# THERMOPTIM®

# **GETTING STARTED**

Gas turbine example

**JAVA VERSION 1.5** 

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## **GETTING STARTED**

This document intends to allow a user to get quickly used to THERMOPTIM (in less than half an hour), by using the basic elements of the software. Subsequently he or she will be able to deal with more complicated problems, especially those making use of nodes or heat exchangers.

You will find additional information in Thermoptim's reference manuals available through the Help menu of the simulator.

The following points will be addressed:

- presentation of some basic notions which must be understood before using the software
- analysis of a simple example: the calculation of a simple gas turbine.
- plot of the cycle on an entropic interactive chart.
- analysis of more complex examples: the steam injection gas turbine and a two stage regenerative gas turbine with intercooling and reheat

## **Basic notions**

The study of a thermodynamic system can be divided into five main tasks:

- 1) the analysis of the structure of the system under investigation, which identifies its main components and their connections: for instance, a thermal machine consists of heat exchangers, compressors, turbines or expansion devices, combustion chambers...
- 2) for each component, the identification of the thermodynamic fluids which are used: for instance, the fluid compressed in a gas turbine is air, which burns with a fuel in the combustion chamber. The resulting flue gases expand in a turbine.
- 3) for each component, the selection of the kind of system to be considered (open or closed): for instance, the study of the compression in a piston compressor must be made in closed system, while that of the expansion in a gas turbine is to be made in open system.

Let us recall that a closed system (respectively an open system) is characterized by the absence (respectively the existence) of mass transfer through its boundaries.

- 4) the description and the calculation of the processes undergone by the different fluids in the components, taking into account their interconnections.
- 5) the calculation of the overal balance of the system analysed.

THERMOPTIM has been designed in order to facilitate the calculation of complex thermodynamic systems, but it cannot replace the user for making the detailed analysis of the system under investigation, which corresponds to the three first steps above.

Before entering his project in the software, the user must have made this analysis. Otherwise there is a risk that the description will be done improperly.

Once this analysis is made, each component can be easily defined with the points, processes, nodes and heat exchangers described below, which together form a project.

THERMOPTIM makes use of four kinds of **substances**: pure ideal gases, composed ideal gases, condensable vapors (which are pure substances), and ext ernal substances. Perfect gases are ideal gases whose specific heat is independent of the temperature. A given substance may exist (under different names) as an ideal gas and a condensable vapor.

The substance can be pure, in which case its properties are predefined in the software, or it can be compound. In the case of gases, the user has to define the composition from the other gases present in the database, by indicating for each of them, its name and its molar or mass fraction. Properties of the composed substance are then determined from those of its constituents.

A **point** designates a particle of a substance and allows the user to define intensive state variables: pressure, temperature, specific heat, enthalpy, entropy, internal energy, exergy, and quality. A point is identified by its name and the name of the associated substance. To calculate it, one may either:

- enter the values of at least two state variables, generally its pressure and temperature for open systems, and its volume and temperature for closed systems.
- automatically calculate them by using for instance one of the processes defined below.

**Processes** correspond to thermodynamic evolutions undergone by a substance between two states. A process associates therefore two points such as defined previously, an inlet and an outlet point. Moreover, it indicates the mass flow rate involved, and therefore allows one to calculate extensive state variables, and notably to determine the variation of energy involved in the course of the process.

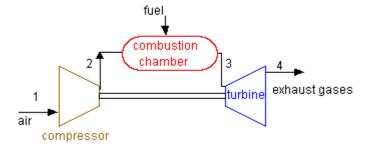
Processes can be of several types: compression, expansion, combustion, throttling, heat exchange, water vapor / gas mixtures (the latter includes six different categories of evolutions), and external ones. According to each case, various characteristics of the process have to be specified, for example, in a compression, its isentropic or polytropic efficiency.

A cycle can thus be described as a set of points connected by processes. To the extent that the mass flow rate fluid is the same in all the evolutions, processes and points are sufficient. If this is not the case, it may be necessary to at least partially describe the network of the fluids involved. Then the first elements to define are the network **nodes** which are described in the documentation.

# Calculation of a gas turbine

A gas turbine burning natural gas without dissociation sucks 1 t/s of air at 15 °C and 1 bar and compresses it at 16 bar in a 0.85 polytropic efficiency compressor, and expands the burnt gases in a 0.85 polytropic efficiency turbine. The temperature of the gases at the turbine inlet is 1150 °C.

#### simple gas turbine

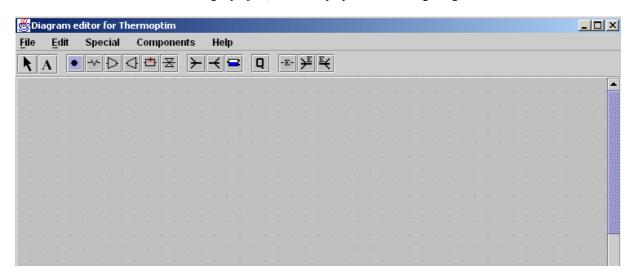


The objective is to model the gas turbine and calculate its efficiency.

## Creation of the diagram

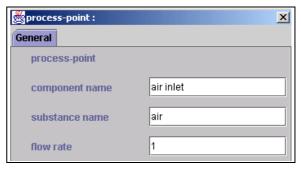
#### Placement of the components

Run THERMOPTIM without loading a project, which displays the following Diagram Editor screen:



On the palette appear the components available: processpoints, exchange, compression, expansion and throttling processes, mixers, dividers, separators, external sources and external components.

The gas turbine block diagram clearly shows which components should be selected: the compressor , the combustion chamber , and the turbine, which is an expansion device .



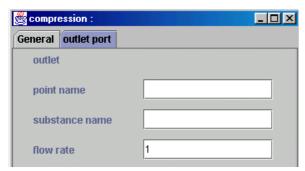
Furthermore, we shall add a fuel inlet, an air inlet and a burnt gas outlet, all represented by process-points. The two latter ones are not compulsory, but they allow to better display the cycle as we shall see later. A process-point mainly allows to associate a flow-rate to a point.

Begin by selecting a process-point component on the palette and place it on the editor by clicking the crosshair cursor at the appropriate location. The property editor is opened. For process-points, it is particularly simple, as the component's name is the same as those of the inlet and outlet points (if you wish you may however choose different names for the point and for the component). Enter its name (air inlet), then that of the subsatnce (air), and the flow rate (1 t/s).

To validate and close the property editor, click on "Apply". The component appears on the diagram editor, with its name below it and the outlet point above on the right.

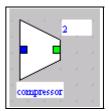


Select then the compressor, name it "compressor", then click on the "outlet port" tab:



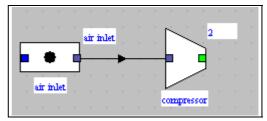
THERMOPTIM-Java Getting Started

Name the point "2". The substance name (air) will be automatically propagated from the upstream component (air inlet) when you connect it to the compressor. To validate and close the property editor, click on "Apply". The component appears on the diagram editor.



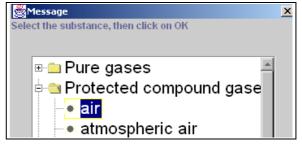
#### **Connection of the components**

To connect the two components, click on the outlet port of the process-point. The cursor becomes a crosshair and a line extends from the port if you drag the cursor. Drag the cursor to the inlet port the destination component (the compressor) while keeping the mouse clicked, and release the mouse. A link is established and the substance name of the compressor is updated, as you can check by displaying the component properties (menu Edit/Show properties or key F4).



To enter the substance name, you may either type it if you know it, or get it from the list of available substances which can be displayed by double-clicking in the substance name field and expanding the type folder (here expand Protected compound gases then click on « air »).

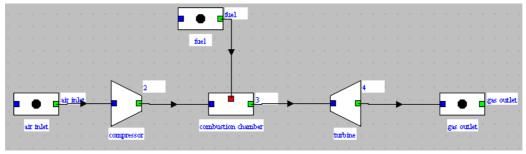
You can now create the other elements of the cycle, namely two process-points corresponding to the fuel and the gas outlet, one combustion chamber (outlet



point 3), and one expansion component corresponding to the turbine (outlet point 4). It is not necessary to select the substance in those components, except for the combustion chamber, as it will be automatically propagated when the components will be connected.

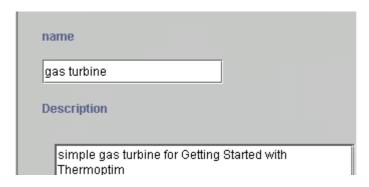
The fuel substance is chosen from among the fuels in the data base, for instance "Montoir natural gas", and the burnt gases substance can be either chosen from among the non protected gases or created as a new gas (you just indicate the name you wish and Thermoptim automatically creates it).

When you have connected them (you connect the fuel to the red port of the combustion chamber), you obtain a diagram which looks like this, which can be refined by using the keyboard arrows to better align the



components.

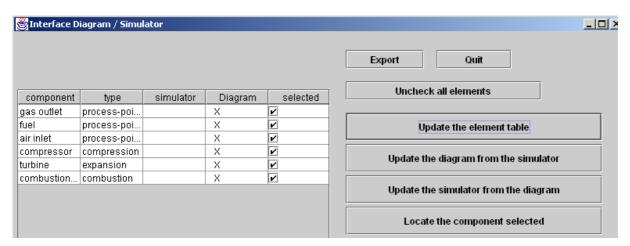
At this stage, the diagram definition is made. In order to facilitate the management of your archives, you may give it a name and a short description which can be subsequently displayed in the diagram libraries (item Description of menu File):



Save the diagram file as "GT.dia" by selecting item "Save As" of menu File of the Diagram Editor.

#### Transfer to the simulator

The diagram is now completed and you may transfer it in the simulator. To do that, select item "Interface Diagram/Simulator" in menu View, which opens a new frame. Click on button "Update the element table":

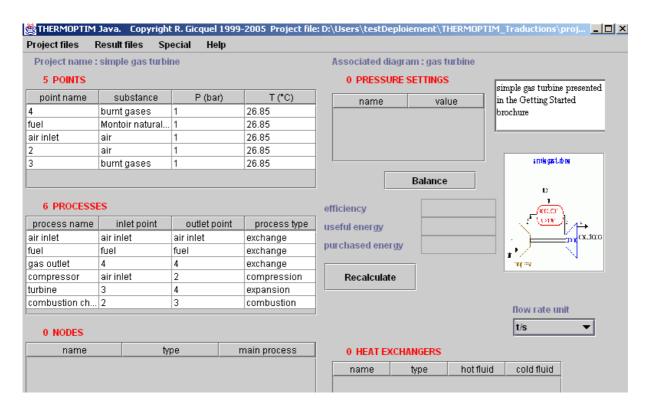


The different components you have created appear in the table. A "x" in the "simulator" or "Diagram" column indicates that the element belongs to this environment (here all elements belong to the diagram, and none to the simulator).

Click the on button "Update the simulator from the diagram". As the project has not yet been named, the following message is prompted:

Name the project and click on "OK". The different points and processes are then created.





The whole structure of the project is created, but the detailed settings have still to be made (by default, all points have the same pressure (1 bar) and temperature (26.85  $^{\circ}$ C = 300 K)). First, select the flow rate unit in the list located in the lower right part of the screen (t/s).

## Definition of the points

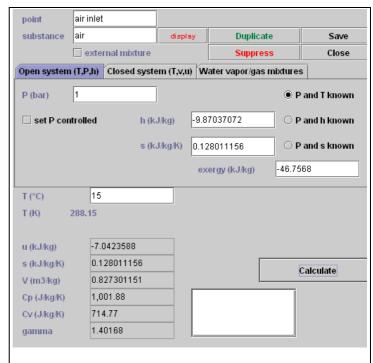
To define point 1, double-click on it in the table or on the link between the air inlet and the compressor. Then enter the state of the substance at this point. Its pressure is known (1 bar), as well as its temperature (15 °C).

Point 1 is now defined. Similarly define the other points.

For point "2", indicate the only information known about it, its pressure p = 16 bar. In the current definition state of the cycle, both its temperature and its enthalpy are not yet known.

For point 3 enter 16 bar and 1150 °C. However, as the composition of the burnt gases is not known, you cannot calculate it.

The fuel can be defined as being at the pressure 20 bar and the temperature 15 °C. It can be calculated.



The last point to define is point 4. Only its pressure is known: 1 bar.

## Definition of the processes

To define the processes, open their frames by double-clicking in the process table or in the diagram editor.

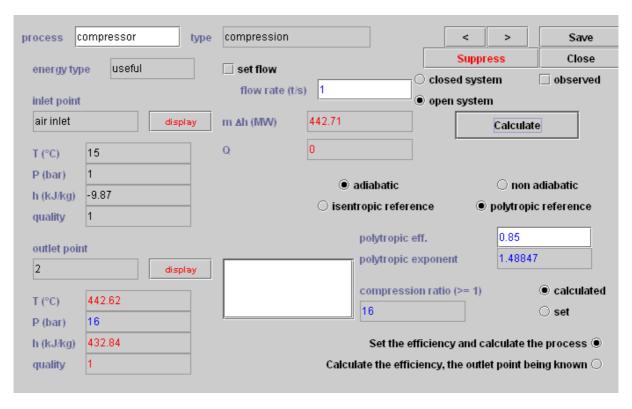
Open the compression screen. By default, its energy type is "useful", which is correct, as this energy is taken from the turbine shaft (see Reference Manual para. "Process screen").

You have the choice between different modes of compression: adiabatic or not, with an isentropic or polytropic reference. For open systems, the compression ratio is that of pressures, for closed systems, that of volumes. It can be either calculated, as it is the case here, where the outlet pressure is known, or set, in which case the latter is calculated from the inlet pressure.

You can select two calculation modes. In the first case ("Set the efficiency and calculate the process"), the outlet point state is calculated from that of the inlet point and the efficiency value. For the second one ("Calculate the efficiency, the outlet point being known"), the efficiency value is calculated on the basis of both inlet and outlet points considered as set. Choose here the first case, which is selected by default.

Make your selection by clicking on the appropriate checkboxes, and enter the efficiency value (isentropic or polytropic) for compression. Choose here: adiabatic, polytropic efficiency equal to 0.85, and open systems.

Click on "Calculate". Automatically, the state of point 2 is calculated, as well as the corresponding enthalpy variation. The value of the compression ratio is displayed (here 16).

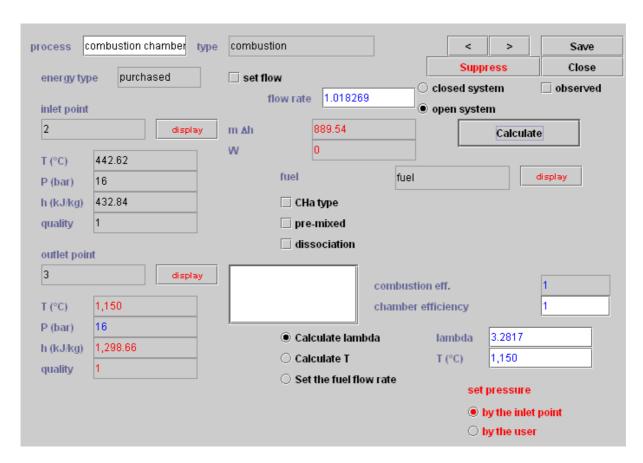


Save the form.

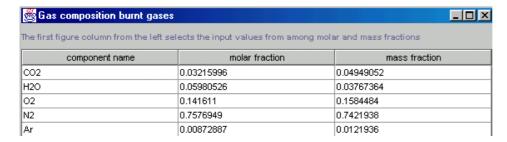
The combustion calculation is more complex: the combustion temperature is set to 1150 °C. Enter this value in the lower right field and select "Calculate lambda".

As the dissociation is not taken into account, there is no need to define its rate nor to enter the quenching temperature. In addition, as we neglect the thermal losses of the chamber, its efficiency is set to 1.

The air factor lambda is calculated, as well as the fuel flow rate, automatically updated in its process-point, and the chamber flow rate is displayed.

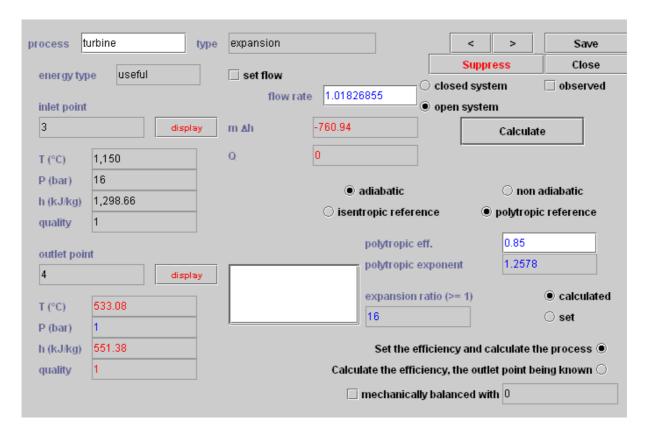


The combustion gas composition is determined. It can be displayed by clicking the red button "display" located to the right of the substance name in the point 3 screen:



Save the form.

The expansion process can now be calculated (here polytropic of efficiency 0.85). The exact state of point 4 and the enthalpy of expansion are then determined:



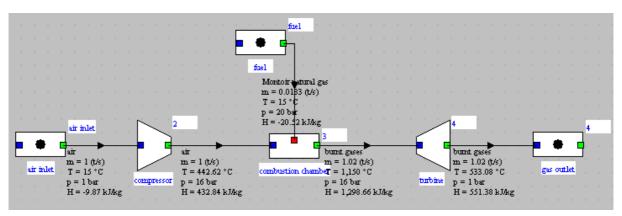
Save the form.

At this stage, the cycle is totally defined, and you can calculate the balance by clicking on the "Recalculate" button in the simulator screen.

efficiency 0.358
useful energy 318
purchased energy 890

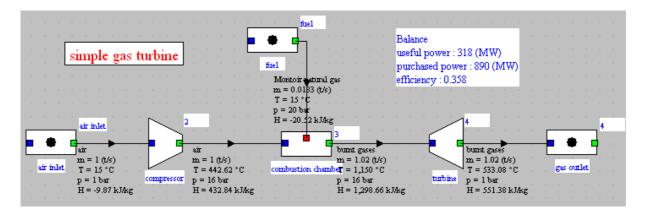
The energy purchased, useful energy, and the efficiency of the cycle are then determined.

The state of the various cycle points can also be directly displayed on the diagram (item Show values of menu Special or key F3):



This is why we have introduced the two process-points "air inlet" and "gas outlet": they allow to show the state of the corresponding points.

In order to improve the appearance on the diagram, you can add a text, as well as a "Balance" type component which allows you to display the balance values (the latter component only appears in menu "Components").



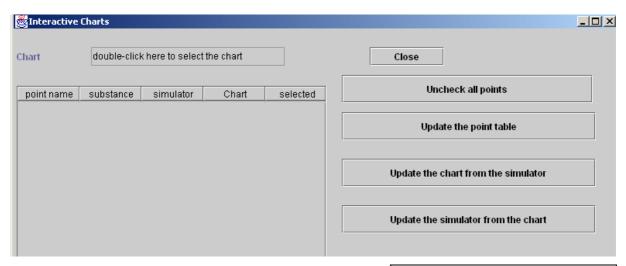
Lastly save the project file, for instance as GT.prj.

## Cycle plot

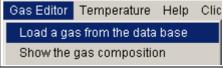
The cycle can now be plotted in the Interactive charts in the following way. In the simulator frame, select item Interactive Charts of menu Special, or type Ctrl C.



The following screen appears:



Double-click in the field labeled "Chart" and select "Ideal gases" from among the proposed list and the interactive chart frame is shown. If the substance selected is not air, load it through menu "Gas editor". Then go back to the "Interactive Chart" frame, and



click on "Update the point table". All the project points are displayed in the table:

point name	substance	simulator	Chart	selected
air inlet	air	Х		ľ
2	air	Χ		ľ
fuel	Montoir nat	Х		ľ
3	burnt gases	Χ		ľ
4	burnt gases	Х		ľ

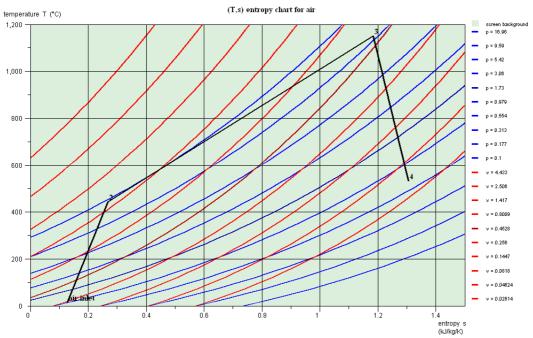
The two first columns show the names and the substances of the points. When a point is part of the simulator project, a "X" appears in the third column, and when it is part of the Chart cycle points, a "X" appears in the fourth one. Here, there are only simulator points.

The last table column titled "selected" shows the point status: if a "X" appears, the point is selected for being taken into account in the transfers between the simulator and the charts, otherwise not. To change a point status, double-click on the corresponding line. Here we want to plot all points but the fuel, so we deselect this one.

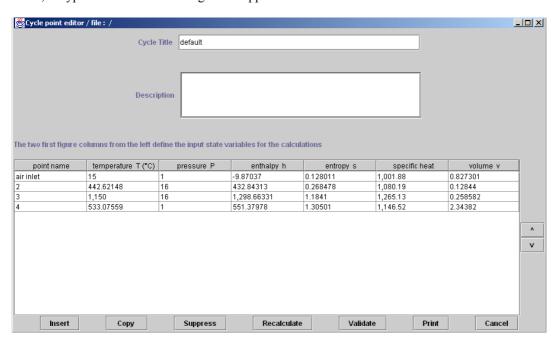
Now, click on "Update the chart from the simulator" to have the points transferred to the chart. The points are transferred while trying to order them as well as possible, but it can be necessary to reorder them to obtain a correctly connected layout. The cycle point editor allows to do it in this case as we will see it.

You also have to change the chart parameter settings. In menu "Chart", choose temperature and pressure boundaries compatible with the problem studied: 0 to 1200 °C, and 0,1 to 30 bar. If necessary, change the axis layout in menu "Chart".

Select "connected points" in menu Cycle. You get the following result:



You can now use the features provided by the interactive charts, which are presented in the chart reference manual, such as editing the points in the cycle editor. In order to do that, select item "Edit a cycle" in the "Cycle" menu, or type Crtl C. The following frame appears:



You can now change the cycle, add new points...

### Improvements in cycle plotting

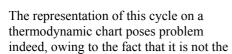
A number of improvements have been recently made in the plotting of cycles:

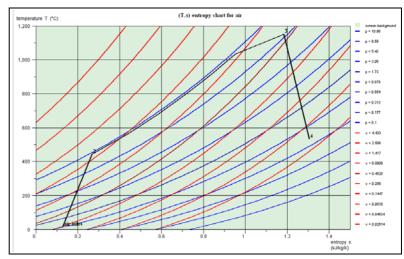
- first, it is possible to link points by various iso-value lines (iso-pressure, isentropic...)
- second, each cycle color may be changed according to the user desire
- third, it is now possible to plot several cycles on the same chart

#### Linking points by iso-value lines

When the cycle is first plotted on the (T, s) chart, the points are connected by straight lines. Opening the cycle point editor displays the cycle elements as shown in above.

It is now possible to connect points 2 and 3 by an iso-pressure line: select both lines 2 and 3 at the same time, and click on "Insert". A combo box with various iso-value choices is shown. Select "iso-pressure". You are requested to give the number of points you want to insert. The default value of 5 is adequate here. 5 new points are created in the cycle point editor. Click on "Validate": the plot now follows the 16 bar line from point 2, but then there is a setback up to point 3.



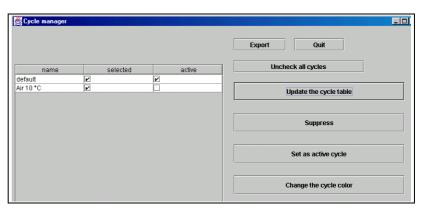


same fluid which flows through the whole machine: the change of composition in the combustion chamber prohibits in theory to plot the cycle in only one chart. On the air entropic chart, points 3 and 4 thus do not appear on the good isobars, because of the change of fluid. The setback observed is explained thus very well.

If you want to save this cycle, just open the cycle point editor, enter any title and description you may wish and save the cycle.

#### Changing cycle color

Until version 1.5, all cycles were plotted in black. It is now possible to select any color in the same way as you do it for the chart curves. In order to do that a new menu line named "Cycle manager" has been added in menu "Cycle". If you select it you open the frame shown here. If you click on "Update the cycle table", all cycles already loaded are displayed. Here, two cycles are loaded: the default one which is

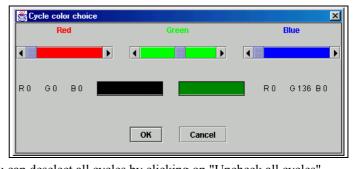


active, and a second one which has been loaded from a file.

You select the active cycle by choosing its line and clicking on "Set as active cycle". The active cycle has the following properties:

- it is connected to the simulator
- it is the one on which the "Cycle" menu lines operate, i.e. it can be erased, saved, its points can be edited in the cycle point editor...

If you double-click on a line, you change the column "selected" status: if it is checked, the



cycle is plotted on the chart, otherwise not. You can deselect all cycles by clicking on "Uncheck all cycles".

You can suppress a cycle in the list by selecting its line and clicking on "Suppress". Its plot is also suppressed from the chart.

To change a cycle color, select its line and click on "Change the cycle color". A frame allowing you to choose its color is displayed. If you want to save the new color, set the cycle as the active one and save it.

Suppressing the active cycle is equivalent to erasing it from the chart menu. You generate a new active cycle either by setting another cycle as the active one, or by interactively creating points in the chart, opening the cycle point editor and validating.

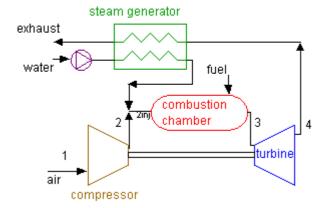
## Superposition of several cycles on a chart

To plot several cycles on a chart, just load them together and set them as selected in the cycle manager screen. They automatically appear on the chart as shown here.

## Steam injection gas turbine

Let us consider now a steam injection gas turbine operating in the Brayton cycle:

#### Steam injection gas turbine



A mass flow rate of 1 t/s of air enters the compressor at 1 bar and T1 = 294 K. It is compressed to 16 bar with a polytropic efficiency of 0.85. At the inlet of the combustion chamber, 20 bar and 400 °C water is injected. The mix is burnt in the combustion chamber with natural gas.

At the inlet of the turbine, technological constraints limit the gas temperature to 1400 K. The CO2 dissociation degree is set equal to 10%, the quenching temperature being 1400 K.

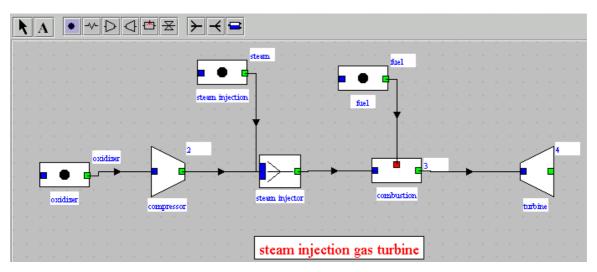
Burnt gases are expanded at 1 bar in a 0.85 polytropic efficiency turbine.

Determine, for  $\alpha = 0.1$  kg/s, the cycle efficiency.

## Creation of the diagram

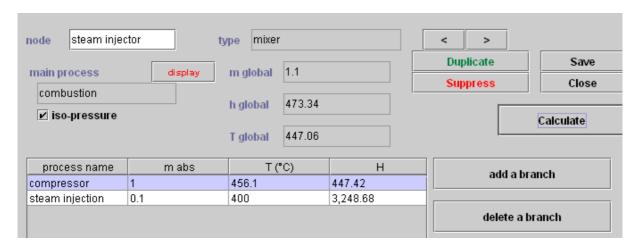
We shall start from the example previously built for the simple gas turbine (files GT.prj and GT.dia) and make the appropriate changes and additions to model this problem.

The cycle diagram is similar to that of the simple gas turbine. In addition to the components of the latter there is a need for a mixer at the inlet opf the combustion chamber. To build it you need to add a process-point named for example "steam injection" and a mixer whose branches are this process point and the compressor, and whose main vein (outlet process) is here "combustion".



On this diagram, some points and processes have been renamed as compared to that of the simple gas turbine. Once the diagram is designed, the simulator elements can be built and their parameters set.

Let us have a look at the mixer:

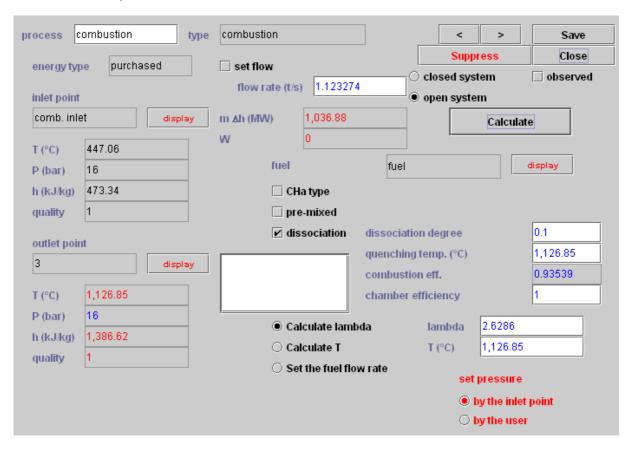


When you calculate the mixer, the "comb. inlet" point state is calculated and the point updated and the molar fractions of the oxidizer mix are determined.

component name	molar fraction	mass fraction
N2	0.6728466	0.6868457
Ar	0.007753674	0.0112876
02	0.1809191	0.2109577
H2O	0.1384806	0.09090909

Before calculating the combustion, you have to check its settings, which are a little more complex than in the previous example because of the dissociation. As the combustion chamber is assumed to be adiabatic, the thermal efficiency is set equal to 1. Due to the existence of a 10% CO2 dissociation degree, click on the corresponding checkbox and enter 0.1. Set the quenching temperature equal to 1400 K.

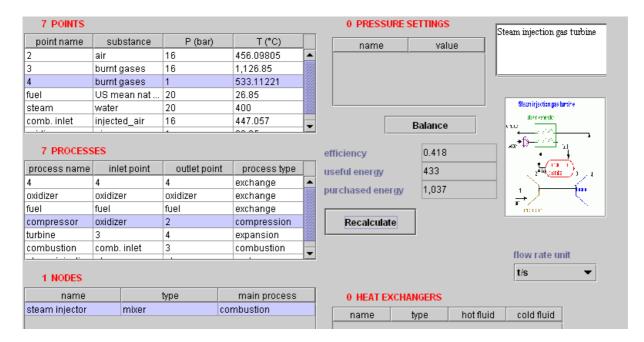
The combustion may then be calculated:



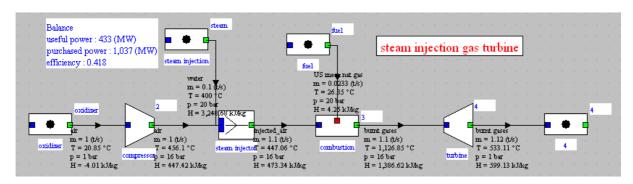
The burnt gas composition is the following:

component name	molar fraction	mass fraction
CO2	0.03015976	0.04933442
H2O	0.1884476	0.126184
02	0.1141161	0.135723
N2	0.6468368	0.6734934
со	0.003351084	0.003488811
H2	0.009644454	0.0007226285
Ar	0.007444216	0.01105372

The rest of the cycle is valid. To recalculate it, you have but to click the "Recalculate" button of the main project screen and iterate until the indicator values converge. Finally the cycle efficiency is obtained: 41.8%.



The point state values can be displayed on the diagram:

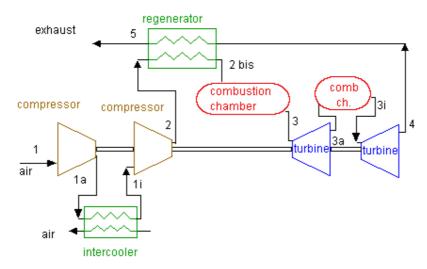


The project file is STIG\_US.prj and the diagram file STIG\_US.dia.

## Two stage regenerative gas turbine with intercooling and reheat

The simple gas turbine that we studied initially is a very simple one. Its cycle can be improved it by splitting in two steps the compression with an intermediate cooling and the expansion with an intermediate reheat. In addition, as the temperature difference between points 4 and 2 becomes significative, it is possible to use the enthalpy of the exhaust gases to preheat the compressed air before entering the combustion chamber in a heat exchanger called a regenerator. The corresponding cycle block diagram is the following:

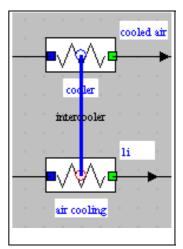
### two stage regenerative gas turbine with intercooling and reheat



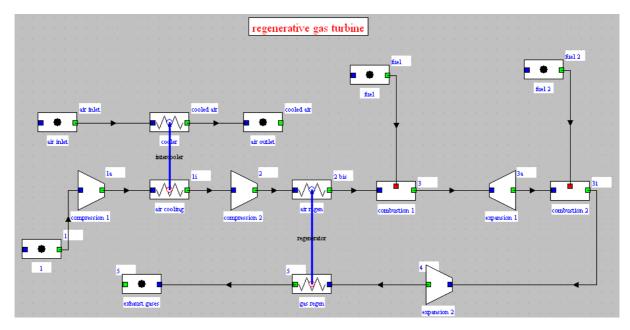
To build this cycle, you have to add a few points and processes in the same way as you did it previously, and to connect the exchange processes to create the two heat exchangers.

To create the heat exchanger, place the mouse on the cooler or the "air cooling" process. In the middle of the component appears a small blue circle which is a heat exchanger connection port. Click on it and drag the mouse above the corresponding port of the other component (the "air cooling" process or the cooler).

The name of the heat exchanger ("intercooler") is asked for. Once you have entered it, the exchanger is symbolized by a link between the two processes:



Apart from that, creating the diagram of the regenerative turbine is rather straightforward, and you end up with a design which is similar to this:



To create the heat exchanger in the simulator environment, double-click on the link. The heat exchanger screen is opened.

First select in the "type" field the heat exchanger type (for instance "mixed crossflow mCp max").

In order to design the heat exchanger, it is now necessary to specify which temperatures and flow rates have to be calculated, the others ones being set.

One can show (see the reference manual) that the problem has five degrees of freedom and that at least one of the two flow rates has to be set.

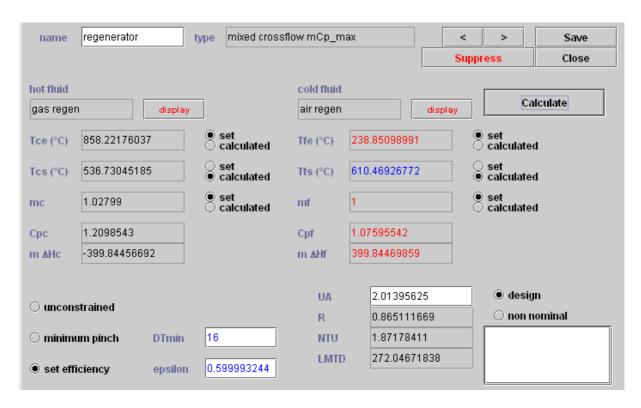
For temperatures, one can define explicit constraints (set values) or implicit constraints: one sets a value for the heat exchanger efficiency, or the pinch is set equal to a minimal value.

To set an efficiency value, it is necessary to enter it in the "epsilon" field and to select the "set efficiency" checkbox. To set a "minimal pinch", select on the corresponding checkbox; in this case, the software calculates the minimal pinch as being equal to the half-sum of the minimal pinches set in each of the processes that the heat exchanger matches.

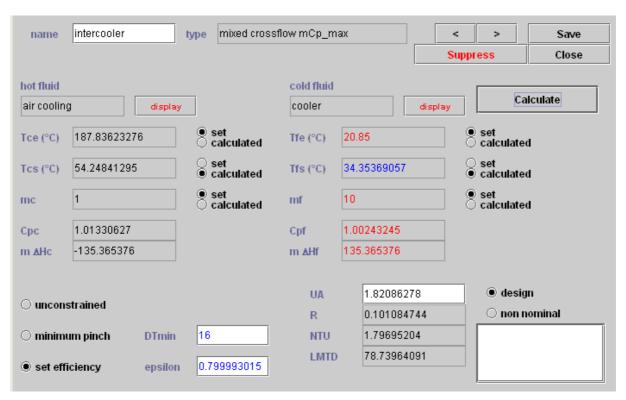
In this example you can for instance select the following constraints: the streams inlet points and flow rates are set. The outlet temperatures are to be calculated by Thermoptim.

Select the calculation mode (here "set efficiency" (to 0.6) and "design" as the heat exchanger has not yet been calculated), and click twice or three times the "Calculate" button until the enthalpy variations DHf and DHc of both fluids are the same (you may have to click several times because the heat exchanger calculations are made with the assumption that the specific capacities of the fluids are constant, whereas Thermoptim calculates them accurately, as indicated in the reference manual, para. "Heat Exchanger screens").

The result is the following:



Create similarly the intercooler, with a set efficiency of 0.8:

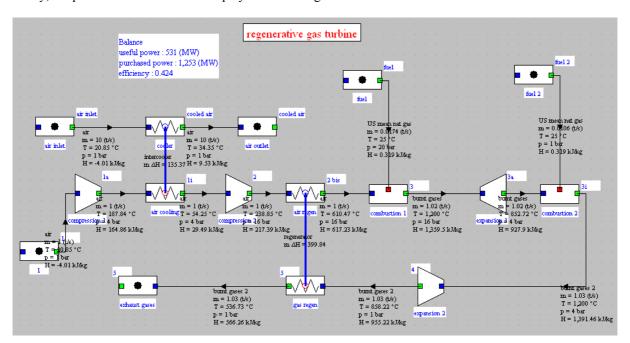


This cycle is indeed quite complicated, as it includes two heat exchangers, one of which creates an internal loop: the regenerator. Calculating the overall balance of the cycle is quite complex, as the temperature at point 2 bis depends on the regenerator behaviour, which itself depends on the gas composition and temperature at point 4, which themselves depend on the states of points 3i, 3a, 3 and 2bis...

This problem demonstrates the power of the recalculation engine: once you have built the cycle and connected all the elements, you can change any parameter of the cycle, such as the air inlet temperature or the combustion

temperature, and run the recalculation. In a few iterations, THERMOPTIM recalculates everything and converges towards the solution.

Lastly, the point state values can be displayed on the diagram:



The project file is named "regenGT.prj" and the diagram fiel "regenGT.dia".