ASIMPTOTE Advanced SIMulation Programs for TOTal Energy systems

Technical Notes

A program for thermodynamic modeling
and optimization of energy conversion systems

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Chapter 1

Introduction

Energy production processes are becoming more and more complex because of the increase in the size of the power of production units and an increasing need for a higher overall efficiency in order to save primary energy.
Combinations of processes (STAG) and processes in which chemical reactions play an important part (fuel cells and fuel gasification) also result in complex calculations.
For such calculations where the process variables are considered in detail, a computer program is required.

In the Laboratory for Thermal Power Engineering of the Delft University of Technology the computer program Cycle-Tempo has been developed to calculate mass flows, thermodynamic variables, chemical equilibrium and compositions of mixed flows for the following processes or combinations of processes:

1. Steam/water cycles
2. Gas turbine cycles
3. Potassium topping cycles
4. Fuel cell systems
5. Coal gasification systems
6. Vapor compression refrigeration machines and heat pumps
7. Absorption refrigeration machines and heat pumps

The computer program can be used for a variety of purposes.
Firstly process variables for new units can be calculated and optimised.
Secondly for existing production units the consequences of a change in operation, for example relating to the thermal efficiency, can be easily calculated.
Finally the computer program can be used for the evaluation and testing of results.

Chapter 2

Basic concept of Cycle-Tempo

Cycle-Tempo was developed for computing thermodynamic properties, gas compositions and mass flows in energy systems for the production of electricity, heat and refrigeration. These can be calculated with:

- mass balances;
- molar balances;
- energy balances;
- relations for thermodynamic properties.

In Cycle-Tempo relations are available for computing thermodynamic properties for:

- steam and water (in accordance with the IFC equations of 1967 [7]);
- a set of 50 gases which may occur as an ideal mixture in a pipe (also for chemical equilibrium calculations);
- refrigerants;
- potassium;
- ammonia/water mixtures.

Predefined compositions for air, natural gas, flue gas, coal and a large number of refrigerant mixtures are also available.

2.1 Principle of the calculation method

The principle of the calculation method of Cycle-Tempo is explained in the light of a simple example (see Figure 2-1).
For the water cycle process mass and energy balances can be prepared for the systemmatrix (see Figure 2-2). With the systemmatrix the mass flows are calculated simultaneously.
The equations prepared are:

Equation:

1. Mass balance of the boiler.
2. Mass balance of the turbine.
3. Total mass balance of the condenser.
4. Mass balance of cooling water side of the condenser.
5. Mass balance of the deaerator.
6. Mass balance of the feedwater pump.
7. Mass balance of the cooling water pump.
8. Energy balance of the deaerator.
9. Energy balance of the condenser.
10. Energy balance of the turbine.

For each closed cycle a mass balance must be eliminated in order to obtain an independent set of equations. This is the reason why the mass balance of the pump with apparatus number 4, and the mass balance of the cooling water sink with apparatus number 7 are missing. The program itself determines which mass balances are eliminated.
The systemmatrix is solved and the mass flows of the system are calculated. With equation 9 the cooling water mass flow is fixed. With equation 10 the size of the mass flows is established by the specified power of the turbine. Where the coefficients in the energy equation of the system matrix are dependent on the mass flows, an iterative calculation is necessary. In the example the turbine efficiency may be dependent on the mass flow through the turbine. In this way the enthalpies of pipes 2 and 7, which occur in the energy balance of equation 10, are also dependent on the mass flow.
The calculation with Cycle-Tempo is included as example 1 in part “Examples” of the manual.

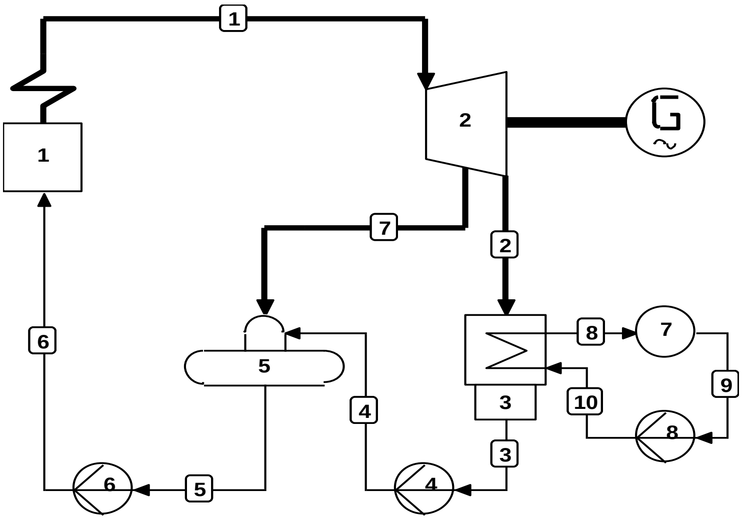


Figure 2-1: example of a simple Cycle-Tempo scheme

pipe numbers ⟶

component	**nr.**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**				
boiler	1	–1					–1						m_1		0
turbine	2	1	–1					–1					m_2		0
condenser	3		1	–1					–1		1		m_3		0
condenser (cooling)	3								–1		1		m_4		0
deaerator	5				1	–1		1				*	m_5	=	0
feedpump	6					1	–1						m_6		0
coolwater pump	8									1	–1		m_7		0
deaerator	5				h_4	$-h_5$		h_7					m_8		0
condenser	3		h_2	$-h_3$					$-h_8$		h_{10}		m_9		0
turbine	2	h_1	$-h_2$					$-h_7$					m_{10}		P_{tur}

Figure 2-2: system matrix of the Cycle-Tempo scheme

2.2 Calculation run of Cycle-Tempo

The process scheme may consist of a closed or an open system or of a combination of these systems.
For preparing the input data for a process scheme all the pipes, apparatuses and cycles must be numbered for the purposes of the identification.
The calculation procedure is broken down into twelve steps. The calculation run for Cycle-Tempo is set out in Figure 2-4.

Step 1 Reading in

The order for reading in is:

a. Parameters which determine the size of the system, such as number of apparatuses, pipes, turbines etc.
b. Apparatus data. Data may be specified which may differ for each apparatus. The apparatus number and apparatus type are compulsory.
c. Topology of the system. It is made clear to the program how the pipes are linked between the apparatuses.
d. Medium data per pipe.
e. Reading in the optional data.

In each step the input data are where possible checked for accuracy. For each error which is discovered, an error message is given. The program stops in that case after the whole input phase has been completed.

Step 2 Creation of system matrix

The calculation starts with the creation of the system matrix for the mass flow calculation. A check is made that the number of equations corresponds with the number of pipes. If this is not the case, then an error message follows and the program stops.

Step 3 Calculating compositions

In this step the medium types and gas compositions in the pipes are determined. There are several apparatus routines for this, depending on the apparatus types used.

Step 4 Difference in compositions

If the main iteration has been carried out a minimum of twice *and* medium types occur in the system which consist of a mixture, then it is determined in which pipe the largest molar fraction change occurs in the succeeding main iterations. It is also determined how many pipes do not meet the break-off criterion. The break-off criterion is:

$$| C_j(i) - C_j(i-1) | < \in$$

The result of this test is always printed out in the "Text Output" and during the calculation process on the screen.

Step 5 Calculating p, T, h

The pressures, temperatures and enthalpies are calculated with the help of apparatus routines. The next order is followed:

1. Turbines (type 3) in order of increasing apparatus number
2. Condensers (type 4) in order of increasing apparatus number
3. Flashed heaters (type 5) in order of increasing apparatus number
4. Heat exchangers (EEQCOD=2, type 6) in order of increasing apparatus number
5. Heat exchangers (EEQCOD=1, type 12) in order of increasing apparatus number
6. Moisture separators (type 22) in order of increasing apparatus number
7. Other apparatus types in order of increasing apparatus number

If after such a passage not all properties are known, the apparatus routines are called again, but then in reversed order. This procedure is repeated until the number of known properties doesn't increase any more. Either the properties in all pipes are known, or not enough input data are specified by the user to calculate these properties.

Step 6 Solving system matrix

In the system matrix, the enthalpies calculated in step 5 are substituted in the relevant energy equations. The solving of this system using the Gauss elimination method gives the mass flows for the system.

Step 7 Difference in mass flows

After the main iteration has been carried out a minimum of twice, for each pipe the relative and absolute difference is determined in the mass flows for the previous main iteration. *For each pipe* a check is made as to whether it meets the break-off criterion:

$$\left| \frac{\phi_m(\mathrm{i}) - \phi_m(\mathrm{i-1})}{\phi_m(\mathrm{i})} \right| < \in \quad \underline{\text{or}} \quad \left| \phi_\mathrm{m}(\mathrm{i}) - \phi_m(\mathrm{i-1}) \right| < 0.001$$

For each pipe the printout shows how many pipes do <u>not</u> meet the criterion and in which pipe the maximum relative and in which the maximum absolute difference occurs.

Step 8 Break-off criterion compositions/mass flows

The break-off criterion for the main iteration is: All the pipes must meet both the criterion for the compositions and the criterion for the mass flows.
If both conditions are met, the required accuracy is reached and the last mass flows calculated are regarded as the solution of the system. If one or both of these conditions is not met, then there is a return to step 3.

Step 9 Calculating compositions

In the solution of the mass flows the relevant compositions are calculated. These compositions are then regarded as the solution of the system. The result is printed out in the table “Composition of fluids”.

Step 10 Calculating p, T, h

With the solution for the mass flows and compositions once again all the unknown pressures, temperatures and enthalpies are calculated. All the pipe data are printed out in the table “Data for all pipes” with for each pipe:

- Medium type.
- Mass flow.
- Molar flow.
- Volume flow at inlet and outlet.
- Pressure at inlet and outlet.

- Temperature at inlet and outlet.
- Enthalpy at inlet and outlet.
- Entropy at inlet and outlet.
- Vapor fraction at inlet and outlet (if fluids are present for which 2-phase states are allowed).
- Exergy at inlet and outlet (if an exergy calculation is made).
- Mass fraction (if binary mixtures are present).

Step 11 Output

As a control for each apparatus the energy balance is calculated with:

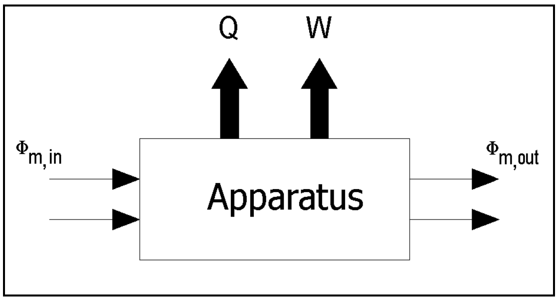


Figure 2-3: Energy balance of an apparatus

$$\sum_{j=1}^{n} \phi_{m,in}(j)\, h_{in}(j) \; - \; \sum_{i=1}^{n} \phi_{m,out}(i)\, h_{out}(i) = Q + W$$

For apparatuses with streams exchanging heat the internal heat transfer is also calculated. The values are printed out in the table “Heat exchanging equipment” and give an idea of the accuracy of the solution.

Step 12 Exergy analysis

In this step, which is optional, an exergy analysis is given for each apparatus and for the whole system.

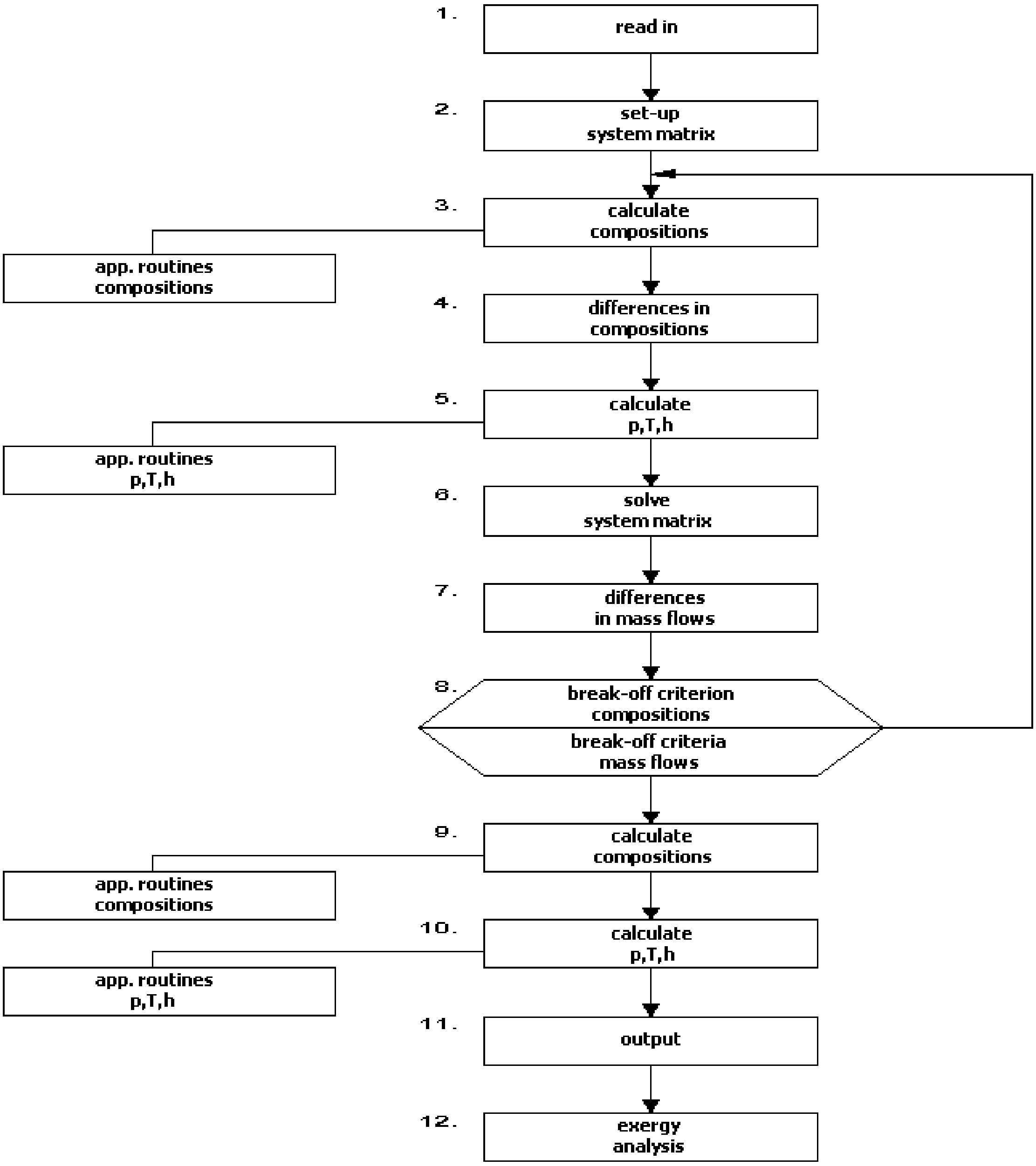
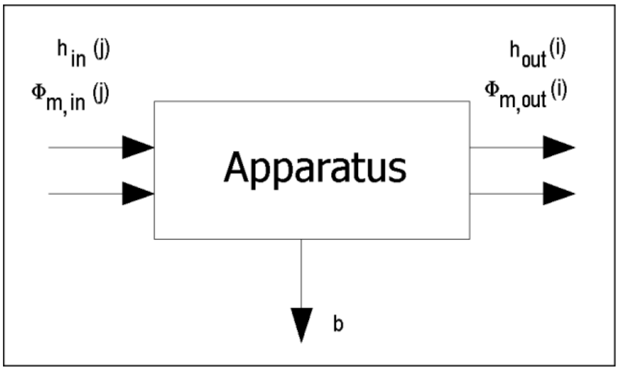


Figure 2-4: Calculation run Cycle-Tempo

2.3 Creating the system matrix

Mass flows are calculated from:

- mass balances of an apparatus
- energy balance of an apparatus



Φ_m = mass flow
h = specific enthalpy
b = mass or energy loss

Figure 2-5: Energy and mass balance of an apparatus

Mass balances are of the type:

$$\sum_{j=1}^{n_i} \phi_{m,in}(j) - \sum_{i=1}^{n_o} \phi_{m,out}(i) \quad = \quad b(k)$$

(k = number of equations)

Energy balances are of the type:

$$\sum_{j=1}^{n_i} \phi_{m,in}(j) \times h_{in}(j) - \sum_{i=1}^{n_o} \phi_{m,out}(i) \times h_{out}(j) \quad = \quad b(l)$$

(l = number of equations)

The mass balances can also be prepared from:

- atomic balance of an apparatus
- prescribed mass flows
- prescribed mass flow ratios

The equations drawn up (mass and energy balances) are written in matrix form:

$$A\,\underline{m} = \underline{b}$$

The solution to this system gives the mass flow for each pipe in the system. The calculation must however meet three conditions:

1. **The matrix must be square, which means that the number of equations must be equal to the number of pipes in the system.**
2. **The matrix must be independent.**
3. **If there are coefficients in the matrix which are dependent on the mass flows, an iterative calculation is necessary. This iteration process must be converging.**

2.3.1 Closed processes

To obtain an independent system of equations for a closed cycle for each closed cycle 1 mass balance of an apparatus must be eliminated. The reason is that 1 mass balance for an apparatus can always be deduced from the other mass balances. This is explained by the example in Figure 2-1.

If we leave out the cooling water cycle, equations 1, 2, 3, 5 and 6 can also be written as:

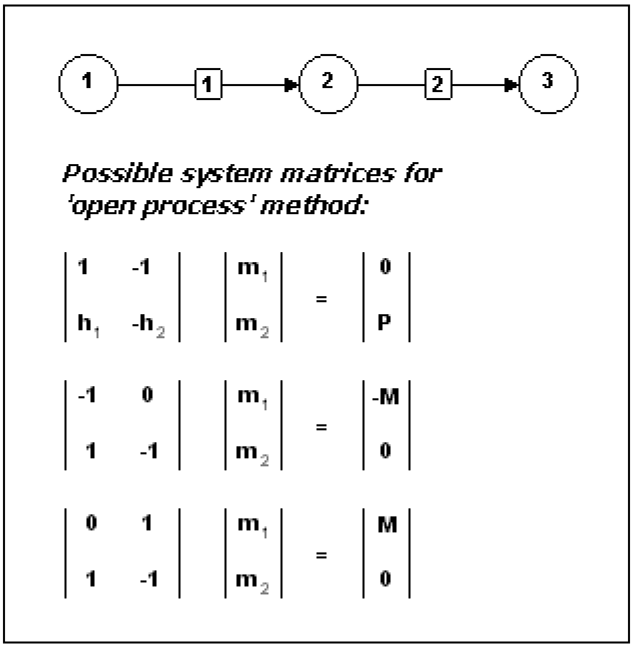
Equation	1	–m1 + m6	= 0	
Equation	2	m1 – m2 – m7	= 0	
Equation	3	m2 – m3	= 0	
Equation	5	m4 – m5 + m7	= 0	
Equation	6	m5 – m6	= 0	+
		m4 – m3	= 0	

The resulting equation is the same as the mass balance of pump number 4.
Thus, adding this mass balance would cause a dependent matrix. For the same reason the mass balance of sink number 7 is left out of the matrix. The program itself eliminates 1 mass balance per closed cycle.

The user is free to specify the energy equations with a right hand side. These are the so-called production functions. It is important to choose these equations such that they are not dependent on the mass balances.

2.3.2 Open processes

For an open process several possibilities are available for selecting mass balances. This is illustrated from an example, see Figure 2-6.



Possible system matrices for 'open process' method:

$$\begin{vmatrix} 1 & -1 \\ h_1 & -h_2 \end{vmatrix} \begin{vmatrix} m_1 \\ m_2 \end{vmatrix} = \begin{vmatrix} 0 \\ P \end{vmatrix}$$

$$\begin{vmatrix} -1 & 0 \\ 1 & -1 \end{vmatrix} \begin{vmatrix} m_1 \\ m_2 \end{vmatrix} = \begin{vmatrix} -M \\ 0 \end{vmatrix}$$

$$\begin{vmatrix} 0 & 1 \\ 1 & -1 \end{vmatrix} \begin{vmatrix} m_1 \\ m_2 \end{vmatrix} = \begin{vmatrix} M \\ 0 \end{vmatrix}$$

Figure 2-6: Example 'open process' method

For an open process *no* mass balance of an apparatus is eliminated in the chain. All the mass balances are necessary in the system matrix so that the solution for the system will meet the boundary conditions for the apparatuses.

The following possibilities are available for preparing the system matrix (worked out for Figure 2-6 but this is to be extended to larger systems):

1. Specify the power for an apparatus in the chain and calculate the mass flows (1 mass balance and 1 energy balance).
2. Specify the incoming mass flow of the system and calculate the outgoing mass flow of the system (2 mass balances).
3. Specify the outgoing mass flow of the system and calculate the incoming mass flow of the system (2 mass balances).

Also for open processes one must select energy equations to be specified with a right-hand side such that these are independent of the mass balances. In this example possibility 1 alone gives an independent system if $h_1 \neq h_2$.

Chapter 3

Apparatus models

3.1 Turbine (type 3)

3.1.1 Introduction

The apparatus type 3, the turbine, is used to model an expansion process, irrespective of the medium expanding in the turbine. Each turbine can, in addition to an inlet and an outlet, have a maximum of 8 extractions, as indicated in Figure 3-1. The outlet pressure and the extraction pressures of a turbine cannot be specified with the parameter POUT, but must be calculated from data which are specified for apparatuses or pipes downstream. For off-design calculations the extraction pressures are calculated on the basis of Traupel's formulae [8] (a refinement of Stodola's cone law), provided the following data are known for the turbine, which means specified or calculated by other apparatuses:

- the outlet pressure; this will in general be calculated in off-design situations from data for the condenser;
- a number of results from the design case; these must be specified as "Off-design input data" for the relevant apparatuses. These design data can also be found at the end of the output file (under option View | Text Output).

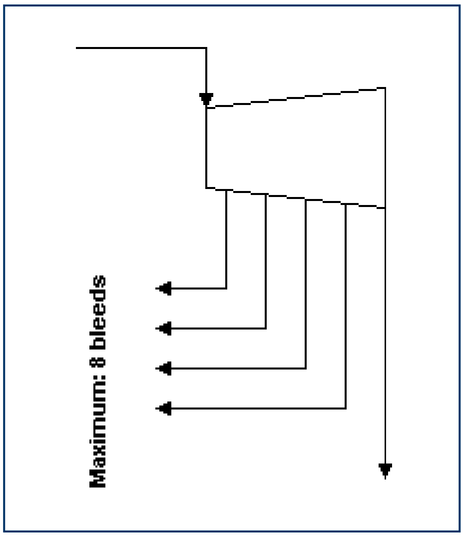


Figure 3-1: Diagram of apparatus type 3, the turbine

The turbines and turbine sections distinguished by the program can be classified in two categories, distinguished from each other by the turbine code TUCODE:

general turbines	TUCODE = 0
specific steam turbines	TUCODE = 10000 and higher

The general turbine type can where necessary also be used as a steam turbine, but is intended more as an expansion section of a gas turbine installation, and as turbine type for various media. The user will have to specify the internal efficiency of the turbine himself, or this must be calculated from the conditions at the inlet and outlet of the turbine.

For a number of types of steam turbine data are available from which the internal efficiency is calculated by the program. If one wants to use these data then one must select the relevant turbine type in accordance with Table 2-2 of part "Reference Guide" of the manual. This is dealt with in more detail in the next paragraph.

3.1.2 The calculation of the isentropic efficiency

As stated in the previous chapter, the isentropic efficiency of a turbine can either be specified by the user or calculated by the program. For a limited number of types of steam turbines the isentropic efficiency can be calculated from data which are incorporated in the turbine code TUCODE, possibly supplemented with data which relate to the geometry of the last stage: DIAOUT and SLENG.

The turbine code TUCODE is a numeric code consisting of five numerals t_1, t_2, t_3, t_4 and t_5. The first numeral t1 typifies the turbine, as set out in Table 3-1; the other numerals are explained in Table 2-2 of part “Reference Guide” of the manual.

Tabel 3-1: The available turbine types

Turbine code (t_1)	**Turbine type**	**Basic value isentr. efficiency (ETHAID)**	**Factor A 1)**
0	general type turbine (gas turbine etc, turbine to drive feed pump)	N/A	N/A
1	intermediate-pressure turbine section (between two reheaters with double reheating)	N/A	N/A
2	high-pressure section (HP) with one-row governing stage	0.8700	$\frac{0.0790669\ N}{\Phi_v}$
3	high-pressure section (HP) with two-row governing stage	0.8400	$\frac{0.106188\ N}{\Phi_v}$
4	non-reheat turbine (combined HP + MP + LP) with two-row governing stage	0.8948	$\frac{0.0338434\ N}{\Phi_v}$
5	condensing section without governing stage, to be used as MP + LP or as LP	0.9193	$\frac{0.0998955\ N}{\Phi_v}$
6	back-pressure section, constant back-pressure, governed by the pressure	0.80	N/A
7	back-pressure section, constant back-pressure, governed by the mass flow	0.80	N/A
8	Condensing section, (cross-compound) MP with 3000 rpm 2) and LP with 1500 rpm 3)	0.9193	$\frac{0.0998955\ N}{\Phi_v}$
9	Condensing section, (cross-compound) MP + LP with 1500 rpm 3)	0.9295	$\frac{0.0998955\ N}{\Phi_v}$

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1) A: correction for the volume flow ; Φ_v: volume flow in m^3/s; N: number parallel flows, for HP-turbines mostly 1, for MP 1 or 2, LP mostly several (For the program maximum 9, practical maximum 6, in exceptional cases 8).

2) 3000 rpm for 50 Hz and 3600 rpm for 60 Hz installations.

3) 1500 rpm for 50 Hz and 1800 rpm for 60 Hz installations.

The efficiencies for the turbine types t1 = 1, 2, 3, 4, 5, 8 and 9 are based on data from General Electric [1]. The efficiencies of the turbine types t1 = 6 and 7 are based on data from Stork (nowadays Stork Energy from Hengelo, the Netherlands). In order to run through the procedures correctly, the required data in accordance with Table 2-2 of the input description are necessary. A summary and brief description of the different turbine types, with the relevant turbine code, is given in

Table 3-1. The basic values given in the table for the isentropic efficiency (ETHAID) are default values in the program: the user can where necessary specify another value, so that developments in the turbine efficiency can be followed, or one can work towards a known internal efficiency.

For turbines or turbine sections with turbine code t1 = 0 the user can himself specify the isentropic efficiency. This can be specified by the user, or must be calculated from the inlet and outlet conditions found. A specified internal efficiency ETHAI can if necessary be amended with user subroutine APSUB. The parameter in the header of this subroutine RESULT corresponds for turbines with the internal efficiency (see example 1 in part "Examples" of the manual as a simple example).

Data of General Electric

For turbine sections with turbine code t_1 = 1 the isentropic efficiency is calculated from the geometry of the turbine using an expression from General Electric, set out graphically in Figure 13 of [1]. Copies of these and other figures used are included in this part of the manual as annex A. In the expression which serves as a basis for Figure 13 the isentropic efficiency is a function of the volume flow in the design situation, and of the pressure ratio between inlet and outlet of the section. Any value specified for the isentropic efficiency (ETHAI), or of the basic value for the isentropic efficiency (ETHAID) in the input data is ignored. The value of the isentropic efficiency in the output of the program includes a pressure drop of 2% over the valves at the inlet of the turbine. In Figure 13 this pressure drop is regarded as external, so that the value printed by the program is somewhat lower than the value found in Figure 13.

For turbines and turbine sections with turbine code t_1 = 2, 3, 4, 5, 8 and 9 correction formulae from General Electric are used to supplement the basic value of the isentropic efficiency ETHAID to the final value ETHAI. These corrections are read off from the figures in [1]. The correction formula looks like the following:

$$\text{ETHAI} = \text{ETHAID} \times (1 - A) \times (1 - B) \times (1 - C) \ldots\text{etc.} \qquad (3\text{-}1)$$

Here:

ETHAI	the calculated isentropic efficiency
ETHAID	basic value of the isentropic efficiency (uncorrected)
A, B, C, etc	correction functions

The basic values for the isentropic efficiency are also the ultimate isentropic efficiency for the conditions, as mentioned in Table 3-2, as no corrections are carried out. For each type of turbine, except for types t1 = 0 and 1, the basic efficiency is corrected for conditions which deviate from the conditions mentioned in Table 3-1, for (the figure numbers refer to the figures in [1]):

- Turbine code $t_1 = 2$ (high-pressure section with single-row governing stage):
    - the volume flow under design conditions;
    - the average diameter (at half blade height) of the row of blades of the governing stage (figure 7);
    - the ratio between the outlet pressure in the design situation and the inlet pressure (figure 6);
    - the mass flow ratio at the inlet, for part load calculations (figures 8 and 9);
    - the number of inlet valves (figure 12).

- Turbine code $t_1 = 3$ (high-pressure section with two-row governing stage):
    - the volume flow under design conditions;
    - the ratio between the outlet pressure in the design situation and the inlet pressure (figure 10);
    - the mass flow ratio at the inlet, for part load calculations (figure 11);
    - the number of inlet valves (figure 12).

Table 3-2: Conditions for which no efficiency corrections are necessary

Turbine-code t_1	$\Phi_{v,d}/t_2$ (m^3/s)	DIAIN (m)	POUTDS / PIN (-)	FMIN / FMIND (-)	t_5 (-)	POUTRT / PIN (-)	Steam inlet-conditions
2	∞	0.965[1]	0.18	1	∞	-	-
3	∞	-	0.18	1	∞	-	-
4	∞	-	-	1	-	0.625	see Figure 3-2
5,8,9	∞	-	-	-	-	-	see Figure 3-2

In this table is:

$\Phi_{v,d}$	volume flow at inlet under design conditions	[m^3/s]
FMIND	mass flow at inlet under design conditions	[kg/s]
FMIN	mass flow at inlet (off-design)	[kg/s]
t_2	number parallel flows in the turbine section (in condensing sections: of the intermediate-pressure turbine	[-]
t_5	number inlet valves for the governing stage of the turbine section (in high-pressure turbines)	[-]

- Turbine code t_1 = 4 (non-reheat turbine, with two-row governing stage):
  - the volume flow under design conditions;
  - the ratio between the pressure at the outlet of the governing stage in the design situation and the inlet pressure (figure 2);
  - the inlet conditions, with a view to the moisture content of the steam at the end of expansion (figure 14);
  - the mass flow ratio at the inlet and the ratio between the inlet pressure and the pressure at the outlet of the governing stage in the design situation, for part load calculations (figure 4);
  - the mass flow ratio at the inlet, for part load calculations (figure 3);
  - the losses over the inlet valves, depending on the mass flow ratio (figure 5).

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[1]) 0.965 m for 60 Hz. For 50 Hz: 1.158 m.

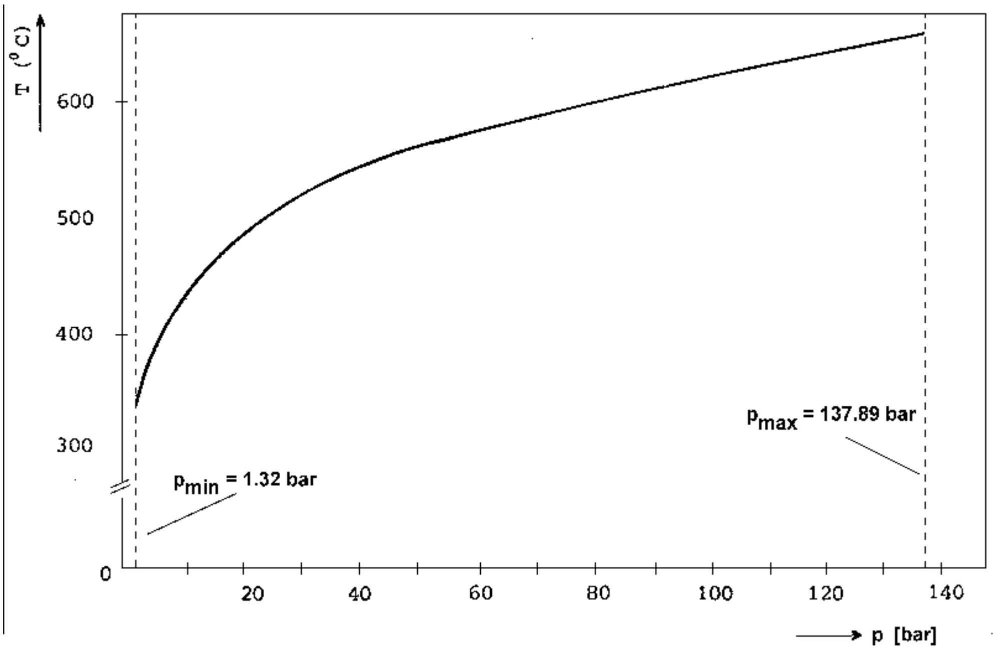

Figure 3-2: Inlet steam conditions for which no efficiency corrections are necessary (see also Table 3-2)

- Turbine code t_1 = 5 (condensing section 3000 or 3600 rpm)
  - the volume flow under design conditions;
  - the inlet conditions of the steam, with a view to the final moisture content (figure 14).

- Turbine code t_1 = 8 (twin-speed condensing section 3000/1500 rpm or 3600/1800 rpm):
  - the volume flow under design conditions;
  - the inlet conditions of the steam, with a view to the final moisture content (figure 14);
  - the expansion in the low-speed part of the section.

- Turbine code t_1 = 9 (condensing section for 1500 rpm or 1800 rpm):
  - the volume flow under design conditions;
  - the inlet conditions of the steam, with a view to the final moisture content (figure 14).

The outlet losses for turbine types 5, 8 and 9 are included in the isentropic efficiency which is printed out by the program, and are also printed out separately, immediately after the isentropic efficiency.

Where the basic value for the isentropic efficiency (ETHAID) is not specified, default values in accordance with Table 3-1 are taken. Since the data date from 1963, and the 1974 update contained no changes to the isentropic efficiencies, the efficiencies calculated are perhaps still on the low side; by selecting a higher basic value for ETHAID than in accordance with the table, one can alter the isentropic efficiency to the state of the technology applied.

If one wants to arrive at a particular value of the isentropic efficiency, then one will have to make an estimate of ETHAID by trial and error. This situation may occur for example when one knows the isentropic efficiency at full load and wants the value for part load to be determined by the program. As shown in (3-1), ETHAI is proportionate to ETHAID; only the outlet loss can cause an alteration here for turbine types 5, 8 and 9. In that case one can, (in different calculations) by having the value of ETHAI calculated for two values of ETHAID, estimate ETHAID by interpolation or extrapolation to arrive at the required value of ETHAI.

Data of Stork

For turbines with turbine code $t_1 = 6$ and 7 (back pressure turbines) a direct method for the calculation of the isentropic efficiency is proposed by VMF Stork (nowadays NEM Hengelo, the Netherlands), and incorporated in the program. For this method corrections are made for part load conditions with respect to the actual value of the isentropic efficiency under design conditions. These corrections are of the form:

$$\mathrm{ETHAI} = \mathrm{ETHAID} \times f\left(\frac{\mathrm{FMIN}}{\mathrm{FMIND}}, \frac{\mathrm{POUTDS}}{\mathrm{PINDS}}\right) \tag{3-2}$$

Here:

FMIN	the mass flow at the inlet	[kg/s]
FMIND	the mass flow at the inlet under design conditions	[kg/s]
POUTDS	the outlet pressure under design conditions	[bar]
PINDS	the inlet pressure under design conditions	[bar]

This relates to different functions for turbines, which are governed with the inlet pressure (for $t_1 = 6$), and turbines which are governed with the mass flow at the inlet (for $t_1 = 7$).

3.1.3 Enthalpies at the extractions

In Figure 3-3 the possible expansion lines for the turbine are set out in the Mollier diagram (h,s diagram). The specific enthalpies at the extractions are determined, by assuming a straight line in the Mollier diagram between inlet conditions and outlet conditions, as in the left-hand figure. For condensing sections with TUCODE = 5mdLe, 8mdLe and 9mdLe a curved expansion line can be selected, by specifying e = 1 (t_5) in the input data. This gives a more absolute value for the specific enthalpy at the extractions; start and end point of the expansion is only affected by the isentropic efficiency, not by the curve of the expansion line. If necessary one can obtain a straight expansion line by specifying e = 0. For the other turbine types the expansion line is always straight.

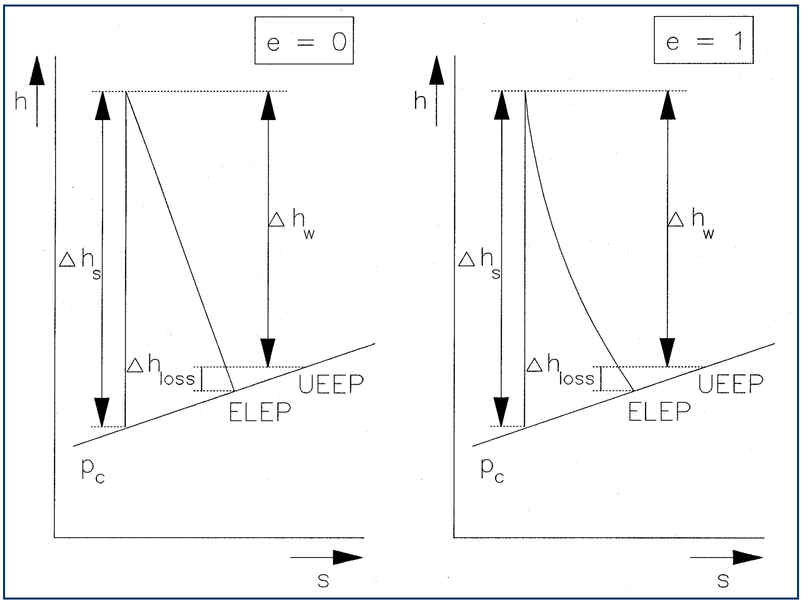

Figure 3-3: expansion lines for condensing sections in the h,s-diagram

e = 0: straight expansion line
e = 1: curved expansion line

The expansion line is fixed, when in addition to the pressures at the inlet and outlet of the turbine another two of the following three variables are known:

- the specific enthalpy at the inlet;
- the specific enthalpy at the outlet;
- the isentropic efficiency.

N.B. The specific enthalpies themselves cannot be specified for turbines; in general the enthalpies will be determined from the pressures and temperatures specified for various apparatuses.

3.1.4 Exhaust losses

Exhaust losses are calculated for the condensing sections t, = 5, 8 and 9, using the procedure of General Electric. The exhaust loss of the non-reheat turbine, type 4, is wrongly not calculated by the program; the calculated power of the turbine is hence too great as the exhaust loss is not deducted from the enthalpy drop over the turbine. For all the other turbine types the exhaust loss is processed in the internal efficiency, as it is a less essential part of the efficiency and because it is not very dependent on the load of the turbine.
The exhaust losses are deduced from the axial speed of the steam at the exhaust of the last row of blades. This speed is calculated from the volume flow and the exhaust area:

$$v_{an} = \frac{\Phi_v}{N \pi D_{out} L_s} \qquad (3\text{-}3)$$

The exhaust loss follows from this with figure 16 (3000/3600 rpm) or 17 (150011800 rpm).

The calculation of the exhaust loss

The value of the exhaust loss is shown in the output under EXHAUST LOSSES in kJ/kg, after the isentropic efficiency of the turbine. The exhaust loss can be read off from figure 16 or 17, depending on the revolutions of the turbine, and must be corrected for turbine efficiency and moisture content, as indicated by Spencer et alia in figure 16 and 17 [11]:

$$UEEP = ELEP + EL \times 0.87 \times (1 - y) \times (1 - 0.65y) \qquad (3\text{-}4)$$

Here:

UEEP	Used Energy End Point: the total enthalpy at the turbine exhaust, also the enthalpy at the inlet of the condenser	[kJ/kg]
ELEP	Expansion Line End Point: the virtual value of the enthalpy at the end of expansion (see Figure 3-3)	[kJ/kg]

EL	Exhaust Loss: the exhaust loss, as read off in figure 16 or 17	[kJ/kg]
y	The mass fraction of moisture in the steam (N.B. in the figures Y is the percentage moisture)	[kg/kg]

The relation with the printed exhaust loss, EXHAUST LOSS, is now:

$$\text{EXHAUST LOSS} = -\,\text{EL} \times 0.87 \times (1 - y) \times (1 - 0.65y) \qquad [\text{kJ/kg}] \qquad (3\text{-}5)$$

In Figure 3-3 the calculation is explained further: the calculated exhaust loss (Δh_{loss} = -EXHAUST LOSS) is added up at the expansion line end point (ELEP) of the condensing section. In this way the specific enthalpy at the turbine exhaust (UEEP) is obtained.

N.B. To calculate the turbine power the specific enthalpy at the turbine exhaust (UEEP) is used in the energy balance. This specific enthalpy is printed as the enthalpy in the pipe at the turbine outlet. The calculated exhaust loss is kept in the program as an enthalpy drop over this outlet pipe of the turbine. A user specified value for DELH in this pipe is ignored by this and overwritten; DELH cannot therefore be specified for outlet pipes of turbines. The enthalpies at the inlet and outlet of the pipe are, in spite of the internal value of DELH, equal to each other, as the printed value of the enthalpy is that of the total enthalpy, that is including the value of the velocity term $\frac{1}{2}v^2$.

Interpretation of the output

The expansion line end point in the turbine cannot be clearly specified. In general the pressure in the condenser is specified, where the velocity of the steam is negligible. At the exhaust of the last row of blades the steam velocity is not negligible (the exhaust of the last row of blades in the program means: the outlet of the turbine). The pressure at this point is dependent on the steam velocity and of the efficiency of the diffusor between the last row of blades and the condenser. The space between the last row of blades of the turbine, including the diffusor, is represented in the scheme by the pipe between the turbine and condenser. The values printed in the output for pressure, temperature, enthalpy and vapor quality for the turbine exhaust must be regarded as notional values (as intended by Spencer et alia). The value of the pressure at the exhaust of the last row of blades will be a little lower than the printed value, as the pressure increases in a diffusor working properly.

The printed value of the enthalpy must be regarded as the total enthalpy, which means that the velocity term is included in the enthalpy:

$$h_{tot} = h_{stat} + ½v^2 \qquad (3\text{-}6)$$

Where:

h_{tot}	the total enthalpy	[kJ/kg]
h_{stat}	the stationary enthalpy	[kJ/kg]
v	the velocity of the steam	[m/s]

The value of the enthalpies for the pipe between the turbine and condenser are equal to each other for this reason: the total enthalpy does not change in the pipe, not even by friction loss or pressure increase in the diffusor. The value of the specific enthalpy at the expansion line end point ELEP is thus not printed, but can if required be calculated from:

$$\text{ELEP} = \text{UEEP} + \text{EXHAUST LOSS} \qquad (3\text{-}7)$$

(EXHAUST LOSS has a value < 0).

The vapor quality (x) at the exhaust from the last row of blades is given at the condenser pressure. The value is hence virtual, but corresponds to the value which Spencer et alia use to calculate the exhaust loss. The printed steam quality in the outlet pipe has a different value for inlet and outlet of the pipe: at the inlet the value of x corresponds with the specific enthalpy at the expansion line end point (ELEP); at the outlet the value of x corresponds with the specific enthalpy at the outlet of the turbine (UEEP), see for example the calculation results of example 6 in part “Examples” of the manual. As a result the user does get a real picture of the steam quality at the exhaust from the last row of blades, which is important in relation to possible erosion of the last row of blades by moisture droplets.

The recovery of pressure in the diffusor after the turbine is included in the calculation of the exhaust loss according to Spencer et alia. Any pressure increase is not however expressed in the method of General Electric, and hence also not in the output of the program (the pressure at the outlet of the turbine and at the inlet of the condenser are equal to each other, as in Figure 3-3). If one wants to deviate from this, then it is possible to simulate the recovery of pressure from the steam velocity in the diffusor, by specifying the pressure at the exhaust from the last row of blades as inlet pressure of the pipe at the outlet of the turbine, in the form of PINL as an extra condition for the relevant pipe. This value must then be lower than

the pressure in the condenser. If necessary a negative value for DELP or DELPR can be specified for the outlet pipe. If one wants to calculate the turbine efficiencies purely with the method of General Electric, then this procedure is not recommended.
The thermodynamic data at the extractions are calculated on the basis of the expansion line, as this results from the conditions at the turbine inlet up to the expansion line end point (ELEP), hence before setting off the exhaust losses. For extractions with a pressure close to the outlet pressure this unfortunately gives an inaccurate value for the enthalpy. In general this inaccuracy will result in a negligible error for the total system, but is marked for extremely low part load fractions.

N.B. Error messages from the programme, relating to turbines, which refer to a figure number, refer to the figures from [1] (see annex A).

Corrections for supersonic annulus velocities

The exhaust loss are calculated on the basis of the exhaust velocity of the steam. If this velocity is above the velocity of sound (approx. 425 m/s), then the pressure at the turbine exhaust is adjusted such that the velocities occurring are subsonic. This method is also described by Spencer et alia [1], and means that the pressure at the outlet from the last row of blades must be increased by the following method:

$$p_{ls} = \frac{v_{an}}{v_s} p_k \tag{3-8}$$

Where:

p_{ls}	pressure at the exhaust of the last row of blades	[bar]
p_k	condenser pressure	[bar]
v_{an}	exhaust velocity of the steam (annulus velocity)	[m/s]
v_s	velocity of sound	[m/s]

Where the annulus velocity even at this higher pressure is still above the velocity of sound, (3-8) is again applied, but then with the previous value of p_{ls} instead of p_k; and this is repeated where necessary until $v_{an} < v_s$. This higher value of the pressure is not however expressed in the output: the value of the condenser pressure specified is retained, and the volume flow is based on this condenser pressure, so that it is simple to later calculate how high the annulus velocity is at this low pressure; one can then quickly calculate how much one must enlarge the passage at the turbine exhaust to obtain subsonic velocities.

The printed value of the exhaust loss is applicabie for the volume flow corrected for the increased pressure, and hence for the corrected velocity. To calculate the isentropic efficiency the increased pressure is assumed for the actual enthalpy drop; for the isentropic enthalpy drop the condenser pressure is assumed. One thus gets a correct picture in the equation (of isentropie efficiencies) with a turbine with a bigger outlet, which does not have a supersonic annulus velocity.

The calculated exhaust losses are applicable for the outlet geometries of General Electric. For other exhaust areas interpolation is carried out between the areas given. This does not result in an exact solution, but is satisfactory.

3.2 Condenser (type 4)

3.2.1 Introduction

The condenser model in accordance with type 4 is carried out as a two-media apparatus. Both media can be chosen at random for a limited design calculation, where the physical data of the media are in the material library of Cycle-Tempo. For the extended design calculation and the off-design calculation the overall beat transfer coefficient (k-value) is calculated. The overall beat transfer equations required for this are available in Cycle-Tempo for a water-cooled steam condenser.

3.2.2 Assumptions

For the model for design calculations

The condenser model is suitable for condensing both superheated and wet vapor of any medium. The vapor can be condensed to saturation, and if necessary the saturated liquid can be aftercooled. It is possible to connect up to 5 inlet pipes for the secondary medium to the condenser, 1 outlet pipe for the condensate must be connected. For the primary medium 1 inlet pipe and 1 outlet pipe must be connected.
With regard to the use of the condenser model two mass equations and possibly 1 energy equation are added to the set of the system equations (see praragraph 3.2.3).

For the model for off-design calculations

The condenser model for off-design is suitable for describing condensation of saturated or wet steam. The heat of condensation must be absorbed by cooling water. In addition the flow on the secondary side must be without pressure drop.

In addition to the two mass equations and the energy equation the overall heat transfer equation is now also available to calculate an extra unknown. The overall heat transfer equation is as follows:

$$Q = U \times A \times \Delta T_{ln} \qquad (3\text{-}9)$$

where:

Q	heat transferred	[kW]
U	overall heat transfer coefficient	[kW/m^2 K]
A	overall heat transfer coefficient	[m^2]
$\Delta T_{\ln}$	log-mean temperature difference	[K]

The heat transfer relations

The overall heat transfer coefficient k is calculated using the instructions as stated in the V.D.I.-Wärmeatlas (edition 1988, 5th impression, parts Gb and Ja). This takes into account:

- the heat transfer of condensing steam to the pipe wall;
- the thermal conduction through the pipe wall;
- the fouling on the cooling water side of the pipe wall and;
- the convective heat transfer from pipe wall to cooling water.

The log-mean temperature difference

The log-mean temperature difference is defined as:

$$\Delta T_{\ln} = \frac{\Delta T_h - \Delta T_l}{\ln \dfrac{\Delta T_h}{\Delta T_l}} = \frac{(T_{cond} - T_{cw,out}) - (T_{cond} - T_{cw,in})}{\ln \dfrac{(T_{cond} - T_{cw,out})}{(T_{cond} - T_{cw,in})}} = \frac{T_{cw,in} - T_{cw,out}}{\ln \dfrac{(T_{cond} - T_{cw,out})}{(T_{cond} - T_{cw,in})}} \qquad (3\text{-}10)$$

When more than 4 pipes are connected to the condenser one looks at the temperatures in the main steam pipe and the temperatures in the cooling water pipes. The effects of other incoming flows on the temperatures in the condenser are ignored.

3.2.3 Calculation options for the design calculation

For the design calculation only the mass balances are used (included in the set of system equations) and the energy equation:

$$\Sigma\,(\Phi_{m,in} \times h_{in}) - \Sigma\,(\Phi_{m,out} \times h_{out}) = \Delta E \qquad (3\text{-}11)$$

The energy equation of the condenser can be used in two ways in the calculation.
The first option, which can be selected by making the EEQCOD (Energy EQuation CODe) 1, uses the energy equation to calculate an unknown mass flow. This possibility can for example be chosen when one wants to calculate the required quantity of cooling water. The energy equation is in this case added to the set of system equations:

$$A\,\underline{m} = \underline{b}$$

The unknown mass flow is then calculated when solving the set.

In the second option, for which the EEQCOD must be 2, the energy equation is used to calculate an unknown enthalpy. When a second state variable (e.g. the pressure) in the relevant pipe is known, the unknown temperature can be calculated.

Calculation of a unknown mass flow (EEQCOD = 1)

Before the set of system equations can be solved, first the coefficients of the energy equation, the enthalpies, are determined. The enthalpies can be calculated when two state variables in the relevant pipe are known. These two state variables can be:

- specified in the apparatus data;
- calculated in the light of the differences specified in the apparatus data (e.g. a pressure difference) over the apparatus;
- specified in or calculated from the apparatus data of adjacent apparatus and transmitted via the connecting pipe, taking into account any pipe losses.

In addition the right hand side of the equation, the energy exchange with the environment, must be known. This must be specified in the apparatus data.
The set of system equations can now be solved, so that the mass flows can be determined.

Calculation of an unknown temperature (EEQCOD = 2)

When the energy equation is used to calculate an unknown temperature, the mass flows must be known from the energy equation. For the first iteration run an initial value is chosen for the mass flow ratio. For the following iteration runs the mass flows are used which are calculated in the previous iteration run. The energy exchange with the environment must be specified in the apparatus data.

The enthalpies from the energy equation can be determined in the same way as described in paragraph 3.2.4, except for the pipe for which the temperature must be calculated. The unknown enthalpy can now be solved from the energy equation. The unknown temperature is then known as a function of the enthalpy and another state property.

3.2.4 Calculation options for the off-design calculation

Also for the off-design calculation the two mass equations and the energy equation is used. The energy equation can be used again to calculate either an unknown mass flow (EEQCOD=I) or an unknown enthalpy (EEQCOD = 2). In addition the thermal transfer equation is also availabie to calculate an extra unknown temperature. Below the possible calculation options are described which result from this.

Calculation of an unknown mass flow (EEQCOD = 1)

The energy equation is in this case added to the set of systemequations and is used to calculate an unknown mass flow. In addition it is possible with the heat transfer equation to calculate an unknown temperature. The following options are thus possible:

Mass flows		**Temperatures**		
Cooling water	Steam	$T_{cw,out}$	T_{cond}/p_{cond}	Other
u	K	u	K	K
u	K	K	u	K
K	u	u	K	K
K	u	K	u	K

K = known, specified for an apparatus or to be determined from another apparatus

u = unknown, to be calculated with the equations of the condenser model

Calculation of an unknown temperature (EEQCOD = 2)

The energy equation is in this case not added to the set of system equations but is used to calculate an unknown enthalpy. In addition it is possible with the heat transfer equation to calculate an extra unknown temperature. The following option is then possible:

Mass flows		**Temperatures**		
Cooling water	Steam	$T_{cw,out}$	T_{cond}/p_{cond}	Other
u	K	u	K	K

K = known, specified for an apparatus or to be determined from another apparatus model

u = unknown, to be calculated with the equations of the condenser model

3.3 Combustor (type 13)

3.3.1 Applications

The combustor model in Cycle-Tempo is suitable for various applications. To get an idea, in setting it up the requirements arising out of three specific applications have been taken into account:

- model for the combustor of a gas turbine;
- model for the furnace of a steam generator;
- model for an additional-firing burner or afterburner.

These applications result in different requirements with regard to the input data and the variables to be calculated. Before going into the possible combinations of input data, first the general assumptions of the model are explained.

3.3.2 Assumptions

Heat transfer in the combustor

In the model no allowance is made for the heat exchanging area in the combustor. However in order for example to model a hearth including heat exchanging area, in Cycle-Tempo one or more heat exchangers can be included after the combustor. In addition it is possible to specify a heat loss Q_{loss}.

Fuels

In the combustor model a number of fuels can be used. With the help of the input window for pipe data, the following fuels can be specified:

- Solid or liquid fuels with unknown chemical composition:
    - mass fractions of the present elements and the lower heating value specified;
    - molar fractions of the present elements and the lower heating value specified;
    - standard composition.

- Gaseous fuels:
    - molar fractions specified;
    - standard Slochteren natural gas.

Flue gas composition

In the combustor a chemical reaction takes place between the fuel and oxidant. The heat released here is determined by the course of the reaction, i.e. the composition of the reaction product (flue gas). In order to determine the heat produced, it is therefore essential to calculate this composition.

Under ideal conditions (residence time, mixture), the composition of the flue gas will be the same as the equilibrium composition corresponding to the composition of the reactants and the reaction conditions (p_{react},T_{react}). Under actual conditions the reactions will however not run to equilibrium. The degree to which the initial composition differs from the equilibrium composition is determined by factors which depend on the design of the combustor, so that a general model for the incomplete course of the reactions within Cycle-Tempo is meaningless. In the combustor model in Cycle-Tempo the equilibrium composition is taken into account. It is however possible to allow the flue gas composition to differ from the equilibrium composition by not letting part of the reactants take part in the reaction. For each component or for a pipe as a whole (oxidant or fuel pipe) a molar or mass fraction is specified which does not react but is passed directly to the flue gas pipe where this bypass flow is mixed with the reaction products (see **Reaction data** in paragraph 4.2 of part “Cycle-Tempo Operation” of the manual). In addition it is possible to specify the equilibrium pressure and temperature entirely independently of the outlet conditions.

Data on the inlet side

One last assumption is that temperatures and compositions on the inlet side must always be specified or calculated in the previous apparatus.

3.3.3 Calculation options for the mass flows

As remarked different applications impose different requirements with regard to the available input data and required output. The most important variables which can be both calculated and specified are:

- outlet temperatures (ash, flue gas);
- mass flows (oxidant, fuel, flue gas, ash);
- pressures and pressure drops;
- air factor (λ).

If we leave the ash pipe out of account for the moment, there are 3 mass flows in the combustor model: oxidant, fuel and flue gas. Since in Cycle-Tempo a total mass balance is prepared for each apparatus, this means that in order to establish the mass flows, 2 further equations are necessary. For this 3 different relations are used:

1. Where a mass flow is calculated in another apparatus, an equation is automatically added to the system matrix.

2. With the specification of the temperature at the outlet, the mass ratio oxidant/fuel is established. Since the inlet temperatures are known, this ratio follows from the energy equation over the combustor.

3. Finally an air factor can also be specified. On the basis of the composition of oxidant and fuel the program in this case determines the mass ratio and again adds this relation to the system matrix.

The specification of both the outlet temperature and λ is not possible, as these both determine the mass ratio oxidant/fuel. This means that 1 mass flow must always be specified using the total mass balance, so that there are three options with regard to the mass flows:

Option 1

Specify or calculate elsewhere 2 mass flows. The third mass flow can now be calculated with the help of the total mass balance. The energy balance can be used to calculate the flue gas temperature.

Option 2

Specify or calculate elsewhere 1 mass flow and the flue gas temperature. The 2 unknown mass flows can then be solved from the total mass balance and the oxidant/fuel ratio calculated from the energy equation.

Option 3

Specify or calculate elsewhere 1 mass flow and specify the air factor λ. To solve the 2 unknown mass flows the mass balance and the calculated oxidant/fuel ratio is used.

In the above the ash pipe is not taken into account. Where the user does not define an ash pipe, all the components are discharged to the flue gas pipe. If however an ash pipe is specified, then the substances which are discharged to the ash pipe are determined in the following way:

- The non-gaseous components Al_2O_3(s), Al_2O_3(l), Fe_2O_3, SiO_2(s) and SiO_2(l), are automatically discharged to the ash pipe. The same happens for the solid carbon formed during the reaction. In order to discharge a solid component or a part of this to the flue gas pipe any way, the “Bypass components” button can be used (see **Reaction data** in paragraph 4.2 of part “Cycle-Tempo Operation” of the manual).
- Via the “Separate components” button one can specify for each component that a particular fraction of the substances supplied via the oxidant or fuel pipe, without taking part in the reaction, is discharged directly to the fuel pipe (see **Reaction data** in paragraph 4.2 of part “Cycle-Tempo Operation” of the manual).

If the ash pipe is connected, the program calculates an ash/fuel ratio and adds this ratio to the system matrix.

For the 3 options we can now prepare the system matrix. For this the following notation is used:

Φ_m = mass flow [kg/s]
OF = **O**xidant/**F**uel ratio [kg/kg]
AF = **A**sh/**F**uel ratio [kg/kg]

Indices:

fu = fuel

ox = oxidant

fg = flue gas

as = ash

Option 1 **2 mass flows specified or calculated elsewhere**

Equation						
1. total mass balance	1	1	1	-1	$\Phi_{m,fu}$	0
2. is placed in system matrix for another apparatus	-	-	-	-	$\Phi_{m,ox}$	-
3. Idem 2	-	-	-	-	$\Phi_{m,fg}$	-
4. mass ratio ash/fuel (AF)	x_{as}	0	0	-1	$\Phi_{m,as}$	0

Note:

- equation 4 is only added where ash pipe is connected
- the energy equation is used to determine the flue gas temperature

Option 2 **1 mass flow and flue gas temperature specified or calculated elsewhere**

Equation						
1. total mass balance	1	1	-1	-1	$\Phi_{m,fu}$	0
2. is placed in system matrix for another apparatus	-	-	-	-	$\Phi_{m,ox}$	-
3. mass ratio oxidant/fuel (OF) calculated from energy equation	OF	0	-1	0	$\Phi_{m,fg}$	0
4. mass ratio ash/fuel (AF)	AF	0	0	-1	$\Phi_{m,as}$	0

Note:

- Equation 4 is only added where ash pipe is connected

Option 3 **1 mass flow specified or calculated elsewhere and air factor specified**

Equation						
5. total mass balance	1	1	-1	-1	$\Phi_{m,fu}$	0
6. is placed in system matrix for another apparatus	-	-	-	-	$\Phi_{m,ox}$	-
7. mass ratio oxidant/fuel (OF) calculated from air factor	OF	0	-1	0	$\Phi_{m,fg}$	0
8. mass ratio ash/fuel (AF)	AF	0	0	-1	$\Phi_{m,as}$	0

Note:

- equation 4 is only added where ash pipe is connected
- the energy equation is used to determine the flue gas temperature

Options regarding the compositions of flue gas and ash

In the combustor model the incoming streams (oxidant and fuel) are split into three separate streams. Part of the oxidant and the fuel is only heated up to the flue gas temperature, but does not take part in the combustion reaction. For each component and pipe, the user may specify what fraction of the added oxidant and fuel remain outside the reaction. The variables in this stream are indicated with the index '**ncec**' (**N**on **C**hemical **E**quilibrium **C**omposition). In the same way a part of the oxidant and fuel stream is passed directly to the ash pipe. Here heating up to the ash temperature takes place. Where this is not specified or calculated elsewhere, this is equal to the flue gas temperature.

The main stream reacts to equilibrium and is therefore marked with the index **cec** (**C**hemical **E**quilibrium **C**omposition). After the reaction this stream is cooled down to the flue gas temperature.

When no data are given by the user with regard to the reaction conditions p_{react} and T_{react}, the program calculates the equilibrium under the outlet conditions p_{out} and T_{out}. The user can also specify the reaction conditions himself or a difference between the calculated outlet conditions and the equilibrium conditions (Δp_{react} and ΔT_{react}). In this latter case the calculation is carried out with:

$$p_{react} = p_{out} - \Delta p_{react}$$

$$T_{react} = T_{out} - \Delta T_{react}$$

3.3.4 Calculations and relations

In this paragraph the different calculations and relations which are used in the combustor model are explained. These are successively:

- calculation of oxidant fraction OF from the flue gas temperature;
- calculation of oxidant fraction OF from the air factor;
- calculation of the flue gas temperature;
- calculation of the equilibrium composition;
- calculation of the pressures.

The following notations are used:

h	specific enthalpy	[kJ/kg]
Φ_m	mass flow	[kg/s]
Q	heat transmitted	[kW]
y	concentration	[mole/mole]

Calculation of the oxidant/fuel ratio from the flue gas temperature

To calculate the oxidant/fuel ratio, the energy equation is used for the calculation. In order to solve this the enthalpy of the flue gases is determined. This enthalpy is, apart from the temperature, also dependent on the composition. This composition is in turn very much dependent on the mass ratio oxidant/fuel (OF).
This means that this ratio cannot be solved explicitly from the energy equation. In order to determine OF an iterative procedure is necessary.

The program therefore calculates for each main iteration a correction to the oxidant/fuel ratio and uses this to calculate a new composition in the following iteration:

$$OF^{(i+1)} = OF^{(i)} + \Delta OF^{(i)} \qquad (3\text{-}12)$$

where: $\Delta OF^{(i)}$ = calculated correction in ith iteration

If in the ith iteration a flue gas temperature $T_{fg}^{(i)}$ is calculated which differs from the required flue gas temperature T_{req}, then an extra quantity of oxidant must be added where $(T_{fg}^{(i)} - T_{req})$ is positive, while with a negative temperature difference, the oxidant/fuel ratio must fall. One can regard ΔOF_{ox} as the extra quantity of oxidant which must be mixed with the flue gases to obtain the required flue gas temperature. Both for and after the correction the energy balance must apply.

In the situation as this is calculated the following applies:

$$h_{ox}(T_{ox}) \times OF + h_{fu}(T_{fu}) = \\ h_{fg}(T_{fg}^{(i)}) \times (1 + OF^{(i)}) + h_{as}(T_{as}) \times AF - Q_{loss} \tag{3-13}$$

Including the extra quantity of oxidant the energy equation:

$$h_{ox}(T_{ox}) \times (OF^{(i)} + \Delta OF^{(i)}) + h_{fu}(T_{fu}) = \\ h_{fg}(T_{fg}^{(i)}) \times (1 + OF^{(i)} + \Delta OF^{(i)}) + h_{as}(T_{as}) \times AF - Q_{loss} \tag{3-14}$$

where: h_{fu}, h_{ox} = enthalpies belonging to the calculated compositions.

h_{fg}^{*} is the enthalpy of the mixture of flue gas and extra oxidant. As the composition is altered by mixing in oxidant, the thermal capacity of the flue gases has obtained a different value. As a result the enthalpy (at the same temperature) of the diluted flue gases differs from the first value calculated. The corrected enthalpy can be calculated from the oxidant and flue gas enthalpy, since for an ideal gas mix the following applies:

$$h_{mixture} = \sum_j x_j h_j$$

where x_j = mass fraction of component j

If we apply this to h_{fg}^{*} we find:

$$h_{fg}^{*}(T_{req}) = \frac{\Delta OF \times h_{ox}(T_{req}) + (1 + OF) \times h_{fg}(T_{req})}{1 + OF + \Delta OF} \tag{3-15}$$

Combining equ. (3-13) and (3-14) gives:

$$h_{ox}(T_{ox}) \times \Delta OF^{(i)} = h_{fg}^{*}(T_{req}) \times (1 + OF^{(i)} + \Delta OF^{(i)}) - h_{fg}(T_{fg}^{(i)}) \times (1 + OF_{ox}^{(i)}) \qquad (3\text{-}16)$$

Filling in here equation (3-15) and making ΔOF explicit gives:

In the ith iteration the temperature $T^{(i)}$ is now calculated as flue gas temperature. On basis of this a correction is calculated for the oxidant/fuel ratio ($\Delta OF^{(i)}$) and a new estimate made for the mass ratio oxidant/fuel ($OF^{(i+1)}$). This is used in the i+1th iteration to calculate the new compositions and temperatures.

Calculation of OF from the air factor λ

Between the air factor λ and the mass ratio oxidant/fuel OF there is the following relation:

$OF = \lambda \times OF_{st}$ where: OF_{st} = stoichiometric mass ratio oxidant/fuel

OF_{st} is the oxidant/fuel ratio where there are just enough oxygen atoms present to let all the fuel react completely. This does *not* include those reactions with oxygen which are the side effects of combustion; formation of sulphur oxides, nitrogen oxides, etc. Decisive for the required O molecules is then the number of H and C molecules.

Say: $\nu_{H,n}$ = number H atoms in component n
$\nu_{C,n}$ = number C atoms in component n
$\nu_{O,n}$ = number O atoms in component n

Then the following applies:

$$OF_{st} = \frac{\sum\limits_{fuel} \left(\nu_{C,n} + \tfrac{1}{2}\nu_{H,n} - \nu_{O,n}\right)}{\sum\limits_{oxid} \left(\nu_{C,n} + \tfrac{1}{2}\nu_{H,n} - \nu_{O,n}\right)} \qquad (3\text{-}18)$$

Use of equation (3-18) now supplies the oxidant/fuel ratio.

Calculation of the flue gas temperature

When the energy equation is not used to calculate a mass flow, then this can be used to determine the temperature of the flue gas. The energy equation over the combustor is :

$$\Phi_{m,ox} \times h_{ox} + \Phi_{m,fu} \times h_{fu} = \Phi_{m,as} \times h_{as} + \Phi_{m,fg} \times h_{fg} = Q_{loss} \tag{3-19}$$

The temperatures and compositions of oxidant and fuel are known, so that the terms in the right hand side can be calculated. Q_{loss} is either specified or has a default value of 0. If the temperature in the ash pipe is known, h_{rg} can now be determined. Where the temperature of the ash is not specified, this is taken as equal to the flue gas temperature. If this must be calculated, then to calculate the term $\Phi_{m,as}h_{as}$, the flue gas temperature is taken from the previous iteration:

$$\Phi_{m,fg} \times h_{fg}(T_{fg}^{(i)}) = \Phi_{m,ox} \times h_{ox} + \Phi_{m,fu} \times h_{fu} - \Phi_{m,as} \times h_{as}(T_{fg}^{(i-1)}) - Q_{loss} \tag{3-20}$$

To determine the temperature of a gas mix at a given enthalpy, pressure and composition, functions are present in Cycle-Tempo. With these the flue gas temrperature can now be determined.

Calculation of the chemical equilibrium

In Cycle-Tempo the following functions are present to calculate the chemical equilibrium:

$y_{cec} = f_1(T_{react},\ p_{react},\ y_{react},\ n_{react})$
$y_{cec} = f_2(H_{react},\ p_{react},\ y_{react},\ n_{react})$
$n_{cec} = f_3(T_{react},\ p_{react},\ y_{react},\ n_{react})$
$n_{cec} = f_4(H_{react},\ p_{react},\ y_{react},\ n_{react})$
$T_{cec} = f_5(H_{react},\ p_{react},\ y_{react},\ n_{react})$

where:

T_{react}	reaction temperature	[°C]
H_{react}	reaction enthalpy	[kJ]
p_{react}	partial reaction pressure	[bar]
y_{react}	composition of the reactants	[mole/mole]
y_{cec}	composition at chemical equilibrium	[mole/mole]
n_{react}	number mole reactants	[mole]
n_{cec}	number mole at chemical equilibrium	[mole]

The partial reaction pressure follows from:

$$p_{react} = p_{react} \times \frac{n_{cec}}{n_{cec} + n_{ncec}} \tag{3-21}$$

where:

n_{cec}	number mole gaseous reaction product
n_{ncec}	number mole non-reacting gas

The number mole released in the reaction is not yet known when computing p_{react} An iterative process is then necessary. For this the main iteration process of Cycle-Tempo is taken. . This means that for n_{cec} the value from the previous iteration is used:

$$p_{react}^{(i)} = p_{react} \times \frac{n_{cec}^{(i-1)}}{n_{cec}^{(i-1)} + n_{ncec}} \tag{3-22}$$

The reaction enthalpy follows from:

$$H_{react} = \Phi_{m,fg} \times h_{fg} - \Phi_{m,ncec} \times h_{ncec} \qquad (3\text{-}23)$$

Here h_{fg} can be determined from the energy balance over the combustor (see above).
To calculate the enthalpy of the non-reacting gases, the flue gas temperature must be known. This does however depend on the equilibrium composition and is hence not yet known. For this reason the flue gas temperature from the previous iteration is used:

$$H_{react}^{(i)} = \Phi_{m,fg} \times h_{fg}^{(i)} - \Phi_{m,ncec} \times h_{ncec}(T_{fg}^{(i-1)}) \qquad (3\text{-}24)$$

If the reaction temperature is specified, the equilibrium composition on the basis of this value is known. If this is not the case, then the reaction enthalpy is used. In addition to the composition, the reaction temperature is then also calculated.

3.4 MCFC and SOFC fuel cell (type 21)

3.4.1 Introduction

Cycle-Tempo includes models for five types of fuel cells: among which molten carbonate fuel cells (MCFC) and solid oxide fuel cells (SOFC). Figure 3-4 presents the principles of both types diagrammatically.

Various types of design can be modelled for both fuel cell types:

- reforming : external or internal reforming
- flow type : co-flow or counter flow

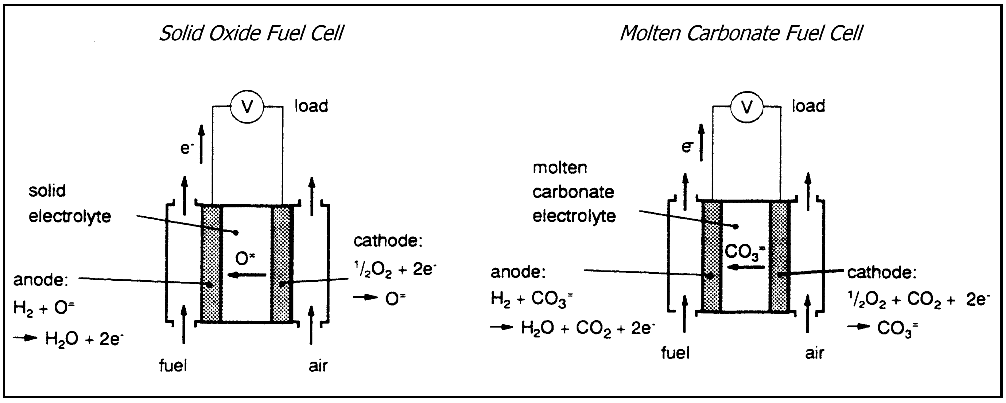

Figure 3-4: Principle of the SOFC and MCFC

3.4.2 Mass equations

The fuel cell model adds two, three or four equations to the system matrix, depending on the number of mass flows that is established by the processes in the fuel cell.

The mass balance over the apparatus is added automatically:

$$\Phi_{m,\, a,\, in} + \Phi_{m,\, c,\, in} - \Phi_{m,\, a,\, out} - \Phi_{m,\, c,\, out} = 0 \qquad (3\text{-}25)$$

The second equation, which is automatically added to the system matrix, is the equation that describes the mass exchange between cathode and anode ($\Phi_{m,\, c \rightarrow a}$):

$$\Phi_{m,\, a,\, in} - \Phi_{m,\, a,\, out} = - \Phi_{m,\, c \rightarrow a} \tag{3-26}$$

If the mass flow fuel ($\Phi_{m,\, fuel}$) has not been calculated elsewhere, it is determined from the generated electrical power, the fuel utilisation and the efficiency of the DC/AC conversion. In this case, the following equation is added to the system matrix:

$$\Phi_{m,\, a,\, in} = \Phi_{m,\, fuel} \tag{3-27}$$

If the mass flow oxidant is not calculated in another apparatus, it can be established by specifying:

1. the outlet temperature of the fuel cell, or
2. the oxidant utilisation.

In the first case (EEQCOD=1), the energy balance is added to the system matrix:

$$\Phi_{m,\, a,\, in} \times h_{a,\, in} + \Phi_{m,\, c,\, in} \times h_{c,\, in} - \Phi_{m,\, a,\, out} \times h_{a,\, out} - \Phi_{m,\, c,\, out} \times h_{c,\, out} = P_{DC} + Q_{loss} \tag{3-28a}$$

If the oxidant utilisation (the second case) has been specified, the oxidant/fuel ratio X_{OF} [kg/kg] is calculated in the model and used in the system matrix:

$$X_{OF} \times \Phi_{m,\, a,\, in} - \Phi_{m,\, a,\, out} \tag{3-28b}$$

If the oxidant utilisation has been specified or the mass flow oxidant is calculated elsewhere, the energy balance is used to calculate the outlet temperature (EEQCOD=2), in which case identical temperatures are assumed for anode and cathode outlets.

3.4.3 Modelling of the process in the fuel cell

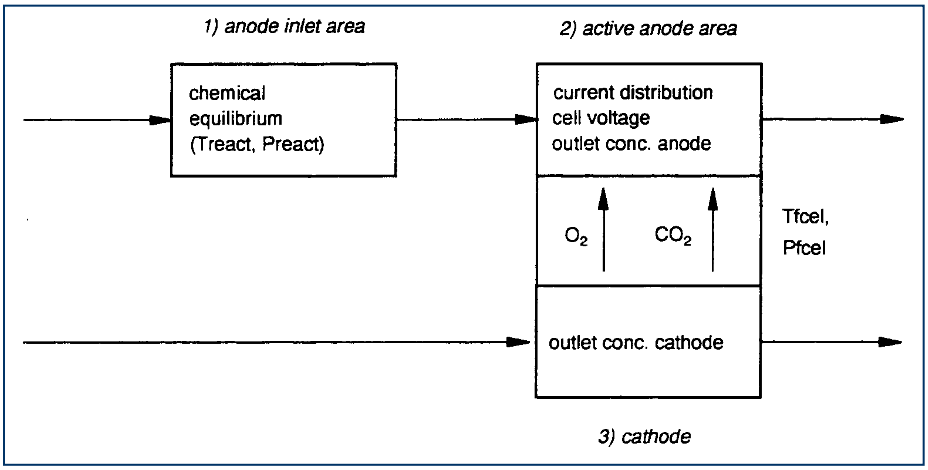

Figure 3-5: Framework of the model

Figure 3-5 shows how the process is modelled in the fuel cell.

Block 1

If the reaction temperature is specified, the fuel is supposed to react to chemical equilibrium at (p_{react}, T_{react}). This calculation block can be used, for instance, to model a (pre)reforming reaction in the cell stack. This process is assumed to occur at a constant temperature; it is assumed that the necessary heat is taken from the reactions in the fuel cell.

Block 2

In this block that models the active cell area, the cell voltage V, the cell flow I and the electrical output power P_e are calculated. It is supposed that the processes occur at a **constant temperature** and **pressure:** the average cell temperature and pressure (p_{fcell}, T_{fcell}) specified by the user.

If all fuel components [1] in the fuel cell are converted, the flow through the fuel cell is equal to:

---

[1] H_2, CO and CH_4 are considered to be fuel components: the contribution of higher hydrocarbons is neglected.

$$I_F = \frac{\Phi_{m,a,in}}{M_{mol,a}} \times 2F \times (y^0_{H_2} + y^0_{CO} + 4y^0_{CH_4}) \qquad (3\text{-}29)$$

in which y^0_i are the concentrations at the inlet, and $M_{mol,a}$ is the mole mass of the anode gas. In reality, only part of the fuel in the fuel cell is converted; the ratio between the real and the maximum conversion is specified by the **utilisation level** U_F. The real cell flow I follows from:

$$I = I_F \times U_F \qquad (3\text{-}30)$$

The relations that are used to calculate the cell voltage will be dealt with in section 3.
The electrical output power of the fuel cell stack is identical to:

$$P_e = V \times I \times \eta_{DCAC} \qquad (3\text{-}31)$$

Apart from cell voltage and cell flow, the composition at the anode outlet is also calculated in this block. The quantities of H_2 and CO that are converted on the cell area are calculated from the cell flow I, using Faraday's law. It is assumed that the shift reaction (and at internal reforming (IR) also the reforming reaction) always occurs at equilibrium on the electrode area, at the cell temperature and pressure.

Block 3

The mass transport of cathode to anode (O_2 for the SOFC, O_2 and CO_2 for the MCFC) is also calculated from the cell flow I. The total mass flow O_2 from cathode to anode is given by:

$$\Phi_{m,O_2,c\rightarrow a} = M_{mol,O_2} \times \frac{I}{4F} \qquad (3\text{-}32)$$

In addition, CO_2 is also transported from the cathode to the anode in the MCFC. For this mole flow, it holds that:

$$\Phi_{m,CO_2,c\rightarrow a} = M_{mol,CO_2} \times \frac{I}{2F} \qquad (3\text{-}33)$$

From the mole balances for the components at the cathode, the composition at the cathode outlet can now be calculated.

Energy balance

Using the energy balance over the apparatus (blocks 1 to 3), the temperature at the outlet is calculated: the temperatures at the anode and cathode outlets are assumed to be identical.

3.4.4 Relations for calculating the cell voltage

Figure 3-6 shows two designs of fuel cells diagrammatically: the tubular monocell (Figure 3-6a) that is applied in several SOFC designs, and the flat-plate cell (Figure 3-6b), the usual MCFC design.

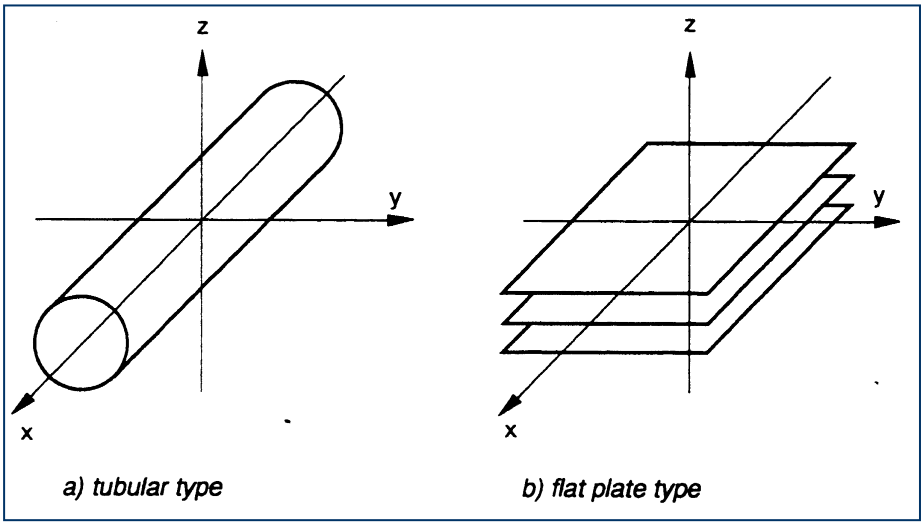

Figure 3-6: Types of design of fuel cells

To calculate i_m, V and P_e, use is made of a one-dimensional model of the active surface. That is, the temperatures, pressures and compositions are supposed to be constant in a cross-section, perpendicular to the direction of the fuel cell flow. In the model of the cell area, the distribution of the flow density is calculated in the x-direction along the cell area (i.e. in the direction of the flow of the fuel). The following **local variables** (indicated with index x) are calculated:

- reversible voltage E_x
- current density i_x
- concentrations y_x (H_2, CO, H_2O, CO_2 and CH_4)

This section states the relations (in an implicit form) from which these variables are solved.

If the processes in a cross-section x of the fuel cell occur without losses, the cell voltage is identical to the **reversible voltage** or **Nernst voltage** E_x. For the SOFC, the reversible voltage, if the gases are supposed to behave ideally, is identical to:

$$E_x = E^0{}_T + \frac{RT_{cell}}{2F} \ln\left\{ \frac{y_{O_2,c}^{1/2}\ y_{H_2,a}}{y_{H_2O,a}} \times p_{cell}^{1/2} \right\} \tag{3-34a}$$

And for the MCFC:

$$E_x = E^0{}_T + \frac{RT_{cell}}{2F} \ln\left\{ \frac{y_{O_2,c}^{1/2}\ y_{H_2,a}\ y_{CO_2,c}}{y_{H_2O,a}\ y_{CO_2,a}} \times p_{cell}^{1/2} \right\} \tag{3-34b}$$

$E^o{}_T$ is the standard reversible voltage for hydrogen, that only depends on the temperature, and is calculated from the change in the Gibbs energy ΔG:

$$E^0{}_T = + \frac{\Delta G_T^0}{2F} \tag{3-35}$$

The second term in the equation (3-34) is a corrective term for the real partial pressures.

In reality, the processes in the cell occur irreversibly, so that the cell voltage V_x (the real voltage difference between the electrodes) is smaller than the reversible voltage. The difference between reversible and real voltage is indicated with the voltage loss ΔV_x:

$$V_x = E_x - \Delta V_x \tag{3-36}$$

In the model, it is assumed that the voltage losses on the level of the electrodes are negligible in the x-direction. This means that the cell voltage is supposed to be constant over the fuel cell. Thus, equation (3-36) becomes as follows:

$$V = E_x - \Delta V_x \tag{3-37}$$

The voltage loss can be regarded as the driving force for the reactions in the fuel cell, and thus for the current density. On the basis of [1] it is now assumed that the current density is proportional to the voltage loss. By analogy with Ohm's law, the proportionality constant is indicated with the **equivalent cell resistance** R_{eq} [ohm m^2]. It then follows for the current density in the cross-section x that:

$$i_x = \Delta V_x / R_{eq} \tag{3-38}$$

Finally, the velocity with which H_2 is converted in a cross-section x, can be calculated from the current density:

$$\frac{dn_{H_2}}{dx} = \frac{i_x}{2F} \tag{3-39}$$

The changes in the concentrations of the components can be calculated using this equation, the mole balances for the components and the reaction balances for shift and (possibly) reforming reactions.
On the basis of the given equation, the voltage and current density can be calculated in a cross-section. Use is made of numerical routines to calculate the course of these quantities over the cell.

List of symbols

A	=	cell area	[m^2]
E	=	reversible voltage	[V]
Eo	=	reversible voltage at standard pressure (1 bar)	[V]
F	=	Faraday's constant	[C/mole]
i	=	current density	[A • m2]
I	=	current	[A]
n	=	number of moles	[mole]
Φ_m	=	mass flow	[kg/s]

M_{mol} = mole mass [kg/mole]
p = pressure [bar]
P = power [kW]
Q_{loss} = heat loss [kW]
R = universal gas constant [kJ/moleK]
R_{eq} = cell resistance [ohm • cm^2]
T = temperature [K]
V = cell voltage [V]
U_F = fuel utilisation [-]
x = distance from inlet [m]
X_{OF} = oxidant/fuel ratio [-]
y_j = mole fraction component j [-]
$y^o{}_j$ = mole fraction component j at the inlet [-]
ΔG = change in Gibbs energy [kJ/mole]
ΔG_o = change in Gibbs energy at standard pressure (1 bar) [kJ/mole]
ΔV = voltage loss [V]
η_{DCAC} = efficiency of DC/AC-conversion [-]

Indices

a = anode
c = cathode
$c \rightarrow a$ = from cathode to anode
DC = direct current
e = electric
F = fuel
m = mean
T = at given temperature T
x = cross-section at distance x = x

3.5 Moisture separator (type 22)

3.5.1 The operation of a moisture separator

Apparatus type 22 is a moisture separator. The incoming gas is cooled by a cooling medium flowing in the opposite direction, as a result of which water vapour condenses. The condensate formed is collected and discharged via a separate pipe.

3.5.2 Assumptions of the model

In the model it is assumed that the pressures of the moisture separated and the outgoing gas are equal and that the temperature of the moisture separated is 1 C lower than that of the outgoing gas. The gas leaves the separator saturated.

3.5.3 Options in the calculations

Pressures and temperatures can be specified both by the user or obtained from apparatus located upstream or downstream. If the outlet pressure or temperature of the gas is not specified by the user, then the user must give an estimate of these parameters with ESTPGS or ESTTGS in order to calculate the quantity of moisture separated in the first iteration. For other iterations the pressure and the temperature from the previous iteration are used for this.

In addition for both the cooling medium and gas the pressure drops and temperature increases are specified. For the gas these are always between the gas inlet and outlet pipe. For the condensate discharge pipe no thermodynamic parameters can be specified since these are always related to the gas outlet pipe (see part “Reference Guide” of the manual).

3.5.4 Formulae used

The three mass equations (mass balance, secondary equation of the cooling medium and the equation for the quantity of condensate separated, i.e. the specified mass equation) and the energy equation of the cooler are all used in the system matrix, to calculate mass flows.

The mass equation, which relates to the quantity of condensate separated, looks like the following:

$$XC \times \Phi_{m\,gas,in} - \Phi_{m\,condensate,sep} = 0 \tag{3-40}$$

where:

XC	ratio between the incoming mass flow gas and the mass flow of condensate separated,
$\Phi_{m,gas,in}$	incoming mass flow of gas,
$\Phi_{m,condensate,sep}$	mass flow of condensate separated,

and is also included as such in the system matrix. The coefficient XC is calculated in accordance with:

$$XC = \frac{\overline{M}_{condensate,sep}}{\overline{M}_{gas,in}} \times \frac{C_{gas,in,H_2O} - C_{gas,out,H_2O}}{1 - C_{gas,out,H_2O}} \tag{3-41}$$

where:

$\overline{M}_{condensate,sep}$	mean molar mass of the condensate separated
$\overline{M}_{gas,in}$	mean molar mass of the incoming gas
C_{gas,in,H_2O}	molar fraction water vapour in the inlet pipe of the gas
C_{gas,out,H_2O}	molar fraction water vapour in outlet pipe of the gas

The only unknown in relation (3-41) is the molar fraction of water in the gas outlet pipe. This is calculated with

$$C_{gas,out,H_2O} = \frac{p_{sat}(T_{gas,out})}{p_{gas,out}} \tag{3-42}$$

where:

$T_{gas,\,out}$	outlet temperature of the gas
$p_{gas,\,out}$	outlet pressure of the gas
$p_{sat}(T)$	the saturation pressure of water at a certain temperature T

In order to calculate the molar fractions of the other components in the outlet pipe of the gas, the following relation is used

$$C_{gas,out,i} = C_{gas,in,i} \times \frac{1 - C_{gas,out,H_2O}}{1 - C_{gas,in,H_2O}} \qquad i \neq H_2O \tag{3-43}$$

waarin:

$C_{gas,\,out,\,i}$ the molar fraction of component i in the gas outlet pipe,

$C_{gas,\,in,\,i}$ the molar fraction of component i in the gas inlet pipe.

The ratio between the mass flows of gas and cooling water follows from the energy balance.

For part load situations no additional relations are present. The consequence of this is that even at part load the mass flow of the cooling medium is calculated such that the temperatures laid down are met.

3.6 General separator (type 26)

3.6.1 Starting points

The general separator has the physical meaning of a separator of solid parts. With a view to strongly simplified calculations it is possible to separate arbitrary components from a gas or coal flow; physically this looks like a separation by means of membranes, as far as gases are concerned. The model is set up in order to give the user a flexibility as large as possible for defining what and how much has to be separated. Because of this flexibility no protection is built in against physically impossible processes; only a right mole balance is taken care of, without chemical reactions.
The energy losses that occur during the separation process will have to appear from the energy balance or they have to be specified by the user.
For the separation of water vapour from a gas flow by means of condensation a moisture separator has to be used, type 22 or type 25. For the separation of moisture from steam, according to medium type WATERSTM, a node (type 9 with EEQCOD = 1) has to be used.

3.6.2 Calculation options

From the chemicals to be separated it can be defined which fractions have to be separated (with button “Separate components”, see **Reaction data** in paragraph 4.2 of part “Cycle-Tempo Operation” of the manual) and/or which concentrations may remain in the main outlet pipe (with button “Bypass components”, see **Reaction data** in paragraph 4.2 of part “Cycle-Tempo Operation” of the manual). Also the complete composition of the medium in the main outlet pipe can be specified.

Pressures can be specified or calculated through pressure drops of the apparatus or obtained by other apparatuses. The same applies to temperatures, with an additional option the calculation of one or in some cases two temperatures out of the energy balance, if the energy exchange with the environment DELE is specified. If all pressures are known and of all temperatures only the inlet temperature is known the relation

$$T_{out,5} = T_{out,6} + \text{TEMDIF} \qquad (3\text{-}44)$$

occurs, if TEMDIF is specified (default TEMDIF = unknown, which means that also temperatures of downstream apparatuses can be taken) and both temperatures will be calculated with an iterative procedure from the energy balance. The decomposing criterion is 0.01 K.

Also coal can be processed in the separator in order to abstract water for instance. However, the medium type of the separation pipe will always be GASMIX.

3.7 Chemical reactor (type 27)

3.7.1 Equilibria of individual reactions

In the reactor chemical equilibrium reactions take place. The equilibria are calculated by means of equilibrium constants. These constants are a function of the temperature.

$$K_{reaction} = f(T_{reaction}) \tag{3-45}$$

in which:

$K_{reaction}$ equilibrium constant (dimension depends on reaction)

$T_{reaction}$ temperature at which the equilibrium is calculated (K)

In the reactor the following reactions are standard:

The CO shift or watergas shift reaction:

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

with equation

$$\frac{(\partial p_{CO_2} + x)(\partial p_{H_2} + x)}{(\partial p_{CO} - x)(\partial p_{H_2O} - x)} = KPS \tag{3-46}$$

De CH_4- reforming reaction:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2$$

with equation

$$\frac{(\partial p_{CO} + y)(\partial p_{H_2} + y)^3}{(\partial p_{CH_4} - y)(\partial p_{H_2O} - y)} = KM \tag{3-47}$$

in which:

∂p_x the partial pressure of component x

x	the reaction coordinate of the watergas shift reaction
y	the reaction coordinate of the CH_4 reforming reaction
KPS	the reaction constant of the watergas shift reaction
KM	the reaction constant of the CH_4 reforming reaction

If PREACT is specified it is taken as p_{tot}. If it is not specified, the lowest of the inlet pressures is taken.

Equations (3-46) and (3-47) are polynomes in x and y respectively. By calculating the roots the new gas composition can be calculated.

Equation (3-46) is a second-degree polynome, equation (3-47) a fourth-degree, which means that both have several roots. In order to select the right root, an algorithm is used that requires the following:

- the root must be real;
- no more can react of a chemical than there is present.

If there is no or no univocal solution, an error message occurs and the programme will be stopped.

The iteration process

Because of the fact that more reactions can take place (at different temperatures) the total equilibrium cannot be calculated in one go. Therefore, an iterative process is needed.
For every reaction the new gas composition is calculated separately in such a way, that the result of the first reaction is the input of the second and so on. At the end of the series the result is compared to the gas composition from the previous iteration. If convergence did not yet occur and the maximum number of iterations has not yet been reached, the calculation process is repeated.

Convergence problems

There will be no convergence problems if:

- only one reaction takes place, or
- the reactions are independent, which means that they do not have any components in common.

If the reactions are dependent, the occurrence of convergence problems depends on the original composition and the specified reaction temperatures.

There can be problems if a large shift occurs in the equilibrium of one of the reactions compared to the original composition of the gas. This can take place by the reaction itself, or forced by another reaction the equilibrium of which is too much to one side already. Such a large shift that influences various reactions again and again, will be considered by the iterative process as a number of shifts that gradually becomes smaller. However, this iteration process converges very slowly.

Solutions depend on the problem. Enlarging the maximum number of iterations is only attractive in very small systems, because of the long calculation time (choose MAXIT with a size of 200 or more). It is recommended to balance the original gas mixture in a better way and to choose the reactions in a better way. It can also help to choose another order in which the equilibria for the different reactions are calculated: in such a way that one reaction does not steer the other in the wrong direction at first (starting value problem).

If three or more reactions have to be brought to equilibrium, the above does apply all the more: the less shifts compared to the original gas composition the better.
As a temporary solution the mixture can be brought to equilibrium with a gasifier at first, type 23.

Other possible problems with reactions programmed by the user

Message ’NO GOOD POLYNOME’.
The routine from the NAG library that solves polynomes from the equilibrium equations of the reactions comes across a mistake (IFAIL > 0), see manual of the library. This does not have to mean, that the polynome has not been described properly!

Message 'ERROR: NUMBER OF SOLUTIONS FOUND: xx'
The routine that selects the root, which has to be the reaction coordinate, does not find a or an univocal solution. Check whether or not the polynome has been described properly.

3.7.2 Thermodynamic calculations

In the apparatus routine an unknown temperature is calculated out of the energy balance; in many cases this will be the outlet temperature. A temperature is calculated out of the pressure, the enthalpy and the gas composition. The reactor only influences the gas composition, during which energy of formation of the components will be released or absorbed. If this results in a reaction, the calculated temperature will be clearly influenced by it.

Behaviour during the first iteration of Cycle-Tempo

In the first iteration of Cycle-Tempo pressures, temperatures, enthalpies and mass flows will not yet be known during the calculation of the gas composition, whilst a pressure and mass flows are needed. If the inlet pressure, an estimation of it or PREACT is specified, a new composition will be calculated; if not, the composition at the outlet will be considered to be equal to that at the inlet.
When an unknown temperature is calculated, DELE is put on zero in the first iteration, unless ESTMAS is specified.
If various inlet pipes are connected, the composition of the total original gas mixture has to be calculated. This requires the mass flows in the inlet pipes or the ratios between them. For the first iteration RMASS can be specified. If RMASS is not specified, the mass flows in the inlet pipes are considered to have the same size.

3.8 Saturator (type 28)

3.8.1 Functioning of the model of the saturator

The model of the saturator is based on a counterflow saturator. It is used to moisturize a gas with water vapour. The composition of the gas to be moisturized is free to be chosen and can be defined by the user himself.

The composition of the outgoing gas is calculated with the inlet pressure and inlet temperature and the relative humidity (RELHUM) specified by the user.

3.8.2 Calculation of the gas composition in the gas outlet pipe

The molar fraction water vapour in the gas outlet pipe can be calculated in three ways.

It can be specified with MLFH2O. The molar fraction water vapour ($x_{out,gas,H2O}$) is considered to be equal to MLFH2O. Then the molar fractions of the other components are calculated, see below.

Or the amount of water to be evaporated can be specified with DELMW. If PIPE is also specified, DELMW is relative compared to another mass flow. The amount of water to be evaporated is DELMW $\times \Phi_{m,PIPE}$.

In order to calculate the molar fraction water vapour in the gas outlet pipe, the number of moles water to be evaporated are calculated, after which

$$x_{out,gas,H_2O} = \frac{\Phi_{mol,in,gas,H_2O} + \Phi_{mol,watertobeevaporated}}{\Phi_{mol,in,gas,total} + \Phi_{mol,watertobeevaporated}} \qquad (3\text{-}48)$$

The mole flows are calculated by dividing the mass flows by the mole mass.

If MLFH2O nor DELMW are specified, the molar fraction water vapour is calculated out of the pressure and the temperature in the gas outlet pipe.

In order to calculate the composition of the outgoing gas, first the partial pressure of the water vapour is determined at the temperature of the outgoing gas:

$$p_{out,gas,H_2O} = RELHUM \times p_{sat}(T_{out,gas}) \tag{3-49}$$

Then the molar fraction water vapour can be calculated:

$$x_{out,gas,H_2O} = \frac{p_{out,gas,H_2O}}{p_{out,gas}} \tag{3-50}$$

Subsequently the molar fractions of the other components can be calculated:

$$x_{out,gas,i} = x_{in,gas,i} \times \frac{1 - x_{out,gas,H_2O}}{1 - x_{in,gas,H_2O}} \qquad (for\, all\ i \neq H_2O) \tag{3-51}$$

3.8.3 Calculation of the mass flows

The saturator adds two mass equations to the system matrix

- mass balance of the apparatus
- ratio of the mass flows in the inlet and outlet pipes of the gas

That ratio from the last equation (GRATIO) is determined by the amount of water, absorbed in the gas.

$$GRATIO = \frac{\overline{M}_{out,gas}}{\overline{M}_{in,gas}} \times \frac{1 - x_{in,gas,H_2O}}{1 - x_{out,gas,H_2O}} \tag{3-52}$$

in which $\overline{M}$ is the average mole mass.

The second mass equation will then be:

$$GRATIO = \Phi_{m,in,gas} - \Phi_{m,out,gas} = 0 \tag{3-53}$$

In this form the equation is added to the system matrix.

3.8.4 Calculation of temperatures and use of the energy balance

As far as the temperatures in the connected pipes are not already determined by data of other apparatus, they can be specified by the user. It is also possible to specify the differences in temperature between the pipes. The energy balance of the saturator can, if desired, be used to determine one of the temperatures by specifying the energy exchange with the environment with DELE. The mass flows that are used in this energy equation are determined as follows:

Because of the fact that the composition of the gas for the current iteration is already known in this stage of the calculation, the ratio between the inlet and outlet mass flows of the gas (GRATIO) is also known. With this ratio the matching outlet mass flow of gas is calculated out of the old inlet mass flow, and the outlet mass flow water is then calculated out of the inlet mass flow from the mass balance that occurred. These mass flows are used in the energy balance to calculate the unknown enthalpy and the temperature that belongs to that.

If the inlet mass flows are the same for every iteration, this will result in the fact that the energy balance is used for the current iteration.
During the first iteration mass flows are not yet known and, therefore, the energy balance cannot be used. That is the reason why an estimation of the unknown temperature has to be given with parameter ESTTEM for this iteration.

If the energy balance is not used for the calculation of an unknown temperature (or enthalpy) it is available to calculate an unknown mass flow. For this purpose a production function &PROFUN has to be specified. Generally, the energy exchange with the environment will be negligible, which means that POWER has to be specified as 0.0.

If no enthalpy or mass flow is calculated out of the energy equation, then the energy exchange with the environment will result. However, in practice this situation will hardly occur.

3.9 Compressor (type 29)

3.9.1 Fields of application

There are three types of compressors:

1. GENERAL
2. SULZER-A
3. SULZER-AV

For the GENERAL compressor there are no specific calculation methods and no facilities for off-design calculations present. In fact, the calculational rules for the GENERAL compressor are equal to those for the pump (type 8). The GENERAL compressor can be used for each type of compressor.

The SULZER compressors can be applied in a less general way. For these types isentropic efficiencies can be calculated for design as well as off-design conditions. However, the field of application is limited to the medium air, pressures between 2 and 7 bar and inlet volume flows between 20 and 350 m^3/s.
There are two types of SULZER compressors available:

1.	type A (SULZR-A):	An axial compressor without adjustable guide vanes. Regulation takes place by changing the number of revolutions.
2.	type AV (SULZR-AV):	An axial compressor with adjustable guide vanes. Regulation takes place by turning the vanes at a constant speed.

3.9.2 Calculation procedure

Establishing pressures, temperatures and enthalpies at inlet and outlet of the compressor can take place by specification of data for apparatuses upstream and downstream in the process or by specification of data for the compressor involved. The mass flow through the compressor can be calculated out of the energy balance. The energy balance can be determined in a production function or in a turbine-pump/compressor combination. It is standard to add 1 mass balance to the system matrix.

An additional possibility for the calculation of an enthalpy value is present if it appears during the calculation that above mentioned procedure does not contain sufficient data. The programme will then try to calculate the inlet enthalpy out of the outlet enthalpy or the outlet enthalpy out of the inlet enthalpy by means of the Mollier diagram through an isentropic efficiency (ETHAI) that has been specified in the input. This is illustrated in Figure 3-7.

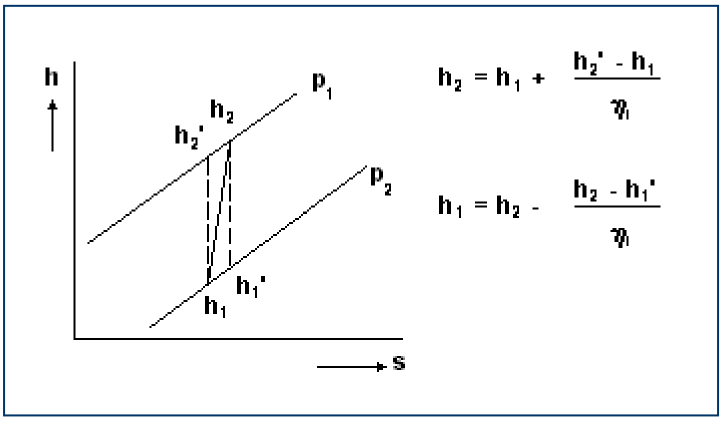

Figure 3-7: Calculation ofenthalpies

No additional possibility exists for the SULZER compressors at the moment. In case of a design calculation the isentropic efficiency can be calculated out of the inlet volume flow and in case of an off-design calculation from the inlet volume flow and the pressure ratio. For type A it is also possible to calculate the isentropic efficiency with off-design calculations from the inlet volume flow and the number of revolutions. This calculation preceeds the enthalpy calculation via the Mollier diagram.

3.9.3 Calculation isentropic efficiency with design conditions (SULZER compressors)

For the calculation of the isentropic efficiency with design conditions a direct relation is determined between the inlet volume flows and the isentropic efficiency. This relation is shown in Figure 3-8.

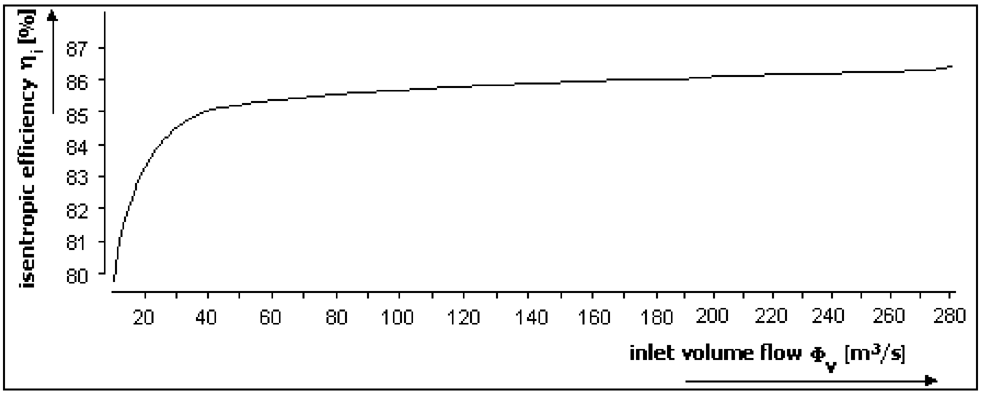

Figure 3-8: Isentropic efficiency with design conditions

From the data supplied by the manufacturer the design conditions are determined for a number of compressors of different sizes. Subsequently an univocal relation is determined by means of a weighted average. The influence of the pressure ratio is ignored in this.
In reality, the isentropic efficiency will not be completely independent of the pressure ratio: higher final pressures will make the volume flow smaller in the last stages, through which leakage and clearance losses will increase. However, from the available data no univocal relation with the pressure ratio could be derived.

3.9.4 Calculation isentropic efficiency with off-design conditions (SULZER compressors)

For the calculation of the isentropic efficiency in an off-design calculation the starting point is dimensionless characteristics. Figure 3-9 shows the characteristic for type A.

Point NP in Figure 3-9 indicates the design point. All conditions in the characteristic are relative values, which means values expressed in percentages of the design point.
Figure 3-10 shows a similar characteristic for type AV.

In both figures a new operating point can be determined by means of a volume flow and a pressure ratio percentage. This results in an efficiency percentage. Moreover, this results in a speed percentage for type A and an angular position percentage for type AV. Both figures are valid for the medium air and a constant inlet temperature.

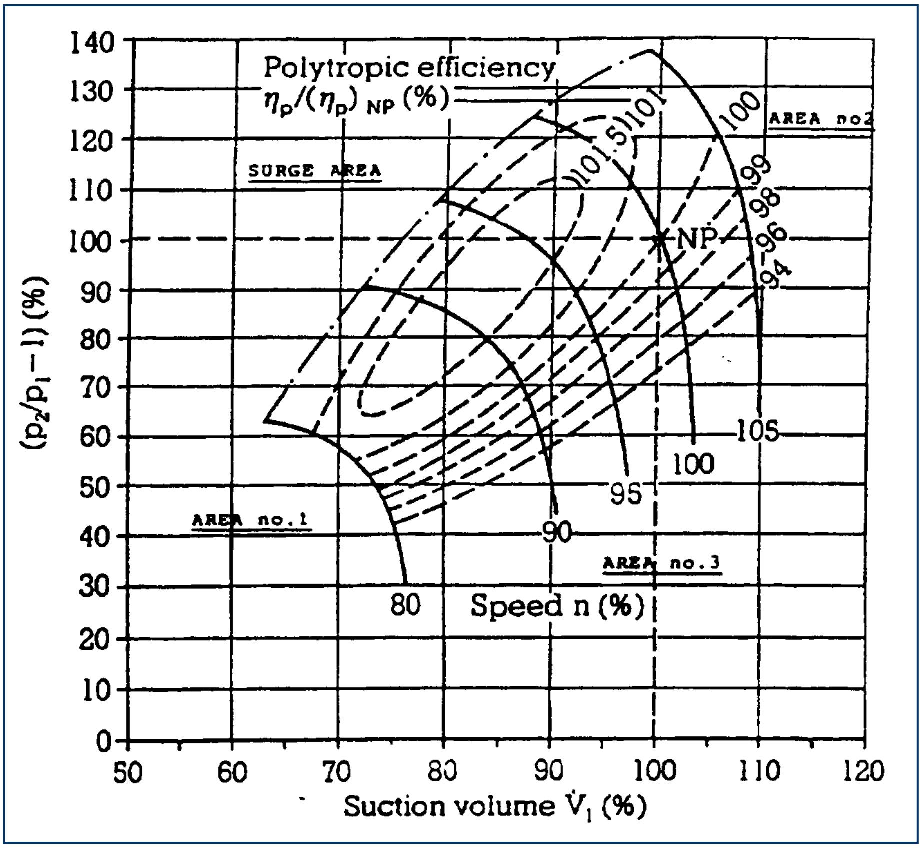

Figure 3-9: Off-design characteristic SULZER type A

In Cycle-Tempo the following method is applied for both types:

Input design data for off-design calculations:

- VOLDES = inlet volume flow with design conditions
- PRATID = pressure ratio with design conditions

From the calculation results:

- $\Phi_{v,\text{off-des}}$ = inlet volume flow with off-design conditions
- $\pi_{\text{off,des}}$ = pressure ratio with off- design conditions

(the pressure ratio can also be specified as PRATI (=POUT/PIN))

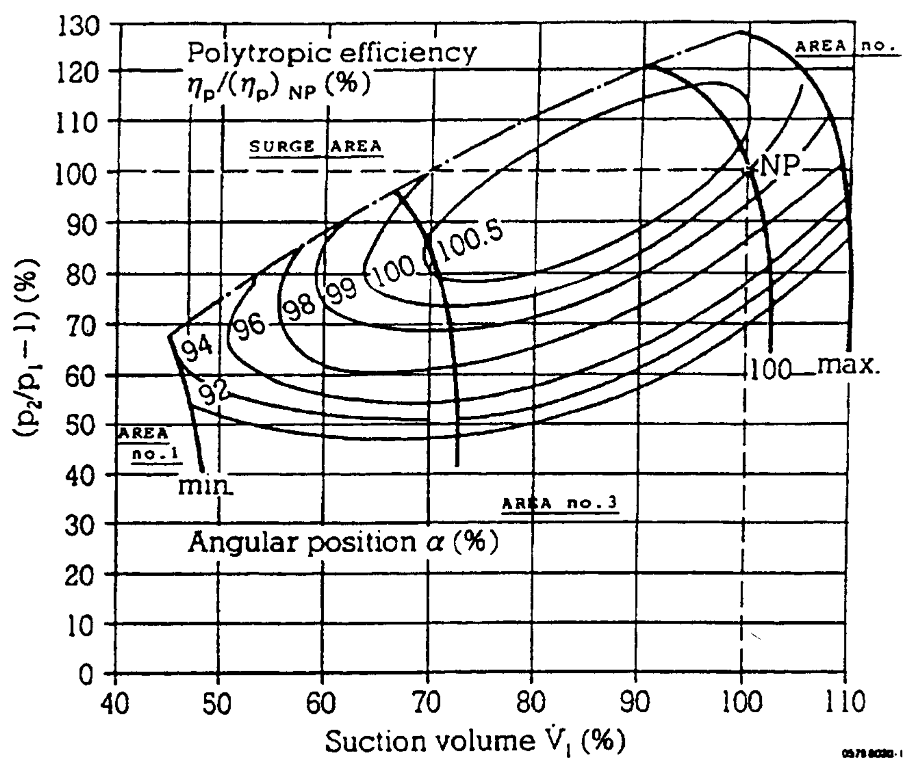

Figure 3-10: Off-design characteristic SULZER type AV

From these data the percentage inlet volume flow $\%\Phi_v$ and the percentage pressure ratio $\%\pi$ of off-design compared to design can be derived:

$$\%\Phi_v = \frac{\%\Phi_{v,off.des}}{DESVOL} \times 100\% \tag{3-54}$$

$$\%\pi = \frac{\pi_{off.des} - 1}{PRATID - 1} \times 100\% \tag{3-55}$$

From the characteristics the polytropic efficiency percentage $\%\eta_p$ will then result.

The polytropic efficiency with design conditions η_p is calculated out of the isentropic efficiency η_i (parameter: ETHAID at “off-design input data”) with the formula:

$$\eta_p = \frac{PRATID^{\frac{k-1}{k}} - 1}{PRATID^{\frac{k-1}{k}\times\frac{1}{\eta_i}} - 1} \qquad (k = 1{,}4) \tag{3-56}$$

The polytropic efficiency with off-design conditions $\eta_{p,off.des}$ with:

$$\eta_{p,off.des} = \frac{\%\eta_p}{100} \times \eta_p \tag{3-57}$$

Finally, the isentropic efficiency with off-design conditions $\eta_{i,off.des}$ is determined as follows:

$$\eta_{i,off.des} = \frac{\ln \pi_{off.des}^{\frac{k-1}{k}}}{\ln\left(1 + \frac{\pi_{off.des}^{\frac{k-1}{k}} - 1}{\eta_{p,off.des}}\right)} \qquad (k = 1{,}4) \tag{3-58}$$

For SULZER type A it is also possible to specify a speed percentage in stead of the design pressure ratio. The calculation method is the same as above.

Chapter 4

Pressure losses in pipes

Pressure losses in pipes may arise from:

- differences in height
- flow resistances

Pressure losses caused by height differences are calculated with the following relation:

$$\Delta p_h = \frac{g\Delta h}{\bar{v}} \times 10^{-5} \qquad [bar]$$

With:

Δp_h	:	pressure change in the pipe as a result of a height difference	[bar]
v	:	average specific volume of the fluid in the pipe	[m^3/kg]
g	:	gravitation constant (9.80665 m/s^2)	[m/s^2]
Δh	:	height difference between inlet and outlet of the pipe	[m]

The average specific volume is the average of the specific volume at the inlet (v_{in}) and the outlet (v_{out}) of the pipe:

$$\bar{v} = \frac{v_{in} + v_{out}}{2} \qquad [m^3/kg]$$

At design, the pressure loss as a result of flow resistance (Δp_f) is specified in the input. At off-design, it is assumed that the flow in the pipe is always turbulent. Furthermore it is assumed that the friction factor ξ is independent of the velocity in the pipe. These assumptions lead to the following relation:

$$\Delta p_{f,o.d.} = \Delta p_{f,d} \times \frac{\bar{v}_{o.d.}.\Phi^2_{m,o.d.}}{\bar{v}_{d}.\Phi^2_{m,d}} \qquad [bar]$$

with:

$\Phi_{m,d}$	:	mass flow in the pipe at design	[kg/s]
v_d	:	average specific volume in the pipe at design	[m^3/kg]
$\Delta p_{f,d}$	:	pressure loss in the pipe by flow resistance at design	[bar]
$\Phi_{m,o.d.}$	:	actual mass flow in the pipe	[kg/s]
$v_{o.d.}$	:	actual average specific volume in the pipe	[m^3/kg]
$\Delta p_{f,o.d.}$	:	pressure loss in the pipe by flow resistance	[bar]

The total pressure loss Δp, both at design and off-design, can be determined according to:

$$\Delta p = \Delta p_h + \Delta p_f \qquad [bar]$$

Chapter 5

Processing the results

5.1 Calculation of the system efficiency

In the calculation of system efficiencies four steps can be distinguished:

1. Determination of the total energy input
2. Determination of the total energy production
3. Determination of the total own energy consumption
4. Calculation of system efficiencies

In the program the variable PH is used to determine the energy exchange with the environment. PH (abbreviation of Power/Heat) of an apparatus i, which has n inlet pipes and m outlet pipes, is defined as follows:

$$\mathrm{PH(i)} = \sum_{j=1}^{n} \left(\mathrm{h}_{in}(j) \times \Phi_{m,in}(j) \right) - \sum_{i=1}^{n} \left(\mathrm{h}_{out}(i) \times \Phi_{m,out}(i) \right)$$

Here h is the enthalpy (kJ/kg) of the medium in a pipe (at the side) connected to apparatus i, and Φ_m the mass flow (kg/s) in the pipe.

A positive value of PH(i) means that apparatus i rejects energy to the environment.

5.1.1 Calculation of the heating value

The lower and higher heating value (henceforth indicated as LHV and HHV, respectively) of all pipes of the medium type GASMIX are calculated. For this calculation, the definitions established in DIN 5499 ('Brennwert und Heizwert, Begriffe', January 1972) were assumed. The heating value is defined as the energy that must be discharged when heating 1

kilogramme of fuel, when the fuel, oxidant and flue gas are all supplied or discharged at a pressure of 1 atm and a temperature of 25°C. In gaseous fuels, it is assumed for the HHV that the water generated by the heating reactions (i.e. not the water that is already present in the gas or in the air) fully condenses. At the LHV, this water is fully present as vapour in the flue gas. Apart from the water generated at the heating, the water present in the fuel is also taken along in the event of solid and liquid fuels. Oxygen is used as oxidant.
No heating value can be calculated for pipes of the medium type FUEL, as the component composition is not known. The LHV must therefore always be stated (through the parameter LHV). The HHV is calculated by determining the humidity of the flue gas and calculating its condensation heat. The HHV is then equal to the LHV plus the condensation heat.
In the event of deviating pressure and temperature, the heating values can be calculated at the conditions specified by the user at General Data | Environment Definition.

5.1.2 Energy input

For the energy input the following apparatuses are considered:

a. Boiler/reheater (type = 1/type = 2)

For the energy input in a boiler or reheater the following formula is used:

Energy input = Σ {-PH(i) / ETHAB(i)}

(for all the apparatuses i of the type boiler/reheater)

b. Source (type = 10)

For a source there are three possibilities:

I. In case of medium type GASMIX the lower heating value (LHV) is calculated (see paragraph 5.1.1):

Energy input = Σ {LHV(i) $\times$ $\Phi_{m,out}$(i) }

(for all the apparatuses i of the type 10 with one connected pipe which is outgoing and for which a LHV greater than 0 is calculated)

II. In case of medium type FUEL the lower heating value is specified by the user (parameter LHV):

Energy input = Σ {LHV(i) × $\Phi_{m,out}$(i) }

(for all the apparatuses i of the type 10 with one connected pipe which is outgoing and which is of medium type FUEL)

III. If LHV is specified for a source with one connected pipe which is outgoing, this value will be used. A calculated LHV for medium type GASMIX or a specified LHV for medium type FUEL will be overwritten.

The total energy input is now

Total energy input = (a) + (b)

Remark: Energy input other than above will not be taken into account in the calculation of the system efficiency.

5.1.3 Energy output

For the energy output the following apparatuses are considered:

a. **Turbines (type = 3)**

Blade power	$PH(i)$
Mechanical power	$PH(i) \times \eta_m(i)$
If the turbine drives a generator:	
Electric power:	$PH(i) \times \eta_m(i) \times \eta_{gen}(i)$

b. **Turbine driven pumps/compressors**
(type = 8 or type = 29 in combination with one or more turbines on a shaft)

Blade power pump/compressor	$-PH(i)$	$(PH(i) < 0)$
Mechanical power pump/compressor	$[-PH(i) / \eta_m(i)]_{pump\ /\ compressor}$	
Blade power turbine	$PH(j)$	$(PH(j) > 0)$
Mechanical power turbine	$[PH(j) \times \eta_m(j)]_{turbine}$	
Surplus mechanical power turbine-pump / compressor combination	$[PH(j) \times \eta_m(j)]_{turbine} - [-PH(i) / \eta_m(i)]_{pump\ /\ compressor}$	

If the turbine-pump/compressor combination drives a generator:

Electric power: $\{ [PH(j) \times \eta_m(j)]_{turbine} - [-PH(i) / \eta_m(i)]_{pump\ /\ compressor} \} \times \eta_{gen}(ij)$

c. Fuel cell (type = 21)

If DELE, the energy loss to the environment, is specified:

HEATLOSS(i) = DELE(i)

If DELEP, relative energy loss to the environment with respect to the power input, is specified:

$$\text{HEATLOSS}(i) = \frac{\text{DELEP}(i) \times \text{PH}(i)}{\text{DELEP}(i) + 1}$$

If both DELE and DELEP are not specified then:

HEATLOSS(i) = 0

DC power generated:	PH(I) – HEATLOSS(i)
AC power generated:	PH(I) – HEATLOSS(i) x DCAC(i) (DCAC(i) is efficiency of conversion of DC power in AC power of apparatus i)

d. Sink/source (type = 10); only heat production

If for a sink/source SUBTYP = 1 is specified, the energy exchange with the environment is considered as useful heat. The number of connected pipes determines the way how the amount of exchanged energy is defined:

I. A “Heat Sink” (or a sink/source with one connected pipe and with subtype = 1 specified): the energy exchange with the environment equals the mass flow multiplied by the difference between the actual enthalpy and the enthalpy at ambient conditions. In case of medium types GASMIX and WATERSTM the water component is considered as liquid at ambient conditions.

II. A “Heat Sink” (or a sink/source with two connected pipes and with subtype = 1 specified): the energy exchange with the environment equals PH(i) (see paragraph 5.1).

The total energy production is now

Total power production = (a) + (b) + (c)

Total heat production = (d)

5.1.4 Own consumption

For the energy consumption two different cases are considered. Firstly the electricity driven pumps/compressors (not turbine driven pumps/compressors) and secondly values specified via the namelist &AUXPOW.

a. Electricity driven pumps or compressors (type = 8 or type = 29)

Power absorbed by medium = –PH(i) (for an apparatus i of the type 8 or 29 which is not turbine driven)

Electrical power = –PH(i) /) / $\eta_{drive}(i)$

The efficiency of the pump/compressor drive $\eta_{drive}(i)$ is built up by two efficiencies: the mechanical efficiency $\eta_m(i)$ and the electric efficiency $\eta_e(i)$. The total efficiency is then determined as follows:

I. If both efficiencies are specified then:

$$\eta_{drive}(i) = \eta_m(i) \times \eta_e(i)$$

II. If one of the efficiencies is not specified then the efficiency which is not specified is set equal to 1. Hence η_m is specified and η_e not, then:

$$\eta_{drive}(i) = \eta_m(i)$$

And vice versa if η_e is specified and η_m not, then:

$$\eta_{drive}(i) = \eta_e(i)$$

III. If none of both efficiencies are specified then the total efficiency is calculated by interpolation from Figure 5-1.

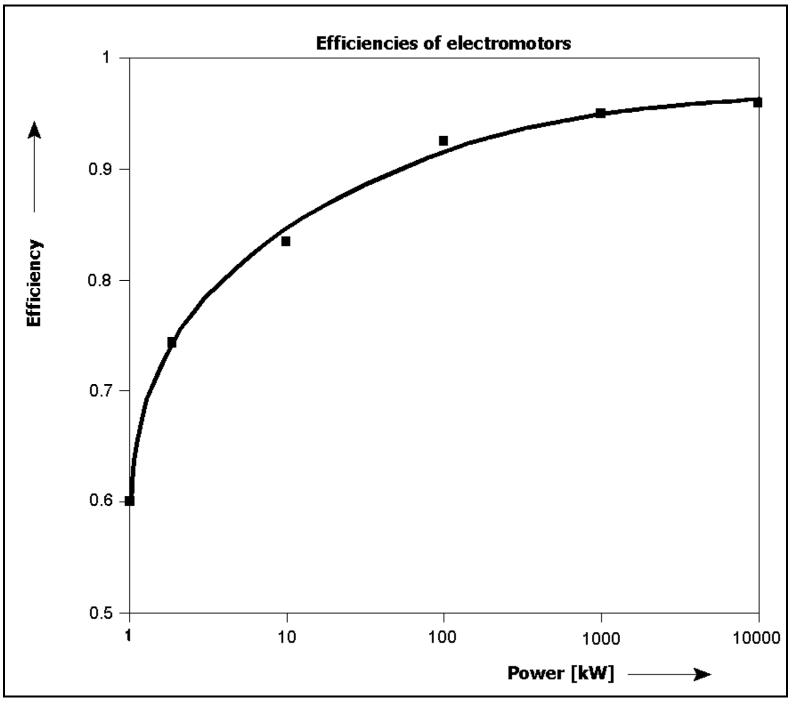

Figure 5-1: The efficiency of electromotors including the mechanical efficiency of the motor and pump/compressor as a function of the power at the shaft of the pump/compressor

b. Auxiliary power consumption

The user may specify additional power consumption of not-modelled consumers at General Data | Auxiliary Power Consumption. For these just the name chosen and the (electric or mechanical) power consumption are used.

The total own energy consumption is now

Total own consumption = (a) + (b)

5.1.5 Efficiencies

1. Gross thermal efficiency $= \dfrac{\text{Total produced electric/mechanical power}}{\text{Total energy input}}$

2. Net thermal efficiency $= \dfrac{\text{Total produced electr./mech. Power} - \text{total own consumption}}{\text{Total energy input}}$

Only if a “Heat Sink”, or a sink/source with subtype = 1 specified, has been defined:

3. Heat efficiency $= \dfrac{\text{Total heat production}}{\text{Total energy input}}$

4. Total net efficiency = net thermal efficiency + heat efficiency

5.2 Calculation of exergy efficiencies

5.2.1 Introduction

Besides system calculations, Cycle-Tempo can perform exergy calculations, the results of which form the basis for an exergy analysis of the system under consideration. For such an exergy analysis, it is important to have available exergy values of process flows and exergy losses in apparatuses, as well as exergy efficiencies of apparatuses.

The evidence has shown that for exergy efficiencies, a variety of definitions is conceivable, which in turn may result in strongly differing efficiency values for a given process or system. Using uniform definitions for these efficiencies will strongly improve the usefulness of exergy efficiencies.

There are no internationally recognized definitions available for exergy efficiencies; however, various authors (among others, [9], [10] and [11]) have made propositions to this end. These propositions show mutual differences, but have been insufficiently worked out for application in practice. The efficiencies used in Cycle-Tempo should be regarded as a proposition to define exergy efficiencies that can be used in practice.

5.2.2 Possibilities for using exergy efficiencies

In the thermodynamic analysis of processes and systems we try to obtain a good picture of the place, the size and the cause of losses. Losses may occur as a result of undesired "drainage" of energy to the environment, for example in the form of heat losses; but also as a result of energy degradation caused by irreversible processes at the energy conversion level. In many cases, the losses prevail as a result of degradation. Both energy drainage (external losses) and energy degradation (internal losses) involve loss of exergy. The seriousness of these losses can be determined by using exergy efficiencies for processes, apparatuses, or systems.

In general, the use of efficiencies is accompanied by interpretation problems. Specifically in the case of complex systems, it is not always clear how efficiencies have been defined, which effects have been considered and which not. In energy conversion systems, it is quite often unclear whether an efficiency is based on the lower heating value (LHV) or on the higher heating value (HHV) of the fuel, and whether the plant's own electricity consumption has been deducted from the power produced. The use of efficiencies only makes sense if such interpretation problems can be solved and prevented.

Exergy efficiencies can be used for varying purposes. For example, it is conceivable that the authorities use exergy efficiencies in granting permits or levying taxes, e.g. by requiring specific conversion efficiencies to be achieved at plant construction or operation. Such an application, however, requires a thorough understanding of the potentials and limitations of exergy efficiencies and can only be realized if there is sufficient experience with these efficiencies.
A more obvious application is to use them for assessing, analyzing and optimizing processes and systems. We can think here of processes and systems for converting material balances in chemical process plants, and of processes and systems for converting energy. Below, we will specifically deal with their application in energy conversion systems.
Exergy efficiencies have only minor importance for a rough evaluation of electricity production units: the electricity produced is also the efficiently produced exergy, while usually the exergy of common fuels for electricity production differs only a few percentages from the LHV. For that reason, a power plant's exergy efficiency will differ only slightly from its thermal efficiency and will, therefore, not provide additional information.
The situation is completely different for combined heat and power (CHP) plants. An exergy efficiency there also visualizes the thermodynamic significance of the heat produced. Since the exergy of heat depends on the temperature, and is for finite temperatures always smaller than the energy quantity, exergy efficiencies of combined heat and power plants will usually be lower than comparable thermal efficiencies. The difference is determined specifically by the temperature level of the heat produced. The exergy efficiency may provide additional information about the quality of the conversion in the CHP plant; the interpretation of exergy efficiencies, however, is still ambiguous.

Exergy efficiencies are particularly valuable in analyzing and optimizing systems. An exergy analysis is usually composed of a detailed calculation of the exergy values of the process flows and the exergy losses in the system. Such a calculation shows the places in the system where losses occur and the seriousness of these losses. In the analysis, an answer must be found to the question of how to limit exergy losses. Based on the absolute value of exergy loss, it is usually difficult to assess whether an exergy loss in an apparatus is unnecessarily large. An exergy efficiency in which the exergy loss is judged from the added or transferred exergy gives a better picture of the quality of the processes in the apparatus, and thus also gives a better impression of whether exergy losses can be reduced.

Exergy efficiencies of apparatuses (or parts of installations) can also be valuable in checking process calculations. Unusual efficiencies can point to the calculation being based on unreal data or incorrect assumptions. Obviously, only frequently occurring apparatuses are eligible for such a checking.

Since exergy efficiencies are important in analyzing and optimizing energy conversion systems, we looked initially at the efficiencies of frequently occurring apparatuses in such systems.

5.2.3 General definition of exergy efficiency

Several authors have provided definitions for exergy efficiency [9], [10], [11]. A complete overview of the published definitions and a discussion of the pros and cons of the various definitions fall outside the scope of this manual. Figure 5-2 which presents a rough division is further elucidated below.

Generally, efficiencies (and thus also exergy efficiencies) for practical use must meet a number of conditions.

1. The sensitivity for changes in the system involved must be large. Efficiencies must be defined in such a way that all values between 0 and 1 are possible, and no other values.
2. Preferably, the definition of efficiency must be applicable in practice. This means that the definition, without additions, must be practicable to a large number of different systems.
3. It must be possible to calculate efficiency values quickly, using available data. Preferably, one should avoid the necessity of making very detailed additional calculations.
4. Efficiencies are a measure for a system's quality. Such a standard is only reliable if based on data that amply take into account the influence of all relevant variables. The quality of the process calculation performed determines whether this condition is satisfied.

As stated above, an efficiency definition not only concerns a theoretically sound choice, but also how to calculate, without over-exerting, the exergy values needed for the efficiencies.

The preference for a specific efficiency definition is thus also determined by the way in which exergy values are available.

The evidence shows that it is not possible to simultaneously satisfy all conditions stated. Depending on the significance attached to the various conditions, it is possible to define exergy efficiencies in various ways. Figure 5-2 distinguishes two different definitions of efficiencies, i.e. *universal efficiency* and *functional efficiency*[1]. Universal efficiency is based on a generally workable definition for exergy efficiency. Due to the relative insensitivity to changes in the system, it is rejected as insufficient in the publications stated. Functional efficiency is preferred, but requires further specification, depending on the type of system. For certain systems, relevant specifications are difficult or completely inconceivable.

Both definitions of efficiency are introduced here in order to emphasize the significance of functional efficiency and to show the impossibility of specifying functional efficiency for certain systems.

We can define *universal efficiency* as follows:

$$\eta_{Ex,u} = \frac{\sum Ex_{out}}{\sum Ex_{in}} \qquad (1)$$

In which:

$\sum Ex_{out}$ is the exergy of the outgoing process and energy flows

$\sum Ex_{in}$ is the exergy of the ingoing process and energy flows

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1) The name 'exergy efficiency' is not derived from literature. In the literature stated, we did not find a name for universal efficiency; various names, however, are used for functional efficiency: rational efficiency, efficiency with transiting exergy, etc.

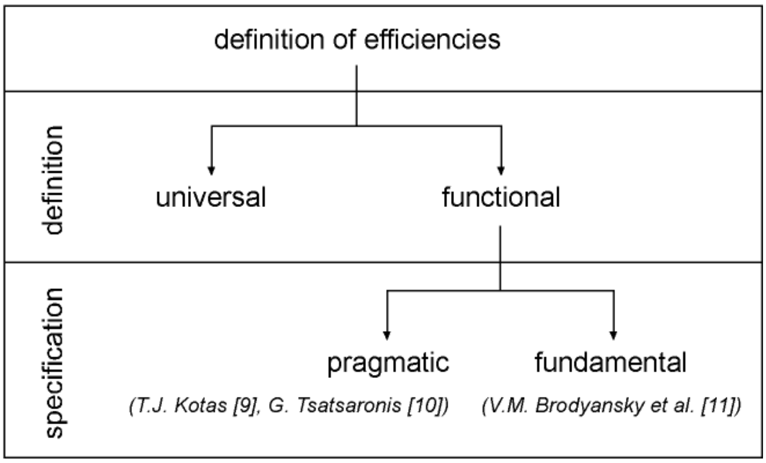

Figure 5-2: rough division of exergy efficiencies

The difference in exergy between the ingoing and outgoing process and energy flows is identical to the exergy loss, i.e.

$$\sum Ex_{in} = \sum Ex_{out} + \sum Ex_{loss} \tag{2}$$

For (1), we can also write:

$$\eta_{Ex,u} = \frac{\sum Ex_{out} + \sum Ex_{loss}}{\sum Ex_{in}} \tag{3}$$

The universal efficiency offers a clear definition for a variety of systems. A disadvantage of this definition, however, is that the efficiency values obtained can be insensitive to changes in the system. This occurs, for example, when only part of the flows undergo a change or when the flows undergo only minor changes. The exergy loss is then small compared to the exergy of the ingoing process and energy flows. We then deal with comparatively large “ballast flows”: exergy flows that are actually fed to the process, but not directly involved in the intended conversion. As a result of these ballast flows, the universal efficiency may be insensitive to changes in exergy loss.

This is the reason for defining functional efficiency, in addition to universal efficiency. With functional efficiency, we try to eliminate the influence of ballast flows as much as possible in order to achieve the best possible sensitivity to changes in the system.

A general definition of *functional efficiency* is:

$$\eta_{Ex,f} = \frac{\sum Ex_{product}}{\sum Ex_{source}} \qquad (4)$$

In which:

$\sum Ex_{product}$ is the exergy of that part of the outgoing process and energy flows that can be considered to be a product of the system;

$\sum Ex_{source}$ is the exergy of that part of the ingoing process and energy flows that can be considered necessary for making the product in the present process.

Basically, $\sum Ex_{source}$ must be identical to the supplied exergy minus the exergy of the ballast flows, or:

$$\sum Ex_{source} = \sum Ex_{in} - \sum Ex_{ballast} \qquad (5)$$

Similarly, we can write for $\sum Ex_{product}$:

$$\sum Ex_{product} = \sum Ex_{out} - \sum Ex_{ballast} \qquad (6)$$

Since by definition, the exergy of ingoing and outgoing ballast flows is the same, the difference in exergy value between "source" and “product” must also be identical to the sum of the exergy losses in the system, i.e.:

$$\sum Ex_{source} = \sum Ex_{product} + \sum Ex_{loss} \qquad (7)$$

The comparisons (4) through (7) are insufficiently clear about how to calculate the functional efficiency of a specific system. First, we will have to establish which flows (or sub-flows) are part of $Ex_{product}$, Ex_{source} or $Ex_{ballast}$. In addition to the definition given, we also need a more detailed elaboration/specification (see also Figure 5-2) of the functional efficiency. It appears, however, that it is not possible to provide a generally valid specification of $Ex_{product}$, Ex_{source} or $Ex_{ballast}$. Thus we must establish for each individual systemhow to specify the exergy of product and source.

The various authors do not use uniform methods and names to specify functional efficiencies. The fundamental approach, as supported by Brodyansky [11], is preferred, but produces large practical problems since it requires a drastic breakdown of exergy values. For this reason, we chose for a more pragmatic approach that is closely linked to the propositions made by Kotas [9] and Tsatsaronis [10].

In paragraph 5.2.5 the functional efficiency of a large number of apparatuses has been specified. Considering the limited breakdown of exergy values required here, this specification is generally workable.
The size of exergy values – and thus of exergy efficiencies – is dependent on the environment definition chosen. Strictly speaking, exergy efficiencies can only be mutually compared if the same environment definition is assumed.

5.2.4 Explanation of efficiency definitions

The difference between universal efficiency and functional efficiency can be illustrated with a simple example: the process of heat transfer in a heat exchanger.
As a given, the purpose of the heat exchanger is to heat a process flow – called primary flow – by withdrawing heat from another process flow – called secondary flow. The exergy of the primary flow will increase as a result of the absorbed heat, and the exergy of the secondary flow will decrease. Figure 5-3 visualizes the exergy change in the process flows.

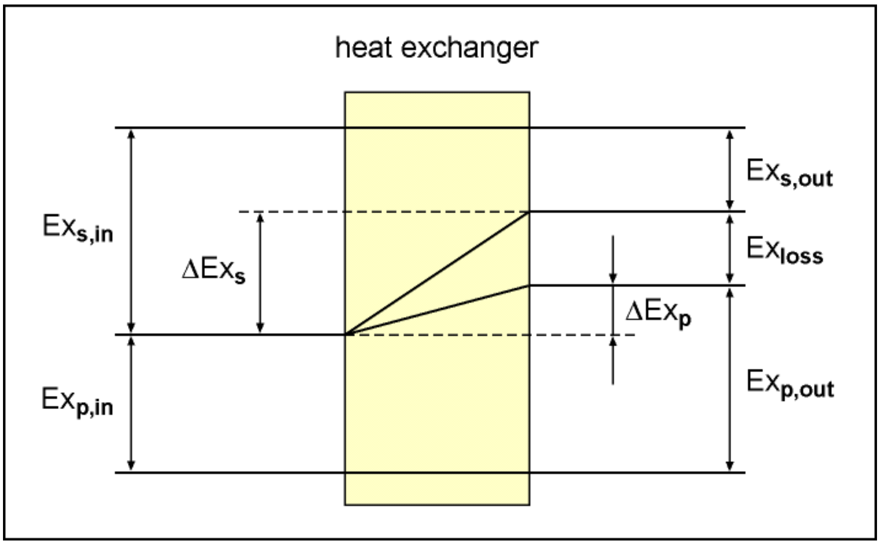

Figure 5-3: change in exergy quantities at heat transfer

The universal exergy efficiency for this heat exchanger follows from comparison (1):

$$\eta_{Ex,u(heatexchanger)} = \frac{Ex_{s,out} + Ex_{p,out}}{Ex_{s,in} + Ex_{p,in}} \tag{8}$$

If we look only at the exergy quantities involved in the process, we see the exergy quantities $Ex_{p,in}$ and $Ex_{s,out}$ flowing through the process without any change. These flows can be regarded as ballast flows that are not part of the process and thus need not be considered in the process assessment.

If possible, the specification of a functional efficiency should relate only to changes in exergy quantities. It is assumed that the purpose of the heat exchanger is to heat the primary flow. The exergy change ΔEx_p of the primary flow can be regarded as $Ex_{product}$ from comparison (4). The secondary flow provides the supply of exergy. The exergy change ΔEx_s of the secondary flow can thus be regarded as Ex_{source}. For the functional exergy efficiency of the heat transfer process, we can then write:

$$\eta_{Ex,f(heatexchanger)} = \frac{\Delta Ex_p}{\Delta Ex_s} = \frac{Ex_{p,out} - Ex_{p,in}}{Ex_{s,in} - Ex_{s,out}} \tag{9}$$

In this comparison, the exergy flows seen as ballast are not taken into consideration. Actually, in comparison (8) the exergy loss is related to the total exergy supplied ($Ex_{s,in}$ + $Ex_{p,in}$), while in comparison (4) the exergy loss is related to the exergy change in the secondary medium (ΔEx_s). Since ΔEx_s is always smaller than ($Ex_{s,in}$ + $Ex_{p,in}$), the functional efficiency (9) is more sensitive to changes in exergy loss than the universal efficiency (8).

5.2.5 Specification of functional exergy efficiencies of apparatuses

In general, functional exergy efficiency is defined as:

$$\eta_{Ex,f} = \frac{\sum Ex_{product}}{\sum Ex_{source}} \tag{10}$$

In order to be able to apply this efficiency to specific systems, a further specification of $\Sigma Ex_{product}$ and ΣE_{source} is required. We must then establish for all ingoing and outgoing process flows which part of the exergy of the process flow must be attributed to product or source. If only part of the exergy of a process flow is attributed to a source or product, a breakdown is required into an active part (source or product) and a passive part (ballast). How to make such a breakdown depends on the desired accuracy with which exergy efficiencies must be determined.

In practical situations, it is usually allowed to neglect the kinetic and potential energy of process flows. Initially, we also started from this assumption to specify exergy efficiencies. In a reversible process, kinetic and potential energies can be fully converted into power; if not insignificant, they can be added to the relative exergy values.

Below, we have chosen for a limited breakdown of exergy values for process flows into thermo-mechanical exergy and chemical exergy. *Thermo-mechanical exergy* is the power produced if the process flow is brought in thermo-mechanical balance with the environment in the prescribed manner. The chemical composition remains unchanged in this process. *Chemical exergy* is the power delivered if the process flow is brought in chemical equilibrium with the environment in the prescribed manner. Chemical equilibrium with the environment means that the components composing the process flow are converted into environment components and expand to the partial pressure of the relative component in the environment.

The sum of the two exergy terms is identical to the exergy of the process flow, i.e.:

$$Ex_{processflow} = Ex^{tm}_{processflow} + Ex^{ch}_{processflow} \qquad (11)$$

Breaking down the exergy of a process flow into a thermo-mechanical and a chemical component offers ample opportunity to distinguish between the active part (source, product) and the non-active part (ballast). On the basis of practical applications, we will have to establish the adequacy of such a breakdown for different situations.

Below, we have specified functional exergy efficiencies for a number of frequently occurring apparatuses; these efficiencies can be used in analysing varying processes. In this specification we have found that sometimes arbitrary choices cannot be avoided and that functional efficiencies cannot be stated for each apparatus.

For example, the function of a condenser in a steam cycle, in which the condenser discharges heat to the environment, only becomes clear if we look at the combination of turbine + condenser, in which case the condenser must be assessed based on the exergy efficiency of this combination. Considering the specific character of such combinations of apparatuses and the many possibilities, we confine ourselves here to efficiencies for individual apparatuses. We expect that with the given examples, the user will be able to specify functional efficiencies in an analogous manner for combinations of apparatuses which have a joint function.

On the following pages, in stating the functional efficiency of each apparatus, we will also briefly describe the process, and elucidate the choice of exergy product and source.

Turbine

In a turbine, a working fluid is expanded so as to deliver mechanical energy via a shaft. During the expansion process, part of the process medium is sometimes extracted; in the case of steam turbines, for example, extraction steam is used to pre-heat boiler feedwater. We may have to deal here with various outgoing flows.

The shaft power produced is regarded as the product of the process in the turbine, so:

$$Ex_{product} = P_{shaft} \tag{12}$$

The thermo-mechanical exergy produced by the working fluid is available as an exergy source. Since the chemical exergy of the working fluid does not change, the change in thermo-mechanical exergy is identical to the change in total exergy of the working fluid. We may suppose:

$$Ex_{source} = Ex_{in}^{tm} - \sum Ex_{out}^{tm} = Ex_{in} - \sum Ex_{out} \tag{13}$$

The turbine's functional efficiency is then:

$$\eta_{Ex,f\,(turbine)} = \frac{P_{shaft}}{Ex_{in-} \sum Ex_{out}} \tag{14}$$

Heat exchanger

In a heat exchanger, a process flow (the primary flow) is generally heated by withdrawing heat from another process flow (the secondary flow).

It is assumed that the purpose of the heat exchanger is to heat the primary flow. The increase in thermo-mechanical exergy of the primary flow is then the product of the heat transfer process. If the chemical composition of the working fluid remains unchanged, the increase in thermo-mechanical exergy is identical to the total exergy:

$$Ex_{product} = Ex_{p,out} - Ex_{p,in} \tag{15}$$

The secondary flow supplies the exergy. The exergy produced by this flow is identical to the exergy change of the secondary fluid in the heat exchanger. For the secondary fluid, it also applies that the chemical composition –and thus the chemical exergy—remains unchanged.

$$Ex_{source} = Ex_{s,in} - Ex_{s,out} \tag{16}$$

The functional exergy efficiency of the heat exchanger is then as follows:

$$\eta_{Ex,f(heatexchanger)} = \frac{Ex_{p,out} - Ex_{p,in}}{Ex_{s,in} - Ex_{s,out}} \tag{17}$$

It occurs, for example in the case of feedwater preheaters, that various ingoing flows are involved at the secondary level; these flows are mixed in the heat exchanger and leave the apparatus as one secondary process flow. In this case it holds true for the functional efficiency:

$$\eta_{Ex,f(heatexchanger)} = \frac{Ex_{p,out} - Ex_{p,in}}{\sum Ex_{s,in} - Ex_{s,out}} \tag{18}$$

Note If heat losses are considered in process calculations, these are automatically taken into account in the above efficiency.

Pump

In a pump, a medium considered incompressible is increased in pressure using shaft power. The exergy increase in the medium is regarded as the product. Shaft power is available as a source for this exergy increase.
The pump's functional efficiency is then:

$$\eta_{Ex,f(pump)} = \frac{Ex_{out} - Ex_{in}}{P_{shaft}} \tag{19}$$

Electromotors are often used for driving pumps. If the losses with respect to driving are also taken into account, it applies:

$$\eta_{Ex,f\,(pump)} = \frac{Ex_{out} - Ex_{in}}{P_{electric}} \tag{20}$$

Condenser

There are various ways to consider the exergy efficiency of condensers. In the case of a condenser that is intended to discharge heat to the environment, it is difficult to speak of a "product" since it is impossible to specify a functional efficiency.
However, there are also situations in which the exergy absorbed by the primary medium in a condenser can be utilized elsewhere in the system. This, for example, applies to warm condensers for the heating of district heating water and to circuits connected in series. We can then use the same wording for functional exergy efficiency as in the case of heat exchangers.
Also with condensers, we may have to deal with various ingoing process flows on the secondary level. For the condenser's functional efficiency we will have to write:

$$\eta_{Ex,f\,(condenser)} = \frac{Ex_{p,out} - Ex_{p,in}}{\sum Ex_{s,in} - Ex_{s,out}} \tag{21}$$

Note Usually in condensers, non-condensable gases are sucked off, along with a certain vapor quantity. If this discharge is considered in the process calculation, the exergy of the discharged steam in the above comparison is attributed to the condenser's exergy loss.

Feedwater preheater

For feedwater preheaters, we can use the same specifications as for heat exchangers and condensers.

De-aerator

In a de-aerator, condensate is heated and de-aerated using steam. Usually, in steam turbine circuits, other –relatively small—condensate flows are fed to the de-aerator. After de-aeration, the liquid mixture is discharged to the boiler feed pump.

The de-aerator can be regarded as a contact heater. The condensate flow is regarded as the primary, heat-absorbing flow. This flow is heated by mixing it with steam and condensate of higher temperatures; these warmer flows can be regarded as the secondary, heat-producing medium flows. Analogous to the heat exchanger, we can write for the product:

$$Ex_{product} = \phi_{m,p} \times \left(ex_{out} - ex_{p,in}\right) = \phi_{m,p} \times ex_{out} - Ex_{p,in} \qquad (22)$$

in which $\Phi_{m,p}$ is the mass flow condensate heated in the de-aerator.

Similarly, we can write for the source:

$$Ex_{source} = \sum\left(\phi_{m,s} \times ex_{s,in}\right) - ex_{out} \times \sum\phi_{m,s} = \sum Ex_{s,in} - ex_{out} \times \sum\phi_{m,s} \qquad (23)$$

The functional exergy efficiency then becomes:

$$\eta_{Ex,f\,(de-aerator)} = \frac{\phi_{m,p} \times ex_{out} - Ex_{p,in}}{\sum Ex_{s,in} - ex_{out} \times \sum\phi_{m,s}} \qquad (24)$$

Note The de-aerator is usually connected with the storage tank of the boiler feed pump. The function of the storage tank is of no significance in considering stationary conditions.

In the top of the de-aerator the non-condensable gases are sucked off, along with a small amount of steam. If the discharge of this quantity of steam is included in the process calculation, then –according to comparison (15)—the exergy of this flow is part of the exergy loss of the de-aerator (assuming that the discharged steam is not utilized elsewhere).

Compressor, fan

In a compressor or fan, by means of shaft power, a compressible medium is increased in pressure. Functional efficiency for compressors is specified in the same way as for pumps, i.e.:

$$\eta_{Ex,f\,(compressor)} = \frac{Ex_{out} - Ex_{in}}{P_{shaft}} \qquad (25)$$

Mixer, splitter, valve

Mixers, splitters and valves are tools that are frequently used in energy conversion systems but are not intended for energy conversion or energy transfer. They may cause loss of exergy, but it is impossible to speak of it in terms of a product. Therefore, it is not possible to define their exergy efficiency.

Note In system calculations it occurs that one uses splitters to separate components. In that case, there is in fact a separator involved. It is not possible to give a meaningful definition for the functional exergy efficiency of a separator.

Drum

A circulation evaporator consists of a heat exchanger and a drum. Heating and partial evaporation of the medium occur in the heat exchanger. In the drum, liquid and vapor are separated and the recirculated liquid is mixed with the feed. If drum and heat exchanger are distinguished as individual apparatuses, the drum can be regarded as an apparatus in which a liquid flow is evaporated using heat withdrawn from the heat exchanger.
The exergy absorbed during heating and evaporation of the feed is then regarded as the product. The exergy produced by the flow circulating in the heat exchanger is the source of this product. It then holds for the functional efficiency that:

$$\eta_{Ex,f(drum)} = \frac{Ex_{steam,out} - Ex_{feedwater,in}}{Ex_{evaporator,out} - Ex_{evaporator,in}} \tag{26}$$

Combustion chamber

In a combustion chamber, fuel is combusted using an oxidant. The flue gases formed during the combustion are discharged. Aside from heat losses as a result of imperfect isolation, the process is adiabatic.
The purpose of the combustion is to produce a gas (flue gas) of which only the thermo-mechanical exergy is utilized. The thermo-mechanical exergy produced can thus be regarded as the product of the combustion chamber.

The fuel and oxidant are fed to the combustion chamber, often at elevated temperature and pressure; the thermo-mechanical exergy of the fuel and oxidant flows is then larger than zero. This thermo-mechanical exergy cannot be regarded as a product of the combustion process and must therefore be deducted from the thermo-mechanical exergy of the flue gas. Therefore, the increase in thermo-mechanical exergy is chosen as the product:

$$Ex_{product} = Ex^{tm}_{fluegas} - Ex^{tm}_{fuel} - Ex^{tm}_{oxidant} \tag{27}$$

As the source for the production of this exergy, the chemical exergy of the fuel and oxidant is used. The chemical exergy of the flue gas flow is discharged to the environment and thus does not become available as a product. As an exergy source, the net availability is:

$$Ex_{source} = Ex^{ch}_{fuel} + Ex^{ch}_{oxidant} - Ex^{ch}_{fluegas} \tag{28}$$

The functional exergy efficiency of the combustion chamber is then specified as follows:

$$\eta_{ex,f\,(combustion\,chamber)} = \frac{Ex^{tm}_{fluegas} - Ex^{tm}_{fuel} - Ex^{tm}_{oxidant}}{Ex^{ch}_{fuel} + Ex^{ch}_{oxidant} - Ex^{ch}_{fluegas}} \tag{29}$$

The above does not account for the presence of non-combustible components in the fuel that are separated in the combustion chamber in the form of ash or slag. The chemical exergy of these substances is not utilized for heat production and must, therefore, be deducted from the chemical exergy of the fuel.

In general, ash and slag are discharged from the combustion chamber at high temperature. It is possible to still utilize the thermo-mechanical exergy of these substances; the thermo-mechanical exergy of ash and slag is, therefore, regarded as the product of the process in the combustion chamber. In that case, the functional efficiency is:

$$\eta_{ex,f\,(combustion\,chamber)} = \frac{Ex^{tm}_{fluegas} + Ex^{tm}_{ash} - Ex^{tm}_{fuel} - Ex^{tm}_{oxidant}}{Ex^{ch}_{fuel} + Ex^{ch}_{oxidant} - Ex^{ch}_{ash} - Ex^{ch}_{fluegas}} \tag{30}$$

Note In practice, not all of the fuel is converted in the combustion chamber. If the non-converted fuel (also in modeling) is discharged in the ash or the flue gas, the chemical exergy of this quantity of fuel is regarded as a ballast flow, according to the comparisons (18) and (19).

Boiler

Usually, a boiler is a complex installation, consisting of various apparatuses such as a combustion chamber, several heat exchangers, pumps and fans. In a detailed analysis of a boiler, we deal with each individual part and use the exergy efficiencies for the apparatuses involved.

In some situations a rough consideration of the boiler suffices; the boiler is then regarded as just an apparatus in which a process flow absorbs heat. The quantity of fuel required can then be determined using a stated thermal efficiency. This makes a complete system calculation possible without detailed boiler calculations. In such a consideration, the flue gas flow to the stack is not calculated individually; the heat discharged with the flue gases is included in the thermal efficiency of the boiler, in which case the exergy of the flue gas when leaving the boiler is also unknown.

The purpose of boiler and optional reheater is to supply thermo-mechanical exergy to the medium in the circuit. The change in thermo-mechanical exergy of the circuit medium can, therefore, be regarded as the product of the processes in the boiler. The chemical composition of the circuit medium in the boiler remains unchanged; the change in thermo-mechanical exergy is identical to the change in total exergy or:

$$Ex_{product} = Ex_{steam}^{tm} - Ex_{water}^{tm} = Ex_{steam} - Ex_{water} \tag{31}$$

Exergy is supplied to the boiler in the form of fuel. The chemical exergy of the fuel actually functions as a source. In fact, the chemical exergy of the oxidant and flue gas must be considered in the same way as with the combustion chamber. Since these flows are not considered in modeling, they are also neglected here in the exergy efficiency. The chemical exergy of the oxidant and flue gas, however, is small compared to the chemical exergy of fuel. Roughly, we can say:

$$Ex_{source} = Ex_{fuel}^{ch} \tag{32}$$

We can write for the functional efficiency of boiler or reheater:

$$\eta_{Ex,f\,(boiler)} = \frac{Ex_{steam} - Ex_{water}}{Ex_{fuel}^{ch}} \tag{33}$$

Note When speaking of fuel exergy, we generally mean chemical exergy. We implicitly assume that the fuel is available at ambient temperature and pressure.

Moisture separator, flue gas condenser

In a moisture separator or flue gas condenser, a flue gas flow is cooled down to below the water dewpoint, causing part of the vapor present in the gas to condense. The condensate is separated from the gas flow and discharged separately. In order for the gas flow to be cooled, another flow must be heated.
A moisture separator can be regarded as a heat exchanger, provided that vapor is condensed from the secondary cooling flow and individually discharged. The exergy change in the primary flow as a result of the heating is to be regarded as the product. The source for this exergy change is, in principle, the exergy change in the secondary flow. The heat in the condensate can possibly still be utilized. The condensate flow is, therefore, regarded as an outgoing secondary flow. In that case, several outgoing flows are concerned and the functional efficiency is:

$$\eta_{Ex,f\,(moisture\,separator)} = \frac{Ex_{p,out} - Ex_{p,in}}{Ex_{s,in} - Ex_{s,out}} \qquad (34)$$

Gasifier

In a gasifier, a solid fuel (usually at elevated temperature and elevated pressure) is converted into a gaseous fuel. For this, use is made of an oxidant (air or oxygen) and, possibly, steam as a gasification means. Usually, the product gas leaves the gasifier at an elevated temperature. It may be necessary to cool the gasifier, for example, in the form of jacket cooling. Ash and slag can also be discharged at an elevated temperature. It is possible to utilize the thermo-mechanical exergy of these flows elsewhere in the system.
Analogous to the thermal cold-gas and hot-gas efficiency, we can think of two ways to formulate functional exergy efficiency.

a. The gasifier is regarded as a device that supplies only fuel. The thermal energy is not utilized elsewhere and is considered a loss. The installation will then be assessed as to its cold-gas efficiency. In that case, the chemical exergy of the gas produced can be regarded as the product of the gasifier. The chemical exergies of the ingoing flows function as a source; the chemical exergy of the discharged ash or slag is regarded as a ballast flow and must be deducted from the chemical exergy of the fuel. The functional efficiency becomes then:

$$\eta_{Ex,f\,(gasifier)} = \frac{Ex^{ch}_{productgas}}{Ex^{ch}_{solid\,fuel} + Ex^{ch}_{steam} + Ex^{ch}_{oxidant} - Ex^{ch}_{ash}} \tag{35}$$

b. The gasifier is part of a system in which also the thermo-mechanical exergy in the product gas can be utilized, as can the thermo-mechanical exergy of other process flows that are part of the gasification process. The product of the gasification process, in that case, becomes the total exergy of the product gas, with the addition of the thermo-mechanical exergy of discharged ash or slag flows and the exergy increase in the cooling agent; the thermo-mechanical exergy of the supplied process flows, solid fuel, steam, and oxidant must be deducted from this. We then have the following formula:

$$Ex_{product} = Ex_{productgas} + Ex^{tm}_{ash} + (Ex_{out} - Ex_{in})_{cooling} - (Ex^{tm}_{solid\,fuel} + Ex^{tm}_{steam} + Ex^{tm}_{oxidant}) \tag{36}$$

Also in this case, the chemical exergy of the ingoing process flows minus the chemical exergy of the ash or slag is the source. The functional efficiency then becomes:

$$\eta_{Ex,f\,(gasifier)} = \frac{Ex_{productgas} + Ex^{tm}_{ash} + (Ex_{out} - Ex_{in})_{cooling} - (Ex^{tm}_{solid\,fuel} + Ex^{tm}_{steam} + Ex^{tm}_{oxidant})}{Ex^{ch}_{solid\,fuel} + Ex^{ch}_{steam} + Ex^{ch}_{oxidant} - Ex^{ch}_{ash}} \tag{37}$$

Reformer

A reformer can be seen as a device that aims at bringing about a change in the chemical composition of a process flow. In order to make the conversion into the desired product gas possible, steam is fed to the feed; while heat is supplied, conversion takes place. The heat required is usually obtained by placing the reformer pipes in a furnace where a certain amount of fuel is combusted. In the calculation, the reformer and combustion chamber are regarded as individual apparatuses, where the heat required for the reforming process is supplied by cooling down the flue gas flow.

It is assumed that the change in chemical exergy of the product gas forms the product of the reforming process, i.e.:

$$Ex_{product} = Ex^{ch}_{productgas} - Ex^{ch}_{steam} - Ex^{ch}_{feed} \tag{38}$$

The change in the thermo-mechanical exergy of the flue gas is considered to be the source. However, not only the chemical exergy of the product gas flow changes, but also the thermo-mechanical exergy as a result of the heating of the product gas. As it is assumed that this thermo-mechanical exergy can be beneficially utilized, it may be deducted from the exergy produced by the flue gas, i.e.:

$$Ex_{source} = Ex^{tm}_{fluegas,in} - Ex^{tm}_{fluegas,out} - (Ex^{tm}_{productgas} - Ex^{tm}_{steam} - Ex^{tm}_{feed}) \tag{39}$$

It is assumed that the chemical composition of the flue gas during cooling in the reformer does not change. The change in thermo-mechanical exergy is then identical to the change in total exergy. The functional efficiency then becomes:

$$\eta_{Ex,f\,(reformer)} = \frac{Ex^{ch}_{productgas} - Ex^{ch}_{steam} - Ex^{ch}_{feed}}{(Ex^{tm}_{fluegas,in} - Ex^{tm}_{fluegas,out}) - (Ex^{tm}_{productgas} - Ex^{tm}_{steam} - Ex^{tm}_{feed})} \tag{40}$$

Fuel cell

In a fuel cell, electricity is produced by making a fuel react (combust) with an oxidant. Both flows are individually fed to the anode and the cathode of the fuel cell, respectively. In practice, usually the fuel and oxidant also contain components that do not take part in the reactions in the cell; these must be removed together with the reaction products. Anode flow and cathode flow leave the cell separately.

The fuel cell produces electricity in the form of direct current. The electrical energy produced can be regarded as the product of the fuel cell. The change in chemical exergy of fuel and oxidant is available as an exergy source. The thermo-mechanical exergy of the fuel and oxidant flow, however, also changes as a result of the heating in the cell. The thermo-mechanical exergy absorbed by these flows can be utilized elsewhere in the system and may therefore be deducted from the change in chemical exergy of the flows, i.e.:

$$Ex_{soure} = (Ex_{in} - Ex_{out})^{ch}_{fuel} + (Ex_{in} - Ex_{out})^{ch}_{oxidant} - (Ex_{out} - Ex_{in})^{tm}_{fuel} - (Ex_{out} - Ex_{in})^{tm}_{oxidant} \tag{41}$$

This comparison shows that the source is formed by the change in total exergy of fuel and oxidant flows. The functional efficiency then becomes:

$$\eta_{Ex,f\,(fuelcell)} = \frac{P_{electric,directcurrent}}{(Ex_{fuel,in} - Ex_{fuel,out}) + (Ex_{oxidant,in} - Ex_{oxidant,out})} \tag{42}$$

Note In the fuel cell, the chemical exergy supplied is converted partly into electricity and partly into thermo-mechanical exergy (heat). In the above comparison, the part converted into thermo-mechanical exergy can be regarded as ballast flow. The larger the ballast flow, the smaller the quantity of exergy that can be converted into electricity. With the fuel cell, one tries to convert the largest possible part of the chemical exergy into electricity. Comparison (33) does not directly indicate the extent to which the fuel cell has succeeded in this.

Scrubber, separator, saturator

Considering exergy, we cannot speak of a product when dealing with scrubbers, separators and saturators. Therefore, it is impossible to give a meaningful specification of functional efficiency.

Reactor

As for reactors, we can only specify functional efficiency after establishing the function of the reactor. For specific designs of reactors (for example, a combustion chamber and a reformer), strongly varying specifications have been given. For the specifications given, we distinguish on the basis of how heat is fed to the process and how the outgoing process flow is used (for chemical or thermo-mechanical purposes). Therefore, it is not possible to define a generally workable functional efficiency.

Note In cases in which functional efficiency cannot be specified, one can always get an impression of the quality of the conversion using the universal efficiency. In drawing conclusions, one must bear in mind that the universal efficiency always has a value larger than, or identical to, the functional efficiency.

List of symbols

ex	specific exergy	[kJ/kg]
Ex	exergy flow	[kW]
P	power	[kW]
ΔEx	exergy change in a flow	[kW]
η	efficiency	
Φ_m	mass flow	[kg/s]

subscripts

Ex	exergy
f	functional
p	primary
s	secondary
u	universal

superscripts

ch	chemical
tm	thermo-mechanical

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