Energy Metrics and Measurements

Introduction

The energy demand for a production process affects the environmental impact substantially. Reasons for this are the emissions and wastes generated during the energy production (e.g. burning of fossil fuels). These have a great environmental impact. It is possible to find nuclear waste within a harmless laboratory reaction[1]. That´s why the decrease of energy consumption of industrial chemical reactions is an important aim. In view of environmental protection and sustainable development it is important as a teaching objective in laboratory, too.

In order to achieve this aim it is necessary to measure and to evaluate energy consumption with help of energy metrics. Thus the progress of optimizing the synthesis can be assessed. In the laboratory the measurement and evaluation of energy consumption can be easily achieved using relatively cheap devices. In the following the strategy of measuring energy consumption is described.

Measuring Energy Consumption

The electric energy used for a conversion can be measured with relative small effort. Cost-effective energy counters with sufficient accuracy for laboratory reactions are available. Examples are:

Figure 1: example device 1

Figure 2: example device 2

Figure 3: example device 3

[1] The source of nuclear waste is purchasing electrical current from typical sources in Germany. The energy generation takes place in hard coal, brown coal, fuel oil, gas, nuclear or hydro-electric plants.

During the preparation of the measurement it is necessary to attach all consumers needed for a single step of the conversion to the energy counter. If more than one consumer is involved this can be simply realized with a multiway connector. In order to ensure comparable measurements it is advisable to put all devices into operating conditions before starting the measurement. This means that e.g. the desired oil bath or cryostat temperature is already reached. This is necessary because the energy consumption to heat or to cool down depends on the initial temperature. Once all devices are set up in their operating conditions the measurement may start. As soon as the reaction has ended, the energy consumption can easily be read off. The energy consumption may differ depending on the laboratory worker, the devices used and the initial size. Of course, the setup of the test equipment must not be changed for comparable measurements.

The energy counters usually measure the energy consumption in Wh. By using the conversion factor 3.6 this value can be converted to the SI-unit kJ. Some energy characteristics can be computed via the energy consumption. These characteristics can be interpreted to reveal high energy consumers during the synthesis and to indicate optimization potential.

Energy Metrics

Environmental metrics are defined in analogy to economical metrics as "a environmental relevant variable which can be an absolute or relative figure providing insight into some issue" [1]. A set of appropriate environmental metrics can be -like the economical metrics - a suitable instrument for a decision-oriented data preparation and processing. One type of environmental metrics are energy metrics. In the context of chemical syntheses, they describe the connections of energy and substance consumption or the ratio of the energy consumption in the reaction and processing, respectively. They may indicate weak points and can be used for result-oriented optimizations. The validity of a metrics depends on the quality of acquired data. The more exactly the measurement is accomplished, the more meaningful metric can be achieved and thus more effective improvements are possible. For example, it is possible to consider both the entire reaction or only the processing. When evaluating the generated metrics it has to be kept in mind that only the electric energy consumption is taken into account. The consumption of primary energy, e.g. from burning of fossil fuels, is significantly larger. Depending on the type of power plant a factor of up to 3 can be assumed for the calculation of the primary energy needed.

Energy Efficiency

The energy efficiency is the ratio of the electric energy used in a synthesis and the isolated product of the reaction.

$$E_E = \frac{m_{product}}{E_{consumpt.}}$$

E_F	= energy efficiency [kg/kJ]
$m_{product}$	= mass of the product [kg]
$E_{consumpt.}$	= consumption of energy of the synthesis (reaction and processing) [kJ]

Taking into consideration the environmental burden refer to energy production, these burden decrease with increasing energy efficiency. When working with the characteristic energy efficiency it has to be noted that different reactions must not be compared with each other, since they have a different theoretical energy consumption. Therefore it is only valid to compare same reactions. The energy efficiency is a very rough characteristic, which is similiar to a "black-box-view". By means of it it is only possible to determine whether the consumption of electric energy within the synthesis has improved or not. To get more detailed information you have to refine the characteristic.

Energetic Work up Expenditure (A_E)

The work up of a reaction mixture takes a substantial part of the work within a chemical synthesis. Apart from the quantities of necessary chemicals, which is often larger in comparison to the reaction, there is often also a large amount of electricity needed for isolation and cleaning. The characteristic "energetic work up expenditure" makes it possible to get information about the amount of energy needed per unit of product. It can be calculated from the ratio of the energy needed for the work up and the mass of the product:

$$A_E = \frac{E_{proc.}}{m_{product}}$$

A_E	= energetic work up expenditure [kJ/kg]
$E_{proc.}$	= energy needed for work up [kJ]
$m_{product}$	= mass of the product [kg]

Ratio reaction/processing

The energy consumption of reaction and work up contributes substantially to the total environmental impact of laboratory reactions. It is interesting that very often an imbalance of the energy consumption is on the side of work up. The cause of this are parallel- and follow-up reactions as well as catalysts and solvent remaining in reaction mixture. These have to be separated often over many stages. By comparing energy consumption of reaction and processing it is possible to get information on the amount of work up needed after the reaction.

$$E_{r/p} = \frac{E_{proc.}}{E_{reaction}}$$

$E_{r/p.}$ = ratio energy consumption reaction/processing

$E_{proc.}$ = energy consumption for work up [kJ]

$E_{reaction.}$ = energy consumption of the reaction [kJ]

The smaller the ratio, the better the reaction. The bigger the metric, the more it is necessary to optimize the reaction to simplify the work up.

Energy-induced Methane Equivalents

The characteristic "energy-induced methane equivalents" allows depicting the energy demand of a reaction and its work up. The basic principle is that the majority of electric energy in Germany is obtained by burning fossil fuels. For determining the methane equivalents it is assumed that electricity is currently only gained from burning methane (H_U[2] = 47.5 MJ/kg). The model power plant does not work with the method of power-heat coupling and provides electricity with an efficiency of 43 %. Now the amount of methane in mol is calculated, which is needed to supply the energy for the reaction, in the synthesis or in a holistic view over the reaction (1 MJ = 3.052 mol methane). Therefore the actual energy is not any longer the focus of attention, but the reaction

$$CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O + \text{energy}$$

[2] H_U (net calorific value): usable portion of the energy generated within a combustion

for energy production is compared to the laboratory synthesis. This abstraction emphasises the significance of energy consumption for the environmental burden of chemical reactions. In order to enable a chemical reaction in the laboratory, fossil fuels must be converted to energy at the same time in another reaction. The characteristic “methane equivalents K_M“ is calculated by dividing the yield of the reaction in mol by the calculated amount of methane.

$$K_M = \frac{n\ methane}{n\ product}$$

$K_{M.}$	= energy-induced methane equivalents
n methane	= amount of methane for energy supplying [mol]
n product	= amount of product [mol]

This metric depicts the unit of electric energy kJ or Wh (which may be too abstract for chemists). Additionally, the characteristic tells us something about the contribution of the reaction to the anthropogenic greenhouse effect.

[1] Loew, Thomas und Kottmann, Heinz, 1996. Kennzahlen im Umweltmanagement Ökologisches Wirtschaften 2/96, S. 10-12.