# 8. Category Chemical

8.1. Chemical Dosing

8.1.1. Purpose (What can it be used for? What can it not be used for?)

The program is part of category 3 – chemical. The dosing of chemicals is required for many different treatment purposes. In almost every case there is a storage tank or vessel that is filled with a chemical. Rarely the chemicals are high concentrated, so that in most cases chemical solutions are used for the treatment process. In order to achieve a defined concentration at the corresponding point of use, different circumstances and criteria are mandatory to be taken into consideration. First of all the general required compounds of a dosing line are mentioned. A storage tank with the corresponding chemical is required. To transfer the chemical solution from the storage tank to the point of use a dosing pump is used, usually. The chemical in the storage tank has a defined concentration. This concentration will be constant, as long as the chemical is on its way passing through the chemical pipeline. At the point of use, where the chemical is dosed into the main flow it will be diluted according to the relation of the flow rates in the chemical pipeline (dosing line) and the main pipeline. The following parameters are mandatory for the calculations: the concentration of the chemical in the storage tank respectively in the chemical pipeline, the flow rate for the dosing pump, the flow rate in the main pipeline at the point of use and the target concentration in the main pipeline at the point of use. Depending on the unit selection for the concentration of the chemical the density of the chemical in the storage tank can be required as given variable.

The variables concentration in chemical line, flow rate in chemical line, concentration in main pipeline and flow rate in main pipeline can be selected either as an input or an output variable. Therefore the selected variable will be the calculated output parameter. The residual three variables are input parameters. Beside the general internal routine that is checking up the entered input values regarding their defined limits, for this program there is also an internal plausibility crosscheck provided for the concentrations in coherence with the given density. Due to practical considerations the density of the chemical is provided as an input variable, only. At the end of the calculation the total flow rate in the main pipeline is calculated, which is the sum up of the flow in the main pipeline before the dosing point and the flow of the dosing pump respectively the flow in the chemical line.

The given and the calculated variables are shown in the sketch on the left side of the form in order to achieve a clear overview. Additionally there are four buttons arranged which allow the used to switch the color of the chemical respectively the liquid inside the storage tank. There are four colors provided: orange for the acid, violet for the base or caustic liquids, blue for water (e.g. with a concentration of matter like salt) and none for other use cases. The color selection has no influence on the calculations.
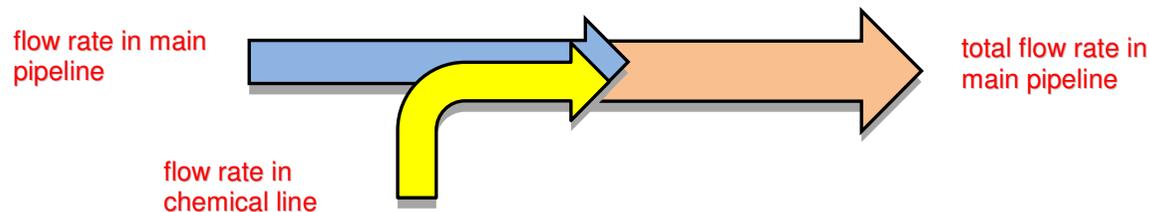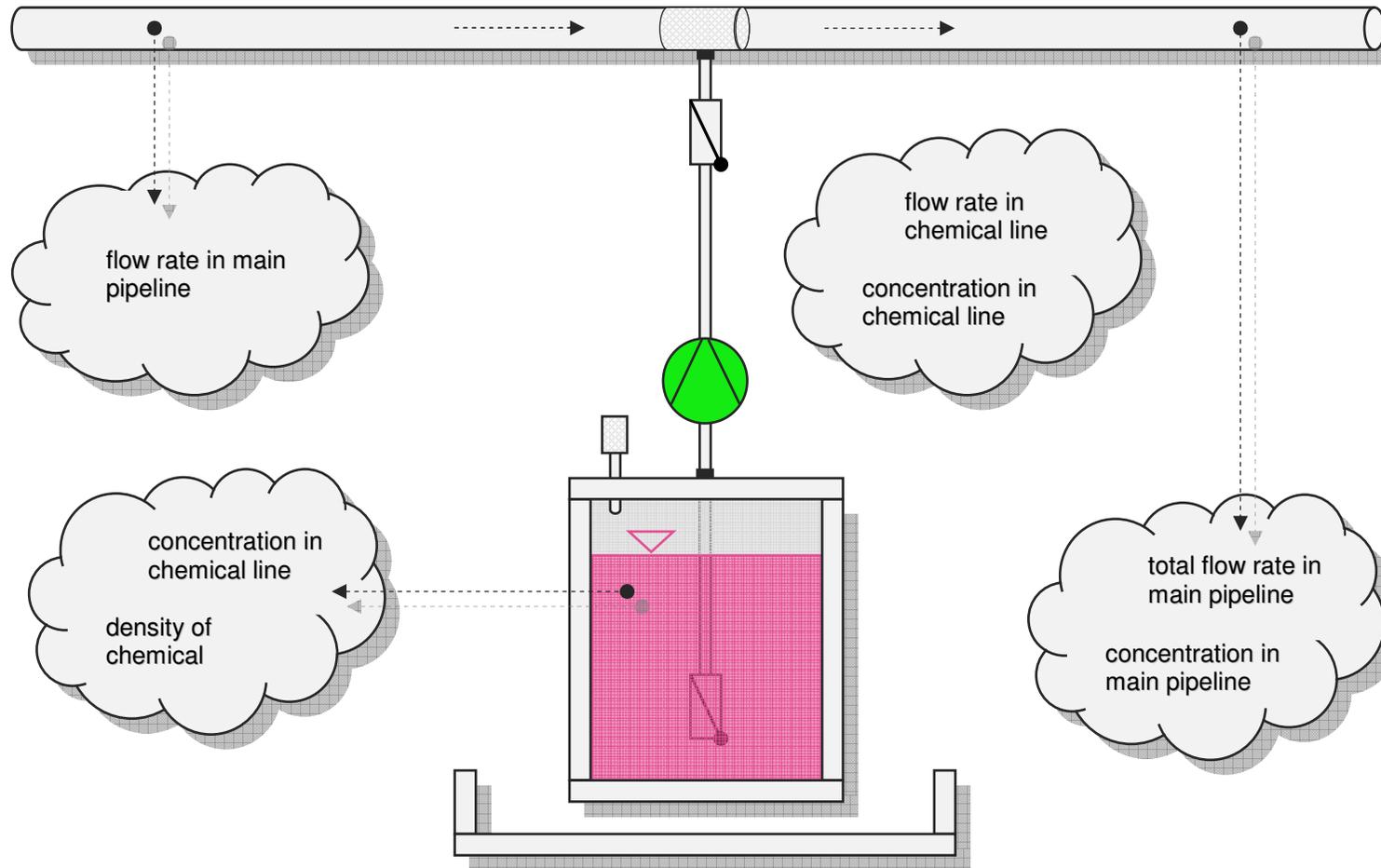
Figure 57: sketch chemical dosing

8.1.2.   Variables (What are the input and output values? What are their limits?)

concentration in chemical line

It is the concentration of the chemical in the dosing tank and in the chemical line. The chemical line is going from the dosing tank into the main pipeline. The chemical is dosed into the main pipeline in order to reach the required concentration in the main pipeline.

The variable type is Input or Output.
For this variable a selection of different units is provided:

- parts per quadrillion [ppq],

- parts per trillion [ppt],

- parts per billion [ppb],

- parts per million [ppm],

- per mille [per mille],

- percent [%],

- microgram per liter [µg / l],

- milligram per liter [mg / l],

- gram per liter [g / l],

- gram per meter cube [g / m³],

- kilogram per meter cube [kg / m³].

The minimum limit is 0.0001.
The maximum limit is variable. The concentration is not allowed to exceed 100% or the density value.
The replacement value is 100.
The number of digits is 10.

flow rate in chemical line

It is the flow rate for the chemical, which is transferred from the chemical tank into the main pipeline. The chemical is dosed into the main pipeline with the required flow rate in order to reach the required concentration in the main pipeline.

The variable type is Input or Output.
For this variable a selection of different units is provided:

- meter cube per hour [m³ / h],

- liter per second [l / s],

- liter per minute [l / min],

- liter per hour [l / h].

The minimum limit is 0.0001.
The maximum limit is 9999999999.
The replacement value is 100.
The number of digits is 10.

concentration in main pipeline

It is the concentration of the chemical in the main pipeline, which results out of the following parameters: the concentration in the chemical line, the flow rate in the chemical line and the flow rate in the main pipeline.

The variable type is Input or Output.
For this variable a selection of different units is provided:

- parts per quadrillion [ppq],

- parts per trillion [ppt],

- parts per billion [ppb],

- parts per million [ppm],

- per mille [per mille],

- percent [%],

- microgram per liter [µg / l],

- milligram per liter [mg / l],

- gram per liter [g / l],

- gram per meter cube [g / m³],

- kilogram per meter cube [kg / m³].

The minimum limit is 0.0001.
The maximum limit is variable. The concentration is not allowed to exceed 100% or the density value.
The replacement value is 100.
The number of digits is 10.

flow rate in main pipeline

It is the flow rate in the main pipeline before the chemical is added. The chemical is transferred from the chemical tank into the main pipeline. The chemical is dosed into the main pipeline with the required flow rate in order to reach the required concentration in the main pipeline.

The variable type is Input or Output.
For this variable a selection of different units is provided:

- meter cube per hour [m³ / h],

- liter per second [l / s],

- liter per minute [l / min],

- liter per hour [l / h].

The minimum limit is 0.0001.
The maximum limit is 9999999999.
The replacement value is 100.
The number of digits is 10.

density of chemical

It is the density of the chemical, which is transferred from the chemical storage tank into the main pipeline. The density is taken into consideration automatically, where the selected concentration unit is without dimensions. Related concentration values are assumed to be mass related values. These units are:

- parts per quadrillion [ppq],

- parts per trillion [ppt],

- parts per billion [ppb],

- parts per million [ppm],

- per mille [per mille],

- percent [%].

The variable type is Input.
The unit is kilogram per liter [kg / l].
The minimum limit is 0.0001.
The maximum limit is 29.
The replacement value is 1.
The number of digits is 10.

mass flow of chemical

It is the mass flow for the chemical, which is transferred from the chemical tank into the main pipeline. The chemical is dosed into the main pipeline with the required flow rate in order to reach the required concentration in the main pipeline. The mass flow is constant at every point of the system. Where the selected concentration unit is without dimensions the density of the chemical is considered accordingly. Related concentration values are assumed to be mass related values.

The variable type is Output.
For this variable a selection of different units is provided:

- kilogram per hour [kg / h],

- gram per second [g / h],

- gram per minute [g / min],

- gram per hour [g / s].

There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

total flow rate in main pipeline

It is the total flow rate in the main pipeline after the chemical is added. First there are two flow rates. One for the chemical line and one for the main pipeline. The chemical is dosed into the main pipeline with the required flow rate in order to reach the required concentration in the main pipeline. At the position where the chemical is dosed into the main pipeline both flow rates are added to a total flow rate.

The variable type is Output.
For this variable a selection of different units is provided:

- meter cube per hour [m³ / h],

- liter per second [l / s],

- liter per minute [l / min],

- liter per hour [l / h].

There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

8.1.3. Operation (How can it be used? How to proceed?)

Step 2:
Select the variable to be calculated
By clicking on the corresponding *RadioButton* I can choose the variable to be calculated. It is like executing an internal conversion of the equation.

Step 5:
Calculate result
After I entered the input values I can calculate the result. Before the calculation starts, all the input values are checked by an internal routine. Whenever entered values decrease the corresponding min limits or increase the corresponding max limits or are not numeric there will be a message according to the fault. The values will be corrected automatically by the internal routine.

Step 3:
Fill the Input-TextBoxes
I enter the values for the input variables. I should respect the variable limits and take care that the entered values are numeric.

Step 4:
Enter the number of decimal places
I enter the number of decimal places for the variables. It is valid only if the corresponding variable is selected as output. The input variables can get more or less decimal numbers according to the number of digits.

Step 7:
Further actions
After the calculation I can have the following options:
Print Data, Erase Data, Program Information, Notes, Save or Restore Values. While printing a new calculation is done automatically.
Clicking the Erase-Button will empty all the *TextBoxes* at once.

Step 6:
Check result
After clicking the Calculate-Button I can check the result.

Step 1:
Select the units
There is a choice of different units for each variable.

Figure 58: form chemical dosing

8.2. Water Hardness

8.2.1. Purpose (What can it be used for? What can it not be used for?)

The program is part of category 3 – chemical. Sometimes it is useful to evaluate the grade of water hardness in order to have a basis for the design criteria for the right water treatment or to find an explanation for the actual circumstances. Although there are only two kinds of matter as hardness compounds available in the water which are calcium and magnesium, there are many different international units describing the grade of water hardness. At least the total hardness is a measure for dividing up the water into mainly three degrees of hardness, which are: soft, medium and hard.

The program is divided up into two parts. It provides a calculation for the total water hardness which results from the concentrations of calcium and magnesium. The concentration is at least the mass of the single hardness component contained in a defined volume of water. One of the variables calcium concentration, magnesium concentration or total hardness can be chosen as result by selection. The residual two are input variables. Via the transfer button the value for the total hardness can be transferred to the unit conversion part. In this case a calculation for the unit conversion will be executed automatically.

Further the program provides a conversion of the different hardness units. These are German Hardness, English Hardness, French Hardness, CaCO3, parts per million, alkaline earth ions as mval / l and alkaline earth ions as 1 mmol / l. One of these variables can be chosen as input parameter by selection. The residual variables will be calculated accordingly.
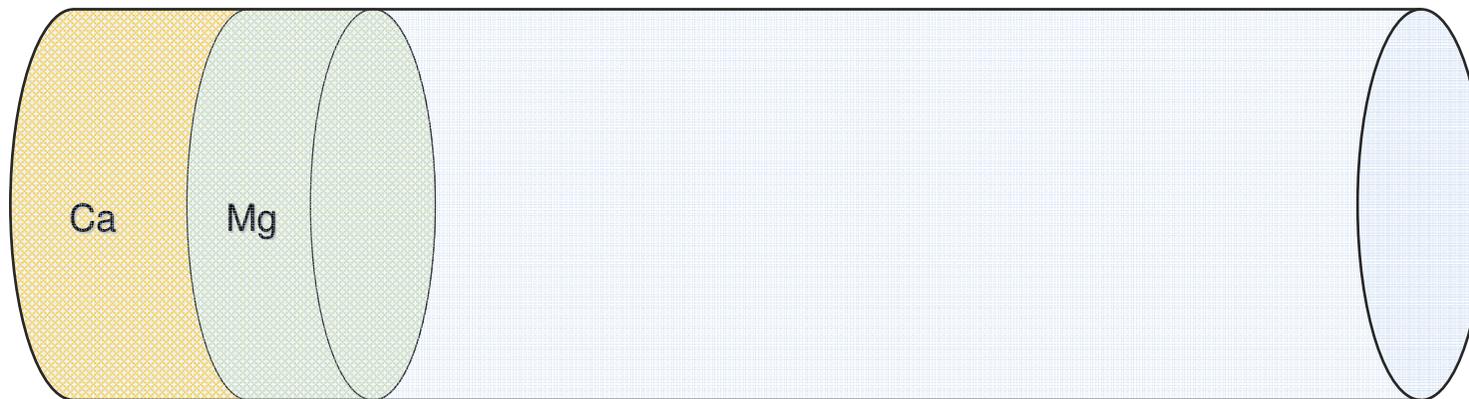

Figure 59: sketch water hardness

8.2.2.   Variables (What are the input and output values? What are their limits?)

concentration of Ca

It is the effective concentration of calcium, which is predominantly available by the calcium carbonate. It is at least the mass of calcium components contained in a defined volume of water.

The variable type is Input or Output
The unit is milligram per liter [mg / l].
The minimum limit is 0.0001.
The maximum limit is 1000.
The replacement value is 10.
The number of digits is 10.

total hardness

It is the total water hardness that results from the concentrations of the contained hardness components as calcium and magnesium in the water. The total hardness can be transmitted into many different units. It is a measure for dividing up the water into mainly three degrees of hardness, which are: soft, medium and hard.

The variable type is Input or Output.
The unit is milligram per liter [mg/l].
The minimum limit is 0.0001.
The maximum limit is 999.
The replacement value is 10.
The number of digits is 10.

concentration of Mg

It is the effective concentration of magnesium, which is predominantly available by the magnesium carbonate. It is at least the mass of magnesium components contained in a defined volume of water.

The variable type is Input or Output.
The unit is milligram per liter [kg / l].
The minimum limit is 0.0001.
The maximum limit is 1000.
The replacement value is 10.
The number of digits is 10.

The values for the three degrees of hardness are as follows:

- soft means < 1.5 mmol / l or < 8.4 °dH

- medium is 1.5 .. 2.5 mmol / l or 8.4 to 14 °dH

- hard means > 2.5 mmol / l or > 14 °dH

German Hardness

It is the water hardness as multiple of the unit German Hardness, that results from the concentrations of the contained hardness components as calcium and magnesium in the water.

The conversion factors for the residual units are as follows.

English Hardness: 1 °eH = 1.253 °dH
French Hardness: 1 °fH = 1.78 °dH
ppm CaCO3: 1 ppm = 17.8 °dH
alkaline earth ions: 1 mval / l = 0.357 °dH
alkaline earth ions: 1 mmol / l = 0.1783 °dH

The variable type is Input or Output.
The unit is degree German Hardness [°dH].
The minimum limit is 0.0001.
The maximum limit is 9999999999.
The replacement value is 10.
The number of digits is 10.

English Hardness

It is the water hardness as multiple of the unit English Hardness, that results from the concentrations of the contained hardness components as calcium and magnesium in the water.

The conversion factors for the residual units are as follows.

German Hardness: 1 °dH = 0.798 °eH
French Hardness: 1 °fH = 1.43 °eH
ppm CaCO3: 1 ppm = 14.3 °eH
alkaline earth ions: 1 mval / l = 0.285 °eH
alkaline earth ions: 1 mmol / l = 0.142 °eH

The variable type is Input or Output.
The unit is degree English Hardness [°eH].
The minimum limit is 0.0001.
The maximum limit is 9999999999.
The replacement value is 10.
The number of digits is 10.

French Hardness

It is the water hardness as multiple of the unit French Hardness, that results from the concentrations of the contained hardness components as calcium and magnesium in the water.

The conversion factors for the residual units are as follows.

German Hardness: 1 °dH = 0.56 °fH
English Hardness: 1 °eH = 0.702 °fH
ppm CaCO3: 1 ppm = 10 °fH
alkaline earth ions: 1 mval / l = 0.2 °fH
alkaline earth ions: 1 mmol / l = 0.1 °fH

The variable type is Input or Output.
The unit is degree French Hardness [°fH].
The minimum limit is 0.0001.
The maximum limit is 9999999999.
The replacement value is 10.
The number of digits is 10.

ppm CaCO3 – precipitated calcium carbonate

It is the water hardness as multiple of the CaCO3-units in ppm as precipitated calcium carbonate. It is the Hardness that results from the concentrations of the contained hardness components as calcium and magnesium in the water.

The conversion factors for the residual units are as follows.

German Hardness: 1 °dH = 0.056 ppm CaCO3
English Hardness: 1 °eH = 0.07 ppm CaCO3
French Hardness: 1 °fH = 0.1 ppm CaCO3
alkaline earth ions: 1 mval / l = 0.02 ppm CaCO3
alkaline earth ions: 1 mmol / l = 0.01 ppm CaCO3

The variable type is Input or Output.
The unit is parts per million of CaCO3 [ppm].
The minimum limit is 0.0001.
The maximum limit is 9999999999.
The replacement value is 10.
The number of digits is 10.

alkaline earth ions – mval / l

It is the water hardness as multiple of the alkaline earth ions unit in mval / l (val is similar to Eq). It is the Hardness that results from the concentrations of the contained hardness components as calcium and magnesium in the water.

The conversion factors for the residual units are as follows.

German Hardness: 1 °dH = 2.8 mval / l
English Hardness: 1 °eH = 3.51 mval / l
French Hardness: 1 °fH = 5 mval / l
ppm CaCO3: 1 ppm = 50 mval / l
alkaline earth ions: 1 mmol / l = 0.5 mval / l

The variable type is Input or Output.
The unit is milli-equivalent per liter [mval / l].
The minimum limit is 0.0001.
The maximum limit is 9999999999.
The replacement value is 10.
The number of digits is 10.

alkaline earth ions – mmol / l

It is the water hardness as multiple of the alkaline earth ions unit in mmol / l. It is the Hardness that results from the concentrations of the contained hardness components as calcium and magnesium in the water.

The conversion factors for the residual units are as follows.

German Hardness: 1 °dH = 5.6 mmol / l
English Hardness: 1 °eH = 7.02 mmol / l
French Hardness: 1 °fH = 10 mmol / l
ppm CaCO3: 1 ppm = 100 mmol / l
alkaline earth ions: 1 mval / l = 2 mmol / l

The variable type is Input or Output.
The unit is milli-mol per liter [mmol / l].
The minimum limit is 0.0001.
The maximum limit is 9999999999.
The replacement value is 10.
The number of digits is 10.

MANUAL

8.2.3. Operation (How can it be used? How to proceed?)

Step 1:
Select the variable to be calculated
By clicking on the corresponding *RadioButton* I can choose the variable to be calculated. It is like executing an internal conversion of the equation.

Step 2:
Fill the Input-TextBoxes
I enter the values for the input variables. I should respect the variable limits and take care that the entered values are numeric.

Step 4:
Check result
After clicking the Calculate-Button I can check the result.

Step 3:
Calculate result
After I entered the input values I can calculate the result. Before the calculation starts, all the input values are checked by an internal routine. Whenever entered values decrease the corresponding min limits or increase the corresponding max limits or are not numeric there will be a message according to the fault. The values will be corrected automatically by the internal routine.

Figure 60: form water hardness

Step 5:
Further actions
After the calculation I can have the following options: Print Data, Erase Data, Program Information, Notes, Save or Restore Values. While printing a new calculation is done automatically. Clicking the Erase-Button will empty all the *TextBoxes* at once.

8.3. Crystalization Diagram NaOH

8.3.1. Purpose (What can it be used for? What can it not be used for?)

The program is part of category 3 – chemical. Caustic soda (NaOH) is used in the field of plant and process engineering for many different tasks and purposes. For the different use cases caustic soda is available in different concentrations. While transportation, storage and using the caustic soda one point is mandatory to consider: the crystallization temperature. The crystallization temperature depends on the concentration of the caustic soda solution. Be aware that if the crystallization temperature is disrespected harmful, time-consuming and expensive damages can occur by blocked pipe work due to crystallized caustic soda. It is an important fact that the crystallization temperature is in a not linear relation to the concentration. It is a curve. The curve provided in this program has six nodes. In between the nodes the values are determined by interpolation. The concentration can be entered as a given input variable. The crystallization temperature is calculated. Additionally the density for the caustic soda solution at the given concentration is calculated. It is obvious, that the density of the solution, beside other criteria, also depends on its concentration. The density can also be an important value regarding transportation and storage of the caustic soda solution.
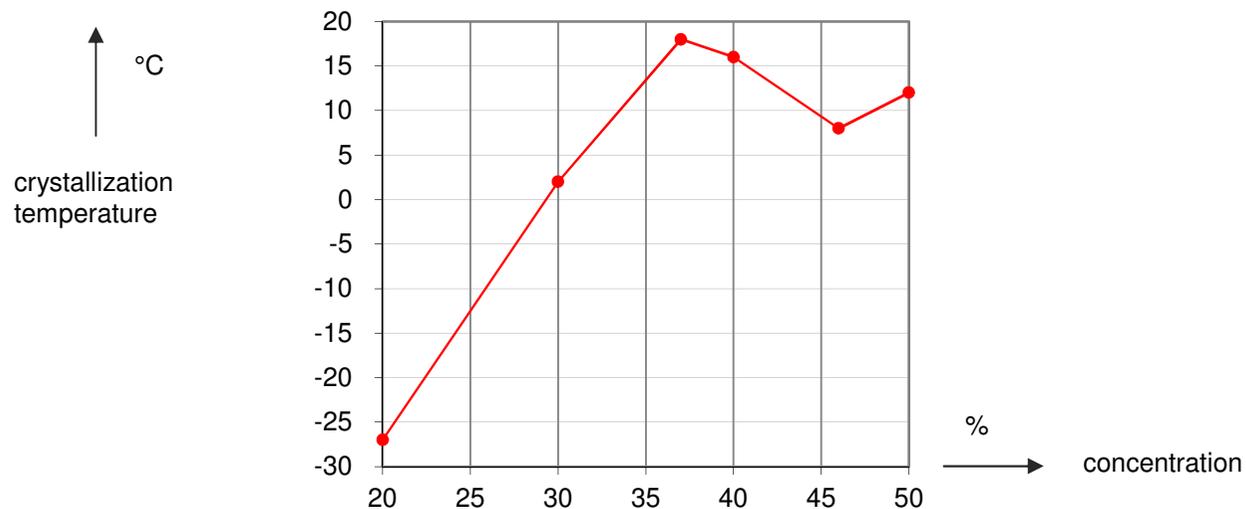

Figure 61: sketch crystallization diagram NaOH

8.3.2. Variables (What are the input and output values? What are their limits?)

concentration NaOH

It is the specified concentration of the instant NaOH-solution. For industrial purposes NaOH-solution can be ordered in different concentrations. Usually these are 4%, 10%, 20%, 30%, 40% and 50%. In practice concentrations in the range from 20% to 50% are used.

The variable type is Input.
The unit is milligram per liter [mg / l].
The minimum limit is 20.
The maximum limit is 50.
The replacement value is 30.
The number of digits is 10.

temperature of crystallization

It is the temperature at which the crystallization of the NaOH-solution will start under consideration of its actual concentration. While storing a NaOH-solution the crystallization temperature should not be decreased to avoid crystallization effects.

The variable type is Output.
The unit is degree Celsius [°C].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

density of the solution

It is the calculated density of the solution which is depending on the concentration of NaOH. The base temperature which is considered here is 20°C.

The variable type is Output.
The unit is milligram per liter [kg / l].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

8.3.3. Operation (How can it be used? How to proceed?)

Figure 62: form crystallization diagram NaOH
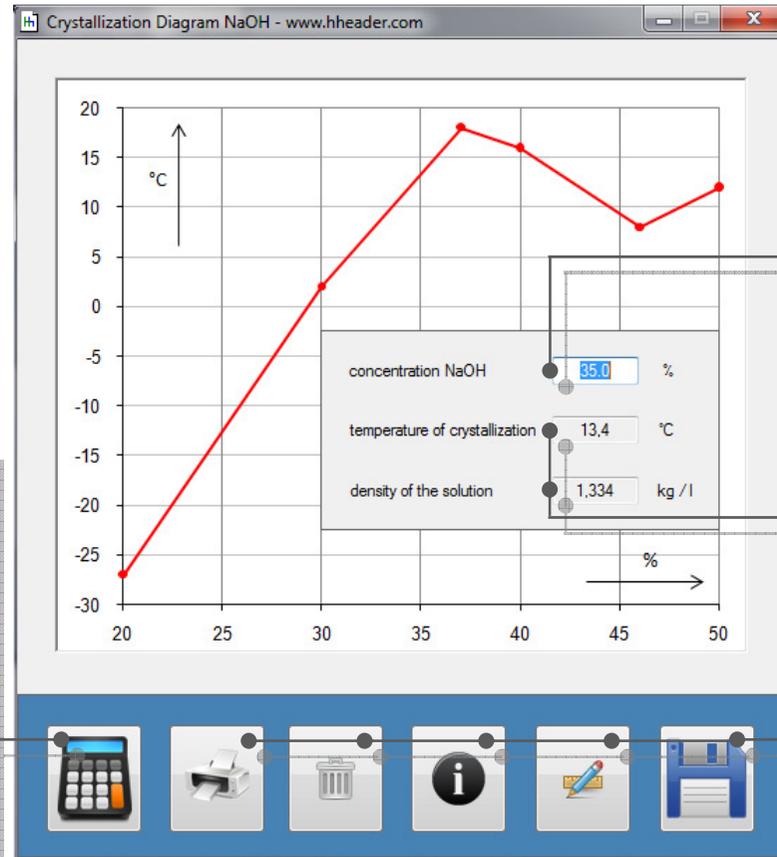
Step 1:
Fill the Input-*TextBoxes*
I enter the values for the input variables.
I should respect the variable limits and
take care that the entered values are
numeric.

Step 3:
Check result
After clicking the Calculate-Button I can
check the result.

Step 2:
Calculate result
After I entered the input values I can
calculate the result. Before the
calculation starts, all the input values are
checked by an internal routine.
Whenever entered values decrease the
corresponding min limits or increase the
corresponding max limits or are not
numeric there will be a message
according to the fault. The values will be
corrected automatically by the internal
routine.

Step 4:
Further actions
After the calculation I can have the
following options: Print Data, Erase
Data, Program Information, Notes, Save
or Restore Values. While printing a new
calculation is done automatically.
Clicking the Erase-Button will empty all
the *TextBoxes* at once.

8.4.   Stoichiometry

8.4.1.   Purpose (What can it be used for? What can it not be used for?)

The program is part of category 3 – chemical. Working in the field of plant and process engineering sometimes requires handling with chemical reactions. An equation for the chemical reaction is one way to describe the process of reaction. Not all the elements of the Periodic Table of Elements have an affinity to react with others. The program provides a selection of elements and molecules that are able to react with other elements and molecules. The selection is also divided up according to the aggregation state and the ionic charge. Regarding this (g) is for the gaseous, (l) for the liquid and (s) for the solid state of aggregation. Further plus (+) is for a positive and minus (-) for a negative ionic charge. If there is neither a plus nor a minus the charge of corresponding element or molecule is neutral. For each side of the chemical equation there are five reactants provided. For each selected reactant the molar mass and the enthalpy of formation is shown below the reactant if the stoichiometric factor is greater than zero. Be aware that the enthalpy of formation depends on the state of aggregation and the ionic charge. The stoichiometric factor can be adjusted via a numeric field to the right of the reactant selection. Below each reactant there are two buttons arranged: a short button that is arranged direct below the numeric field for the stoichiometric factor and a longer one that is arranged direct below the reactant selection. Both buttons are for showing up the composition of the elements for the selected reactant. Therefore via the long button a stoichiometric factor of one is taken into consideration and via the small button the actual adjusted stoichiometric factor is taken into consideration. The element composition is shown in the middle panel of the form between the right and left side of the chemical equation. The included elements are displayed by the colored blocks with the corresponding given amounts. It is also possible to display the total composition of the left or right side of the chemical equation. This is done by the buttons direct below the label "Left Side" respectively the label "Right Side". Each reactant has a button "X" which is for deactivation of the reactant. Therefore the stoichiometric factor will be set to zero and the reactant and the content of the text boxes for molar mass and the enthalpy of formation will be erased. Above the reactants the sum up for the molar mass and the enthalpy sum up of the total left and right side of the chemical equation are shown. Beside this also the difference between the summed up enthalpies for both reaction sides is calculated. Thereby the left side value is subtracted from the right side value. The enthalpy difference will be equal to the reaction enthalpy if the products are arranged on the right side and the educts are arranged on the left side. It is obvious that a correct result can be displayed, only if the reaction parameters have been entered correctly by the user.

After the reactants with their stoichiometric factors are defined for both sides of the chemical reaction (equation), the compounds and the stoichiometric factors can be checked. Therefore corresponding buttons in the tool strip menu are provided. The checks are initialized by clicking on the buttons. The checks can be evaluated as successful in case if the compounds and the stoichiometry are equal on both sides of the chemical equation.

Examples for some simple stoichiometric equations:

$$NaOH + HCl \rightarrow H2O + NaCl$$
$$Fe2O3 + 3CO \rightarrow 2Fe + 3CO2$$
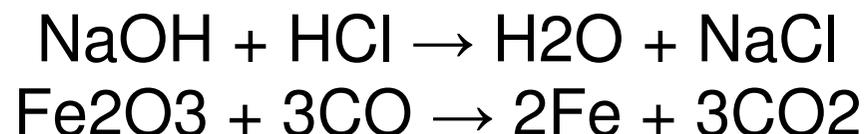
Left side of the reaction:

Right side of the reaction:
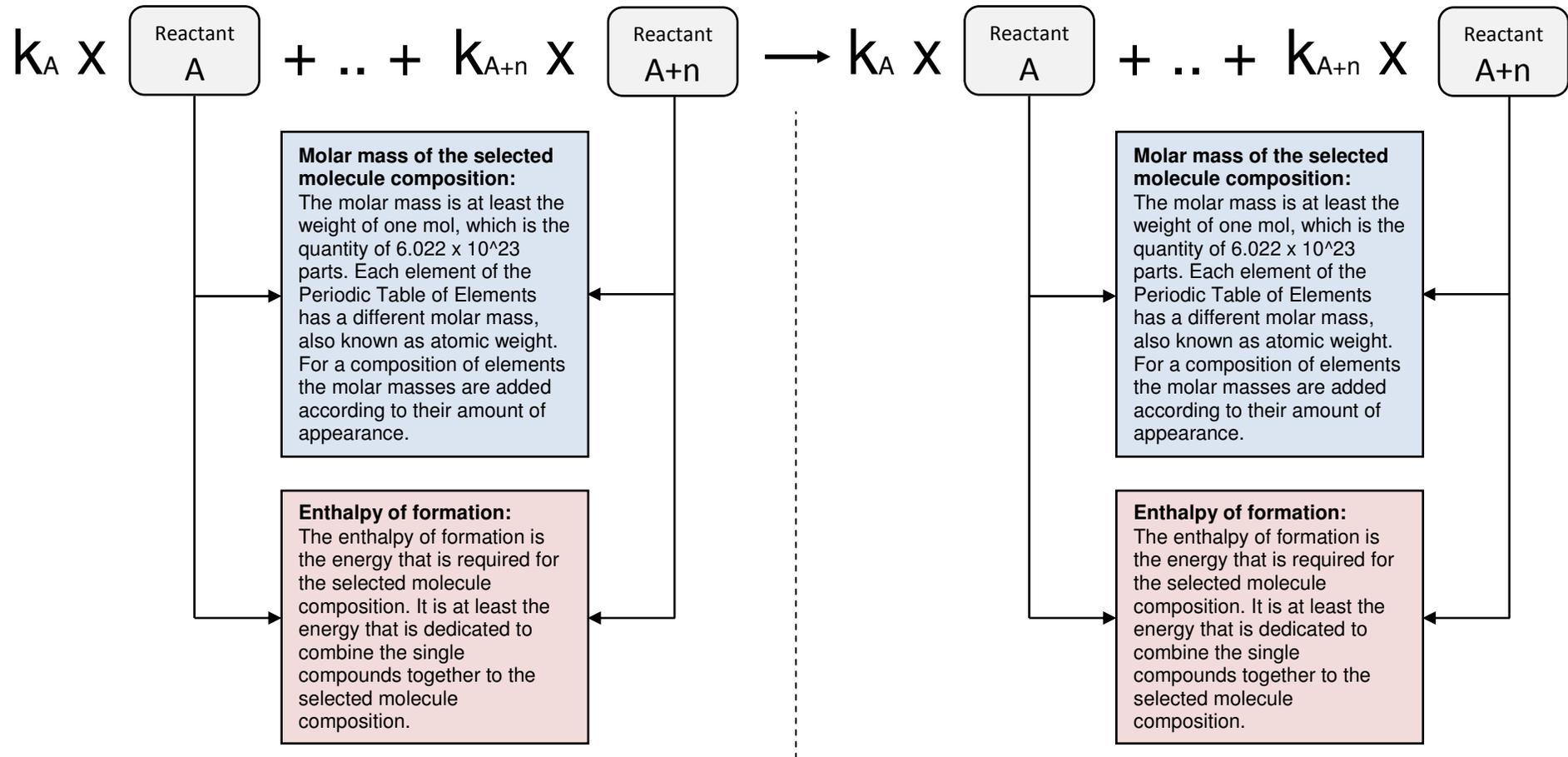
Figure 63: sketch stoichiometry

Item 1 to 22	Item 23 to 44	Item 45 to 66	Item 67 to 88
- Ag(s)	- AlCl3(g)	- CH4(g,methane)	- C6H12(l,cyclohexane)
- Ag(g)	- Al2O3(s,alumina)	- C2H2(g,ethyne)	- CaO(s)
- Ag+(g)	- Al2(SO4)3(s)	- C2H4(g,ethene)	- Ca(OH)2(s)
- Ag+(l)	- B(s)	- C2H6(g,ethane)	- CaCO3(s,calcite)
- Ag2CO3(s)	- BF3(g)	- C3H6(g,propene)	- CaCO3(s,aragonite)
- Ag2O(s)	- BaCO3(s,witherite)	- C3H8(g,propane)	- CaC2O4(s)
- Ag2S(s,argentite)	- BaC2O4(s)	- C4H10(g,n-butane)	- CaF2(s)
- AgCN(s)	- BaCrO4(s)	- C5H12(g,n-pentane)	- Ca3(PO4)2
- AgCNS(s)	- BaF2(s)	- C8H18(g,octane)	- CaSO4(s,anhydrite)
- AgCl(s,cerargyrite)	- BaSO4(s)	- CH3OCH3(g)	- Cd(s)
- AgBr(s)	- Bi(s)	- CH3OH(g,methanol)	- Cd(g)
- AgI(s)	- Bi2S3(s)	- CH3OH(l,methanol)	- Cd++(g)
- AgNO3(s)	- Br2(l)	- C2H5OH(g,ethanol)	- Cd(OH)2(s)
- Ag3PO4(s)	- Br2(g)	- C2H5OH(l,ethanol)	- CdS(s)
- Ag2CrO4(s)	- Br(g)	- CH3COOH(l,aceticacid)	- Cl2(g)
- Ag2SO4(s)	- Br-(g)	- (CH3)2O(g)	- Cl(g)
- Al(s)	- C(s,graphite)	- CH3CHO(l)	- Cl-(g)
- Al(g)	- C(s,diamond)	- CH3Cl(g)	- ClO2(g)
- Al+++(g)	- C(g)	- CHCl3(g)	- Cu(s)
- Al+++(l)	- CO(g)	- CCl4(l)	- Cu(g)
- Al(OH)3(s)	- CO2(g)	- C6H6(g,benzene)	- CuC2O4(s)
- AlCl3(s)	- COCl2(g,phosgene)	- C6H6(l,benzene)	- CuCO3*Cu(OH)2(s,malachite)

Item 89 to 110	**Item 111 to 132**	**Item 133 to 154**	**Item 155 to 176**
- Cu2O(s,cuprite)	- H+(g)	- I-(g)	- NH4+(l)
- CuO(s,tenorite)	- H2O(g)	- ICl(g)	- NH4Cl(s)
- Cu(OH)2(s)	- H2O(l)	- K(s)	- (NH4)2SO4(s)
- Cu2S(s,chalcocite)	- H2O2(g)	- K(g)	- NO(g)
- CuS(s,covellite)	- H2O2(l)	- K+(g)	- NO2(g)
- F2(g)	- H2S(g)	- KF(s)	- N2O(g)
- F(g)	- H2SO4(l)	- KCl(s)	- N2O4(g)
- F-(g)	- HF(g)	- KBr(s)	- N2O4(l)
- Fe(s)	- HCl(g)	- KI(s)	- N2O5(g)
- Fe(g)	- HBr(g)	- KClO4(s)	- N2O5(s)
- Fe++(g)	- HI(g)	- KNO3(s)	- NOCl(g)
- Fe+++(g)	- HCN(g)	- Mg(s)	- NOBr(g)
- FeO(s,wuestite)	- Hg(l)	- Mg++(g)	- Na(s)
- Fe2O3(s,hematite)	- HgCl2(s)	- MgF2(s)	- Na(g)
- Fe3O4(s,magnetite)	- Hg2Br2(s)	- MgCO3(s,magnesite)	- Na+(g)
- Fe(OH)3(s)	- Hg2Cl2(s)	- Mg(OH)2(s)	- Na+(l)
- Fe3C(s,cementite)	- HgS(s,red)	- Mn(s)	- NaF(s)
- FeCO3(s,siderite)	- HgS(s,black)	- MnO2(s)	- NaCl(s)
- FeS(s,pyrrhotite)	- Hg2SO4(s)	- MnS(s,green)	- NaBr(s)
- FeS2(s,pyrite)	- I2(s)	- N2(g)	- NaI(s)
- H2(g)	- I2(g)	- N(g)	- Na2CO3(s)
- H(g)	- I(g)	- NH3(g)	- NaNO2(s)

Item 177 to 198	Item 199 to 220	Item 221 to 223
- NaNO3(s)	- Pb(OH)2(s)	- ZnO(s)
- NaOH(l)	- PbS(s,galena)	- ZnS(s,wurtzite)
- Na2O(s)	- PbSO4(s)	- ZnS(s,sphalerite)
- Na2SO4(s)	- S(s,rhombic)	
- NiS(s)	- S(s,monoclinic)	
- O2(g)	- S(g)	
- O3(g,ozone)	- SF6(g)	
- O(g)	- SO2(g)	
- OH-(l)	- SO3(g)	
- P(s,white)	- SO3--(l)	
- P(g)	- SO4--(l)	
- PH3(g)	- SO2Cl2(g)	
- PCl3(g)	- Sn(s,white)	
- PCl5(g)	- Sn(s,grey)	
- Pb(s)	- SnO(s)	
- Pb(g)	- SnO2(s,cassiterite)	
- PbBr2(s)	- SnS(s)	
- PbCl2(s)	- Ti(s)	
- PbO(s,red,litharge)	- Ti+(g)	
- PbO(s,ye,massicot)	- Ti+++(g)	
- PbO2(s)	- Zn(s)	
- Pb3O4(s)	- Zn++(g)	

8.4.2.   Variables (What are the input and output values? What are their limits?)

molar mass

It is the molar mass of the selected molecule composition. The molar mass is at least the weight of one mol, which is the quantity of 6.022 x 10^23 parts. Each element of the Periodic Table of Elements has a different molar mass, also known as atomic weight. For a composition of elements the molar masses are added according to their amount of appearance.

The variable type is Output.
The unit is gram per mol [g / mol].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

enthalpy of formation (ΔH0)

It is the enthalpy of formation that is specified for the selected molecule composition. It is at least the energy that is dedicated to combine the single compounds together to the selected molecule composition.

The variable type is Output.
The unit is kilo-Joule per mol [kJ / mol].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

enthalpy sum up

It is the enthalpy sum up for all reactants on the corresponding reaction side. It is obvious that a correct result can be displayed, only if the reaction parameters have been entered correctly by the user.

The variable type is Output.
The unit is kilo-Joule per mol [kJ / mol].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

delta enthalpy

It is the difference of the enthalpies on the left side and the right side of the equation. Thereby the left side value is subtracted from the right side value. The enthalpy difference will be equal to the reaction enthalpy if the products are arranged on the right side and the educts are arranged on the left side. It is obvious that a correct result can be displayed, only if the reaction parameters have been entered correctly by the user.

The variable type is Output.
The unit is kilo-Joule per mol [kJ / mol].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

8.4.3. Operation (How can it be used? How to proceed?)

Step 5:
Check compounds and stoichiometry
After both sides of the reaction are entered completely, I can check the reaction for the equal compounds and the correct stoichiometry.

Step 3:
Show the element combination
The element combination can be shown for the single reactant, under consideration of the stoichiometric factors or for the total reaction side.

Step 1:
Specify the reactants
I choose the required reactants from the corresponding lists. The lists provide a selection of elements and molecules that have a chemical affinity to undergo reactions.

Step 4:
Check result
After the selection of the reactants and the adjustment of the stoichiometric factors I can check the results.

Step 6:
Further actions
After the calculation I can have the following options: Print Data, Erase Data, Program Information, and Notes.

Step 7:
(option)
Reset the reactants
I can reset not required reactants.

Step 2:
Adjust the stoichio-metric factors
I adjust the stoichiometric factors according to the reaction.

Figure 64: form stoichiometry

8.5. Periodic Table of Elements

8.5.1. Purpose (What can it be used for? What can it not be used for?)

The program is part of category 3 – chemical. In the Periodic Table of Elements the known elements are arranged according to their atomic number. The Periodic Table of Elements contains information about the elements which describe their chemical and physical properties or allow conclusions to their chemical and physical properties.

This program provides, if known, the following information:

- atomic number,
- symbolic,
- atomic weight,
- melting point,
- discovered in,

- element / type,
- elec. configuration,
- density,
- boiling point,
- discovered by.

The elements are divided up into ten different groups:

- Transitions,
- Metalloids,
- Halogens,
- Inert Gases,
- Actinides,

- Lanthanides,
- Alcaline Metals,
- Alcaline Earth Metals,
- Metals,
- Non-Metals.

For each element there is a button provided. By clicking the button for an element, the corresponding information are shown in a table in the top of the form. For some elements some information are not known exactly yet or there are up to now still doubts regarding these points. This is why some information are replaced by a question mark (?).

The sketch below shows the arrangement of the results which are displayed in a colored box. The color is according to the group where the selected element belongs to.

atomic number	1	Hydrogen / non metals	element / type
symbolic	H	1s1	elec. configuration
atomic weight	1.01 u	0.0000899 kg/l	density
melting point	-259 °C	-253 °C	boiling point
discovered in	1766	Cavendish	discovered by

Figure 65: sketch Periodic Table of Elements

8.5.2.   Variables (What are the input and output values? What are their limits?)

atomic number

It is the atomic number of the selected element. Each element of the Periodic Table of Elements has its own atomic number. It is equal to the number of protons in the nucleus of the atom. This is why the atomic number is also known as proton number.

The variable type is Output.
This variable has no unit [-].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

symbolic

It is the symbolic of the selected element. It is an abbreviated form for the element consisting of one or two letters. Each element of the Periodic Table of Elements has its own symbolic.

The variable type is Output.
This variable has no unit [-].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

atomic weight

It is the molar mass of the selected element. The molar mass is at least the weight of one mol, which is the quantity of 6.022×10^{23} parts. Each element of the Periodic Table of Elements has a different molar mass, also known as atomic weight. For a composition of elements the molar masses are added according to their amount of appearance.

The variable type is Output.
The unit is gram per mol [g / mol].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

melting point

It is the melting point of the selected element. The melting point is the temperature at which the corresponding element changes from the solid to the liquid state of aggregation at an atmospheric pressure.

The variable type is Output.
The unit is degree Celsius [°C].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

discovered in

It is the year in which the selected element was discovered - in all conscience.

The variable type is Output.
This variable has no unit [-].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

elec. config

It is the electron configuration of the selected element. Each element has its own configuration of electrons. It declares how many electrons the element has in total and how many sojourn in which atom orbital - with a high probability.

The variable type is Output.
This variable has no unit [-].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

element / type

This variable is at least consisting of two different parts. Number one, element, is the name of the element in normal form. Number two, type, is the type of the element. It declares to which kind, to which group of elements the selected element belongs. Elements of the same group or type have similar properties.

The variable type is Output.
This variable has no unit [-].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

density

It is the density of the selected element at an atmospheric pressure and a temperature of 20°C.

The variable type is Output.
The unit is kilogram per liter [kg / l].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

boiling point

It is the boiling point of the selected element. The boiling point is the temperature at which the corresponding element changes from the liquid to the gaseous state of aggregation at an atmospheric pressure.

The variable type is Output.
The unit is degree Celsius [°C].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

discovered by

It is the name of the person who discovered the selected element - in all conscience.

The variable type is Output.
This variable has no unit [-].
There is no defined minimum limit for output variables.
There is no defined maximum limit for output variables.
There is no defined replacement value for output variables.
There is no defined number of digits for output variables.

Be aware that the methods for determining properties and the techniques for measuring values are improving by time. Due to this fact values are updated quasi permanently in such data bases. Thereby values can deviate from data base to data base. Keep this in mind.

8.5.3. Operation (How can it be used? How to proceed?)

Step 1:
Select an element
I select the element which I need to be informed about.

Step 3:
Check result
After selecting an element I can check the result.

Step 4:
Further actions
After the calculation I can have the following options: Print Data, Program Information, Notes and Hint.

Step 2:
Check the element type
I can check the element type by color in order to make sure that the choice is according to the case.

Figure 66: form periodic table of elements

8.6. Chemical Resistance

8.6.1. Purpose (What can it be used for? What can it not be used for?)

The program is part of category 3 – chemical. For the plant design criteria, especially for the selection of a proper pipe work and gasket material, it is important to consider the chemical resistance of the material to be selected in coherence with the used chemicals. The program can give support regarding this subject. Therefore an extensive selection of chemicals is provided. The chemicals can be selected via lists, which are arranged in an alphabetic order. For each letter of the alphabet there is a button provided which will link to the corresponding list of chemicals. By selecting a chemical the evaluation of the chemical resistance is started for different standard materials, which are used predominantly in the field of plant and process engineering. The evaluation is done for two different temperature ranges: one is around 20°C and two is around 50°C. Regarding the results of the evaluation there are six groups defined by text and color code.

The results are defined as follows:

- not specified (gray),

- excellent resistance (green),

- good resistance (green),

- limited resistance (orange),

- no proper resistance (red),

- danger of local corrosion or cracks (red).

The results for both temperature ranges are shown at once in one row. They are separated by a slash "/". The color code always refers to the worse of both results.
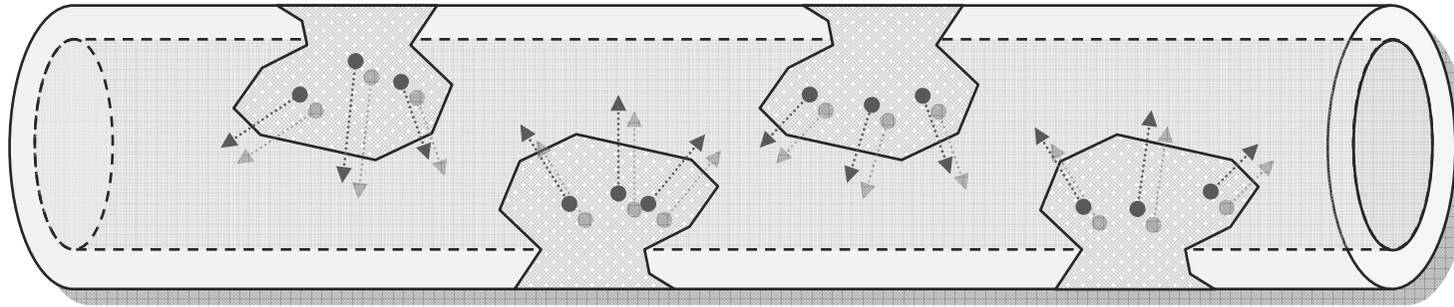
Figure 67: sketch chemical resistance

8.6.2. Variables (What are the input and output values? What are their limits?)

HDPE: High-density polyethylene

LDPE: Low-density polyethylene

PA: Polyamide

POM: Polyoximethylene

PP: Polypropylene

PVC – HARD: Polyvinyl chloride hard

PVC – SOFT: Polyvinyl chloride soft

PTFE: Polytetrafluoroethylene

EPDM: ethylene propylene diene monomer rubber

FPM: Viton (synthetic rubber and fluoropolymer elastomer)

NBR: Nitrile rubber

AL: Aluminum

V2A: stainless steels like 1.4301 (X5CrNi18-10), AISI 304

V4A: stainless steels like 1.4401 (X5CrNiMo17-12-2) AISI 316

8.6.3. Operation (How can it be used? How to proceed?)

Step 2:
Select a chemical
I select the chemical that should be evaluated in coherence with the materials.

Step 1:
Select a list of chemicals
I select a list of chemicals that should be evaluated in coherence with the materials.

Chemical Resistance - www.hheader.com

Chemicals

Sodium carbonate Na 2 CO 3
Sodium carbonate Na 2 CO 3 (aqueous)
Sodium carbonate Na 2 CO 3 (saturated)
Sodium chlorate NaClO 3 (aqueous)
Sodium chlorate NaClO 3 all kinds
Sodium chloride NaCl (aqueous)
Sodium chloride NaCl all kinds
Sodium cyanide / refer to: sodium cyanide
Sodium cyanide CNNA (aqueous)
Sodium cyanide CNNA (saturated)
Sodium dichromate / refer to: sodium dichromate
Sodium dichromate Na 2 Cr 2 O 7
Sodium dithionite Na 2 S 2 O 4
Sodium dithionite Na 2 S 2 O 4 (10%)
Sodium dodecylbenzenesulfonate C 18 H 29 NaSO 3
Sodium ferrocyanide / refer to: Natriumhexacyanoferrat (II)
Sodium fluoride NaF (saturated)
Sodium hexametaphosphate (NaPO 3) 6 (saturated)
Sodium hydrogen sulfite / refer to: sodium bisulfite
Sodium hydrosulfite / refer to: sodium dithionite
Sodium hydroxide / refer to: sodium hydroxide
Sodium hydroxide NaHO (1%)
Sodium hydroxide NaHO (30%)
Sodium hydroxide NaHO (45%)
Sodium hydroxide NaHO (50%)
Sodium hydroxide NaHO (60%)
Sodium Hypochlorite / refer to: sodium hypochlorite
Sodium hypochlorite / refer to: sodium hypochlorite
Sodium hypochlorite NaClO (12.5% Cl)
Sodium hypochlorite NaClO (15%)
Sodium hypochlorite NaClO (saturated)
Sodium iodide NaI all kinds
Sodium Na 2 S 2 O 5 all kinds
Sodium NaBO 2 (HO) 2 × 3H 2 O (aqueous)
Sodium NaBO 2 (HO) 2 × 3H 2 O (saturated)
Sodium nitrate / refer to: sodium nitrate
Sodium nitrate NaNO 3 (aqueous)
Sodium nitrate NaNO 3 (saturated)
Sodium nitrite NaNO 2 (aqueous)
Sodium nitrite NaNO 2 (saturated)

Material	Evaluation of Resistance
HDPE:	excellent resistance at 20°C / excellent resistance at 50°C
LDPE:	excellent resistance at 20°C / excellent resistance at 50°C
PA:	excellent resistance at 20°C / not specified at 50°C
POM:	excellent resistance at 20°C / limited resistance at 50°C
PP:	excellent resistance at 20°C / excellent resistance at 50°C
PVC - HARD:	excellent resistance at 20°C / good resistance at 50°C
PVC - SOFT:	not specified at 20°C / not specified at 50°C
PTFE:	excellent resistance at 20°C / excellent resistance at 50°C
EPDM:	excellent resistance at 20°C / not specified at 50°C
FPM:	limited resistance at 20°C / no proper resistance at 50°C
NBR:	limited resistance at 20°C / limited resistance at 50°C
AL:	no proper resistance at 20°C / no proper resistance at 50°C
V2A:	excellent resistance at 20°C / limited resistance at 50°C
V4A:	excellent resistance at 20°C / limited resistance at 50°C

A B C D E F G H I J K L M
N O P Q R S T U V W X Y Z

Step 3:
Check result
After selecting an element I can check the result. The evaluation is done for two different temperature ranges: one is around 20°C and two is around 50°C. Regarding the results of the evaluation there are six groups defined by text and color code. The results for both ranges are shown at once in one row.

Step 4:
Further actions
After the calculation I can have the following options: Print Data, Erase Data, Program Information, and Notes.

Figure 68: form chemical resistance