch method and the exergy analysis, to reduce the process energy consumption.

These two methods are implemented through process modelling carried out in the ProSimPlus process simulation software. The Pinch method and the exergy analysis are made possible by simply adding a dedicated unit operation into the process simulator, which then automatically performs the energy efficiency calculations.

The Pinch unit operation calls a fully-automated method that carries out the energy analysis (minimal requirement calculation for hot and cold utilities, calculation of the maximum quantity of recoverable energy) and that creates hot and cold streams, which become the input data for Simulis Pinch, a software that automatically creates heat exchanger networks.

The exergy analysis unit operation carries out the exergy balance for each unit operation of the process, as well as the global exergy balance. The exergy calculations include both the physical exergy, and also the chemical exergy.

These two methods are complementary, where the Pinch technology is a systematic and well-known method, while the exergy method provides improvements when the Pinch method may fail, in particular for processes under pressure, or for separation processes that require more than a single stage, i.e., a cascading separation system.

2. Process modelling

2.1. Collecting data

Data collection is a prerequisite for an accurate plant energetic optimization: erroneous information on hot and cold streams will systematically lead to wrong process heat integration. Even if the heat integration methods can be considered as well-known, the fundamental risk is upstream, when stream characteristics are obtained, and data collection is the major step of the study. During this step, engineers identify which streams are to be cooled, heated, evaporated or condensed and then extract, from all of the available information, only the characteristics which are key to the heat integration analysis. Streams with too much uncertainty on temperature or with fluctuating temperature have to be eliminated, hot and cold utilities have to be well identified and their consumption for each equipment has to be compared with the global production of the site. Engineers have also to pay attention to other potential sources of error: batch operations, heat integration networks where the coupling of hot and cold process streams production in the same equipment is adversely affected by different ways of operating the plant, contractual restrictions, equipment technical and operating limitations…

Process simulation is a very good way to improve the quality of the energetic optimization, and can be used to provide the engineer with missing information. The simulation model will also be used to test the heat integration network, change of operating conditions, process modifications, pinch value influence... Steady state process engineering simulation software are tools that perform mass and energy balance calculations for all the operating units of a continuous process in steady state operation. They include models based on first principles and allow the analysis of the behaviour of a complete process. The main functions of these software are the calculation of:

- all process stream characteristics (partial flowrates, temperature, pressure but also all of the physical properties);
- performance of the process equipment;
- all process data required for equipment sizing;
- data required for energy analysis of a process (pinch or exergy analysis).

Today, such software are widely used by process engineers in the design of new units as well as in operations of existing plants for process optimisation, units troubleshooting or debottlenecking, plants revamping, performing front-end engineering analysis… They are used in nearly all process industries: chemicals, pharmaceuticals, petrochemicals, oil and gas, refining, specialty chemicals… Even as similar unit operations (reactors, distillation or absorption columns, heat exchangers, pumps and turbines…) are commonly used in all of these industries, the different chemical mixtures involved may have completely different behaviours. Thus, in addition to a complete unit operations library, process simulation tools have to embed thermophysical properties and phase equilibria calculation servers able to tackle the challenge of correctly representing these mixtures of components.

2.2. Thermodynamic modelling

ProSimPlus® Energy includes the thermophysical properties and phase equilibria calculation server Simulis® Thermodynamics, which generates highly accurate pure component and mixture properties (thermodynamic, transport, compressibility…) and fluid phase equilibria. To obtain reliable thermodynamics calculations, one needs first to have accurate pure component properties. Based on the AIChE's DIPPR database [5], Simulis® Thermodynamics provides access to a property database of more than 2300 pure components. For each component, up to 125 constant properties (molecular weight, critical coordinates…) and 16 temperature dependant properties (vapour pressure, enthalpy of vaporization…) are available. All of these properties can be edited, plotted, modified and Simulis® Thermodynamics makes it very easy to create new components and private databases, offering pure component property estimation methods and experimental data fitting services. For multi-components systems, a major problem encountered in chemical engineering lies in the calculation of phase equilibria and thermodynamic properties (enthalpies, entropies…). Fluid phase equilibria can be calculated using two different methods. A first way of approaching the problem consists in applying to both phases different models: the liquid phase fugacities are calculated from a reference state, which is characterized by the pure component in the same conditions of physical state, temperature and pressure, where the laws of the ideal solutions are corrected by using a model of free excess enthalpy, also called an activity coefficient model (NRTL, UNIQUAC, UNIFAC…). The gas phase fugacities are calculated using an equation of state (ideal gas, SRK, PR…). These methods are used to represent the heterogeneous nature of the considered system and are classically called "heterogeneous" methods. Their application is typically for the domain of low pressures and it is important to note that they do not satisfy the continuity existing in the critical zone between the vapour state and the liquid state. The second way of approaching the problem, grouping together the so-called "homogeneous" methods, applies the same model to both phases that are present. These "homogeneous" methods are generally an equation of state, in order to ensure continuity at the critical point. For example, the equations of state with their classic mixing rules (SRK, PR, LKP…) belong to this second category. However, the domain of application of these models is limited to non-polar or few polar systems. By integrating the excess enthalpy models into the mixing rules of the equations of state, authors managed to combine these two approaches (MHV2, PSRK, NRTL-PR…). This type of model is usually called a "combined model", which is in fact a homogeneous approach with complex mixing rules. Moreover, some specific models were also developed for some domains of application: electrolytic mixtures, aqueous solutions of strong acid, formaldehyde… Simulis Thermodynamics is a unique software that includes all of the above methods and approaches.

3. Exergy analysis

3.1. Description

Exergy is based on simultaneous use of the first and second laws of thermodynamics and can be defined [6] as the maximum amount of work that can be obtained when a system is brought to thermodynamic equilibrium with the environment in terms of temperature, pressure and composition through reversible processes. For the calculation of the exergy of streams, the environmental state, which refers to a state where the conditions of mechanical and thermal equilibrium between the system and the environment are satisfied, is chosen as twenty five Celsius degrees and one atmosphere. The standard chemical exergies of each compound tabulated by Rivero et al. [7] are used. For a given system, the exergy balance is given by the following equation, which, contrary to heat and mass balances, considers internal losses:

$$B_{in}^{matter} + B_{in}^{Heat} + B_{in}^{work} = B_{out}^{matter} + B_{out}^{Heat} + B_{out}^{work} + I$$

with:

$$B^{matter} = [h(T,P,z) - h(T^{00},P^{00},z)] - T^{00}[s(T,P,z) - s(T^{00},P^{00},z)] + \sum_{1}^{N_\varphi} \omega_\varphi \left(\sum_{i}^{N_c} z_i \left[b_i^{0\varphi} + RT^{00} \ln\left(a_i(T^{00},P^{00},z_i)\right)\right] \right)$$

$$B^{Heat} = Q.\left(1 - \frac{T^{00}}{T}\right)$$

$$B^{work} = W$$

The exergy balance can be refined by making the distinction between waste streams (directly rejected to the environment, i.e. external losses) and utilized streams (with a well-defined use, i.e. product streams). Both internal and external losses are sources of inefficiency in a process and one way to improve the energy efficiency of the system is to reduce these losses. Thus, a clear distinction between waste and used streams is required when performing the exergy analysis. From this exergy balance, several diagram types can be used and different performance indicators can be defined.

3.2. Implementation and use in ProSimPlus® Energy

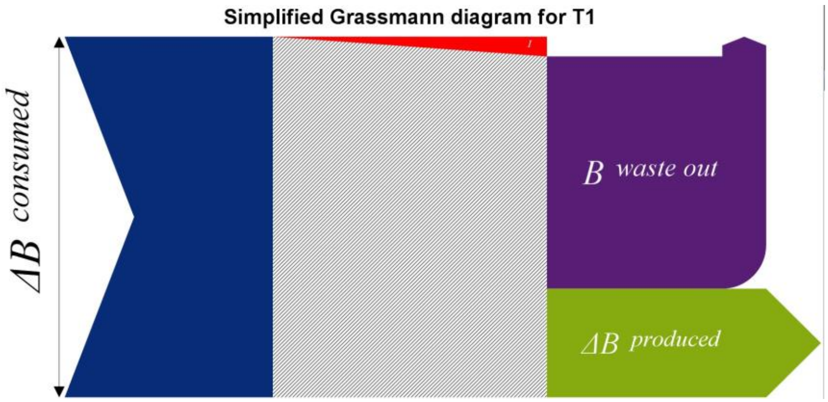
The exergy analysis unit operation is simply added to the simulation process flowsheet, to indicate that the exergy balances will be calculated.

The user provides the data necessary for the analysis, such as:

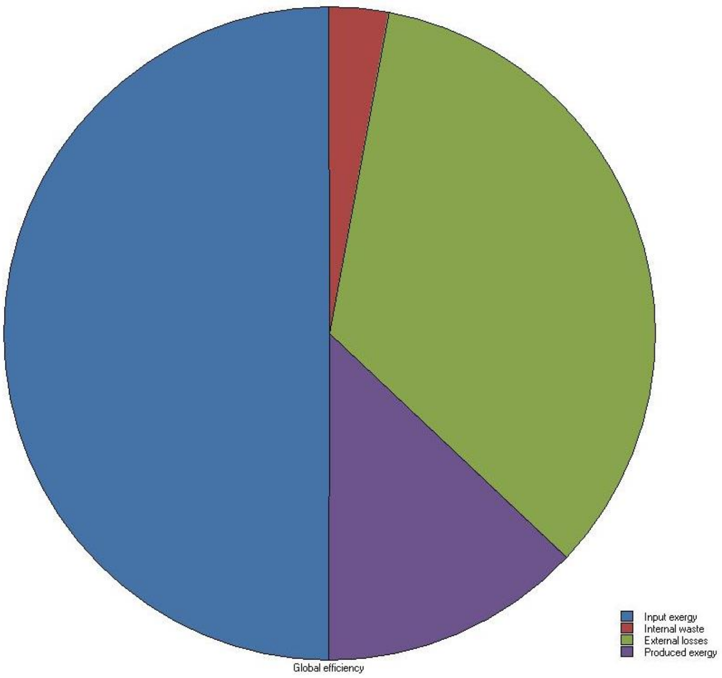
- ✓ the balance area (unit operations to take into account)
- ✓ the calculation type (physical exergy only, or chemical AND physical exergy)
- ✓ the waste streams of the process (to characterize the exergy losses)

The exergy balance calculations are carried out at the same time as the classical material and energy balances of the ProSimPlus simulation.

In terms of results, the unit operation shows the exergy balances of each unit operation, using tables and charts, such as the Grassmann diagram below:



For each unit operation, but also for the whole process, exergy conversion balances appear in pie charts, as shown below:



4. Pinch analysis

4.1. Energy diagnostic

Pinch analysis allows for the determination of the minimum required process utilities consumption. A dedicated pinch analysis unit operation is used in ProSimPlus to carry out energy integration calculations with the pinch method. Based on a chosen pinch that is acceptable for the whole process (minimum temperature difference between the hot streams and the cold streams), the minimum utility needs (hot and cold) are calculated as well as the maximum heat quantity recoverable by energy integration. The pinch analysis unit operation also plots the hot and cold composite curves, as well as the grand composite curve.

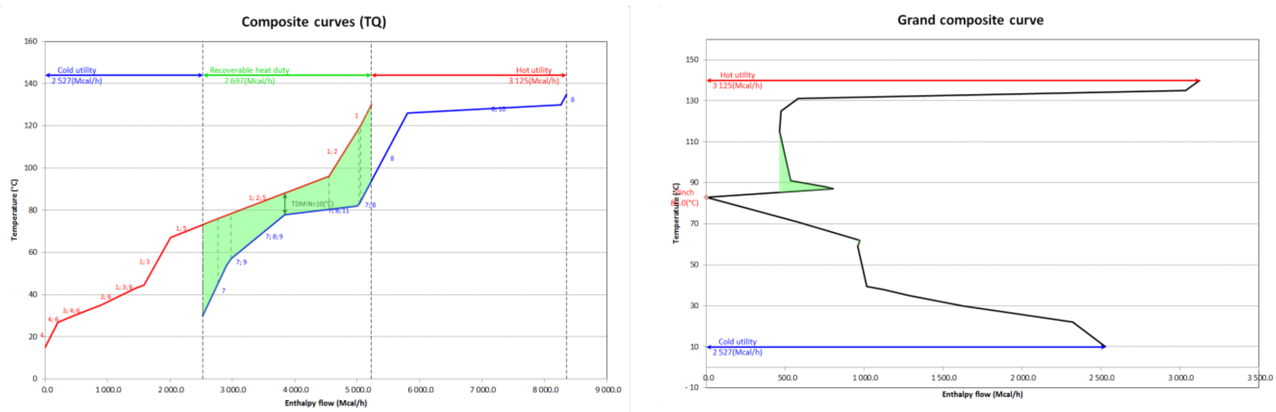


Fig. 1. Composite curves resulting from pinch analysis

The pinch analysis unit operation interacts directly with the other relevant unit operation on the process flowsheet, i.e., those unit operations where a heating or a cooling occurs (boilers and columns condensers, heat exchangers, flashes, reactors...). To take maximum advantage of the pinch analysis unit operation, the following are important to consider during the modelling step:

- Mixers: according to the choice made by the user, the consequences of the heating and the cooling associated to the mixing of streams can be, or not, taken into consideration. In particular, when streams with very different temperatures are mixed. In this case, the implicit cooling of the hottest streams and the implicit heating of the cool streams will automatically be taken into account.
- Pressure drop issues: the unit operations in which both a pressure and a thermal effect occur must be used with care if a pinch study is planned. Indeed, antagonistic effects may appear and may lead to the creation of an outlier stream. For example, for a flash with a significant pressure drop leading to an important temperature drop in the flash, where a slight heating is applied to reduce this temperature drop. For this unit operation, heat is provided, yet the temperature decreases between the inlet and the outlet. The question is the following one: is the stream to take into consideration hot or cold? In such situations, the stream is not taken into consideration and a warning message appears. For the unit operations that give the option to define a pressure drop, this possibility may be used to describe the unit operation pressure drop, but not the pressure drop of a valve located upstream of the unit operation (in particular, for the “simple heat exchanger”, or the “Coolers/Heaters” unit operations defined in the ProSimPlus Energy software). In the same way, to represent the effective pressure drop for the flashes, it is advisable to model this with a valve upstream of the flash for the process simulation.
- Existing heat exchangers: if one wants to keep the existing heat integration exchangers, it is possible to specify that the streams have been integrated, and then they will not be taken into account in the energy diagnostic.
- Process outlets: they can also be heat sources (hot effluents that may possibly be cooled) or on the opposite, cold sources. However, it is necessary to define a cooler/heater on these streams to indicate if an energy recovery is possible or not on this stream.
- Phase change: if a stream changes partly or totally its physical state, the isobar heating capacity of this stream varies greatly along the heat exchanger. It is possible to linearize this variation in order to find a mean isobar heating capacity or to segment it according to the physical states. This segmentation makes it appear as if there are up to three different streams for the same stream. For instance, for a liquid vaporization, the three segments apply to:
  - The liquid heating to the bubble point;
  - The state change to the dew point;
  - The steam superheating.

The pinch analysis calculation can be done after the simulation of the whole process in order to simply achieve an energy balance on the process. For a more sophisticated analysis, it can also be carried out in “On-Run” mode in order to do case studies on some process parameters or to use the pinch unit operation results as a criterion or constraint for an optimization issue.

4.2. Heat exchanger network

The energy integration concept is used to arrive at the optimal synthesis of a heat exchanger network that achieves the maximum energy recovery, i.e. to reach the process operating point with the minimum amount of required energy. This synthesis is subject to construction rules (division of the problem into two sub-problems, one below and the other above the pinch temperature). The ideal point may not be simple to reach (due to partial exchanges on streams, stream divisions…), and the number of heat exchangers needed may be significant. Optimisation tools can help to determine the optimal structure of the heat exchanger networks using MINLP-type algorithms. Even though these tools are powerful, their calculation time can be very long, and their convergence on an industrial scale is not guaranteed.

The approach developed by Simulis Pinch is more pragmatic: the aim is to propose very quickly the right solutions with a limited number of heat exchangers. The method is not an "optimal" method in the mathematical sense of the term, as it systematically aims to exchange the maximum power between two streams. If a hot stream and a cold stream can exchange heat, the algorithm searches for the possible couplings allowing the exchange of the maximal thermal power under certain limitations or "boundary conditions". Between two streams (cold stream and hot stream) that can exchange heat, the combination of the achievable heat exchanges is reduced or limited (maximum of 3 possible couplings between a hot and a cold stream). For a problem with HSN hot streams and CSN cold streams, the number of exchanges is then less than or equal to 3*HSN*CSN, where HSN is the number of hot streams and CSN is the number of cold streams.

The first phase consists in determining the exact number of achievable heat exchanges between the matched hot and cold streams. Each possible exchange is characterized by a certain number of attributes, e.g. the power exchanged, the efficiency…

Efficiency for the exchange is defined by the following formula:

$$Eff = \frac{MRE\_AF + P}{MRE\_BE}$$

where:

P	power exchanged by the coupling considered
MRE_BE	Maximum amount of Recovery Energy BEfore the coupling is considered
MRE_AF	Maximum amount of Recoverable Energy AFter considering the coupling, i.e., it is the MRE obtained by updating the streams with the assumption that the coupling has been carried out.

It has to be noticed that if all the couplings selected have an efficiency equal to 1, the approach is by definition optimal. In other words, the choice of an exchange does not deteriorate the initial recovery potential.

The Simulis Pinch operation algorithm for the synthesis of the heat exchanger network is described in Fig. 2.

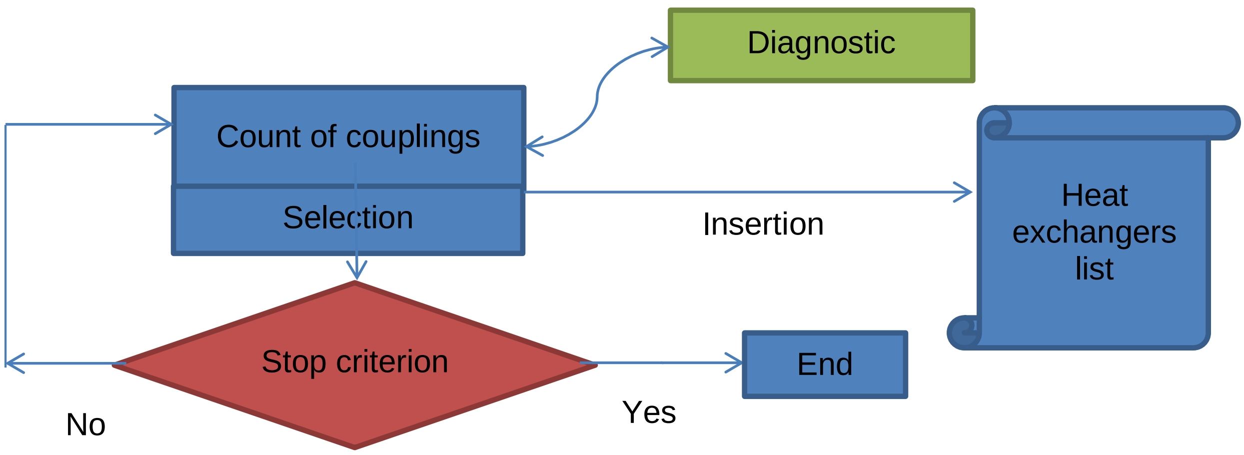


Fig. 2. Simulis Pinch operation algorithm

The counting method provides an exhaustive list of the achievable heat exchanges. In addition to the thermodynamic criteria, the user can specify constraints that will allow only the pertinent exchanges, e.g. minimal power exchanged, a minimum recovery percentage (compared to the initial MRE)…

The selection method consists in selecting an exchanger among all the achievable heat exchanges. Several selection criteria are possible, e.g. maximal heat duty exchanged, maximal efficiency, HeatDuty*MaximalEfficiency… The user can also manually select the heat exchangers at each iteration.

Finally, different stop criterion/criteria can be selected, e.g. maximum number of exchangers reached, recovery percentage reached (% compared to the initial MRE)…

The list of proposed exchangers is the main result of the synthesis and all the selected exchangers are listed with the required information needed to estimate their cost.

5. Specific unit operations and economic evaluation

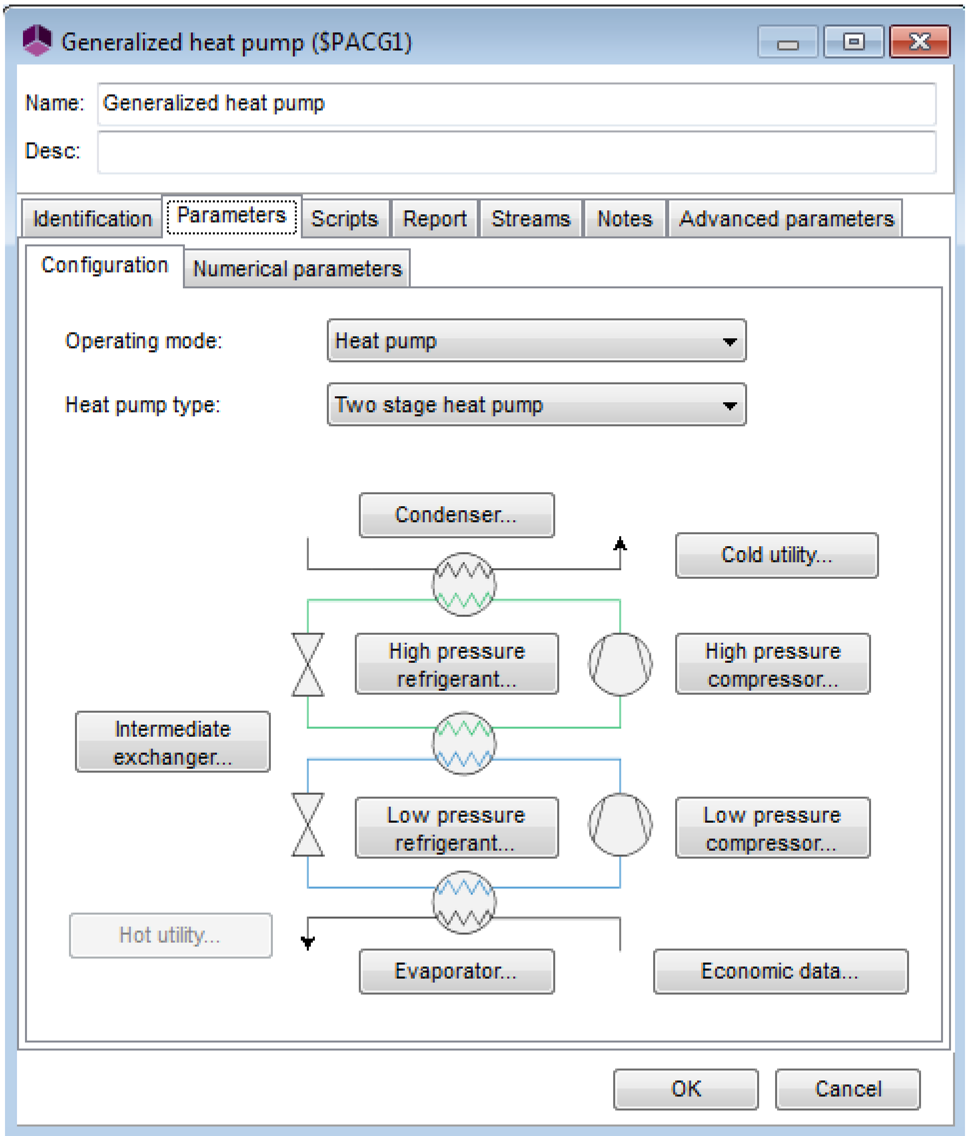
With either the Pinch method or the exergy analysis, the investigations may lead to a consideration of the implementation of specific unit operations to optimize the energy integration of the process.

Obviously, the time of return on investment cannot be compared with the heat exchangers proposed by the automatic synthesis of the heat exchangers networks coming from the Pinch analysis. Nonetheless, in some cases, the energy gain associated with the implementation of a thermal unit operation is such that the time of return on investment may be reasonable and worth considering.

In order to test the insertion of such complex unit operations, specific macro-unit operations have been developed in ProSimPlus:

- Simple heat exchanger
- Two-stage or side-injection heat pump
- Rankine cycle
- Gas engines
- Gas turbines
- …

These macro-unit operations are easily inserted into the simulation process flowsheet. An example of the heat pump unit operation is shown below:



In order to test the economic interest of such an investment, a process economic evaluation unit operation is also available in the latest version of ProSimPlus. This unit operation provides a full economic analysis of the process (operating, maintenance and investment costs). For example, it can be used to calculate the time of return on investment related to the addition of a unit operation, such as a thermal unit operation.

6. Perspectives and conclusions

The two energy balances described above (Pinch analysis and exergy balance) are now easily accessible in the ProSimPlus simulation environment. Engineers at all levels (both senior and junior!), can now use these tools to easily carry out expert analysis and to propose energy improvements for their processes.

Prospects for an improvement are of two kinds:

- ✓ The exergy analysis provides a focus on the irreversibilities of the process, but does not yet provide concrete proposals to the user. The work that remains consists in devising methods to guide the user to formal solutions (in an automated way), or at least, to bring attention to the ideas that are most important to consider for future investigation.

- ✓ Both methods exist in ProSimPlus, but it would make more sense to combine them in a global approach, in order to fully automate the energy efficiency analysis for the process. Work is underway to implement such a methodology.

To conclude, the work performed helped to achieve a significant headway in the areas of decision-making support and fully automatized energy efficiency analysis, from a simple simulation of the process. The ideal method that combines both approaches in a systematic but fully automated approach still remains to be formalized.

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Nomenclature

a	molar activity
B	exergy flow, kW
b	molar exergy, kJ/mol
h	molar enthalpy, kJ/mol
I	irreversibility or internal losses, kW
Nc	number of components
$N\varphi$	number of phases of a stream
P	absolute pressure, atm
R	universal gas constant, kJ/mol K
s	molar entropy, kJ/mol K
T	absolute temperature, K
W	power, kW
z	global molar composition of a material stream

Greek symbols

ω	molar vapour fraction of a stream

Subscripts and superscripts

00	environmental state
φ	related to a phase

References

[1] Linnhoff B., Thermodynamic Analysis in the Design of Process Networks [dissertation]. Leeds, UK: Leeds University; 1979

[2] ProSim web site – Available at:< http://www.prosim.net/en/index.php> [accessed 20.01.2015].

[3] Kotas T. J., The exergy method of thermal plant analysis. Butterworths; 1985

[4] Ghannadzadeh A., Thery-Hetreux R., Baudouin O., Baudet P., Floquet P., Joulia X., General methodology for exergy balance in ProSimPlus® process simulator, Energy 2012; 44: 38-59

[5] Rowley R. L., Wilding W. V., Oscarson J. L., Yang Y., Giles N. F., DIPPR® Data Compilation of Pure Chemical Properties, Design Institute for Physical Properties, AIChE (2011)

[6] Szargut J.,Morris D.R., Stewart F.R., "Exergy Analaysis of Thermal Chemical and Metallurgical Processes". New York: Hemisphere Publishing Corporation; 1988

[7] Rivero R., Garfias M., "Standard chemical exergy of elements updated", Energy 2006; 31(15): 3310-3326