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## SIMULATION OF PROCESS LINES IN MICROSOFT EXCEL - NITRIC ACID PRODUCTION

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### SYMULACJA LINII TECHNOLOGICZNYCH W PROGRAMIE MICROSOFT EXCEL – PRODUKCJA KWASU AZOTOWEGO

#### Abstract

In this contribution, it is explained in the detail how useful Microsoft EXCEL could be for the simulation of process lines. The report contains a manual flowsheet as well as a tutorial case and the results of its application for Nitric acid production can be gained.

*Keywords: program Microsoft EXCEL, simulation*

#### Streszczenie

W artykule szczegółowo przedstawiono jak użytecznym narzędziem do symulacji linii procesowych może być program Microsoft EXCEL. Praca zawiera indywidualne arkusze danych, poradniki przydatne w szczególnych przypadkach (tutoriale) oraz wyniki ich zastosowania w produkcji kwasu azotowego.

*Słowa kluczowe: program Microsoft EXCEL, symulacja*

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## 1. Introduction

I already introduced the usage of Microsoft Excel for process line simulation at the 2012 conference in Berlin.

Now, I would like to explain the main principles of this method on the „Boiler“ example, which demonstrates both enthalpy and mass balances.

First of all, we need to understand the basic principles, which are shortly described in this presentation:

### 1.1. Decision-making

Experience and practice have made us realise that mass and material balances represent effective tools for decision-making. The concept of decision-making shall include the following spheres of action:

- Sizing lines and individual apparatus in designing.
- Adjusting a line to the modified composition of materials.
- Adjusting a line to the modified requirements for quality (composition) of a product.
- Diagnosing failures of operation of lines and locating causes of failure.
- Checking or substituting measured quantities by calculating those quantities and taking advantage of this principle to ensure easier control or to carry out process, or guarantee measurements.
- Optimising operation of a line and searching for alternatives of operation using the method: “What will happen if.....?”
- Training and teaching operating personnel.

This enumeration is certainly not complete; however, it gives us an idea of the content of the concept of decision-making.

### 1.2. Working tools for decision-making

Decision-making that involves any process requires a quantitative model. This decision-making shall mean either proposing a new process, or modifying a process, or controlling an existing process. Such a model should give us an opportunity to study the behaviour of the system if the initial conditions change. In other words, the model should enable one to study changes of the system behaviour after modifying initial conditions, that is to search for an answer to the question: What will happen if...? Such a model constitutes a prerequisite for an objective quantitative economic analysis of the system. It is necessary to bear in mind at all times that the quantitative model should be exact. This means we receive one and only solution for the selected values of the designating parameters. When using empirical coefficients, such as efficiency, yield, or adjustable constants guaranteed by the provider of the equipment, maximum attention must be paid in order to define these coefficients accurately. The use of empirical coefficients is thus limited to cases where those coefficients include deviations from the ideal behaviour, express efficiency of the process, or adjust the theory to the real behaviour of the equipment. These adjustable parameters often constitute the subject of know-how. In any case, however, exact mass and enthalpy balances constitute the basis of the model. Thereby, a quantitative model of a

process establishes a reliable foundation of the system's economic model, which is the final tool for the management in making decisions.

The law of conservation of mass and the law of conservation of energy can be used as an exact model for processes accompanied by a chemical reaction and heat exchange. On the basis of this model, mass and enthalpy balances can be drawn up for the process in question, and subsequently, complete system characteristic can be acquired.

### 1.3. Complete system characteristic

Material balances are used for obtaining a complete characteristic for all streams that are present in the process flow chart. This information is essential both for a designer and for the operation control itself. A complete characteristic contains the following details:

- Where the stream comes from and where it goes – that defines the direction of the stream, i.e. its orientation.
- Size of the stream, expressed as weight per time unit ( $\text{kg}\cdot\text{s}^{-1}$ ) or moles per time unit ( $\text{kmol}\cdot\text{s}^{-1}$ ).
- What components the stream contains and their part, expressed as a weight or mole fraction of the component in the stream in question. The method of expressing the composition of the stream should be invariant to temperature and pressure.
- Temperature and pressure for each stream are added to the above-mentioned in the case of enthalpy balance.

## 2. Basic concepts

If we know the composition, temperature and pressure for a stream, we are able to determine:

- any intensive physical property of the stream – such as density, viscosity, or surface tension,
- whether the stream consists of one or more phases and what these phases consist of.

In general, we can say that all intensive physical properties represent a function of composition, temperature and pressure. With liquid and solid phases, the effect of pressure on the value of intensive properties is mostly negligible. As to ideal gases, the change of enthalpy with pressure is null. A more noticeable dependence of enthalpy on pressure is encountered only with streams, the position of which is in the proximity of a two-phase range. This leads to the following conclusions:

- The composition of the stream must serve the purpose of mass balance.
- The temperature of the stream must serve the purpose of enthalpy balance.
- The pressure of the stream does not constitute the object of balance calculations. If we need to know its value (for instance, in order to calculate in what phase the stream is – whether in a gaseous or liquid phase), its value must be determined.

### 2.1. What is flowsheeting?

Flowsheeting consists of a flow sheet of the process being analysed and the complete system characteristic. It includes neither the dimensions and the structural design of the apparatus, nor the planning of the piping system. Flowsheeting consists in the following steps:

- Drawing up a process flow sheet
- Defining components in individual streams
- Establishing balance equations

By working them out, we obtain the missing information for complete system characteristic. Flowsheeting is a working tool for decision-making.

### 2.2. What is a balance?

Any extensive property – a property, the numerical value of which changes with the size of the system – can be balanced. This class includes mass, volume, internal energy, entropy, and so forth. On the contrary, intensive properties are properties with their value being independent of the size of the system, such as density, temperature, viscosity, specific heat, colour, hardness, and so forth.

Within the defined boundaries of the system being balanced and the limited time for which the balancing is being performed, the following balance relation holds good for the extensive property being balanced:

$$\text{Accumulation} = \text{Input} - \text{Output} + \text{Source}$$

- Input is the quantity of the extensive property being balanced that passes into the system through the balanced system boundaries within the limited time for which the balance is being performed.
- Source is the quantity of the extensive property being balanced that is generated within the system boundaries in the course of the balanced period. Disappearance of the extensive property is expressed as a source with a negative sign.
- Output is the quantity of the extensive property being balanced that gets out of the system through the balanced system boundaries within the limited time, for which the balance is being performed.
- Accumulation is the change in the quantity of the extensive property being balanced within the balanced system boundaries in the course of the balanced period.

The introduction of a source element enables us to balance all extensive properties, even those properties to which the law of conservation does not apply (for instance, entropy, exergy, component subject to a chemical reaction, and so forth). In order to apply a balance relation, it is still necessary to define in greater detail the concepts involved in the balance relation.

At the start of each balancing, three concepts must be defined clearly:

- *Extensive property being balanced*
- *Balanced system boundaries*
- *Limited time for which the balance is being performed.*

### 2.3. What is a component?

An extensive property being balanced will be hereinafter referred to as a component. Components can be:

- pure chemical compounds, such as methane, sulphuric acid, water, oxygen, to which a specific molar mass can be attributed,
- polymers – chemically pure substances, whose molar mass is not clearly defined,
- substances representing a group of chemical compounds, such as fats,  $R_2O_3$ , silicates, hydrocarbons  $C_{4+}$ ,
- substances that cannot be specified chemically, such as water-insoluble residue, substances with density lower than water, substrate in bioreactors.

When defining a component, it is necessary to define in a precise manner the method through which the component is determined. Differences in methods used for determining a component can lead to significant discrepancies. For instance, it is not enough to define a component as water content in a solid phase, it being loose material. Water can be on the surface of particles; in the case of porous particles, it can be bound through adsorption to the inner surface of particles; it can be water of crystallisation if the particles are of crystalline nature, and in the case of some substances it can be chemically bound water. Based on the method of determining the water content, results can differ even in the order of magnitude.

This applies also to a component defined as a particle size. If we determine the proportion of particles of a specific dimension by measuring the particle's largest dimension under the microscope, by separating on sieves, or by measuring the distribution of the particles using the settling method, we will arrive at different results.

### 2.4. What is a balanced system boundary?

A boundary of the system being balanced must be defined in order so that a component can enter or get out of the system only by crossing the system's boundaries. System boundaries do not have to be identical with the apparatus housing. A system can also be an imaginary volume defined within the apparatus. This method is very often used to define differential volume, it being the system with  $dx$ ,  $dy$  and  $dz$  dimensions in rectangular coordinates. Then, the balance relation for the component leads to a partial differential equation.

The system being balanced does not have to be identical with the individual units of apparatus. Units of apparatus can be combined for the purposes of balancing. Admittedly, this reduces the number of input data, required for the performance of the balance calculation, but the possibility of acquiring further information is thereby lost. For instance, if we link, for the purposes of balancing, an evaporating apparatus and crystalliser, we lose the information about the properties of the concentrated solution entering the crystalliser, which is an information necessary for the structural design of the evaporating apparatus. An opposite approach is possible as well. For instance, instead of balancing the whole distillation column, individual levels can be balanced.

### 2.5. What is a limited time of balance?

If we divide all elements of the balance relation by the limited time of balance, we will obtain the component's quantity per unit of time. This quantity can be termed as stream. Then, the balance relation for any one component can be posted as follows:

$$\text{Rate of Accumulation} = \text{Input Stream} - \text{Output Stream} + \text{Source per Unit of Time}$$

Source of component per unit of time (rate of source) can be seen as an imaginary (fictive) stream that enters into the system; however, it does not cross its boundaries at the same time. It can have both positive – a component is formed – and negative – a component disappears – value.

Accumulation per unit of time can be designated as the rate of accumulation; it is the change in quantity of the balanced component in the system with time. Therefore, the final form of the balance relation reads as follows:

$$\text{Input Stream of Component} + \text{Fictive Stream of Component} = \text{Output Stream of Component} + \text{Accumulation Rate of Component.}$$

### 2.6. What is an amount of component?

In order to substitute into the above-mentioned relation, we need to know the stream of the component, which is the quantity of the component per unit of time. However, we do not usually have the opportunity to measure the component stream directly. In most cases, we measure the overall stream and its composition. The component stream can be calculated from these two pieces of information.

If the component is a differential particle size, the size of the stream of this component can be calculated by multiplying the overall flow of particles by the relative frequency of occurrence of the particles within the monitored interval. When reducing the interval of the particle size to zero, we get a differential and integral description known in literature as population balance.

The numerical value of the flow of the component is required to be invariant to temperature and pressure. This requirement excludes the overall stream to be expressed as volume per unit of time. There remains the possibility of expressing the flows of components as mass or amount (number of pieces) – kilograms of flour and number of eggs per unit of time.

Furthermore, it is required to have the opportunity to convert mass to amount (number of pieces) and vice versa. For it is common practice to weigh small screws instead of counting our thousands of pieces. The approach is accurate only if every piece has exactly the same mass as the other ones. This requirement is satisfied strictly only with molecules. Molecules are too small to be counted out. However, we know that one kmol of any substance contains the same number of molecules, corresponding to the Avogadro's number, which is  $6.0221367 \cdot 10^{26} \text{ kmol}^{-1}$ . If we know the molar mass for a component ( $\text{kg} \cdot \text{kmol}^{-1}$ ), we can convert the amount of substance (kmol) to mass (kg) and vice versa. If a component cannot be attributed molar mass, its quantity can be expressed only as mass in kg.

Consequently, we shall express the fraction of the component present in the stream only as a weight fraction or a mole fraction, depending on whether the overall stream is expressed in  $\text{kmol} \cdot \text{s}^{-1}$  or  $\text{kg} \cdot \text{s}^{-1}$ .

### 2.7. What is a continuous process?

The accumulation of a component in the system is the change in the quantity of the property being balanced (hold-up). If a process is run continuously in a steady state, the change in hold-up and its composition with time is null, and therefore, the rate of accumulation is also null.

The accumulation of mass is usually applied in batch systems. If we choose a limited time of balance exceeding the time of a batch process cycle by a long way, we can accept the assumption of a zero rate of accumulation. If we choose no matter how long balance period, the system accumulation will be given by the level of the system hold-up at the end of the balance period minus the system hold-up at the start of the balance period. This can be the difference between the maximum and the minimum hold-up at the most. If we choose the balance period to be just as long so that the maximum accumulation possible is negligible compared with the input and output streams for the balance period, we can regard also the periodical batch processes to be continuous and deem the rate of accumulation to be zero.

Complete system characteristic does not say anything about the dimensions of individual pieces of equipment, and therefore, the relations we use for balancing do not contain any parameters of the equipment. However, in order to calculate the rate of accumulation, it is necessary to know the hold-up, which constitutes a parameter of the equipment. Therefore, our concern will be focused on continuous and periodical batch processes, where the accumulation rate can be ignored.

### 2.8. What is a source stream of reaction?

Just as in the case of accumulation, it is necessary to know the hold-up of the equipment in which the chemical reaction takes place in order to calculate the source of a component directly. The rate of generation of the component being balanced is the amount of component generated at the given place in the unit of capacity of the system per unit of time. That means that an intensive property is involved. Since the source in balances is an extensive property, we have to integrate the intensive property through the capacity of the system being balanced. In the case of an ideal stirred tank, where composition and temperature do not constitute functions of the place, we simply multiply the mentioned intensive property by the capacity of the hold-up, which is, however, a parameter of the equipment. In order to avoid this difficulty, we can substitute the source by a fictive stream of reaction.

For every independent reaction, there will be one fictive stream, which will be denominated as  $nr_k$  for balances of amount of substance and as  $mr_k$  for mass balances, where  $k$  is the serial number of reaction in case that more independent reactions are taking place in the block being balanced.

Instead of posting mole and/or weight fractions into the fictive stream column in the specification table for  $k$ , we:

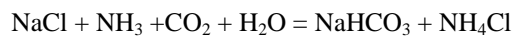
- enter the component's stoichiometric coefficient into the component's row, with a positive sign if the component is a product of the reaction (second term on the right side of the stoichiometric equation), or with a negative sign if the component

is a reactant (first term on the left side of the stoichiometric equation) in the case of material balance;

- multiply, in addition, the stoichiometric coefficient (with the appropriate sign) by the component's molar mass in the case of mass balance.

**Tutorial Problem:**

If we take the stoichiometric equation of formation of sodium hydrogen carbonate in manufacturing soda



as an example, the column for the fictive stream will read as follows:

Table 1

**Stoichiometric coefficients and molecular weight**

		for molar balance in kmols/sec	for mass balance in kg/sec
	components	Nr	Mr
1	H <sub>2</sub> O	-1	-18.02
2	NaCl	-1	-58.44
3	CO <sub>2</sub>	-1	-44.01
4	NH <sub>3</sub>	-1	-17.03
5	NaHCO <sub>3</sub>	1	84.01
6	NH <sub>4</sub> Cl	1	53.49

2.9. Why enthalpy balance and not heat balance?

The change in energy of 1 kg of water upon being heated by 0.5°C corresponds to the change in the mass flow rate of the same by 65 m·s<sup>-1</sup> or raising by 213 m. Such changes in kinetic and potential energy can be hardly encountered in a chemical plant, the exception thereof being power-producing machinery (turbines). For the purposes of balancing, we can therefore ignore potential and kinetic energy of streams and substitute heat balance by enthalpy balance.

This has the same advantage as disregarding the accumulation rate. In order to calculate kinetic and potential energy of a stream at the given place, we need to know the diameter of the piping and its height above the ground, which are parameters of equipment that do not belong into the system characteristic. We do not need this information to calculate the enthalpy of a stream, and therefore, we replace the overall heat balance by enthalpy balance. The mistake that can be thereby caused is negligible in the absolute majority of cases.

2.10. What is the difference between material balance and enthalpy balance?

For a continuous process or a batch process occurring periodically, material balance of a component has the following form:



$$\text{Accumulation Rate of Component} = \text{Input Stream of Component} - \text{Output Stream of Component} + \text{Source.}$$

This applies to every component, which means that for a balanced system, we have as many material balances as there are components present in the system.

The dimension of individual parts of the balance equation is  $\text{kg}\cdot\text{s}^{-1}$ , or  $\text{kmol}\cdot\text{s}^{-1}$ .

The system being balanced can interchange energy with the surroundings not only through the material streams, but also through the exchange across the system boundaries – heat exchangers, or stirrers as the case may be, and so forth.

In this case, the enthalpy balance for a continuous process or a batch process occurring periodically will have the following form:

$$\text{Enthalpy Accumulation} = \text{Input Stream Enthalpy} - \text{Output Stream Enthalpy} + \text{Interchange of Energy with Surroundings} + \text{Source}$$

Individual parts of the balance equation are expressed in kW.

Removal of energy into the surroundings has a plus sign, while power supply has a negative sign. The system in which the interchange of energy with the surroundings is zero, is called *adiabatic*.

Only one enthalpy balance holds good for the balanced block.

### 2.11. Enthalpy balance

To draw up an enthalpy balance, physical and chemical data of individual components must be available. Various databases can serve as sources of data. Data from individual databases may not be quite consistent, and therefore, it is practical to use only one database if possible and not to take data for various components from different databases. A database adapted for Excel from the book by R.C. Reid, J.M. Prausnitz, and T.K. Sherwood – *The Properties of gases and liquids* (Mc Graw Hill 1982) is used for the purposes of teaching at the Czech Technical University.

The database of the National Bureau of Standards or the DECHEMA database can be recommended for industrial applications. The respective Internet addresses are provided at the end.

### 2.12. Formulation of the problem being solved

In order to comply with the law of conservation of mass and enthalpy, the following equations must hold true for every block of the flow sheet:

- material balance for every one component (in other words, the number of balance equations agreeing with the number of different components present in the streams, which pass into or get out of the given block – we take into account both real and fictive streams);
- summation equations for every one stream (in other words, the total of weight or mole fractions of all components in the given stream must equal one);
- other equations, if any, follow from the laws that determine the relations among the composition, pressure, and temperature of individual streams. These are the laws of thermodynamics, chemical and phase balance, or laws of kinetics of processes. These relations are almost always non-linear;

- other equations issue from specifications given by technological regulations (such as yield, selectivity) or in data provided by the producer of the equipment (such as efficiency of machines);
- in the case of changes in temperature, one enthalpy balance is added.

The first two groups form a system of linear equations.

Enthalpy balance is non-linear, which is given by the fact that molar heats represent functions of temperature.

This set of equations forms a mathematical model, for which methods of solving must be established.

### 2.13. How many equations define the system behaviour in full?

A system is defined in full if the sum of balance equations, summation equations, equations for physical laws, specification equations, and enthalpy balance is equal to the number of unknowns in the equations.

### 2.14. Solving possibilities of the governing equations

The issue of simplicity of information transmission plays an important role with the model used. There is specialised software available for these models, such as CHEMCAD, PRO, or MAX. In addition, advantage can be taken of mathematical software, such as MATLAB, Mathematica, MATHCAD, and so forth.

This software has two big disadvantages – firstly, it is very expensive, and secondly, to become proficient in the software requires great efforts and a lot of time. It is necessary to bear in mind that a model set up by means of certain software will be used from a certain level of management upwards. At this level, it is possible to encounter the willingness to sacrifice the financial means to buy the software; however, it is an absolute illusion to expect that someone would be willing to sacrifice the time needed in order to become familiar with the software.

However, there is software available with the following advantages:

- It is installed on every computer in an enterprise – one can assume that Microsoft Office is installed on every PC.
- Almost everyone, who is able to use a computer, has a good command of it. And if the manager is not willing to communicate with a computer, his secretary is bound to have a good command of this programme.
- Operating records and source data are stored by means of this programme. Transmitting source data into our model is therefore possible without even one number being retyped using a keyboard.
- All and any economic and statistical analyses are performed by means of this programme. Transferring data for these analyses is also performed through floppy disks, over the net and through other channels, but not by typing the data on the keyboard.
- Tables and diagrams obtained using this programme can be, without the slightest difficulty, transferred into the most widespread Word processor.

We are talking about Excel. Working with Excel may not be as elegant as working with special programmes, but the above-mentioned advantages are significant to such an extent that, for the time being, Excel cannot be replaced with any other tool – exception perhaps being Lotus II, but it is fully compatible with Excel.

### 3. Methods of setting up and solving a model

The methods of solving have been drawn up to be generally valid and uniform for all types of balance cases. Exactly the same procedure is used for all cases, ranging from the problem of what ratio to use to mix two streams of water with different temperatures so that the resulting stream can have the temperature required, to systems containing dozens of blocks and streams.

These uniform methods have facilitated the elaboration of an exact method of solving, which is available to the engineering public at large, and which consists of the following steps:

The following are required for any process we wish to balance:

1. Process basis and data available with respect thereto.
2. Process flow sheet and definition of balance blocks, incidence matrix.
3. List of components in streams and their definitions.
4. Basis of calculation and conversion of specified flows and compositions.
5. Chemical reactions, determination of number of independent chemical reactions.
6. Specification table and matrix of coefficients.
7. Formulation of additional relations.
8. Conditions of system solvability.
9. Solution of a system of equations using methods of linear algebra, with the advantage of using excel.
10. Table of solutions containing complete system characteristic.

#### 3.1. Solving a system of equations – a model

In general, tasks are not noticeably complicated from the mathematical point of view. Solving a system of equations, most of which are linear, is always involved.

It is important to solve the essential question of whether the system has been overdetermined, that is whether also data that should be the result of the calculation are available for the system characteristic, or whether the system has been determined insufficiently, that means that not enough information is available to enable us to determine the complete system characteristic.

The method of how to proceed from process description to solvable mathematical model has certain logic, which must be adhered to when computing with a calculator as well as when using programmes, such as PRO, MAX, or CHEMCAD. The mentioned programmes obtain the required information from the user using various menus. Formation of and recording in what is known as a specification table is, in fact, making a list of all equations that are available to us to solve the problem.

The methods for EXCEL have exactly the same logical structure as the mentioned programmes, with the difference consisting in that we know exactly why we take the respective steps. Although this method is more laborious, we know the logic and subject-matter of the procedure, and therefore, we are able to eliminate any contingent mistake or error in the specification right at the beginning.

A system can be solved using a calculator only in the cases where it is possible to apply the solution through iterative method by means of substitution.

The following part demonstrates in detail on sample problems the application of the general methods discussed above. Stress is put on the uniform procedure, which must be unconditionally observed for success of the solution to be guaranteed.

### 3.2. General information

In describing the methods, we will proceed by providing the reader with a standard text and with a solution of the problem being described in EXCEL. This file has been provided with quite a detailed description and numerous commentaries, so that the standard text can serve, after the initial working through, only as reference. In addition, series of problems solved in EXCEL have been attached so that the user can review the methods on other problems as well. This file contains problems ranging from the most simple to the larger-scale ones. Commentaries on these problems do not constitute part of the standard text anymore; the commentary, with which the EXCEL file has been provided, should be sufficient for the user.

Let's discuss the individual phases of the procedure in detail. For example we use problem **Boiler**:

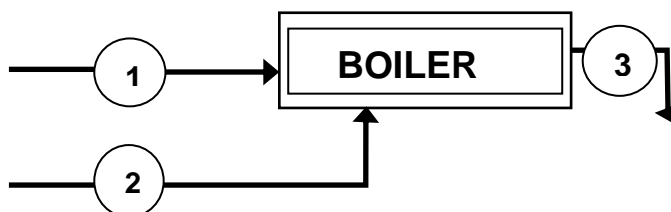
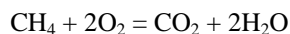


Fig. 1. Input and output flows in a boiler

A pipe oven serves as a source of energy for heating a family house, where power-gas is mixed with air and burned. We assume that power-gas is pure  $\text{CH}_4$ .

The process of combustion runs according to the following stoichiometric equation



Dry air comes into the oven in surplus compared with the stoichiometry of the process. Combustion occurs under an oxygen surplus and the flue gas contains traces of unburned power-gas.

**1. Process input parameters:**

$$R = 8,314 \text{ kW} \cdot \text{s} \cdot \text{Kmol}^{-1} \cdot \text{K}^{-1}$$

$$T = 273,15 \text{ K}$$

$$Q = 20 \text{ kW}$$

$$C_{\text{CH}_4} \text{ in flue gas} = 0,004 \text{ kmol} / \sum \text{kmol}$$

$$C_{\text{O}_2} \text{ in air} = 0,21 \text{ kmol}/\Sigma\text{kmol}$$

Air surplus = 25%

$$T_{\text{stream } 1} = 5^\circ\text{C}, T_{\text{stream } 2} = -15^\circ\text{C}, T_{\text{stream } 3} = 150^\circ\text{C}$$

**2. List of components ,streams and process units:**

$$\text{CH}_4 = 16,04 \text{ kg/kmol}$$

$$\text{O}_2 = 32 \text{ kg/kmol}$$

$$\text{N}_2 = 28,01 \text{ kg/kmol}$$

$$\text{CO}_2 = 44,01 \text{ kg/kmol}$$

$$\text{H}_2\text{O} = 18,02 \text{ kg/kmol}$$

**3. Common basis:**

mol flow kg/kmol

**4. Reference stream & component flows:**

$$Q = 20 \text{ kW}$$

**5. Recalculations:**

Component concentration in Stream:

Stream 3, Component 4

$$C_{3,4} = 0,004 \text{ kmol}/\Sigma\text{kmol}$$

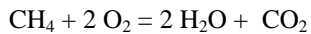
Relation between two Component Flows:

Stream 2, Component 2

$$n_{2,2} = 2,5 \cdot n_{1,1}$$

**6. Chemical reactions:**

Reactants = Products



Stoichiometric Coefficients:

Stoichiometric coefficients are defined in the following way:

- stoichiometric coefficients of reactants have a minus sign and reaction products have a plus sign.
- stoichiometric coefficients of reactants have a minus sign and reaction products have a plus sign.
- single stoichiometric coefficients are used in mol balances.
- In the case of mass balances, we must multiply the stoichiometric coefficients by the corresponding mol masses.

Table 2

**Stoichiometric coefficients (S.C)**

	Element	S.C	Mass [kg/kmol]	Thermodata indexes
1	CH <sub>4</sub>	-1	-16,043	63
2	O <sub>2</sub>	-2	-64	34
3	N <sub>2</sub>	0	0	31
4	CO <sub>2</sub>	1	44,01	48
5	H <sub>2</sub> O	2	36,03	22

*For the calculation of molar enthalpies of individual components, as a function of temperature, we will use a suitable data-base where we could find the necessary information. For our purposes, we will use the data-base Thermodata.*

Now, we have to arrange available data into a suitable form.  
As the first step, we put down the **basic parameters**.

Table 3

**Basic parameters**

number of streams	3
number of chemical reactions	1
number of process units	1
number of components	5

Respecting the recommended form, we put down the **IM** matrix (incidence matrix) and the **TD** matrix (data table):

Table 4

**IM**

process unit	streams			reactions
	1	2	3	r1
1. Boiler	1	1	-1	1

Table 5

**TD**

	process unit	streams			reactions
	1. Boiler	1	2	3	r1
1	CH <sub>4</sub>	1	0	1	-1
2	O <sub>2</sub>	0	1	1	-2
3	N <sub>2</sub>	0	1	1	0
4	CO <sub>2</sub>	0	0	1	1
5	H <sub>2</sub> O	0	0	1	2

**Number of unknown parameters:**

Scalar product of the matrix TD + number of reactions gives the number of unknowns

(**nUKN**):

$$\mathbf{nUKN} = \text{SUMMPRODUCT}(\text{TD}) + 1$$

Table 6

**Number of mass balance equations can be calculated as the product of TD x IM matrixes**

		Number of balances for <b>Boiler</b> for each element
1	CH <sub>4</sub>	2
2	O <sub>2</sub>	2
3	N <sub>2</sub>	2
4	CO <sub>2</sub>	1
5	H <sub>2</sub> O	1

*Balance equations = number of non zero elements.*



After, we need to calculate the determinant of Matrix A (blue area) to control if it is solvable

Det A	146,402
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And finally, we calculate the mol flows for each stream (vector “X”), because  $A \cdot X = B$   
 $\Rightarrow X = B \cdot A^{-1}$

#### 4. Results

Stream	n1,1	n2,2	n2,3	n3,1	n3,2	n3,3	n3,4	n3,5	r1
Flowrate [kmol/sec]	0,028688	0,07172	0,269805	0,001481	0,017306	0,269805	0,027207	0,054414	0,027207

In the same way, we applied this method for simulation of Nitric acid production, where the situation was much more complicated. The matrix of coefficients is the matrix  $145 \times 145$ . A block-diagram is shown in the Fig. 2 and a simulation Excel-file can be sent on request-[ditl@centrum.cz](mailto:ditl@centrum.cz)

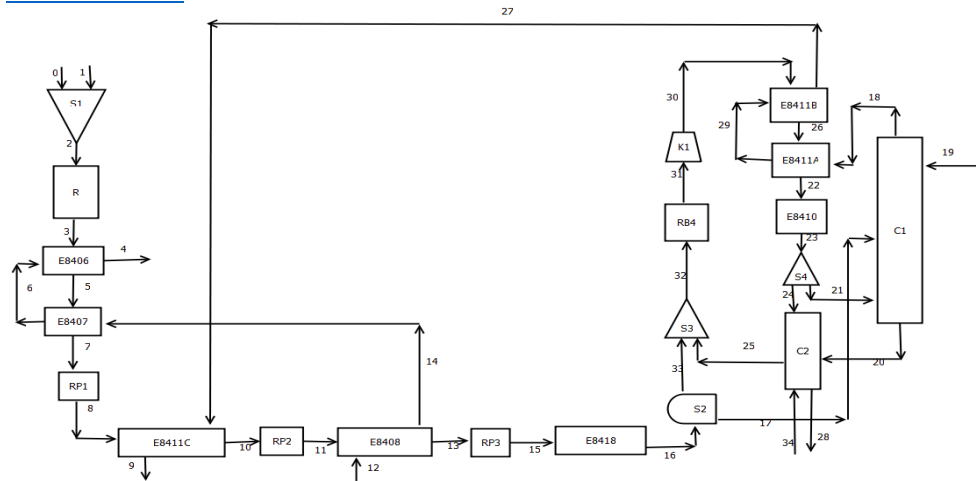


Fig. 2. Block diagram of nitric acid production

For those who are more deeply interested in the methodology we can provide the manual “Flowsheeting in EXCEL” (In Russian, English, German or Czech).

#### References

- [1] <http://www.i-programmer.info/ebooks/automating-excel/1264-getting-started.html>
- [2] <https://studium.fs.cvut.cz/studium/u12118/DITL/PPP/> (access only for staff and students, having university ID)
- [3] <http://4excel.ru/index.php?id=excelbasic>