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A PROPOSAL FOR SOLVING ONE MATHEMATICAL PROBLEM IN THE DESIGN OF CHEMICAL REACTION ENGINEERING BY GRAPHICAL METHOD

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***Abstract*-.** Starting from the main equation for calculation of pipe reactor, in which there are differential, i.e. integral links between values of τ (volumetric time), r_A (reaction rate), X_A (level of conversion of reactant) and C_A (reactant concentration), their graphic dependence has been established using certain mathematical transformations. Basic theorems of differential geometry, i.e. differential and integral calculus were used to prove graphic constructions in this process. Using the previous, based on a known analytic dependence that has been shown graphically, two other characteristic dependencies have been determined by graphic construction. In that way, we obtained more information on the observed process in a relatively simpler way compared to the existing methods. For both of the suggested constructions, a special overview has been given for determining coefficients of proportionality, since they are crucial for practical application of the suggested method. Verification of the method has been performed on a practical example from the area of chemical reaction engineering, where volumetric time for the given output was determined by a graphic procedure. The obtained results were verified with two mathematical methods, with satisfactory accuracy.

Key words - chemical reaction engineering, graphical methods, designing of plug flow reactors, residence time, subintegral and differential functions, scale coefficient

I. INTRODUCTORY DISCUSSION

Theory and design of chemical reactors is an engineering discipline that deals with their application in industry. A chemical reactor is an important and essential processing unit in every chemical process [1, 2]. It always contains a chemical reaction and many physical processes of transfer of matter, energy and heat. The final construction shape of a chemical reactor is determined by reaction conditions, operation type and production capacity. Reaction engineering is a part of chemical engineering which focuses on the study of chemical reactors [3, 4, 5, 6]. An important point at dimensioning of each reactor is an engineering view of the problem. Nowadays, mathematical complexity of reactor models is no longer an obstacle for their use in practice. Numerical methods for solving mathematical problems are especially important in this process and are based on the use of electronic computers and appropriate programs [1, 3, 5, 7]. Here, analytical methods are applicable to a very few problems [1, 4, 6, 8, 10]. Due to the previous, graphic procedures have an important role in reactor design. These procedures will be the subject of the paper.

II. MAIN RELATIONS FOR CALCULATION OF AN IDEAL PIPE REACTOR

In an ideal pipe reactor (piston flow reactor) fluid composition changes from point to point along the flow direction. Therefore, the material balance for a specific reaction component has to be set for the differential volume element dV, according to Fig. 1. [3, 5, 6, 11, 12].

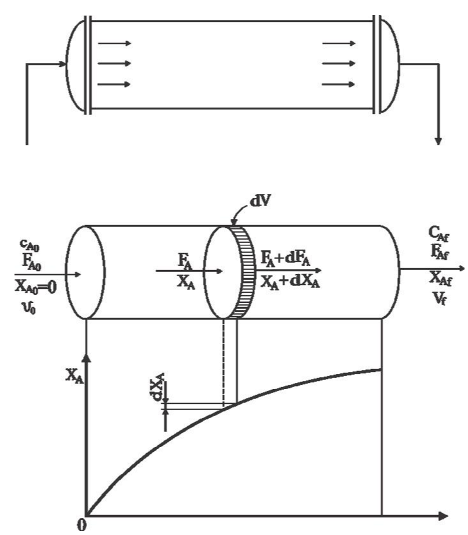

Fig. 1. Values for calculation of ideal pipe reactor

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The level of conversion of reactant A is given depending on the distance from the reactor entrance.
It can be shown that the material balance of reactant A in a differential reactor element, of volume dV [2, 3, 7, 13, 14] is:

$$F_{A_0} dX_A = (-r_A) dV \tag{1}$$

For the reactor as a whole, integration of equation (1) has to be performed. In flow velocity F_{A_0} is constant, while reaction rate r_A in each case depends on the concentration of matter or reaction degree.

By grouping appropriate values, the equation (1) becomes:

$$\int_0^V \frac{dV}{F_{A_0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} \tag{2}$$

i.e.:

$$\frac{V}{F_{A_0}} = \frac{\tau}{C_{A_0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} \tag{3}$$

$$\tau = \frac{V}{v_0} = C_{A_0} \int_0^{X_{Af}} \frac{dX_A}{-r_A} \tag{4}$$

Equations (3) and (4) are used to determine volume of the reactor, i.e. volumetric time τ at the given inflow speed and desired degree of reaction.
If input current (index 0), in relation to which we calculate degree of reaction, flows into the reactor with a certain degree of reaction, marked by index '*i*'' and output current leaves the reactor with degree of reaction described with index '*f*'', we can obtain a more general equation for design of ideal pipe reactors:

$$\frac{V}{F_{A_0}} = \frac{V}{C_{A_0} v_0} = \int_{X_{A_i}}^{X_{Af}} \frac{dX_A}{-r_A} \tag{5}$$

i.e.:

$$\tau = \frac{V}{v_0} = C_{A_0} \int_{X_{A_i}}^{X_{Af}} \frac{dX_A}{-r_A} \tag{6}$$

For a special case of a system with constant density, it follows:

$$X_A = 1 - \frac{C_A}{C_{A_0}} \qquad dX_A = -\frac{dC_A}{C_{A_0}}$$

so the equation for calculation of a reactor can be expressed through concentration:

$$\frac{V}{F_{A_0}} = \frac{\tau}{C_{A_0}} = \int_{X_{A_i}}^{X_{Af}} \frac{dX_A}{-r_A} = -\frac{1}{C_{A_0}} \int_{C_{A_0}}^{C_{Af}} \frac{dC_A}{-r_A} \tag{7}$$

$$\tau = \frac{V}{v_0} = C_{A_0} \int_0^{X_{Af}} \frac{dX_A}{-r_A} = -\int_{C_{A_0}}^{C_{Af}} \frac{dC_A}{-r_A} \tag{8}$$

III. GRAPHIC METHOD FOR PROBLEM SOLVING

From the known diagram $(X_A, -\frac{1}{r_A})$ which is applicable to a general case, we can obtain the diagram $(X_A, \frac{\tau}{C_{A_0}})$ by a graphic procedure which can be used to determine volumetric time [15].
According to relation (8), considering that a constant of integration is $(\frac{\tau}{C_{A_0}})_0$, it follows that

$$\frac{\tau}{C_{A_0}} = \int (-\frac{1}{r_A}) dX_A + (\frac{\tau}{C_{A_0}}) \tag{9}$$

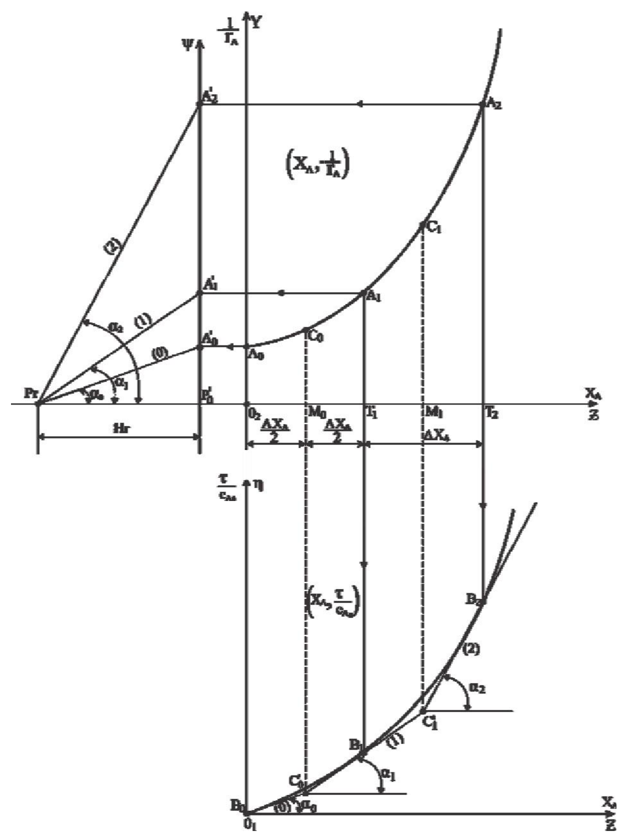

Fig. 2. Graphic construction of diagram (X_A, $\frac{\tau}{C_{A_0}}$) with the use of diagram $(X_{A,} -\frac{1}{r_A})$

Since the curve (X_A, $\frac{\tau}{C_{A_0}}$) is the integral curve of $(X_{A,} -\frac{1}{r_A})$, relation (8), particular integral, i.e. the starting point of the curve has to be known, [2, 9], so only one integral curve goes through it; the curve represents the law of change ($\frac{\tau}{C_{A_0}}$) of X_A, for the given initial condition.

Let us consider that diagram $(X_{A,} -\frac{1}{r_A})$ was drawn in the ratio of μ_{X_A} for reaction degree X_A and μ_{-1/r_A} for reciprocal negative value of reaction rate $(-\frac{1}{r_A})$, Picture 2.

We divide the gap on the abscissa into a number of equal divisions, where:

$$\Delta X_A = \overline{O_2M}_0 = \overline{M_0T_1} = \overline{M_1T_2} = \ldots\ldots.$$

$$\overline{O_2T}_1 = \overline{T_1T}_2 = \ldots\ldots\ldots..$$

Obviously, adopting a larger number of divisions on the abscissa gives a more accurate solution.

In each division we find a mean abscissa M_i such that an ordinate drawn from that point intersects the diagram in point C_i so that the area $T_iA_iA_{i+1}T_{i+1}$ equals the area of the $T_iK_iC_iK_{i+1}T_{i+1}$ rectangle, or, which is the same, that areas of $A_iD_iC_i$ and $C_iG_iA_{i+1}$ are approximately equal, which is separately presented in Fig 3 for better visibility.

Now according to Fig.2 , to the Leith, onto the adopted ordinate, we project the diagram points A_0, A_1, A_2; in that way we get points $A_0^{'}$, $A_1^{'}$, $A_2^{'}$. We choose pole P_r at distance $\overline{P_0^{'}P_r} = \overline{H_r}$ and connect it by rays in points A_i.

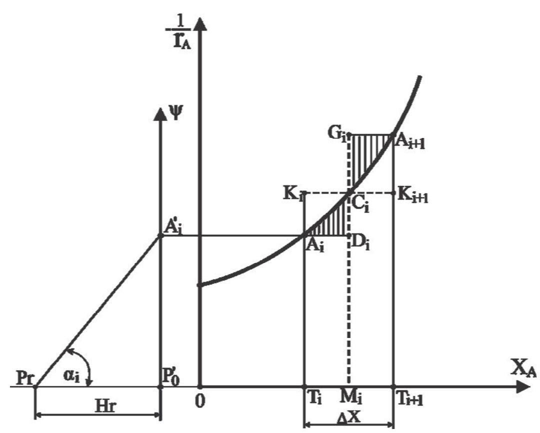

Fig. 3. Division of gap on the diagram $(X_{A,} -\frac{1}{r_A})$ *abscissa*

Now we choose a new system $(O_1\eta z)$ so that vertical axes of both diagrams are collinear. On axis $O_1\eta$ we choose point B_0 that corresponds to initial value of $\frac{\tau}{C_{A_0}}$ and from it we draw a line parallel to the ray (O) to the intersection with the vertical drawn from point C_0; we will get point $C_0^{'}$, Fig. 2. From this point we draw a line parallel to the ray (1) to the intersection with the vertical drawn from C_1; we will get point $C_1^{'}$, etc. Line segments $B_0C_0^{'}C_1^{'}$ form a polygonal line, tangents of the diagram ($X_{A,}$ $\frac{\tau}{C_{A_0}}$), because tangent of the angle of inclination α_i of a tangent drawn onto this diagram is proportional to $(-\frac{1}{r_A})$. Diagram ($X_{A,}$ $\frac{\tau}{C_{A_0}}$) should be drawn into polygon of tangents and it has to go through points B_i that are points of intersection of the verticals drawn from points A_i of the diagram ($X_{A,}$ $-\frac{1}{r_A}$) with these tangents.

At this construction we have to pay attention to proportions, i.e. coefficients of proportionality. Taking into account the ordinate and the scale of the diagram ($X_{A,}$ $-\frac{1}{r_A}$) it follows:

$$-\frac{1}{r_A} = \mu_{-1/r_A} \cdot y = \mu_{-1/r_A} \cdot \overline{P_0^{'}A_i^{'}} \qquad (10)$$

Analogously, for abscissa it is true that:

$$X_A = \mu_{X_A} \cdot z \quad \Rightarrow \quad dX_A = \mu_{X_A} \cdot dz \qquad (11)$$

Replacing (11) and (10) in relation (9)

$$\frac{\tau}{C_{A_0}} = \int(-\frac{1}{r_A})dX_A =$$

$$\int \mu_{-1/r_A} \cdot y \cdot \mu_{X_A} \cdot dz = \mu_{-1/r_A} \cdot \mu_{X_A} \cdot \int y \cdot dz \qquad (12)$$

For an arbitrary point of the diagram ($X_{A,}$ $-\frac{1}{r_A}$), taking into account the angle of the tangent for ($X_{A,}$ $\frac{\tau}{C_{A_0}}$) diagram, it follows:

$$tg\alpha = \frac{y}{\overline{H_r}} = \frac{d\eta}{dz} \Rightarrow y \cdot dz = \overline{H_r} \cdot d\eta \qquad (13)$$

Replacing (13) in (12) it follows that:

$$\frac{\tau}{C_{A0}} = \mu_{-1/r_A} \cdot \mu_{X_A} \cdot \int \overline{H}_r \cdot d\eta \qquad (14)$$

where η is ordinate of the diagram (X_A, $\frac{\tau}{C_{A_0}}$).

Solving the integral in relation (14) it follows:

$$\frac{\tau}{C_{A0}} = \mu_{-1/r_A} \cdot \mu_{X_A} \cdot \overline{H}_r \cdot \overline{\eta} \qquad (15)$$

It can be shown that (15) becomes:

$$\frac{\tau}{C_{A_0}} = \mu_{\tau / C_{A_0}} \cdot \overline{\eta} \qquad (16)$$

Since the coefficient of proportionality for $\frac{\tau}{C_{A_0}}$ axis is:

$$\mu_{\tau / C_{A_0}} = \mu_{-1/r_A} \cdot \mu_{X_A} \cdot \overline{H}_r$$

$$[\mu_{\tau / C_{A_0}}] = \frac{\frac{dm^3 s}{mol}}{dm} \cdot \frac{1}{dm} \cdot dm = \frac{dm^3 s / mol}{dm} \qquad (17)$$

Also, according to (15) dimension for ($\frac{\tau}{C_{A_0}}$) is:

$$[\frac{\tau}{C_{A0}}] = \frac{\frac{dm^3 s}{mol}}{dm} \cdot \frac{1}{dm} \cdot dm \cdot dm = \frac{dm^3 s}{mol} \qquad (18)$$

Relation (16) enables calculation of volumetric time by graphic method.

IV. VERIFICATION OF THE METHOD ON A COMPUTATION EXAMPLE

The rate of homogenous gas reaction, A → 3R, at 215ºC is given by the expression $-r_A = 10^{-2} \cdot C_A^{1/2}$ [mol/dm^{3}s]. Through the presented graphic metod we will determine volumetric time needed to achieve the degree of reaction of 80%. An input mixture that contains 50% A and 50% of inert gas flows into an ideal pipe reactor in which the temperature is 215ºC, and the pressure is 5 bar, where c_{A0} = 0,0625 dm^3/l.

Considering the given stoichiometry and the share of the inert gas in the input mixture of 50%, two volumes of the input gas will produce, after the reaction is completed, four volumes of output gas, which means that the degree of change of reaction system volume is:

$$\varepsilon_A = \frac{4-2}{2} = 1$$

Equation for calculation of ideal pipe reactor (4) can be written as:

$$\frac{\tau}{C_{A_0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} \qquad (19)$$

According to the given expression, reaction rate constant is:

$$k = 10^{-2} \frac{mol^{1/2}}{dm^{3/2} s}$$

considering that $-r_A = k \cdot C_A^{1/2}$

Replacing r_A into relation (19) it follows:

$$\frac{\tau}{C_{A_0}} = \int_0^{X_{Af}} \frac{dX_A}{k C_A^{1/2}} \qquad (20)$$

From dependency relation between concentration of C_A and degree of reaction X_A

$$\frac{C_A}{C_{A_0}} = \frac{1 - X_A}{1 + \varepsilon_A X_A} \qquad (21)$$

it follows that:

$$C_A = C_{A_0} \cdot \frac{1 - X_A}{1 + \varepsilon_A X_A} \Rightarrow C_A^{1/2} = C_{A_0}^{1/2} \left(\frac{1 - X_A}{1 + \varepsilon_A X_A} \right)^{1/2}$$

Now relation (20) becomes:

$$\frac{\tau}{C_{A_0}} = \int_0^{X_{Af}} \frac{1}{k \cdot C_{A_0}^{1/2}} \left(\frac{1 + \varepsilon_A X_A}{1 - X_A} \right)^{1/2} dX_A \qquad (22)$$

In equation (22) it is ε_A = 1, while:

$$\frac{1}{k \cdot C_{A_0}^{1/2}} = \frac{1}{10^{-2} \cdot 0{,}0625^{1/2}} = 400 \cdot \frac{dm^{3/2} s}{mol^{3/2}}$$

According to this, equation (22), considering (21), gets its final form:

$$\frac{\tau}{C_{A_0}} = \int_0^{X_{Af}} 400 \left(\frac{1 + X_A}{1 - X_A} \right)^{1/2} dX_A = \int_0^{X_{Af}} \left(-\frac{1}{r_A} \right) dX_A \qquad (23)$$

By comparison, according to (23) it follows that:

$$-\frac{1}{r_A} = 400 \left(\frac{1 + X_A}{1 - X_A}\right)^{1/2} \qquad (24)$$

According to relation (24), Table 1 was compiled for five characteristic points.

Table 1. Characteristic values of the function

$$-\frac{1}{r_A} = f(X_A)$$

Point	X_A	$-\frac{1}{r_A} = 400\left(\frac{1+X_A}{1-X_A}\right)^{1/2}$	y_i
0	0	400	y_0
1	0,2	491	y_1
2	0,4	611	y_2
3	0,6	800	y_3
4	0,8	1200	y_4

Using the data from Table 1, a dependency diagram $(X_A, -\frac{1}{r_A})$ was constructed in Fig. 4. For a more precise construction of the diagram, several additional points were calculated.

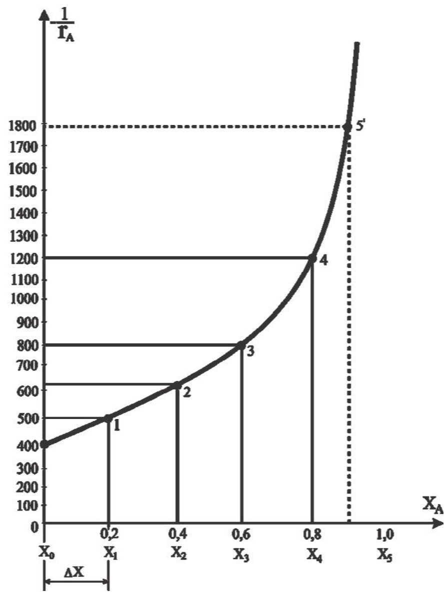

Fig. 4. Diagram of functional dependency $-\frac{1}{r_A} = f(X_A)$ *for the computation example*

Ratio for axis $\frac{\tau}{C_{A_0}}$ is calculated according to relation (17):

$$\mu_{\tau/C_{A_0}} = \mu_{-1/r_A} \cdot \mu_{X_A} \cdot \overline{H}_r =$$

$$\frac{150 dm^3 s/mol}{0{,}1 dm} \cdot \frac{0{,}1}{0{,}1 dm} \cdot 0{,}5 dm =$$

$$\frac{75 dm^3 s/mol}{10 mm} = \frac{7{,}5 dm^3 s/mol}{1 mm}$$

According to this ratio, a division on the ordinate axis of the diagram $(X_A, \frac{\tau}{C_{A_0}})$ is applied.

The value of $\frac{\tau}{C_{A_0}}$ for X_A = 0,8 is calculated according to relation (16):

$$\left(\frac{\tau}{C_{A_0}}\right)_{X_A=0{,}8} =$$

$$\mu_{\tau/C_{A_0}} \cdot \overline{\eta} = \frac{7{,}5 dm^3 s/mol}{1 mm} \cdot 71 mm = 532{,}5\, dm^3 s/mol$$

which is presented in Fig. 5. Obviously, the value of ordinate $\overline{\eta}$ was measured from the diagram.

Volumetric time needed for the given output from this will be:

$$(\tau)_{X_A=0{,}8} = C_{A_0} \cdot 532{,}5 =$$

$$0{,}0625 \frac{mol}{dm^3} \cdot 532{,}5 \frac{dm^3 \cdot s}{mol} = 33{,}28\, s$$

For the given computation example, in Picture 5 the diagram $(X_A, \frac{\tau}{C_{A_0}})$ was constructed, where a known diagram $(X_A, -\frac{1}{r_A})$ was used. The construction was done according to the general procedure given in Fig. 2.

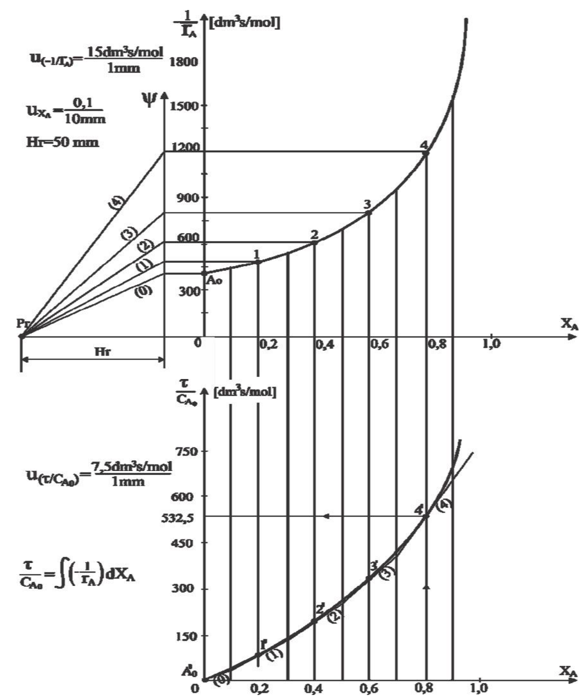

Fig. 5. Construction of diagram (X_A, $\frac{\tau}{C_{A_0}}$) *with the help of diagram* $(X_{A,} -\frac{1}{r_A})$ *for computation example*

The obtained result for volumetric time can be verified using Simpson's rule [2, 9, 10], according to ordinates of points in Table 1:

$$I_s = \int_a^b y dx \approx \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + y_4) \quad (25)$$

$$I_s = \frac{0,2}{3}(400 + 4 \cdot 491 + 2 \cdot 611 + 4 \cdot 800 + 1200) = 532,4$$

$$\tau = C_{A_0} \int_0^{X_{Af}} \frac{dX_A}{-r_A} = C_{A_0} \cdot I_s = 0,0625 \cdot 532,4 = 33,275 \text{ s}$$

In the given case, exceptionally, the solution can also be obtained by analytical integration, relation (23):

$$\frac{\tau}{C_{A_0}} = 400 \int_0^{0,8} \sqrt{\frac{1+X_A}{1-X_A}} dX_A =$$

$$= 400 \int_0^{0,8} \frac{\sqrt{1+X_A}}{\sqrt{1-X_A}} \cdot \frac{\sqrt{1+X_A}}{\sqrt{1+X_A}} dX_A =$$

$$= 400 \int_0^{0,8} \frac{1+X_A}{\sqrt{1-X_A^2}} dX_A =$$

$$= 400 \cdot \left(\int_0^{0,8} \frac{dX_A}{\sqrt{1-X_A^2}} + \int_0^{0,8} \frac{X_A dX_A}{\sqrt{1-X_A^2}} \right) =$$

$$= 400(\arcsin X_A - \sqrt{1-X_A^2}) \Big|_0^{0,8} =$$

$$= 400\left[(\arcsin 0,8 - \sqrt{1-0,8^2}) - (\arcsin 0 - \sqrt{1}) \right] =$$

$$400 \cdot (0,927294 - 0,6 + 1) = 530,9176$$

From this it follows:

$$\tau = 530,9176 \cdot c_{A_0} = 530,9176 \cdot 0,0625 = 33,18235 \text{ s}$$

Let us note that the procedure of analytical integration in practical problems of chemical reaction engineering is mostly not possible, due to complex integrands, so numerical methods are used [2, 9, 14].

V. GRAPHIC CONSTRUCTION OF DIAGRAM $\left(\frac{\tau}{C_{A_0}}, -\frac{1}{r_A}\right)$

From the known analytical dependencies $\frac{\tau}{C_{A_0}} = \frac{\tau}{C_{A_0}}(X_A)$ and $-\frac{1}{r_A} = -\frac{1}{r_A}(X_A)$, eliminating degree of reaction X_A by analytical method, dependency $-\frac{1}{r_A} = f\left(\frac{\tau}{C_{A_0}}\right)$ can be obtained. It should be mentioned that at this elimination there are often certain, more precisely serious, mathematical difficulties, since these are complex functions.

We will show that this elimination of degree of reaction X_A can also be done graphically. Diagram $\left(\frac{\tau}{C_{A_0}}, -\frac{1}{r_A}\right)$ can be directly constructed from diagram $\left(X_A, \frac{\tau}{C_{A_0}}\right)$, which was also obtained by graphic method (Pic.5).

In point A of the known diagram $\left(X_A, \frac{\tau}{C_{A_0}}\right)$, Pic. 6., tangent creates an angle α with OX_A axis, which is proportionate to the value $\left(-\frac{1}{r_A}\right)$, considering that according to (6), i.e. according to Fig.5:

$$tg\alpha = -\frac{1}{r_A} = \frac{d\left(\frac{\tau}{C_{A_0}}\right)}{dX_A} \quad (26)$$

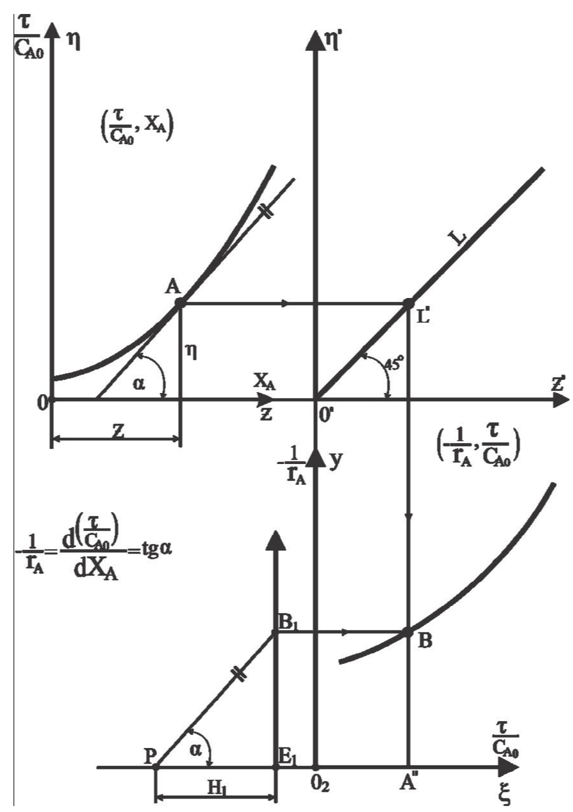

Fig.6. Principal procedure of construction of diagram $\left(\frac{\tau}{C_{A_0}}, -\frac{1}{r_A}\right)$ based on known diagram $\left(X_A, \frac{\tau}{C_{A_0}}\right)$

In point O' on axis OX_A we construct a new system O'η'z', so that axis O'z' matches axis OX_A, and axis O'η' is parallel to axis Oη. Through point O' we draw a line L at 45° on X_A axis. In point O_2 we construct a system $O_2y\xi$ parallel to system η'O'z', which will be system ($\frac{\tau}{C_{A_0}}$, $-\frac{1}{r_A}$). To the left, in an arbitrary point E_1 we draw a line parallel to axis O_2y. Point E_1 is in continuation of axis $O_2\xi$. We choose, at arbitrary distance H_1, pole P_1, so that $\overline{P_1E_1} = \overline{H_1}$. We project point A of the initial diagram onto line L, so that we get point L'. A vertical from this point will intersect axis $O_2\xi$ in point A".

Now in point A of diagram (X_A , $\frac{\tau}{C_{A_0}}$) we draw a tangent that creates angle α with the horizontal. From pole P_1 we draw ray P_1B_1 parallel to tangent. The horizontal from point B_1 intersects the vertical L'A" in point B. Geometric place of such constructed B points is diagram ($\frac{\tau}{C_{A_0}}$, $-\frac{1}{r_A}$). The construction proof follows from a quality of the tangent of the diagram (X_A , $\frac{\tau}{C_{A_0}}$) and tilt angle of ray drawn from pole P_1:

$$\mathrm{tg}\alpha = \frac{\mathrm{d}\eta}{\mathrm{d}z} \tag{27}$$

Considering the proportions of (X_A , $\frac{\tau}{C_{A_0}}$) system, it follows:

$$\frac{\tau}{C_{A_0}} = \eta \cdot \mu_{\tau/C_{A_0}} \qquad X_A = z \cdot \mu_{X_A} \tag{28}$$

From this, by differentiation, it follows:

$$d(\frac{\tau}{C_{A_0}}) = \mu_{\tau/C_{A_0}} \cdot d\eta$$

$$dX_A = \mu_{X_A} \cdot dz$$

i.e.:

$$d\eta = \frac{d(\frac{\tau}{C_{A_0}})}{\mu_{\tau/C_{A_0}}}$$

$$dz = \frac{dX_A}{\mu_{X_A}} \tag{29}$$

Replacing the differential (29) in (27) it follows:

$$tg\alpha = \frac{d(\frac{\tau}{C_{A_0}})}{dX_A} \cdot \frac{\mu_{X_A}}{\mu_{\tau/C_{A_0}}} \tag{30}$$

Considering (26), equation (30) becomes:

$$tg\alpha = -\frac{1}{r_A} \cdot \frac{\mu_{X_A}}{\mu_{\tau/C_{A_0}}} \tag{31}$$

From PB_1E_1 triangle it follows that:

$$tg\alpha = \frac{\overline{B_1E_1}}{\overline{P_1E_1}} = \frac{\overline{B_1E_1}}{\overline{H_1}} \tag{32}$$

From balancing relations (31) and (32) it follows:

$$-\frac{1}{r_A} \cdot \frac{\mu_{X_A}}{\mu_{\tau/C_{A_0}}} = \frac{\overline{B_1E_1}}{\overline{H_1}} \tag{33}$$

From here it follows that:

$$-\frac{1}{r_A} = \frac{\mu_{\tau/C_{A_0}}}{\mu_{X_A} \cdot \overline{H_1}} \cdot \overline{B_1E_1} = \mu_{-1/r_A} \cdot \overline{B_1E_1} \tag{34}$$

We will show that coefficient of proportionality for $-\frac{1}{r_A}$ in relation (34) has dimensions:

$$\mu_{-1/r_A} = -\frac{1}{r_A} = \frac{\mu_{\tau/C_{A_0}}}{\mu_{X_A} \cdot \overline{H_1}}$$

$$[\mu_{-1/r_A}] = \frac{dm^2 s/mol}{1/dm \cdot dm} = \frac{dm^2 s}{mol} \tag{35}$$

Also, dimensions for $-\frac{1}{r_A}$ according to (34) are:

$$[-\frac{1}{r_A}] = \frac{dm^2 s}{mol} \cdot dm = \frac{dm^3 s}{mol}$$

Based on the previous analysis, the known diagram (X_A , $\frac{\tau}{C_{A_0}}$) according to Pic. 5. will be used for obtaining diagram ($\frac{\tau}{C_{A_0}}$, $-\frac{1}{r_A}$) by the suggested graphic method. The construction is shown in Fig.7.

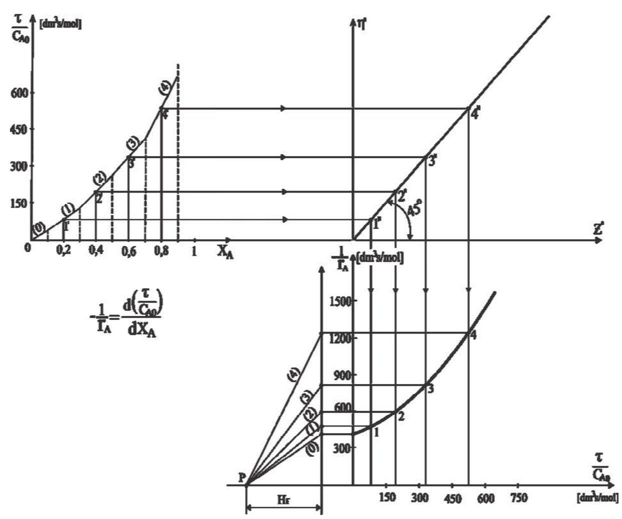

Fig. 7. Construction of diagram ($\frac{\tau}{C_{A_0}}$, $-\frac{1}{r_A}$) based on diagram (X_A, $\frac{\tau}{C_{A_0}}$) for computation example

For better visibility of diagram (X_A , $\frac{\tau}{C_{A_0}}$), only the polygonal line made by tangents on the curved line (which has been omitted in the drawing) is shown. Divisions on the ordinate and abscissa are determined according to coefficient of proportionality.

VI. . GRAPHIC CONSTRUCTION OF DIAGRAM τ = f (C_A)

According to diagram in Fig. 5., function $-\frac{1}{r_A}$ =f (X_A) is upward sloping, which is most often the case in practice, [4, 7, 10]. However, the same function, when it is expressed as depending on concentration C_A will be downward sloping, relation (8). This is the case with systems with constant density, [12, 13, 14]. Pic. 8 shows, in principle, that the same graphic construction developed in chapter 3 can be applied to this case.

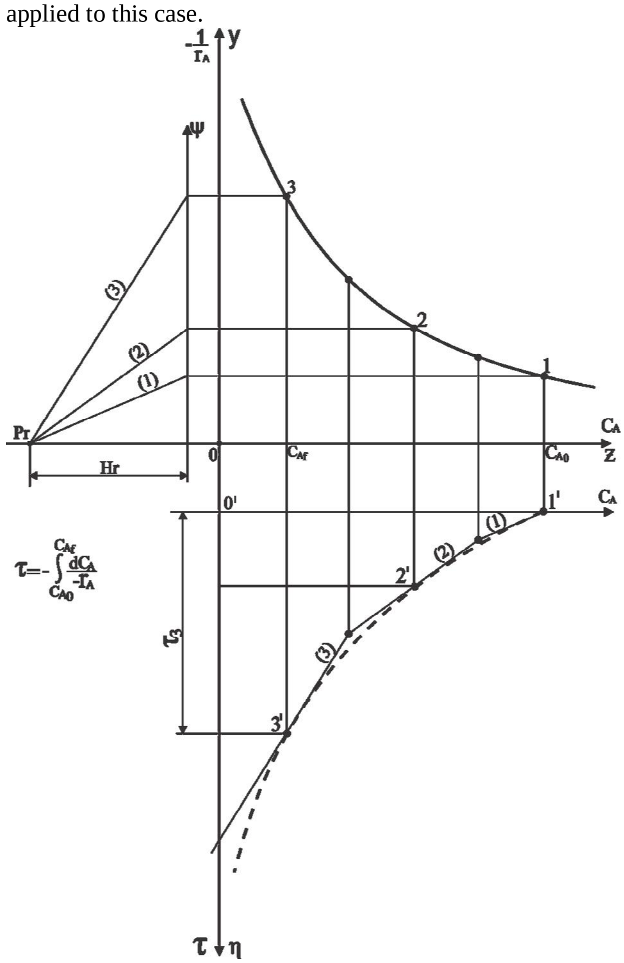

Fig. 8. Graphic construction of diagram τ = f (C_A) based on diagram $-\frac{1}{r_A} = f(C_A)$ when the function is downward sloping

VII. CONCLUSION

Numerical methods, lately, are irreplaceable while solving mathematical problems that necessarily appear at complex models in chemical reaction engineering. Application of those methods is enabled through use of electronic computers and appropriate programs. However, as it has been shown, in some cases the problem can be efficiently solved by graphic methods with satisfactory accuracy.

Also, the advantage of graphic method is obvious when compared to analytical methods that are mostly not applicable in practice due to complex integrands, since integral of the function cannot be solved in its final form. Planimetric methods, which are sometimes used to solve the presented problem, are less efficient than the suggested graphic method, mostly due to longer time needed to solve them and lower accuracy. Analytical integration is possible for a number of simple kinetic expressions.

It should be noted that there is no limit for application of the suggested method, considering the form and complexity of integrand, which speaks of its universal quality.

Apart from obtaining two graphic dependencies based on one known dependency, an inverse task is possible; it comes down to graphic construction of the first, i.e. initial diagram, if the other diagram is known. In this case, the problem comes down to construction of tangents in the points of the known diagram. At this, slightly lower accuracy of the obtained results should be expected.

Graphic methods at designing in chemical engineering should be given special attention and they should be used whenever possible, since they follow the researched process in a clear, transparent and reliable way, while the accuracy of the obtained results, if they are properly conducted, is mostly satisfactory.

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