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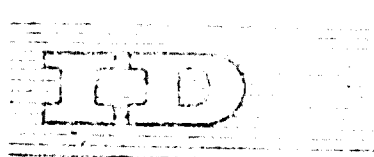
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... Industries in
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... 21-11-1969

PET.SHP. B/4

NUMERICAL MODELLING IN THE DEVELOPMENT
OF PETROCHEMISTRY^{1/}

by

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Petrochemistry is today characterised by the steep increase of the unit capacity of the production plants. The second characteristic feature is the considerable increase of the by-products. Since these two factors affect a major part of production costs, we may draw the conclusion that the construction of petrochemical and very sophisticated large capital investments. It is necessary of course to have sufficient market needs for selling products produced in these plants. The demand of the market depends upon

- the degree of industrial development of the country,
- the level of demands by industry and agriculture,
- the population of the country.

Since the developing countries in some cases have not sufficient capital at their disposal, neither do the market needs justify the construction of big capacities, it becomes increasingly difficult to start a reasonably sized and viable petrochemical industry. It is therefore necessary - when making plans for the development of the petrochemical industry - to consider the possibility of cooperation between the various production facilities planned in the country and to go further and explore cooperation between plants situated in neighbouring countries.

One of the aims of this lecture is to outline some mathematical models, suitable for assessing the economic effect of petrochemical cooperation.

From the technical - economical point of view - cooperation may be realised at various levels. If each of the companies A, B and C / which may be situated in the same country or in neighbouring countries / are considering the construction of a petrochemical complex having a specified assortment of products, then the cooperation may be effected on three levels.

- 1/ The cooperation affects the production of olefines, thus allowing a big capacity naphtha cracker to be constructed. The olefins are transported to the companies A, B and C, but the assortment of products remains unchanged.
- 2/ The cooperation affects the assortment of products too, with the aim that each product should be produced only on one site, thus ensuring the construction of bigger - capacity units.



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Developing Countries

PET.SYM. 3/A

Baku, USSR, 20 - 31 October 1969

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SUMMARY

MATHEMATICAL MODELLING
OF THE DEVELOPMENT OF PETROCHEMISTRY ^{1/}

by

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Petrochemistry in the industrially developed countries is characterised by the steep increase of the unit capacity of the producing equipment. This is due partly to the marked growth of the needs in petrochemical products, partly to the aim at lowering the production costs.

The developing countries on the other hand generally do not have either sufficient market needs, nor in some cases enough capital to construct such petrochemical complexes, which approach the capacities nowadays built and which therefore prove to be competitive in the perspective. When formulating the development conception of a petrochemical industry giving favourable economic results it is advisable to

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$$T = d_1 \cdot S_1 \quad \text{where}$$

$$d_1 = 1,1 \cdot \frac{1}{\sqrt{(x-x_1)^2 + (y-y_1)^2}} \quad \text{The multiplier 1,1}$$

takes into account the deviation of pipelines, roads etc. from the straight connection, it can be changed according to local conditions.

The unit transport cost is computed by a subroutine for each of the necessitated pipelines and for tank-car transport (propylene).

The sum of transport costs is expressed by the following equation:

$$T = \sum_{1=1}^{i+j+p} d_1 \cdot d_1$$

where i - number of naphtha producers,
 j - number of ethylene consumers,
 p - number of propylene consumers.

In order to find the minimum value of the function T , i.e. to find the lowest point of the mentioned surface it is necessary to differentiate partially with respect to x and y and to seek those values of x and y , where the differential is equal to zero.

$$\frac{\partial T}{\partial x} = \sum_{e=1}^{i+j+p} S_e \frac{\partial d_e}{\partial x} = \sum_{e=1}^{i+j+p} \frac{S_e (x - x_e)}{d_e} = 0$$

$$\frac{\partial T}{\partial y} = \sum_{e=1}^{i+j+p} S_e \frac{\partial d_e}{\partial y} = \sum_{e=1}^{i+j+p} \frac{S_e (y - y_e)}{d_e} = 0$$

The following table shows the production of the various types of aircraft engines and the total production of aircraft engines in the United States during the period from 1940 to 1945. The production of aircraft engines is shown in thousands of units. The total production of aircraft engines is shown in millions of units.

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Table 1

	Production in thousands	Production in millions
Total production of aircraft engines	11,14	11.14
One-cylinder engines	-	-
Two-cylinder engines (air-cooled) and piston engines (air-cooled)	-	-
Two-cylinder engines (air-cooled) on site	31,7	31.7
Two-cylinder engines (air-cooled) on site	31,3	31.3
Units cost price of engines on site	10,2	10.2
Units cost price of propellers on site	66,2	66.2
Units cost price of systems on site	59,4	59.4
Units cost price of propellers on site	50,0	50.0
Total production of aircraft engines	26,63	26.63

Table 1 - continued

Investment cost of plant X	-	2,55
Investment cost of plant Y	-	6,0

According to Table 1, in the example presented about 14% of the investment cost of plant X and production costs may be saved.

The cost of utilities on site X are equal to those on site Y. It is not clear if this assumption may not be correct, since the site X defined by the optimal coordinates may be unsuitable for the location of industry. Therefore we carried out a study of the deviation from the optimal coordinates on the total area of the country. We moved the plant X on a circle /radius 100 km/ and determined the total production cost on four sites. The values were 20, 22, 23 and 24. Thereupon we concluded, that the system is not very sensitive to the deviation from an area of ~ 3000 km² a suitable site can be found.

The type of cooperation cannot be determined a priori. The example indicates, that the crucial consumer is the company with the greatest demand. Its distance relative to the smaller consumer is more important, than that of which co-operative activities may take place.

Case 2

If we assume that there is a market for the total quantity of the products figuring in the plans of the companies A, B and C, then further savings in investment cost and production costs are possible by specializing the production. Specialization is only possible if the envisaged production programs of the companies considered in cooperation contain identical products.

To introduce a mathematical model which may be used in such circumstances, let us start from the following suppositions:

- two companies /A and B/ are considering the specialization of their production,
- both companies have envisaged the production of two ethylene - derivatives P_1 and P_2 and two propylene - derivatives P_3 and P_4 ,

June 1

The following information was obtained from records to record significant
events of the month of June 1954. The information was obtained from
the following sources: (1) the records of the State Department connected
with the activities of the Communist Party, U.S.A., and cooper-
ators thereof; (2) the records of the State Department connected
with the activities of the Communist Party, U.S.A., and cooper-
ators thereof.

1. The following information was obtained from records to record significant

events of the month of June 1954.

2. The following information was obtained from records to record significant

Table 2

Index	Demand				Supply			
	1970	1971	1972	1973	1970	1971	1972	1973
D ₁	10.0	11.5	13.0	15.0	10.0	11.5	13.0	15.0
D ₂	4.0	5.0	6.0	7.0	4.0	5.0	6.0	7.0
T ₁	5.0	7.0	9.0	11.0	5.0	7.0	9.0	11.0
T ₂	9.0	13.0	17.0	21.0	9.0	13.0	17.0	21.0
DI: The 2nd	10.0	12.0	14.0	16.0	10.0	12.0	14.0	16.0
Total	30.0	38.0	48.0	60.0	30.0	38.0	48.0	60.0

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The first of these is the fact that the production of goods and services is not a simple process. It involves the use of many different resources, including labor, capital, and land. These resources are combined in various ways to produce different goods and services. The process of production is therefore a complex one, and it is important to understand the different stages of production and the different resources involved.

The second of these is the fact that the production of goods and services is not a static process. It is a dynamic one, and it is constantly changing. This is because the technology used in production is constantly improving, and the resources available are constantly changing. This means that the production process is always evolving, and it is important to keep up with the latest developments in production technology.

The third of these is the fact that the production of goods and services is not a linear process. It is a non-linear one, and it is often characterized by economies of scale. This means that the cost of production often decreases as the quantity of goods and services produced increases. This is because fixed costs are spread over a larger number of units, and variable costs often decrease as the quantity produced increases.

The fourth of these is the fact that the production of goods and services is not a homogeneous process. It is a heterogeneous one, and it is often characterized by different types of production. This means that different goods and services are produced using different resources and different technologies. This is why we have different industries and different types of production processes.

1. The production of goods and services is a complex process that involves the use of many different resources.
2. The production of goods and services is a dynamic process that is constantly changing.
3. The production of goods and services is a non-linear process that is often characterized by economies of scale.
4. The production of goods and services is a heterogeneous process that is often characterized by different types of production.

... should be selected, then /columns 20 -
... enough to give valid some
... of the economic func-
... the selection of a capacity under

... linear programming technique

... computation of each alternative on our
... iterations on necessary and

... different conditional

... we showed only the sal
... that the gain obtained by
... plant if their spare capacity
... level of profitability since the
... (see Table).

... it has been compared exactly
... 4. The output of the system does not
... without

... solution demonstrates, that
... chemical par-
... increasing the profitability of
... plant.

Polystyrene	4%	11,000	1,000	1,000
Polyethylmethacrylate	"	20,000	2,000	2,000
Polyisobutylene	"	30,000	3,000	3,000
Methanol	"	20,000	2,000	2,000
Ethylene oxide	"	10,000	1,000	1,000
PA	"	50,000	5,000	5,000
Polystyrene	"	2,000	200	200
Phenol	"	30,000	3,000	3,000
Propylene sulfide	"	60,000	6,000	6,000
Ethylene from propylene	"	-	300	300
Investments	mill.	10,000	1,000	1,000
Objective function		10,000	200,000	1,000
Average value of objective function, related to 1 unit product		0,1000	2,000	1,000

The first part of the report deals with the analysis of the data obtained from the experiments. It is found that the rate of reaction is first order with respect to the concentration of the reactant. The rate constant is found to be $1.5 \times 10^{-3} \text{ s}^{-1}$. The activation energy is found to be 50 kJ mol^{-1} . The pre-exponential factor is found to be $1.5 \times 10^{10} \text{ s}^{-1}$. The Arrhenius equation is used to determine the activation energy. The plot of $\ln k$ versus $1/T$ is a straight line with a slope of -5000 K . The activation energy is calculated from the slope of the line. The pre-exponential factor is calculated from the intercept of the line. The rate constant is calculated from the Arrhenius equation. The rate of reaction is calculated from the rate constant and the concentration of the reactant. The half-life of the reaction is calculated from the rate constant. The half-life is found to be 77 s . The reaction is first order with respect to the concentration of the reactant. The rate constant is found to be $1.5 \times 10^{-3} \text{ s}^{-1}$. The activation energy is found to be 50 kJ mol^{-1} . The pre-exponential factor is found to be $1.5 \times 10^{10} \text{ s}^{-1}$. The Arrhenius equation is used to determine the activation energy. The plot of $\ln k$ versus $1/T$ is a straight line with a slope of -5000 K . The activation energy is calculated from the slope of the line. The pre-exponential factor is calculated from the intercept of the line. The rate constant is calculated from the Arrhenius equation. The rate of reaction is calculated from the rate constant and the concentration of the reactant. The half-life of the reaction is calculated from the rate constant. The half-life is found to be 77 s .

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Figure 1.

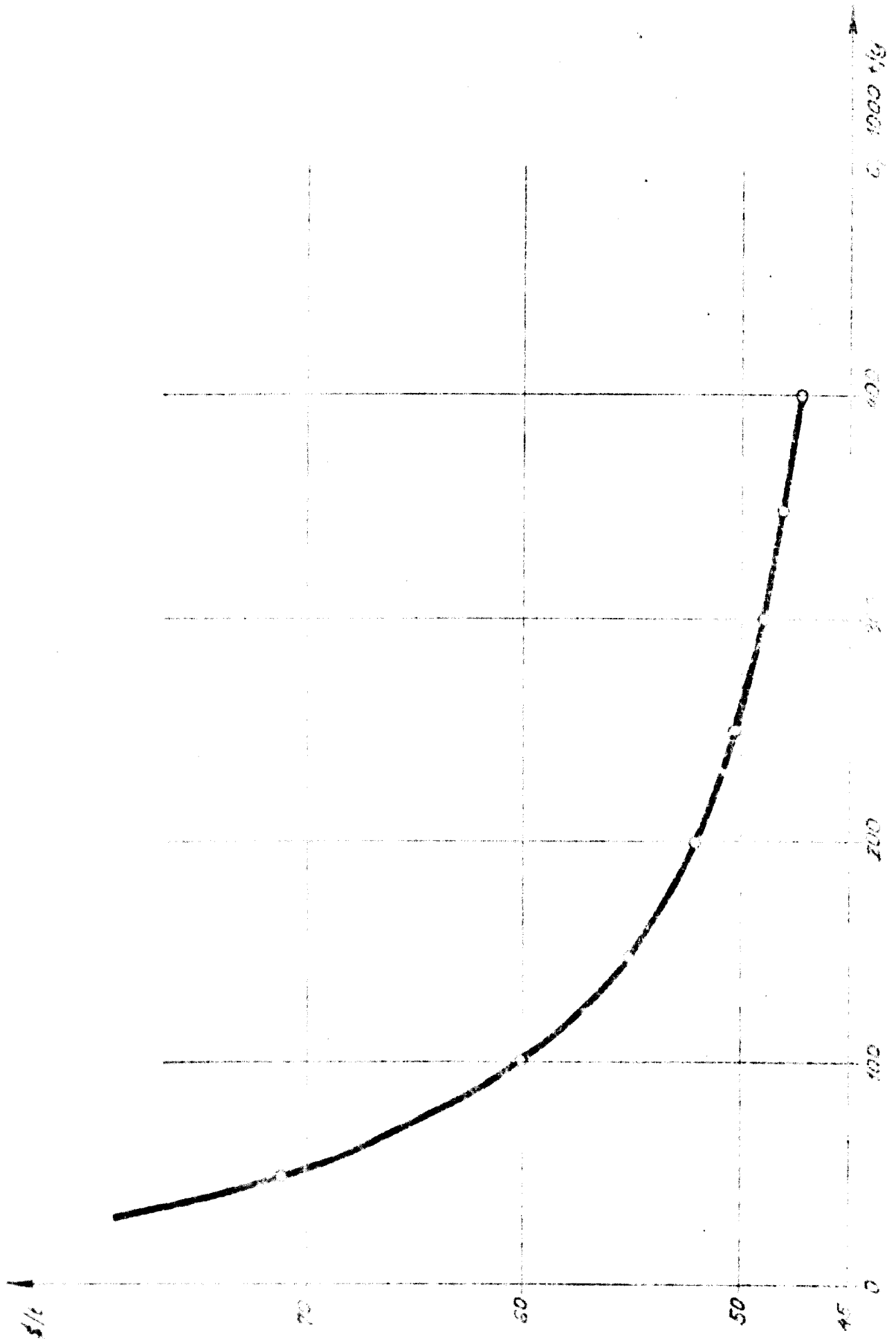
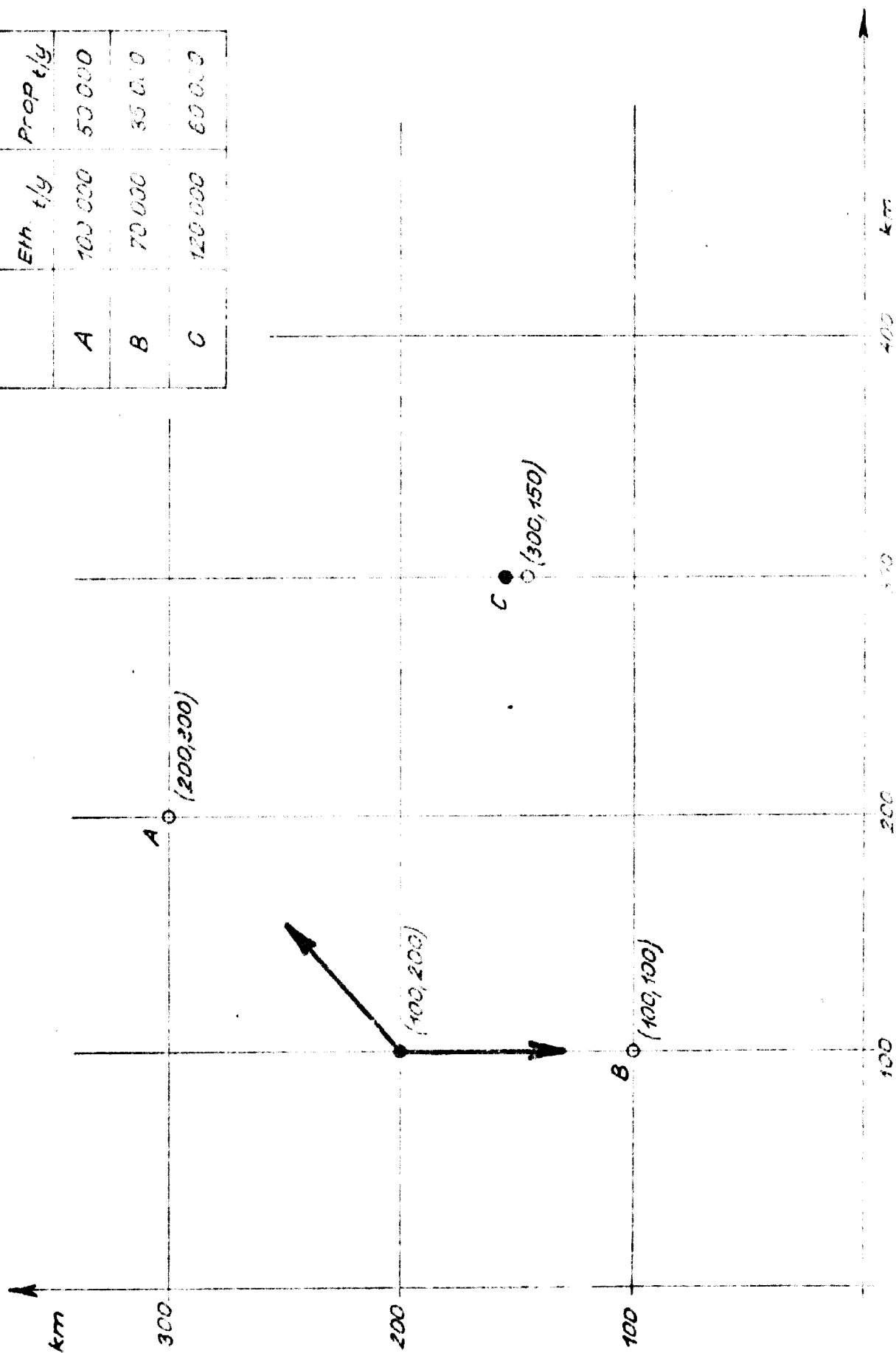
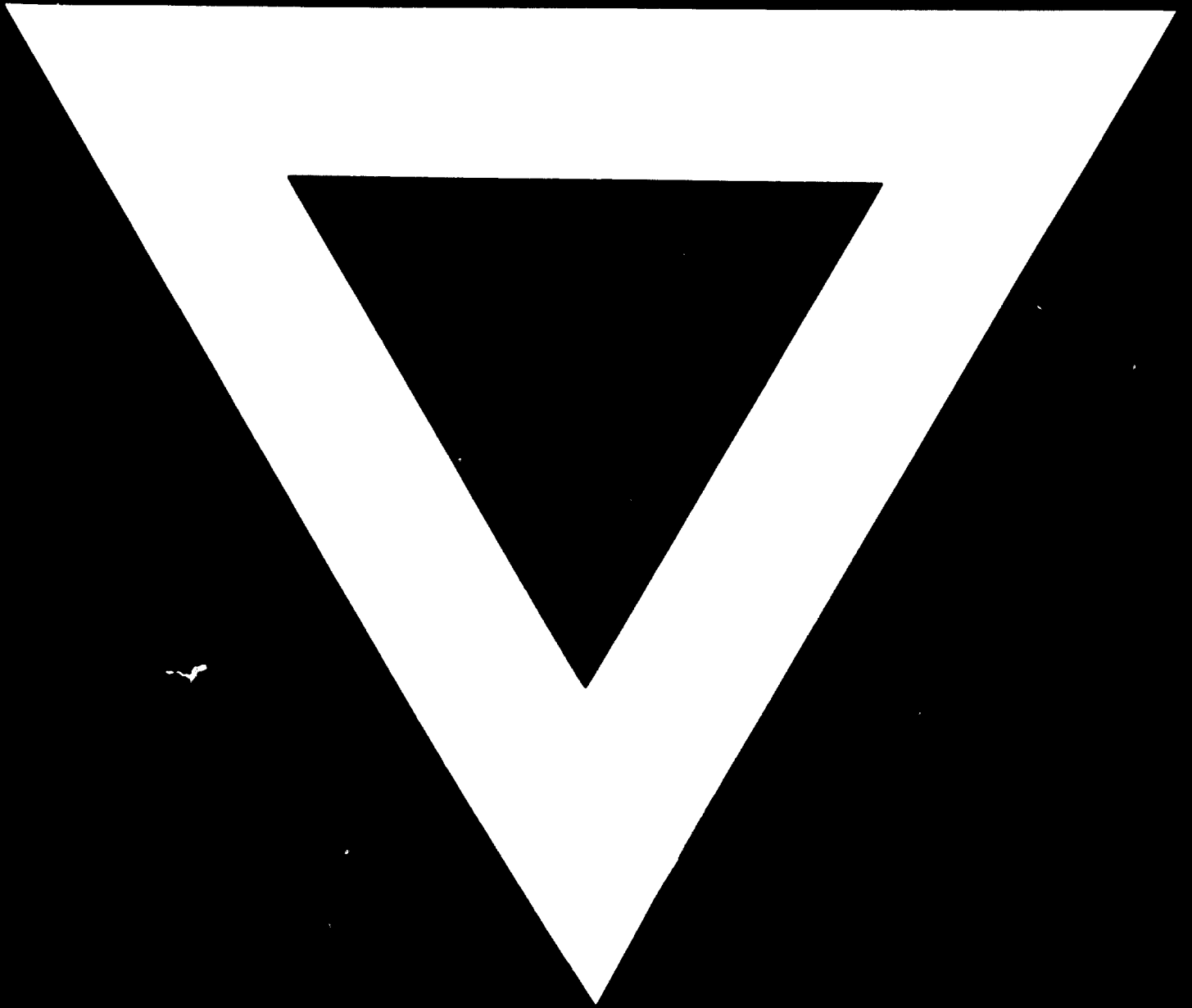


Figure 2.

	Eth. tly	Prop. tly
A	100,000	50,000
B	70,000	35,000
C	120,000	60,000



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33
Ethylene balance																																	
Propylene balance																																	
Investment																																	
Q1 plant lower limit																																	
Q1 plant upper limit																																	
Polyethylene HP I																																	
Polyethylene HP II																																	
Polyethylene LPI																																	
Polyethylene LPII																																	
Ethanol I																																	
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PVC I																																	
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Polypropylene I																																	
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Phenol I																																	
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Economic function																																	



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