

# Guidance page for practical work 7: AZEP (Advanced Zero Emission Power) cycle modeling

## 1) Objectives of the practical work

The project objective is to study one of the innovative power generation cycles using oxy-combustion, called AZEP (Advanced Zero Emission Power), and show how to model it realistically with ThermoOptim.

Achieve oxy-combustion is to replace by pure oxygen the usual oxidizer, ie air, a mixture mainly of oxygen and nitrogen (respectively 21% and 78% by volume). Oxy techniques allow both to get smoke almost exclusively composed of water and carbon dioxide, and to drastically reduce emissions of nitrogen oxides. These are technologies already used in the industry, including glass and steel.

The separation of CO<sub>2</sub> and H<sub>2</sub>O is then easily done by simple condensation of water and the lack of nitrogen significantly reduces NO<sub>x</sub> emissions and the volume of smoke.

Despite these advantages, these technologies have so far hardly been used for electricity generation because of the difficulties and costs associated with the production of oxygen.

The technical solution most developed today, called the Air Separation Unit, is to separate oxygen and nitrogen from the air by cryogenic operation both costly and energy intensive.

This process is not the only one, and innovations are being considered, such as the use of oxygen permeable membranes (AZEP cycle).

This relatively complicated practical work allows students to build two variants of AZEP cycle models. It is for students who already have studied combined cycles. If this is not the case, there should do it first (Session S41En<sup>1</sup>).

This document is an excerpt from the guidance page with complete results, which is reserved for teachers. For this reason, the numbering of figures is flawed.

## 2) References

This work is the result of a collaboration between the Center for Energy Processes (CEP) of the Ecole des Mines de Paris (R. Gicquel) and the EPFL LENI (D. Favrat, F. Marechal). The first two references below relate to innovative processes for CO<sub>2</sub> capture, the following more specifically deals with the behavior of the membrane permeable to oxygen, and the last two with AZEP cycles.

H. M. Kvamsdal, O. Maurstad, K. Jordal, and O. Bolland, benchmarking of gas-turbine cycles with CO<sub>2</sub> capture, GHGT-7, Vancouver, 2004.

L.I. Eide, M. Anheden, A. Lyngfelt, C. Abanades, M. Younes, D. Clodic, A.A. Bill, P.H.M. Feron, A. Rojey and F. Giroudière, Novel Capture Processes, Oil & Gas Science and Technology – Rev. IFP, Vol. 60 (2005), No. 3, pp. 497-508.

A. Maestro, Thermo-economic design of hydrogen production systems using oxygen, LENI-EPFL, juin 2005

R. Bolliger, D. Favrat, and F. Marechal. Advanced power plant design methodology using process integration and multi-objective thermo-economic optimisation. In ECOS 2005, 18th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, volume 2 of ECOS 2005, pages 777–784, 2005.

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<sup>1</sup> <http://www.thermooptim.org/sections/enseignement/cours-en-ligne/seances-diapason/session-s41en-single>

R. Bolliger. A methodology for the conceptual design and optimisation of advanced combined cycles. Master's thesis, Ecole Polytechnique Fédérale de Lausanne, Laboratoire d'énergie industrielle, 2004.

### 3) Main practical work

#### 3.1 Question

The sketch of a AZEP cycle is given in Figure 3.1.

Air is sucked by the compressor of a modified gas turbine, where the combustion chamber is replaced by a chamber with two compartments separated by a ceramic membrane permeable to oxygen (Mixed ionic-electronic Conducting MIEC membrane). In one of the chambers, the air is oxygen-depleted due to the difference in oxygen partial pressure between the two media. In the other takes

place the combustion of fuel with the oxygen in the presence of an inert gas that is an exhaust gas recirculation, composed mainly of  $\text{CO}_2$  and  $\text{H}_2\text{O}$ , more inert gases if the fuel contains.

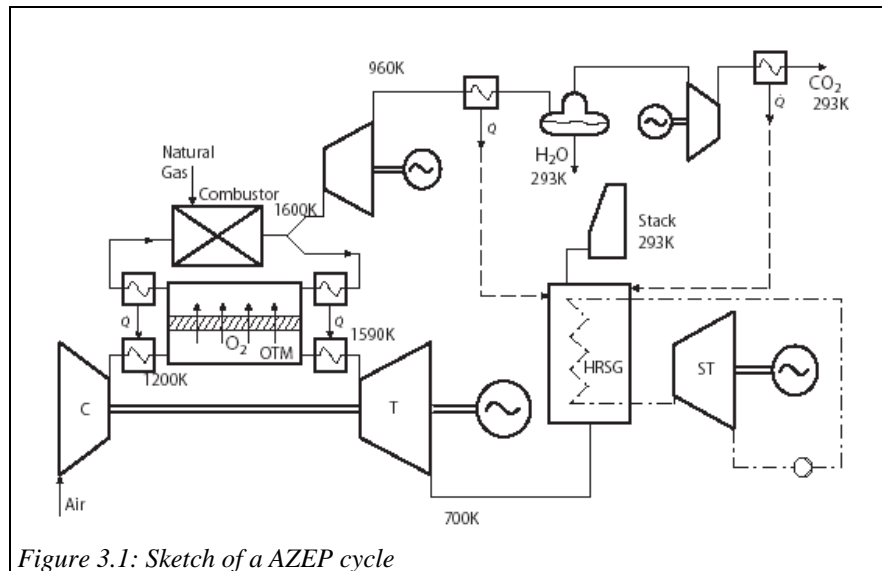


Figure 3.1: Sketch of a AZEP cycle

At high temperatures (above  $700\text{ }^\circ\text{C}$ ), the ceramic membrane (Figure 3.2) is a mixed ionic and electronic conductor, which passes simultaneously  $\text{O}_2$ -ions and electrons, oxygen being adsorbed on the surface.

The depleted air is expanded in a turbine, and used as a heat source for a steam cycle. The portion of the flue gas which is not recirculated is expanded in a turbine, and also used as a source for the hot steam cycle, before being condensed for water extraction. The remaining  $\text{CO}_2$  can then be captured. The portion of the exhaust gas being recirculated is first cooled slightly to ensure air preheating.

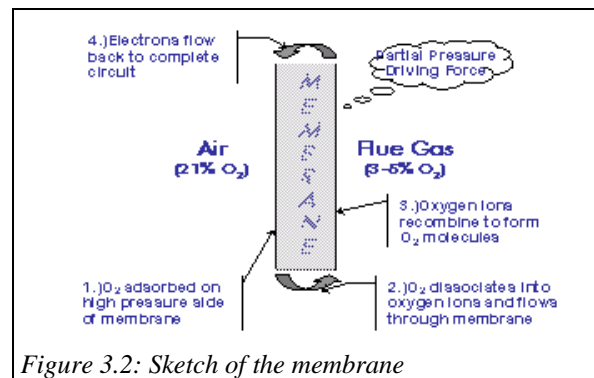


Figure 3.2: Sketch of the membrane

This type of cycle has the following advantages:

- Allow one to capture all the  $\text{CO}_2$  ;
- reduce  $\text{NO}_x$  emissions below 1 ppm ;
- reduce the cost of  $\text{CO}_2$  capture from 25 to 35% ;
- separate the  $\text{CO}_2$  by losing only two points of efficiency ;
- Cycle organs are standard, with the exception of the membrane component.

The objective of the work is to study such a cycle and model it with ThermoOptim, using external components "MIEC\_Inlet" and "MIEC".

### 3.2 Model of the membrane component

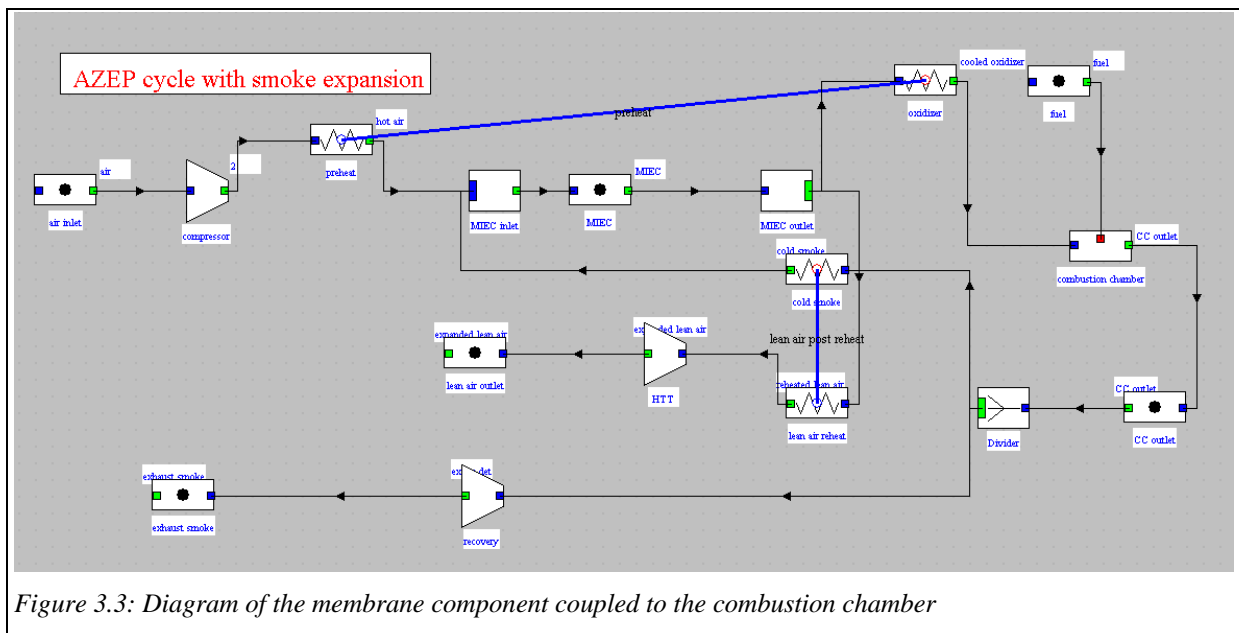
The membrane involves two separate streams which exchange matter through an interface: the oxygen depleted air and fumes out of the combustion chamber that are enriched in oxygen. It behaves like a quadrupole receiving two fluids in input, out of which come the other two.

To represent it in ThermoOptim, the quadrupole is formed by combining the inlet Mixer (class MIEC\_Inlet) and an outlet divider (class MIEC), the two being connected by a process-point playing a passive role. The classes references are "MIEC Inlet" and "MIEC".

For the model to be consistent, it synchronizes the calculations made by the two nodes. More specifically, the outlet divider takes control of the mixer, whose role is to perform an update of the coupling variables associated with the input stream.

The model structure is given in Figure 3.3. The membrane is represented by the three components "MIEC Inlet", "MIEC" and "MIEC outlet." The inlet mixer MIEC Inlet receives the compressed air heated by the combustion before entering the combustion chamber, and a fraction of the recirculated and cooled flue gas. At the output of the external divider, there is firstly the oxygen-depleted air, which is heated by the flue gases leaving the combustion chamber prior to expansion in the HTT turbine, and secondly the oxidizer formed by oxygen enriched fumes, which are cooled before entering the combustion chamber.

In the top right of the figure is the stoichiometric combustion chamber. The stream of smoke coming out, mainly composed of H<sub>2</sub>O and O<sub>2</sub> (plus inert if the fuel contains), is divided into two parts. Almost 90% is recirculated and used to raise the temperature of the depleted air before it is expanded, while the remainder is expanded in the "recovery" turbine.



The membrane model we develop here is that used by the EPFL LENI. The surface molar flow of oxygen through the membrane is given by:

$$j_{O_2} = j_{O_2,0} \cdot e^{-\frac{E_A}{RT}} \left[ p^{n_{O_2}}_{O_2, feedside} - p^{n_{O_2}}_{O_2, permeateside} \right]$$

It is proportional to a reference flow, to  $\exp(-E_a/RT)$ ,  $E_a$  being the activation energy and  $T$  the temperature of the membrane, and the difference in oxygen partial pressure between the two sides of the membrane. Since we can

consider that the partial pressure of oxygen is zero combustion chamber side, this equation can be simplified further.

The model that can be retained is the following:

- 1) the membrane surface, its temperature and surface conductance parameters are read on the screen;
- 2) we first calculate using the equation above the molar flow of oxygen through the membrane;
- 3) we thus determine the composition of the depleted air then that of the oxidizer with which oxygen is mixed and their flow-rates
- 4) we estimate the thermal power transferred between the two sides of the membrane, which provides the enthalpy of combustion and that of the depleted air;

In this model, available in the Thermoptim model library<sup>2</sup>, we do not know the pressure in the combustion chamber, a chamber separate from the air. To prevent damage to the membrane, the pressure difference between both sides must remain low.

Technologically, the fuel, here assumed to be natural gas at 70 bar, pressurizes the circuit, for example through an ejector. In our model, we do not represent this device, we simply set a slightly higher pressure than the air circuit.

In the combustion chamber, we assume that the reaction is stoichiometric and complete.

### 3.3 Solving approach

Given its complexity, this practical work is for students familiar with combined cycles. In addition, the model being somewhat difficult to set, it is recommended that they begin by working on the session Diapason S07\_trucs<sup>3</sup> presenting tips and tricks for modeling with Thermoptim.

In addition, the full model involves a number of elements beyond the limits permitted by the Education version of Thermoptim. Students then build it in two parts, the assembly being realized subsequently by providing them with the appropriate files.

#### 3.3.1 High temperature cycle model

We will start by the model whose diagram is given in figure 3.3, which can be described as high-temperature cycle, the rest of the cycle representing the recovery by the steam cycle.

If one has never done it, a little difficulty exists for the selection of external classes. It is easily lifted by referring to the note Using external classes or by operating as shown in the first nine stages of the Diapason session S07En\_ext<sup>4</sup>.

We must then define two new gas at the outlet of the external divider, one representing the depleted air, which must contain at least oxygen and nitrogen as components, and the second representing the exhaust gas, which the least contains components such as water and carbon dioxide as it is on this basis that the veins will be identified by the external class. These gases will be defined with an approximate composition as substances of upstream and downstream points of processes connected downstream of the external divider. Their exact composition will be recalculated by Thermoptim.

Similarly, gases associated with the processes entering the external mixer will be air, possibly moist, and the burnt gases defined above.

<sup>2</sup> <http://www.thermoptim.org/sections/logiciels/thermoptim/modelotheque/modele-miec>

<sup>3</sup> Session S07\_trucs: [http://www.thermoptim.org/SE/seances/S07\\_trucs/seance.html](http://www.thermoptim.org/SE/seances/S07_trucs/seance.html)

<sup>4</sup> Session S07En\_ext: [http://www.thermoptim.org/sections/enseignement/cours-en-ligne/seances-diapason/s07en\\_ext-introduction](http://www.thermoptim.org/sections/enseignement/cours-en-ligne/seances-diapason/s07en_ext-introduction)

Both exchangers are configured with a set effectiveness equal to 0.75, and turbomachinery as adiabatic with a polytropic efficiency equal to 0.9. The pressure of the air circuit is 15 bar, and that of the combustion chamber 15.5 bar. The flow of intake air is 600 kg/s.

We chose here the following settings: a membrane area of 2500 m<sup>2</sup>, a membrane temperature of 1100 °C and a conductance equal to 0.025 W/m<sup>2</sup>/K.

The thermal power transferred to the air is equal to 16.3 MW and 54.8 kg/s of oxygen go through the membrane, the mole fraction of oxygen-depleted air being equal to 13.9%. The temperature of the membrane, assumed to be the average temperature of the air, is in fine 1018 °C, air entering at 965 °C and exiting at 1072 °C.

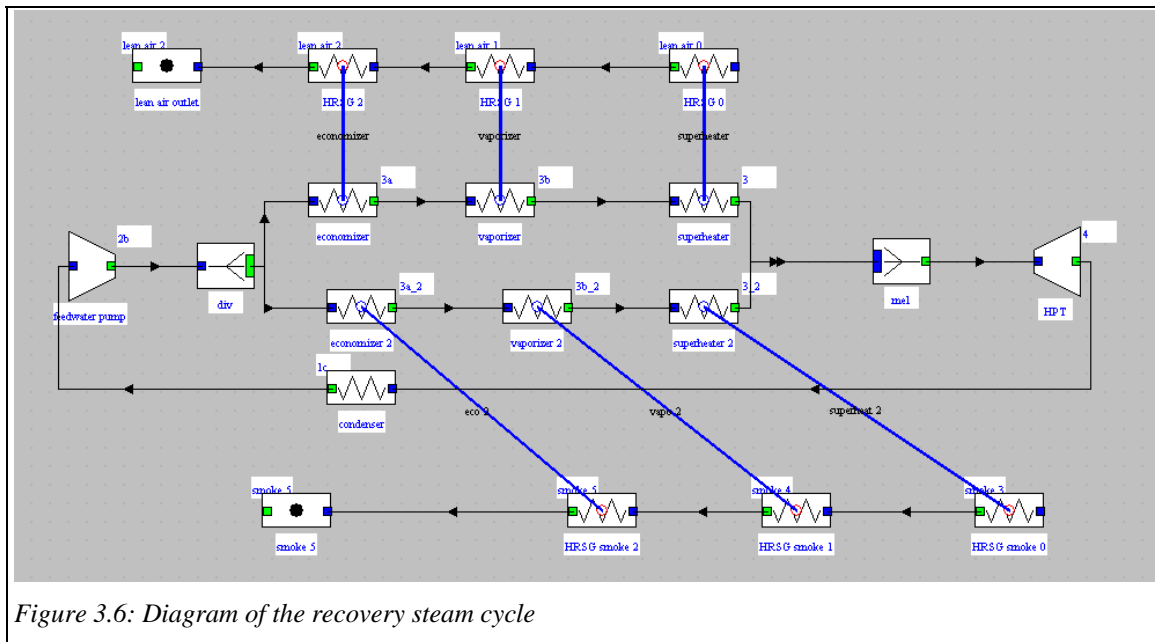
With this setting, the mole fraction of oxygen in the oxidizer is equal to 7%.

The bulk of the gas leaving the combustion chamber is recycled, so in particular that the average molar fraction of oxygen in the combustion is low enough that oxygen can pass through the membrane. We must therefore introduce a divider, which will be set as follows: since it has two branches only, it is possible to set the flow in one of them. In this case, we must set the recirculated flow value (600 kg/s) because the total flow exiting the combustion chamber depends on the flow of oxygen through the membrane, which also sets the fuel flow, combustion being stoichiometric.

Note that the system under study is strongly coupled, which requires to perform many recalculations for results to converge.

### 3.3.2 Steam recovery cycle model

Once the membrane component represented, it remains to model the heat recovery steam cycle. Although this is not the only possible solution, we have chosen here to separate the steam generator into two parts, one heated by the depleted air, and the other by the exhaust gases.



A small problem is the creation and configuration of the dividers and mixers to create the various branches of the circuits. Let us recall that nodes do not propagate automatically point and substance names in the diagram. We must therefore take care to enter this information in the input tabs of processes located just downstream of the divider and the mixer. For the divider, the point is naturally the same as that downstream of the main process. For the mixer, it must of course create a new point which has water as substance as the two upstream branches are crossed by this fluid. The pressure must be set by the modeler, equal to the pressure upstream and the temperature will be recalculated by ThermoOptim.

Once the diagram in figure 3.6 is complete, the setup can be done as shown below.

We will retain for the steam cycle condensation at 0.05 bar (33 °C), a high pressure of 70 bar, and a superheating temperature of 400 °C. These values can of course be changed later in the course of sensitivity studies (section 4.1).

Both veins of gas (depleted air and fumes) should be initialized using the values from the high temperature cycle (545.24 kg/s and 572.99 °C for the depleted air, and 68.49 kg/s and 790.85 °C for smoke). Their compositions must also be the same as those of the other cycle.

To finish the setup, you must set the main flow of the steam cycle and that of the branches, which can only be done by iterations. We initialize the main flow at 100 kg/s, and the flow distribution between the two veins to 75% in the stream cooling depleted air, and 25% in the other. Simply enter this distribution in the upstream divider screen, as flow setting of the various branches, entering 3 and 1 (Figure 3.7).

For students who have modeled a simple steam cycle (if not, they must begin by working on the S26En<sup>5</sup> session), the only difficulty is the construction and configuration of three parts heat exchangers.

How to solve this problem is explained in detail at the end of session S18En<sup>6</sup> on the thermodynamics of heat exchangers in an exercise where are set exchangers representing a boiler for a simple steam cycle.

The setting of heat exchangers is done assuming that are known all values in the steam cycle, as well as the inlet temperature and fluid flow of each heat exchanger. We must set a realistic exit temperature for the heat exchanger can be built by ThermoOptim, the exact value being recalculated.

After all these initializations are made, we must recalculate the cycle until the outlet temperatures of the two gases are stabilized, then play on the value of the main flow and the flow distribution of the branches until these temperatures are as low as possible, knowing that a pinch of ten degrees at least should be respected at the output of economizers.

### 3.3.3 Full model

The complete model is obtained by joining the previous two, with in addition condensation of water.

The fumes coming out of one of two steam generators contain only CO<sub>2</sub> and H<sub>2</sub>O. They are cooled by an external heat sink at a temperature low enough that almost all the water is condensed.

At the output of this cooler, the gas composed mainly of CO<sub>2</sub> is captured. We did not show on the diagram the corresponding compressors.

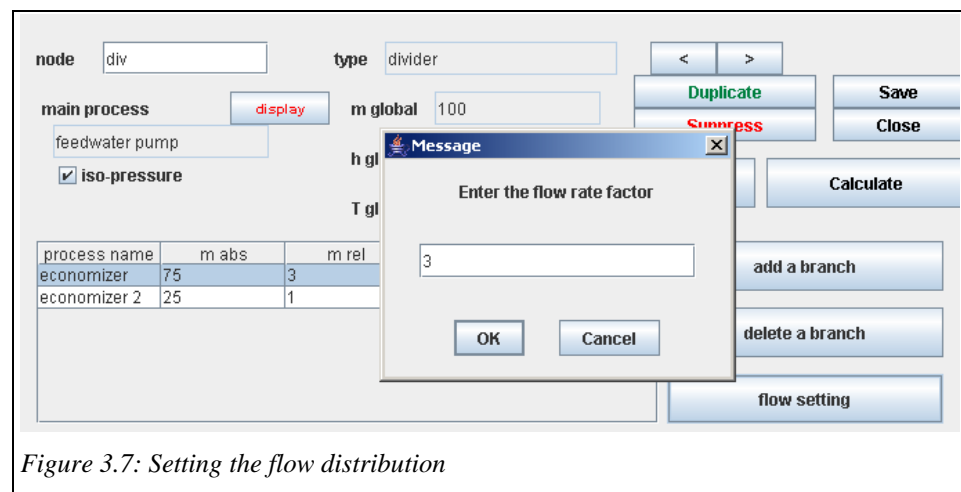


Figure 3.7: Setting the flow distribution

<sup>5</sup> Session S26En: [http://www.thermooptim.org/sections/enseignement/cours-en-ligne/seances-diapason/s26\\_vapor\\_cycle](http://www.thermooptim.org/sections/enseignement/cours-en-ligne/seances-diapason/s26_vapor_cycle)

<sup>6</sup> Session S18En: <http://www.thermooptim.org/sections/enseignement/cours-en-ligne/seances-diapason/session-s18en>

This diagram uses an external divider ("cold battery") to represent the cooling and condensation of water contained in the fumes<sup>7</sup>. This is a simplified model, which has two parameters: the water temperature, which we take equal to 30 °C, and the efficiency of water extraction, which represents the percentage (by volume) of the condensed water from the incoming flow.

We get for the full model the same values as those obtained in calculating the two sides separately.

## 4) Variants

We propose a few variants, but many others can be imagined, depending on the time available, the level of the students, their number, and educational objectives pursued.

### 4.1 AZEP Cycle without smoke expansion (or bypass)

The detailed analysis of the AZEP cycle just built shows that the power of the recovery turbine on flue gases represents only about 20% of that which expands the depleted air. To simplify the cycle, and thus reduce costs, the manufacturer (Alstom Power), considers a slightly modified scheme (Figure 4.1), where a fraction of the compressed air does not pass through the membrane component and is heated by cooling fumes in a heat exchanger of effectiveness equal to 0.9, before being mixed with the depleted air and expanded.

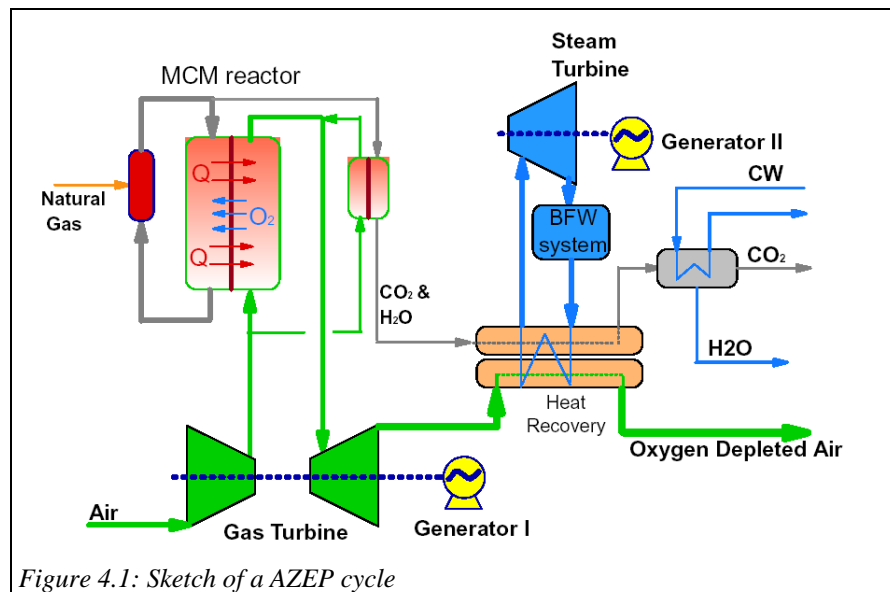


Figure 4.1: Sketch of a AZEP cycle

Figure 4.2 shows a possible model for such a cycle. Instead of splitting in two the steam generator, we merely reheat steam, which does not completely cool the smoke. Despite this, the cycle efficiency is excellent (55% versus 58.7%). Depending on the cost of equipment, the rated power and operating constraints, either cycle may be preferable.

The work proposed to students will be similar to that of the main practical work: they begin by working on the high temperature cycle, including the heat exchanger of warm air through the bypass, and then study the steam recovery cycle, simpler in this case. Since there is only one steam circuit, looking for the steam flow is facilitated.

Setting the air divider is by choosing a flow rate of 600 kg/s in the "preheat" process upstream the membrane component. Do not forget to introduce a new point and a new substance at the outlet of the mixer receiving the initial air and depleted air.

<sup>7</sup> <http://www.thermoptim.org/sections/logiciels/thermoptim/modelotheque/modele-cold-battery>

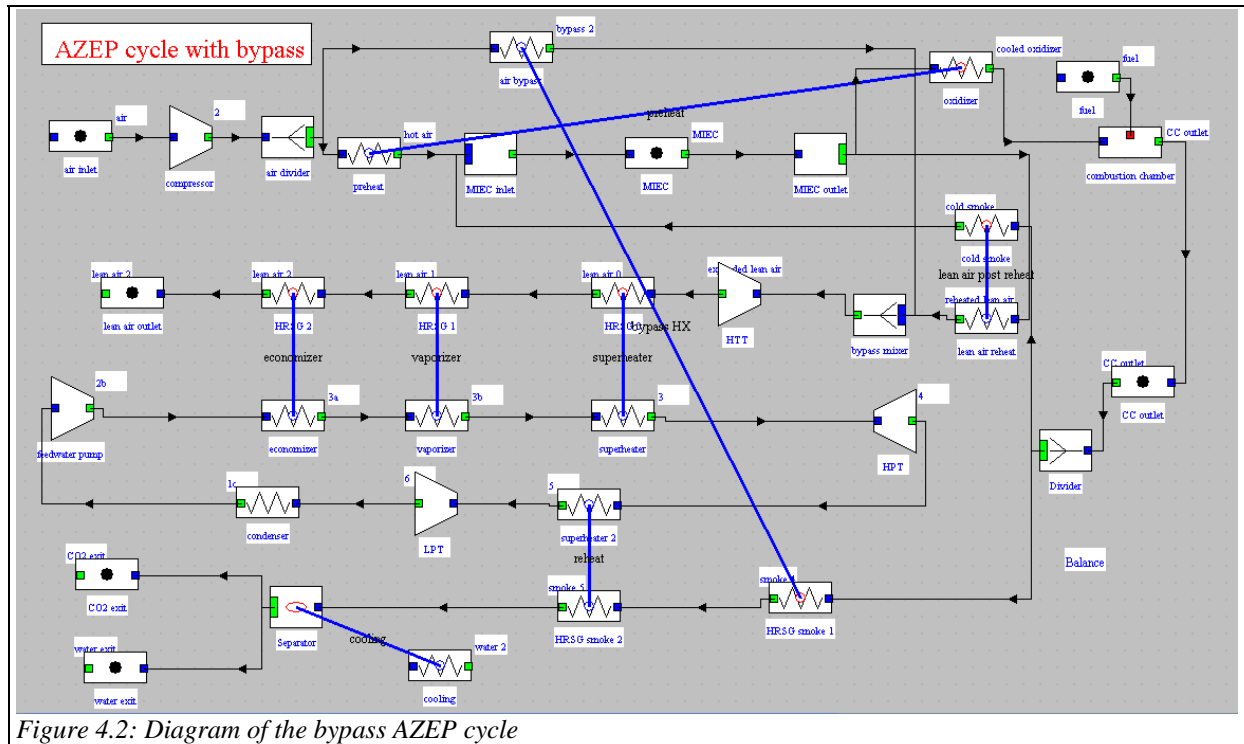


Figure 4.2: Diagram of the bypass AZEP cycle

## 4.2 Sensitivity studies

From the previous model, it is possible to ask students to make sensitivity studies on the values of parameters chosen for the temperatures, pressures, flow rates... They may in particular take into account the pressure drops in the exchangers.

In the example in Figure 4.2, we set the pressure in the combustion chamber at 15.5 bar, as previously. It might be interesting to reduce the pressure a bit to lower the partial pressure of oxygen in the combustion and thus enhance the permeability of the membrane.

## 4.3 Adding a natural gas compressor

In the model with expansion of the fumes, we assumed that the fuel was natural gas at 70 bar. If the facility is not close to the high-pressure gas network, there must be a natural gas compressor upstream of the fuel port of the combustion chamber.

## 4.4 Changing the membrane model

So far we have chosen a particularly simple membrane model, where we considered that the gradient of partial pressure of oxygen was uniform. It might be interesting to refine this model and study the impact of these changes on complete cycles.

## 4.5 Optimization of the steam generator

As we have said, we have chosen in the first model to separate the steam generator into two parts, one heated by the depleted air, and the other by the exhaust gases. This is not necessarily optimal, firstly because it is a single pressure steam cycle, and secondly because another exchanger network might be slightly more efficient.

In the second model, the second steam generator is removed, and a reheat is added.



It would be possible if students have enough time to ask them to optimize, through Thermoptim tools, configuration of the cycle steam by playing on both its architecture (pressure levels, possible reheat) and that of the exchanger network.

## 4.6 Cycle exergy balance

Finally, it is possible to ask students to build up the cycle exergy balance, if they have enough time.

Diapason session S06En<sup>8</sup> will provide necessary explanations on how to proceed.

## 5) Work files, recommendations

### 5.1 Work files

The following work files are attached to the file in the archive AZEP-en.zip:

- extUser.zip file containing these external classes
- Thermoptim project and diagram files of the model

### 5.2 Recommendations

It is necessary that the teacher checks that students have at their disposal in their work environment Thermoptim external classes they need.

The easiest way to this is to run Thermoptim, then open the external class viewer (menu Special of the simulator). Classes will be grouped by type, MIEC\_inlet", "MIEC" et "ColdBattery" should appear among the mixers and dividers, as shown in Figure 5.1.

If a class is missing, replace the extUser.zip or extUser2.zip file by that provided in archive AZEP-en.zip. If present, it is unnecessary to make this change.

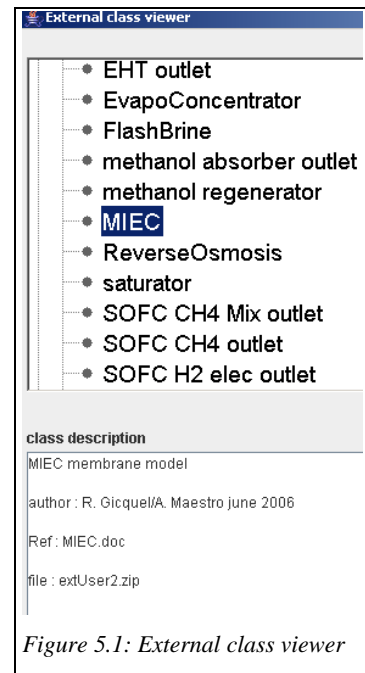


Figure 5.1: External class viewer

<sup>8</sup> Session S06En : <http://www.thermoptim.org/sections/enseignement/cours-en-ligne/seances-diapason/s06en-exergy-balances>