

15. Exergy Balance Module

15.1. Introduction

This module allows the user to calculate exergy, mass and heat balance for a system where there can be multiple input and output streams with multiple species. Exergy calculations can be performed for three different types of streams and the user can see the results for physical, chemical, and total exergy.

Recent concerns about sustainability and global warming have led to stricter environmental standards, which in turn have made exergy a more important property in many of today's industries. Energy analysis can show the energy efficiency of a process but does not give the whole picture of the usability of the energy before or after the process. Exergy analysis is used in industry and industrial ecology to measure the amount of usable energy. The results can be used for example to calculate how efficiently the process uses the available energy.

In practice, an engineer might have two possible designs to complete one process. The two designs may have the same energy efficiency but different exergy efficiency. A lower exergy efficiency would mean that the process is more irreversible and wastes more usable energy than the process with higher exergy efficiency.

15.2. Basic Use

When the user starts the program, only one normal input and output stream with a sample H₂O species is available in the Excel sheet. To insert a new species, you can write or paste the list of species to the “Insert/paste species here” cell and press Enter. The user can also use the database browser to add species to the stream.

The screenshot shows the 'Exergy Balance' software window. At the top, there is a menu bar (File, Edit, Units, Help) and a toolbar with buttons for 'Browse database', 'Insert stream', 'Input', 'Gas stream', 'Delete stream', 'Delete species', and 'Calculate'. Below the toolbar, there are three summary boxes: 'Mass Balance (kg)' with a value of 0.00, 'Heat Balance (kJ)' with a value of 0.00, and 'Exergy Balance (kJ)' with a value of 0.00. A text box on the right provides a disclaimer: 'All exergy calculations are based on Szargut theory with the standard state being 25°C and 1 bar. Normal stream accepts any species. Gas stream accepts gas species and adds pressure S to exergy. Energy stream adds heat and electricity feed/loss. Carnot cycle is used to convert heat to exergy.'

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
	Streams and species	Mass (kg)	Amount (mol)	Molfraction (fraction)	T (K)	P (bar)	H Total (kJ)	Ex_elemental (kJ/mol)	Ex_che (kJ)	Ex_phy (kJ)	Ex_tot (kJ)	Ex_tot_stream (kJ)			
1	Streams and species														
2															
3	Input Stream 1														
4	H2O		1.00												
5	Insert/paste species here														
6															
7	Output Stream 1														
8	H2O		1.00												
9	Insert/paste species here														
10															
11															
12															
13															
14															
15															
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Fig. 1. General layout of the exergy calculator.

The user can enter and edit data in the white cells. These include the name of the species, the title of the stream, the amount and mass of the species, and the temperature. There are two additional editable cells for the other streams which are located in the pressure and H total columns. The user must always enter either the mass OR amount for each species. If no temperature is inserted, the program will calculate using the standard state temperature (298.15 K).

The user can insert new streams, remove streams, and remove species from the streams by using the corresponding buttons in the upper left corner. The type of stream can be selected from the drop-down menu next to the **Insert Stream** button. Pressing **Calculate** calculates all values and also gives the user the mass, heat, and exergy balance at the top, see **Fig. 2** and example file C:\Program Files (x86)\HSC10\Exergy\Exergy_example.exe8.

Exergy Balance														
Mass Balance (kg)			Heat Balance (kJ)			Exergy Balance (kJ)			All exergy calculations are based on Szargut theory with the standard state being 25°C and 1 bar. Normal stream accepts any species. Gas stream accepts gas species and adds pressure S to exergy. Energy stream adds heat and electricity feed/loss. Carnot cycle is used to convert heat to exergy.					
-12.80			57851.57			-271313.81								
A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
Streams and species	Mass (kg)	Amount (mol)	Molfraction (fraction)	T (K)	P (bar)	H Total (kJ)	Ex_elemental (kJ/mol)	Ex_che (kJ)	Ex_phy (kJ)	Ex_tot (kJ)	Ex_tot_stream (kJ)			
Input Stream 1	85.28	900.00	1.00	1100.00	1.00	-10334.22	1725.50	638764.19	22082.34	660846.53	660845.75			
CuS	76.49	800.00	0.89	1100.00	1.00	-5878.05	741.90	550521.58	19443.71	569965.30				
FeS	8.79	100.00	0.11	1100.00	1.00	-4456.17	983.60	88242.61	2638.62	90881.23				
Input Stream 2	3.00	50.00	1.00	200.00	1.00	-45719.19	858.92	123.86	33.46	157.32	157.32			
SiO2	3.00	50.00	1.00	200.00	1.00	-45719.19	858.92	123.86	33.46	157.32				
Input Gas Stream 1	288.10	10000.00	1.00	25.00	1.00	-79350.71	4.59	13200.00	134271.61	147471.61	147459.21			
O2(g)	64.00	2000.00	0.20	25.00	1.00	-15851.92	3.92	7840.00	26583.11	34423.11				
N2(g)	224.11	8000.00	0.80	25.00	1.00	-63498.79	0.67	5360.00	107688.50	113048.50				
Input Energy Stream 1						10000.00					10000.00			
Heat feed				25.00		0.00								
Electricity feed						10000.00								
Output Stream 1	54.04	800.00	1.00	1300.00	1.00	-4299.34	267.16	80552.98	15600.71	96153.69	96152.58			
Cu	38.13	600.00	0.75	1300.00	1.00	16663.23	132.60	79560.00	9557.95	89117.95				
CuO	15.91	200.00	0.25	1300.00	1.00	-20962.57	134.56	992.98	6042.76	7035.74				
Output Stream 2	10.19	50.00	1.00	1300.00	1.00	-65038.99	1611.44	11644.39	5133.50	16777.88	16777.88			
*2FeO*SiO2	10.19	50.00	1.00	1300.00	1.00	-65038.99	1611.44	11644.39	5133.50	16777.88				
Output Gas Stream 1	299.36	9450.00	1.00	1100.00	1.00	-18214.22	617.81	289330.35	130320.99	419651.34	419638.91			
SO2(g)	57.66	900.00	0.10	1100.00	1.00	-230707.39	613.22	281814.35	19378.71	301193.06				
SO3(g)	0.00	0.00		1100.00	1.00	0.00	0.00	0.00	0.00	0.00				
O2(g)	17.60	550.00	0.06	1100.00	1.00	14419.43	3.92	2156.00	7567.96	9723.96				
N2(g)	224.11	8000.00	0.85	1100.00	1.00	198073.74	0.67	5360.00	103374.32	108734.32				
Output Energy Stream 1						20000.00					14579.09			
Heat loss				1100.00		20000.00								
Electricity out						0.00								

Fig. 2. Spreadsheet after calculations.

The three different types of streams are explained in the upper right corner of the screen where the exergy calculation standard state is also mentioned. The type of stream can be recognized from the color of the stream title: a normal stream is black, the ideal gas stream is red, and the energy stream is green.

A normal stream accepts any species and can be used for any stream whereas the ideal gas stream accepts gaseous species. It should also be noted that the ideal gas stream uses pressure for the entropy calculations. The energy stream allows the user to enter heat and electricity amounts for the system. Electricity is calculated directly into the total exergy but the heat value is converted to the exergy value using the Carnot heat engine equation as follows:

$$Ex = q * \left(1 - \frac{T_0}{T}\right) \quad (1)$$

where Ex is exergy, q is heat, T_0 is the temperature in the standard state, and T is temperature of the heat source.

15.3. Errors and Calculation

The program calculates all values for each species and also sums these values to the total values for the streams. Stream total exergy is only for the stream as a whole, because mixing entropy cannot be divided between species in a meaningful way. In the calculations, elemental exergy is part of chemical exergy and the total exergy is the sum of the chemical and physical exergy.

The program will always check that the species are inserted correctly and that they can be found on the database. It also checks that either mass OR amount is inserted so that the different types of streams have the right phase for the species.

15.4. Exergy Theory

Exergy is the maximum amount of work obtainable when an energy carrier is brought from its initial state to a state of thermodynamic equilibrium with the common substances of the natural environment by means of reversible processes, involving interaction only with the above-mentioned substances of nature. The thermodynamic equilibrium is a chosen reference state, and in these calculations the atmospheric and the common lithosphere conditions are used as the reference state for exergy. Exergy is thus a function of the thermodynamic state of the substances under consideration and of the thermodynamic state of the common reference substances in the natural environment¹.

For example, the temperature of seawater (in these calculations 25 °C is chosen) is one reference state used for the calculations. Any substance with a higher or lower temperature than seawater has an exergy value greater than zero. Another example is gaseous molecular oxygen. In atmospheric air the mole fraction of oxygen is 0.21, and it is at this concentration that the exergy of gaseous oxygen is zero. Therefore pure oxygen has an exergy value greater than zero because work can be produced by bringing it to equilibrium with the reference environment. As for the lithosphere, the most common substances are used for the reference state. This means that, for example for iron, oxidized iron is used as a reference state instead of pure iron¹.

According to Szargut's theory which is used in the program, the total exergy of a particular species can be calculated using the following formula:

$$Ex_{tot} = \underbrace{\sum_k n_k b_k^{ref} + \Delta G_{f(25^\circ\text{C}, 1\text{bar}), i}^0}_{\text{Chemical exergy}} + \underbrace{(H_i - H_{i(25^\circ\text{C}, 1\text{bar})}) - T_{25^\circ\text{C}}(S_i - S_{i(25^\circ\text{C}, 1\text{bar})})}_{\text{Physical exergy}}, \quad (2)$$

where

n_k is the stoichiometric amount of element k in the species

b_k^{ref} is the elemental exergy of element k

$\Delta G_{f(25^\circ\text{C}, 1\text{bar}), i}^0$ is the standard formation Gibbs energy of the species

H_i is the total enthalpy of the species at a temperature of T

$H_{i(25^\circ\text{C}, 1\text{bar})}$ is the total enthalpy of the species in the standard state

S_i is the total entropy of the species in the temperature of T , and

$S_{i(25^\circ\text{C}, 1\text{bar})}$ is the total entropy of the species in the standard state.

Szargut's standard state (25 °C, 1 bar) is used in the calculations as well as the elemental exergy values which are defined in his article².

15.5. References

1. Sato, N. Chemical Energy and Exergy: An Introduction to Chemical Thermodynamics for Engineers. 2004. Elsevier Science & Technology Books.
2. Szargut, J. Chemical exergies of the elements. Applied Energy. 1989.