OCCASION

This publication has been made available to the public on the occasion of the 50th anniversary of the United Nations Industrial Development Organisation.

DISCLAIMER

FAIR USE POLICY

CONTACT

Please contact publications@unido.org for further information concerning UNIDO publications.

For more information about UNIDO, please visit us at www.unido.org

UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION
Vienna International Centre, P.O. Box 300, 1400 Vienna, Austria
Tel: (+43-1) 26026-0 · www.unido.org · unido@unido.org

D02841

United Nations Industrial Development Organization

Distribution:
LIMITED

ID/WG.99/15
6 August 1971

ENGLISH
Original: RUSSIAN

Second Interregional Fertilizer Symposium

Kiev, USSR, 21 September - 1 October 1971
New Delhi, India, 2 - 13 October 1971

Agenda item III/1f

LARGE-CAPACITY AMMONIA SYNTHESIS REACTORS AND PLANTS: CONSTRUCTION OF MODELS AND OPTIMIZATION[1/]

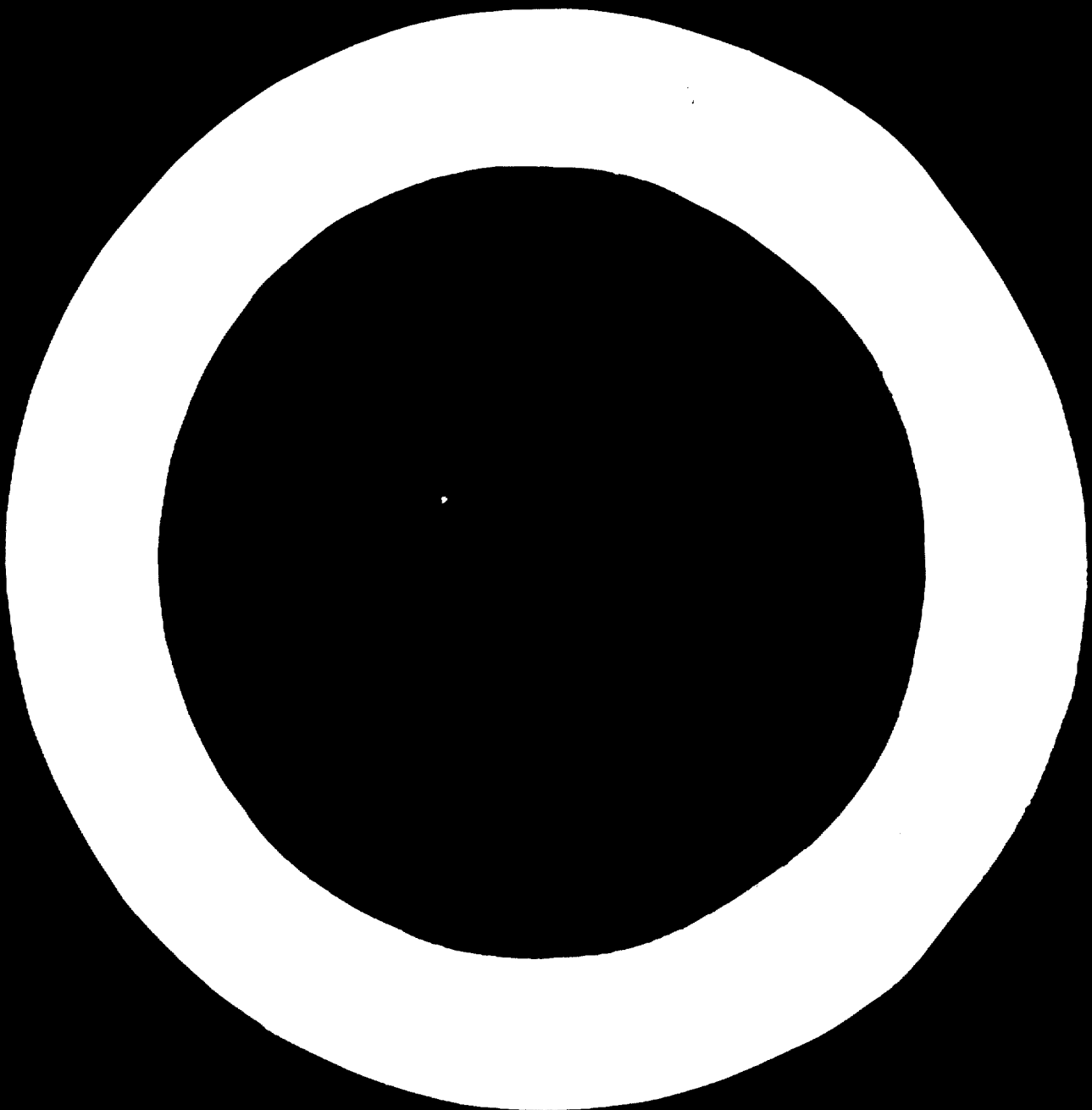
by

M. B. Aizenbud

State Institute for Nitrogenous Fertilizers
Ministry for Chemical Industry USSR

1/ The views and opinions expressed in this paper are those of the author and do not necessarily reflect the views of the secretariat of UNIDO. This document has been reproduced without formal editing.

id.71-6387



Production of synthetic ammonia is continuosly growing throughout the whole world. Within the last years large ammonia synthesis plants ranging from 600 to 1500 t/day capacity have been put into operation leading to considerable capital investments.

The choice of technological systems, apparatuses designs and pressure of the synthesis process is often governed by preceeding experience, market and patent considerations. Modern methods of mothematical modelling provide for objective approach towards optimization problems of ammonia synthesis plants and minimizing capital investments and running cost. Depending on the price level of raw materials, equipment and environment (temperature of cooling water and air) various results can be arrived at. In this connection we have made an attempt to create a complex mathematical model of ammonia synthesis plant covering not only calculations of material streams but all apparatuses for ammonia synthesis, their price and finally investments per 1 ton of ammonia which is accepted as an optimization criterion.

The separate stage of our work was collection, systemizing and carrying out special tests to finalize certain data

of thermodynamic and thermophysical properties of gas mixtures, circulating in the synthesis cycle, process macrokinetics, problems of diffusion, reversible and irreversible poisoning of catalysts, etc. These data were processed as equations, suitable for application in digital computers. Not all the work in this field has been completed and our programmes are corrected as new additional data enter.

Considerable attention was drawn to problems of modelling and optimization of ammonia synthesis reactors. During more than half a century existance period of the nitrogen industry, dozens of designs of ammonia synthesis columns, such as tubular, tray, radial and combined types were developed.

Desire to bring the temperature conditions of the column to the optimum one is known to lead to complicated and sometimes unreliable designs. Upscaling to large capacity plants makes very acute the problem of creating very simple and reliable design alongside with high efficiency.

We have compared different designs of synthesis columns packing both between thenselves and with the so-called "ideal" column, i.e. a column with the optimal temperature conditions.

Mathematical models of ammonia synthesis reactors both with internal heat exchange and adiabatic layers have been worked out. Mathematical description of the reactor took into account the basic processes, occuring in the reactor: heat transfer, kinetics of ammonia synthesis, diffusion in catalyst pores. Phenomena of heat-transfer have been described by classic heat-transfer equations, Tyomkin. Pizhev[1] equation, later

modified by Smirnov[2] was adcpted as a kinetic equation for reversible poisoning of catalyst by water vapours. Stefan-Maxwell's equations of multicomponent diffusion served as the basis for mathematical description of the process using the porous grain catalyst and the digital method for solving equations obtained[3,4] has been suggested.

Mathematical models of the reactor made it possible to computirize calculation and optimization process and design parameters of ammonia synthesis reactors of the indicated types. When, calculating the operating conditions of the reactor varied over a wide range: volume velocity of gas mixture, concentration of ammonia and inerts at the income to the reactor, reaction initial temperature.

Double and single tubes reactor in the catalytic zone (5, 6, 7) - fig. 1 as well as reactors with a number of adiabatic catalyst layers (8, 9, 10) - fig. 2 have been considered.

At the same time calculations of an "ideal" reactor with the optimal temperature conditions have been carried out. In this case the productivity of the catalyst volume unit served as an optimization criterion.

Quantitative determination of approximation degree to the optimum conditions of one of the simpliest designs (double adiabatic catalyst layer reactor) presented special interest alongside with the study of complicated designs of ammonia synthesis reactors.

Requirements of stationary stability conditions for all indicated reactors designs have been considered; optimal stability conditions have been analyzed.

The analysis of the calculation results has proved that one can reach rather high productivity under certain conditions, including composition of synthesis-gas which is as a rule manufactured at modern large capacity plants in the column with two adiabatic layers.

Thus in the column with removal of reaction heat productivity equal to 90 - 93 % of the maximum one (fig. 3a) can be obtained in between the layers of the heat-exchanger.

This value is somewhat lower - 85.90 % in the column with a cold by-pass (fig. 3b). Under these conditions sufficiently complete utilization of heat reaction can be obtained providing that operating conditions in the catalytic zone are satisfactory.

Study of the reactor with three adiabatic layers has shown that the increase of the trays number does not lead to considerable productivity growth compared with a double-tray reactor (fig. 4).

In internal heat-exchange reactors productivity can reach 93 - 95 % (of the maximum possible).

Thus, analysis of various versions of reactor designs, including the simpliest, double tray reactor points out that different designs have no marked difference on their maximum capacity.

As stated above, parametric sensitivity and stability reserve of the chosen operating conditions were determined for all reactor designs studied on the basis of specially worked out methods.[13-14]

Stability reserve on the inlet temperature into the catalyst chamber is understood to be the difference of values of this temperature under chosen and critical operating conditions.

Stability reserve can be determined in a similar way on any other processing parameter.

Analysis of different designs has also proved that optimal conditions are stable for all the types, unless hot point limitation tells. However, stability reserve of the optimal conditions is not large as a rule. Stability reserve on the inlet temperature into a catalyst chamber in all reactors under consideration is very close to each other.

The value of stability reserve ranges between 3° and 6°.

By raising the inlet temperature compared to the optimum, one can increase stability reserve unless limitation on hot point tells. The biggest advantages in this regard can be related to a double-tube reactor. But investigation of parametric sensitivity under fixed conditions (fig. 5) of the simpliest reactor's design with two adiabatic layers has shown that their parametric sensitivity is not high and in the reactor with removal of reaction heat in a heat-exchanger is lower than that of the reactor with a cold by-pass.

Besides, utilization of the reaction heat for heating of external heat-carrier, for example, water under pressure, also increases stability reserve. As a result, the reactor with two adiabatic layers and with a heat-exchanger between them has stability reserve, close to that of the double-tube reactor.

Comparison of an"ideal" and real reactors characteristics taking into account their stability makes it possible to select the most rational design of ammonia synthesis for large capacity plants combining high efficiency and reliability.

Thus, the simpliest designs of ammonia synthesis reactors, such as the reactor with two adiabatic layers and with a heat-exchanger between them, can be recommended for large capacity units.

Such reactors could not be extensively applied before, due to the presence of considerable ammount of catalytic poisons, such as water vapours, CO, CO_2,sulphur in a gas mixture.

It is known that poisonous agents are particularly harmful for a catalyst under low temperatures of about 400°.

When the initial temperature of the reaction in a tray reactor was raised up to 440°C, it caused considerable cut down in the productivity.

Wide application of double-tray synthesis reactors was seriously hindered by absence of thermostable catalyst, which could cause catalyst overheat, especially when working with gas mixture without inerts and with low ammonia concentrations.

At present the system of obtaining and purification of processing gas is simplified and at the same time modified to such an extent that makes it possible to get gas mixture practically without any poisons. In modern designs the content of oxygen containing compounds does not exceed 20 ppm, while sulphur containing compounds are completely absent.

Special interest is drawn by the synthesis process in a double tray reactor where the first layer is in suspension and the second one in a fixed state. Isothermic conditions of ammonia synthesis process in suspension layer provide for avoiding overheat in the first catalytic layer.

Granulated catalyst developed by our institute provides for commercial application of a fluidized bed.

In this reactor design one can use fine-grained catalyst, i.e. to carry out a process under conditions close to kinetic sphere.

Application of a suspended layer enables to carry out operation with increased volume velocity. Calculations proved that such types reactors are quite promising.

At present, a new, high-temperature ammonia synthesis catalyst CA-2[15] able to stand up to 600°C has been developed and commercialized. Activity of CA-2 catalyst under low temperature is somewhat lower than that of a conventional catalyst CA-1, but under high temperatures of 550 - 575°C is practically the same.

Charging in layers of the catalyst CA-2 together with CA-1 into ammonia synthesis columns will provide for commercial application of double tray ammonia synthesis reactors.

Development of thermostable catalyst creates the same possibilities for a double-tray reactor (in terms of increasing stability reserve) as for a reactor with double counter-current pipes.

To calculate optimization of an ammonia synthesis unit as a whole it is necessary to have mathenatical descriptions of other apparatuses included in ammonia synthesis cycle. That is why we have developed mathematical models for heat-exchange[16] and condensation[17] apparatuses.

Mathematical description of a heat-exchange apparatus include equations of heat-balance and heat-transfer. This description was based on the use of heat-content values as functions of temperature, pressure and composition of gas-mixture.

Effective separation of ammonia from gas mixture by a condensation method is of great importance in production of synthetic ammonia.

The right choice of a condenser's design and its sizes acquires special importance due to considerable increase of capacities in synthesis units.

While calculating condensation apparatuses one should take into account not only heat-exchange but mass-transfer processes as well, and also the presence of considerable ammount (up to 80 %) of inert, non-condensable gas: nitrogen--hydrogen mixture.

We have considered a number of methods for calculating the process of ammonia condensation, which cover phenomena of heat-and mass transfer as well as the influence of inert gas. The analysis of methods available has shown that methods

18 and 19 consider in the most complete way the physical essence of steam and steam-gas mixture condensation process. They allow to determine changes of basic values, which characterize heat and mass transfer when both are present. That is why these two methods were taken for granted in developing mathematical description of condensation apparatus in ammonia synthesis cycle.

As a stream flows condensation process is divided into three zones: the cooling zone, the condensation zone at the apparatus walls and the condensation zone in the nucleus of stream - i.e. fog-generation zone. Mathematical description of ammonia condensation process out of gas mixture include differential equations of heat-balance, drawn for counter--flow case. Speed of mass exchange was determined by Stefan's equation[20] according to differential equation as the speed of vapours diffusion through a boundary layer of vapour-gas flow. Besides, parameters of heat-and mass exchange are tied up by an equation of equilibrium curve indicating dependence of equilitrium concentration on the temperature and by a heat--balance equation per unit of surface.

Algorithm and programme of calculating water condensers at digital computers, condensation columns and liquid ammonia evaporators of different design were drawn on the basis of this mathematical model.

Alongside with working over algorithms and programmes for calculating separate apparatuses - algorithms of material

balances for different designs of ammonia synthesis with single-and double stage condensation, with continious purging by gas and without it have been drawn.

Parameter determination meeting stationary conditions of the plant operation serves as the basis of these algorithms.

One of the modern unit systems shown in fig. 6 served as the basis for further study taking into consideration big variaty of synthesis systems; algorithms being specially worked out for this system and the calculation programme on computer M-220 being made out. This methods with certain corrections can be used for calculating other systems.

Initial and variable process parameters, their digital values completely determine operating conditions of ammonia synthesis unit are the following: pressure, volume velocity, content ammonia and inerts at the inlet tc the column, gas temperature after primary condensation, content of inerts in fresh gas, temperature of fresh gas, daily capacity of the unit.

The ready product, liquid ammonia is being continuously taken out in the synthesis cycle. Besides, to prevent build--up of inerts (argon and methane) which are in fresh gas, continuous purging by gas is carried out. One should take into account the ammount of gas which is being dissolved in liquid ammonia and taken away from the cycle by liquid stream both from primary and secondary condensation systems. Ammount of fresh gas supplied into unit should make up for all its losses.

Observing material balance can be actuated through multiple iterations, by consecutive comparison of gas stream at the inlet to the synthesis column (preset and obtained).

When the latter do not coincide one should turn to the purging point, as initially approximating value of dissolved gases ammount in the system of secondary condensation was accepted as the basis for determination of purging and fresh gas consumption.

Flow-diagram of calculating ammonia synthesis is presented at fig. 7.

The programme provides for preparation and computation of information from magnetic tape before each block. Printing of calculated technological and design parameters is carried out after each block.

It stands to reason to begin calculation from the catalyst chamber of an ammonia synthesis column. Inspite of multiple interations in this case the catalyst chamber of an ammonia synthesis column is taken into account only once.

In calculating ammonia synthesis column the following parameters are considered to be variable: content of ammonia and inerts at the inlet to the synthesis column, volume velocity and pressure. In the result of calculating the synthesis column one can obtain data, initial for consequent diagram calculation: composition of gas mixture at the outcome of the synthesis column, volume of the catalyst, temperature at the outcome of the catalytic zone and also at the inlet to heat-exchange pipes of the catalyst chamber.

After calculating the catalyst chamber one passes over to calculating material balance. As distribution of material streams in the synthesis system depends on the temperature of primary condensation, the latter is also a variable parameter.

As a result, one obtains total amount of gas mixture and its composition at the inlet to different apparatuses of the synthesis system, as well as temperatures in the mixing zone of the separation section of the condensation column and at the outcome of the evaporator. After it one proceeds to calculating apparatuses of the condensation-separation system.

In calculating heat-exchange section of a condensation column, ammount of gas mixture in pipe and interpipe spaces, as well as temperature of cooling gas-mixture at the inlet into the apparatus and inlet and outlet temperature of heated gas mixture are known. As a result, surface of heat-exchange section of a condensation column and temperature of cooled mixture at the outlet of the condensation column, i,e, at the inlet to evaporator become available.

After calculation of evaporator, ammount of boiling liquid ammonia and the surface of heat-exchange were determined.

The next apparatus submitted to calculation, is outside heat-exchanger. Ammount of gas mixture, its composition in pipe and interpipe spaces are determined on the basis of material balance. The temperature at the inlet to interpipe space of a heat-exchanger is known from calculation of the

synthesis column, as-according to the algorithm of the catalyst chamber, degree of gas mixture heating during the catalyst chamber shell can be determined. The temperature of gas mixture at the outlet of water-heater, i.e. at the inlet to the outside heat-exchanger is preset. Besides, the temperature at the outlet of the heat-exchanger pipe space is also preset. As the surface of the latter considerably depends on the temperature at the outlet of the heat-exchanger (at the inlet to the condenser), heat-exchange surface is calculated with different variations of the indicated temperature. The temperature at the outlet of an interpipe space in the outside heat-exchanger is being also determined and consequently the temperature at the inlet to interpipe space of the inner heat-exchanger. Temperatures at the outlet of interpipe space and at the inlet to pipes of the inner heat-exchanger are determined due to calculation of a catalyst chamber. Thus, the only unknown values are the surface of heat-exchange and the temperature at the outlet of pipe space in the inner heat--exchanger. These values are determined according to the algorithm of the heat-exchanger calculation. After it one can carry out calculations of a water-heater. Since all four temperature values in a water-heater are known, surface of heat-exchange and ammount of circulating water can be determined in the result of calculation.

The last apparatus in the system is a condenser. Its calculating results in determination the ammount of circula-

ting water and condensation surface. Thus, material streams in all critical points of the cycle as well as the main parameters (dimensions) of all apparatuses are determined according to the described algorithm.

To calculate the cost of apparatuses - we take for granted any project being carried out at the present, for which estimated costs of all apparatuses are known.

On the oasis of information obtained from literature [22][23][24] and investigations which have been carried out by us, we have adopted equations by means of which one can pass over from the cost of known apparatuses of a certain design to the same design but with other operating parameters in the range of changing the initial parameters under study.

In some cases, for example, when pressure of synthesis is compared, it is worthwhile to consider together sections of compression and ammonia refrigeration unit besides section of ammonia synthesis.

Having available the given mathematical description of ammonia synthesis unit, one can solve the optimization problem at the design stage of the whole unit.

Expenditures comprising the product operation cost and investment share taking account of rated efficiency factor have been adopted as an optimum criterion

$$З = C + E\frac{k}{n}$$

where: З - expenditures, roubles/t

C - running cost, roubles/t

k - capital investments, roubles

n - output of an ammonia unit, t/a

E - rated efficiency factor

$Year^{-1}$ (usually adopted in the chemical industry 0.12 - 0.15)

On the basis of the algorithm given above we have written the programme for calculating at the M-220 computer expenses of the synthesis cycle on preset initial data for the flow--sheet of the unit, described in fig. 6.

The programme makes it possible to calculate in several minutes heat and material balance of the synthesis cycle, operating and design parameters of separate apparatuses and units, costs of power material expenses, capital investments and in the long run expenses per 1 ton of ammonia.

Fig. 1. Reactors with internal heat-exchange

I. Reactor with single counter flow pipes

II. Reactor with single straight through pipes

III. Reactor with double counterflow pipes

IV. Reactor with double straight-through pipes

T - temperature in internal pipes

Q - temperature in external pipes

t - temperature in catalytic zone

H - length of reactor, m

X - relative reactor length

Fig. 2. Reactors with adiabatic layers

I. Reactor with two adiabatic layers with removal of reaction heat in the heat-exchanger between layers

II. Reactor with two adiabatic layers and with feeding cold gas between layers

III. Reactor with three adiabatic layers and with cold gas feeding between layers.

t - temperature in the catalytic zone

Δt_k - reducing temperature in heat-exchanger between layers

λ - share of cold by pass

i.r.t - initial reaction temperature

W - volume velocity at the inlet to the column

i, Z_0 - content of inerts and ammonia at the inlet to the column

λ - total share of cold by-pass

λ_1 - share of by-pass in the second layer of the total share of cold - by-pass

Fig. 3. Dependence of degree of bringing capacity to the optimum one on reducing temperature of gas mixture between the first and the second layer (a) and on the share of cold by-pass between the first and the second layers (b) with different ratio of the catalyst volume on trays ($W = 20000\ h^{-1}$, i.r.t=400°C, i.o.= = 10 %, Z_o = 2 %)

Fig. 4. Dependence of the maximum capacity and the degree of bringing to the optimal capacity (C max./C opt) on the ratio of the catalyst volume in the first layer to the catalyst volume in the first and the second layers ($\frac{V}{V_1+V_2}$) under different ratios ($V_1 + V_2$) to the total catalyst volume.

Fig. 5. Dependence of ammonia content at the outlet of the column on changing operating conditions.

a. - changing i.r.t, content of inerts at the inlet to the column i_o, reducing temperature between layers t_k, share of cold by-pass)

b - changing volume velocity W, content of ammonia at the inlet to the column Z_o, ratio of catalyst volume $\frac{V_1}{V}$

Fig. 7.

P - pressure before the synthesis ammonia column

NH_3 - content of ammonia before the synthesis column

i - content of inerts before the synthesis column

W - volume velocity

t_8 - gas temperature after a condenser

t_7 - gas temperature before a condenser

Fig. 6. Schematic diagram of ammonia synthesis unit.

1. Synthesis column
2. Water-heater
3. Outer heat-exchanger
4. Condenser
5. Separator
6. Condensation column
7. Evaporator
8. Circulating compressor

1. Loading of P^{*}, W^{*}, J^{NH3}, $J^{"}$ into operating cells
2. Calculation of the catalyst chamber of the synthesis column
3. Loading of t_8^{*} into operating cell
4. Calculation of heat-material balance of the synthesis cycle
5. Calculation of heat-exchange section of the condensation column
6. Calculation of evaporator
7. Loading of t_7^{*} into operating cell
8. Calculation of outer heat-exchanger
9. Calculation of internal heat-exchanger of the synthesis column
10. Calculation of water-heater
11. Calculation of condenser
12. Calculation of expenditures
13. Check up of cycle termination on t_7 complete
14. Check up of cycle termination on t_8 complete
15. Check up of cycle termination on P, W, J^{NH3}, J^{4} complete Termination

Fig. 7. Flow-diagram of calculation ammonia synthesis unit

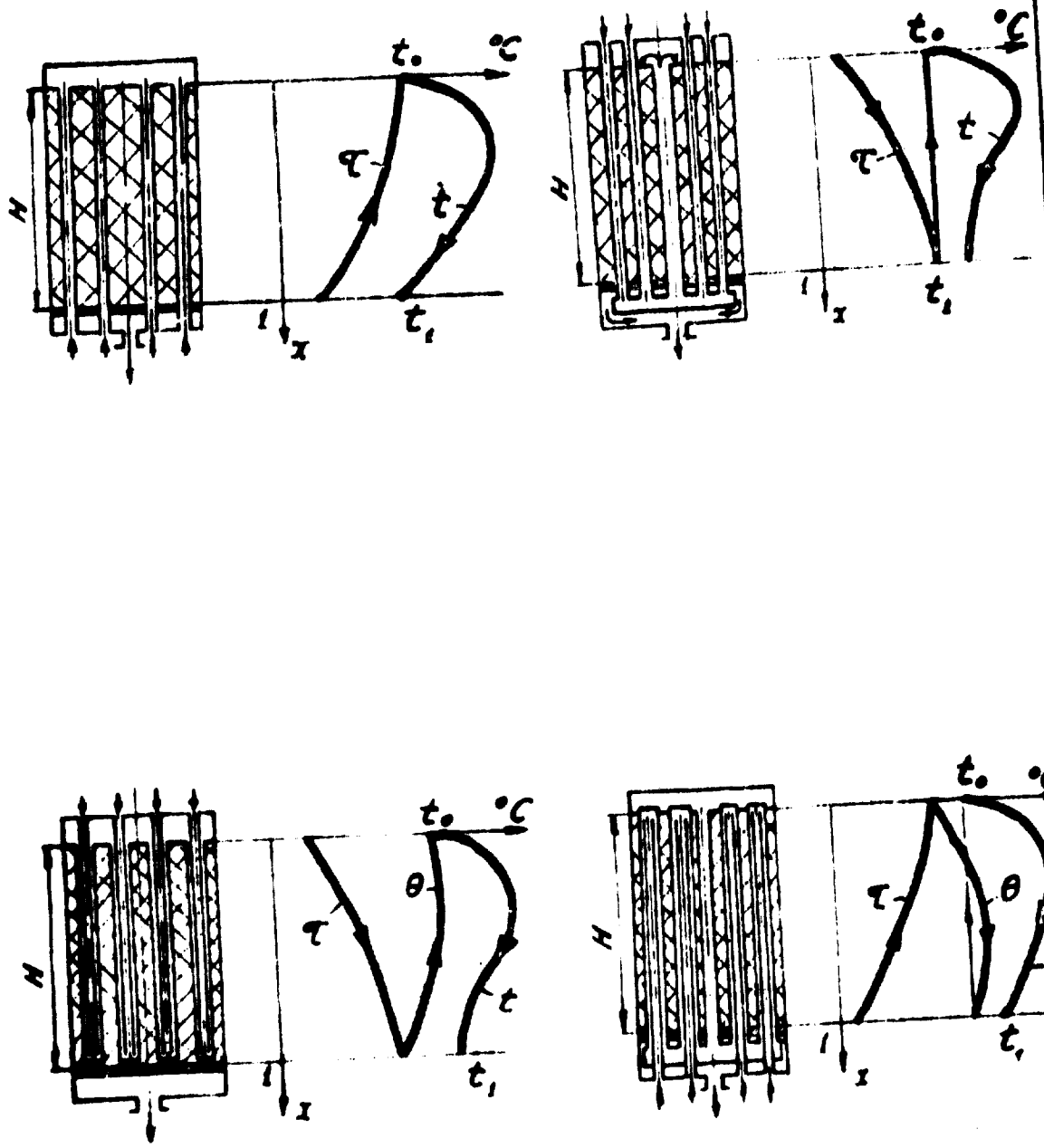


Рис. 1

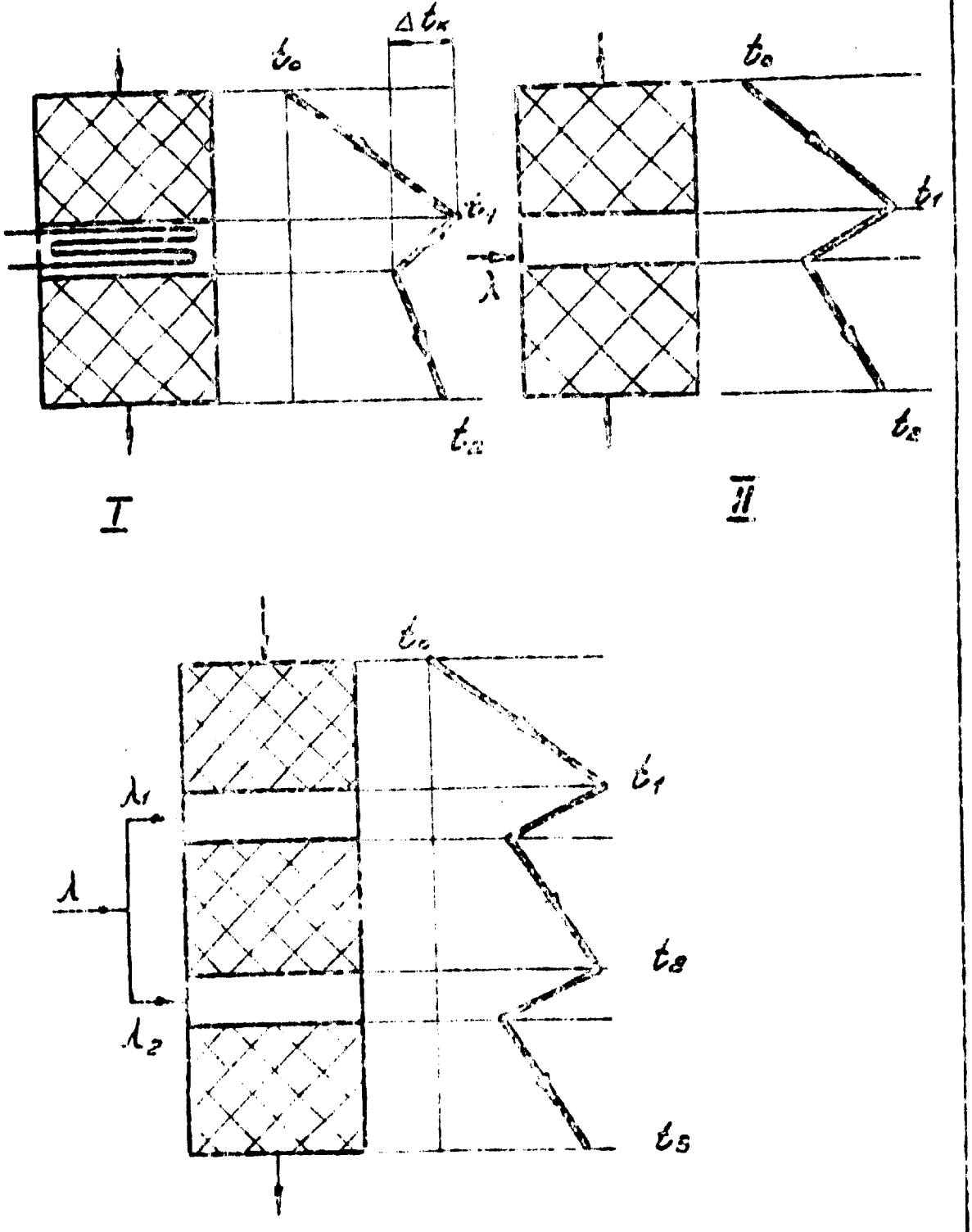
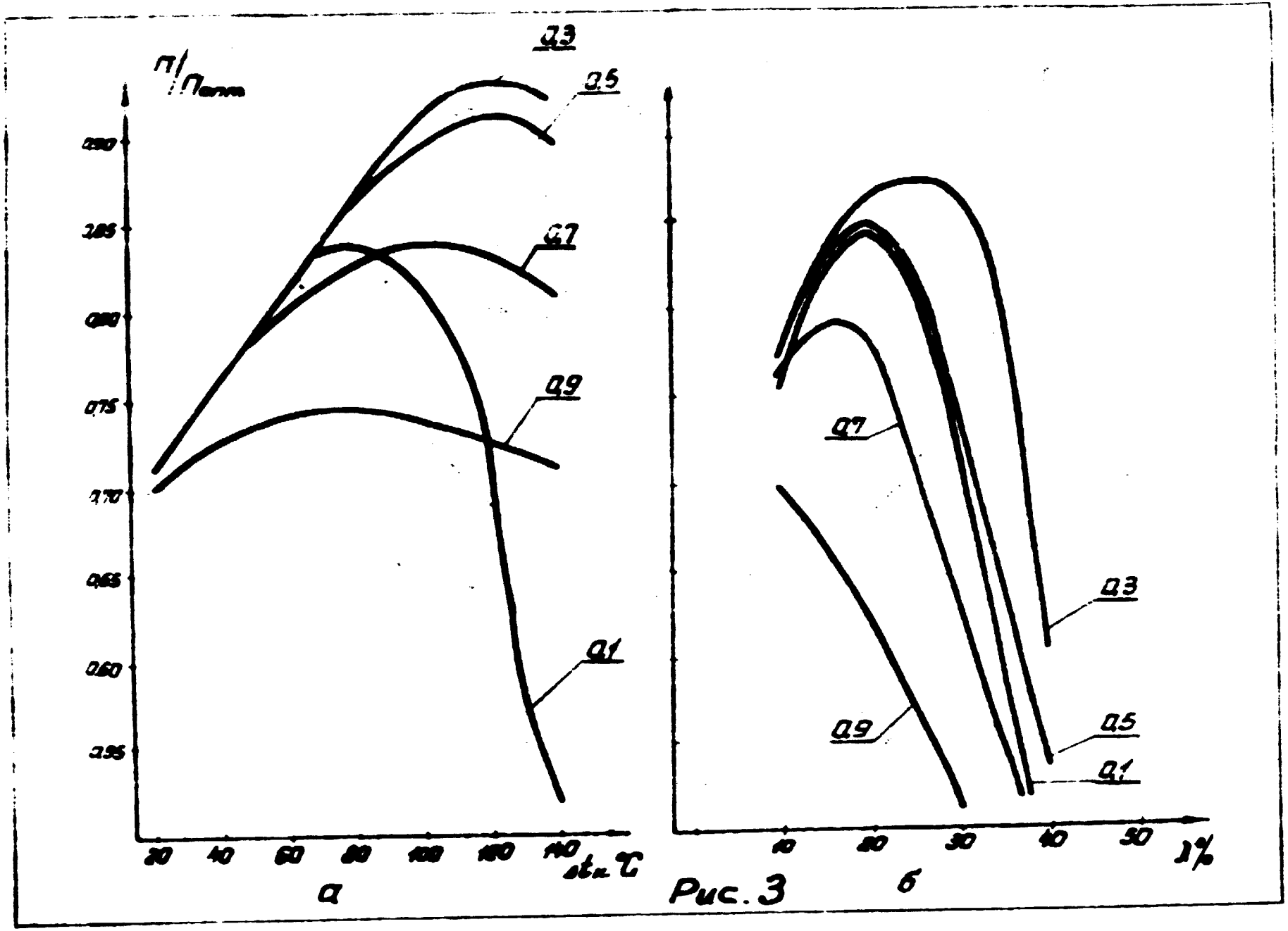


Рис 2


0,3
0,5
0,7
0,9
0,1
n/nном
0,90
0,85
0,80
0,75
0,70
0,65
0,60
0,55
20
40
60
80
100
120
140
Мкр, Т
а
Рис. 3
0,7
0,3
0,5
0,1
0,9
10
20
30
40
50
J%
б

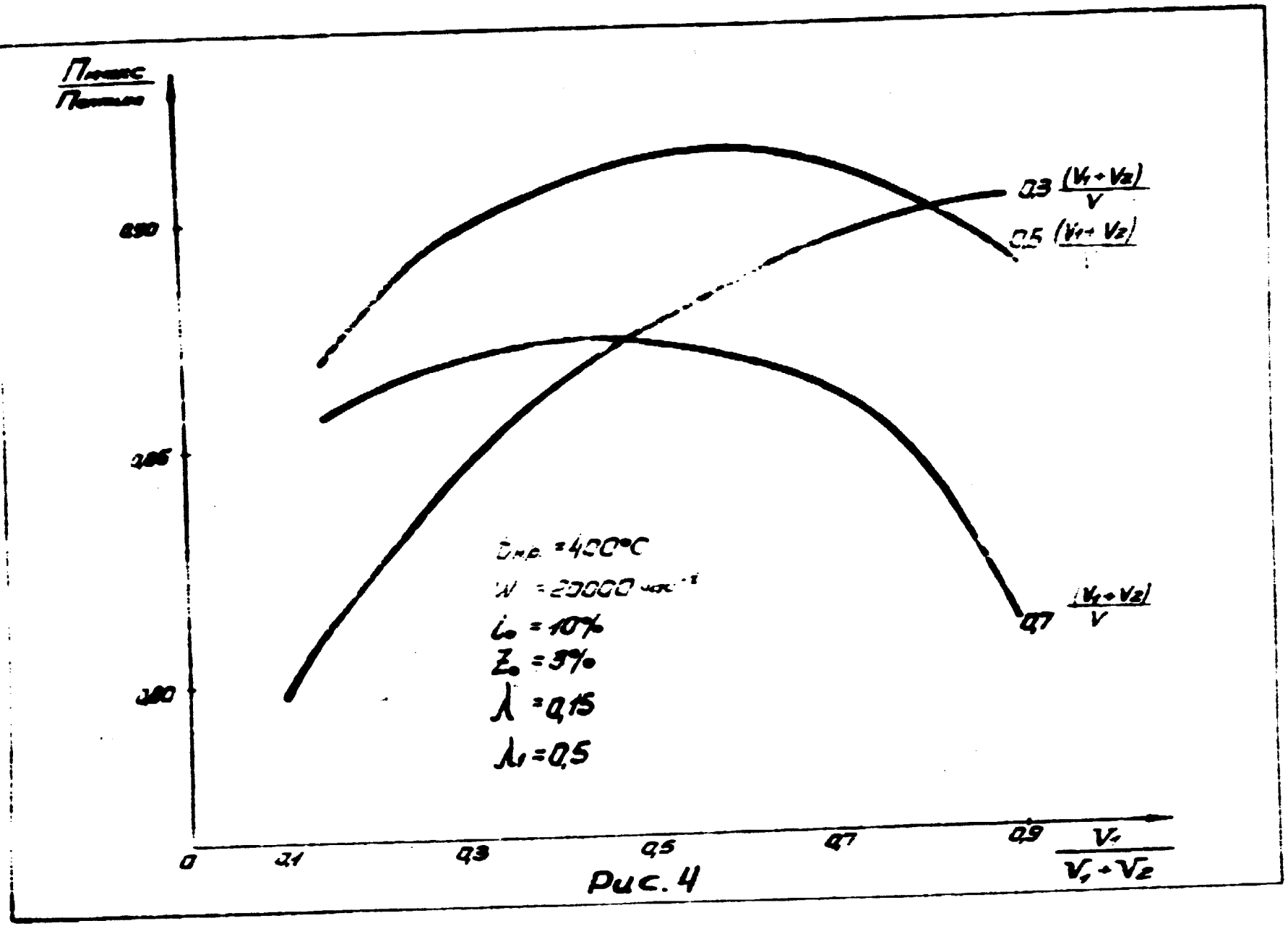

Pmax / Pmin
0,90
0,85
0,80
0,3
0,5
0,7
0,9
0
0,1
0,3
0,5
0,7
0,9
Vэ / V1 + V2
0,3 (V1 + V2) / V
0,5 (V1 + V2)
0,7 (V1 + V2) / V
Tнв = 400°C
n = 20000 мин⁻¹
i0 = 10%
Z0 = 3%
λ = 0,15
λ1 = 0,5

Рис. 4

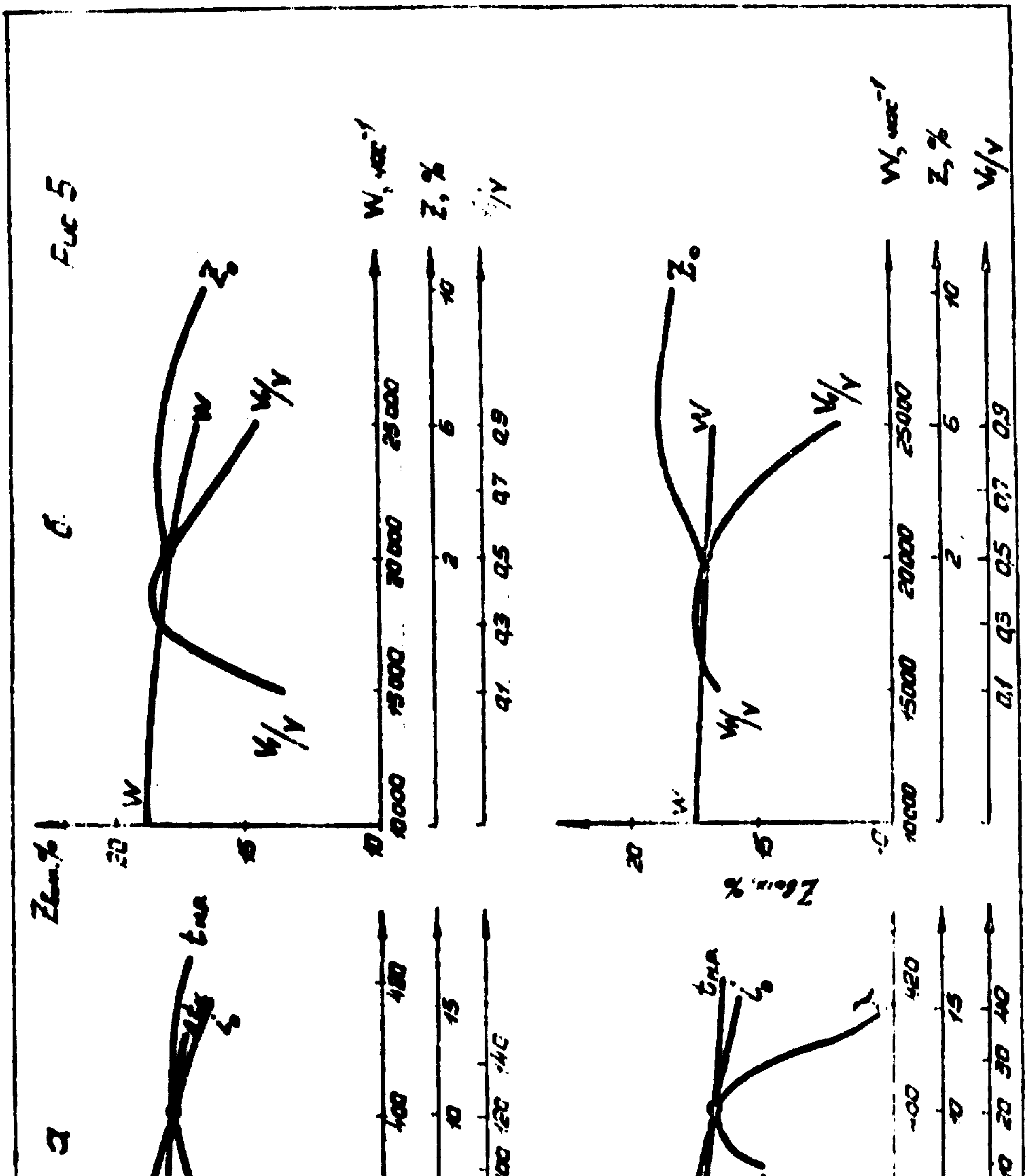


Рис 5
а
б
10000
15000
20000
25000
0,1
0,3
0,5
0,7
0,9
20
15
10

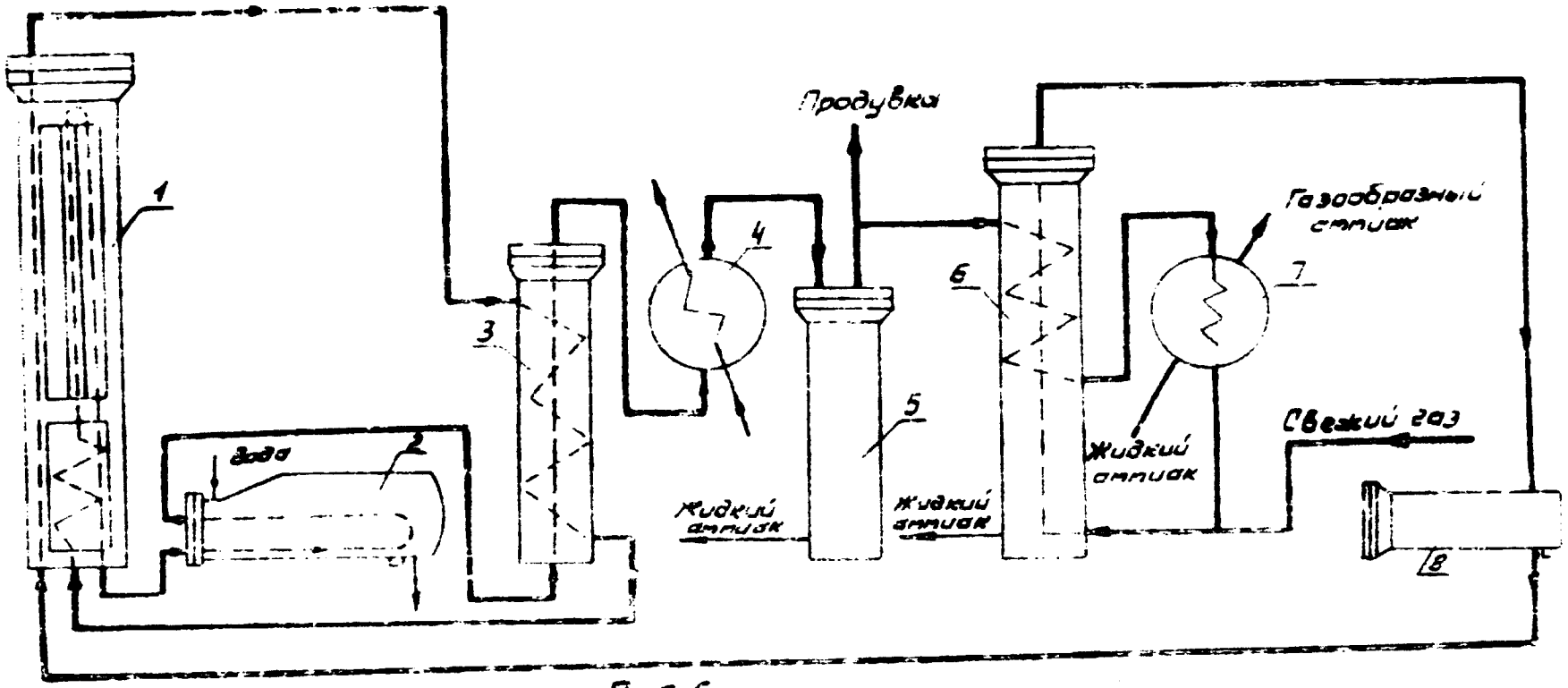


Рис.6.

Схема агрегата синтеза аммиака

1 - колонна синтеза; 2 - водоподогреватель; 3- выносной теплообменник;
4 - конденсатор; 5- сепаратор; 6- конденсационная колонна 7-испаритель;
8 - циркуляционный компрессор.

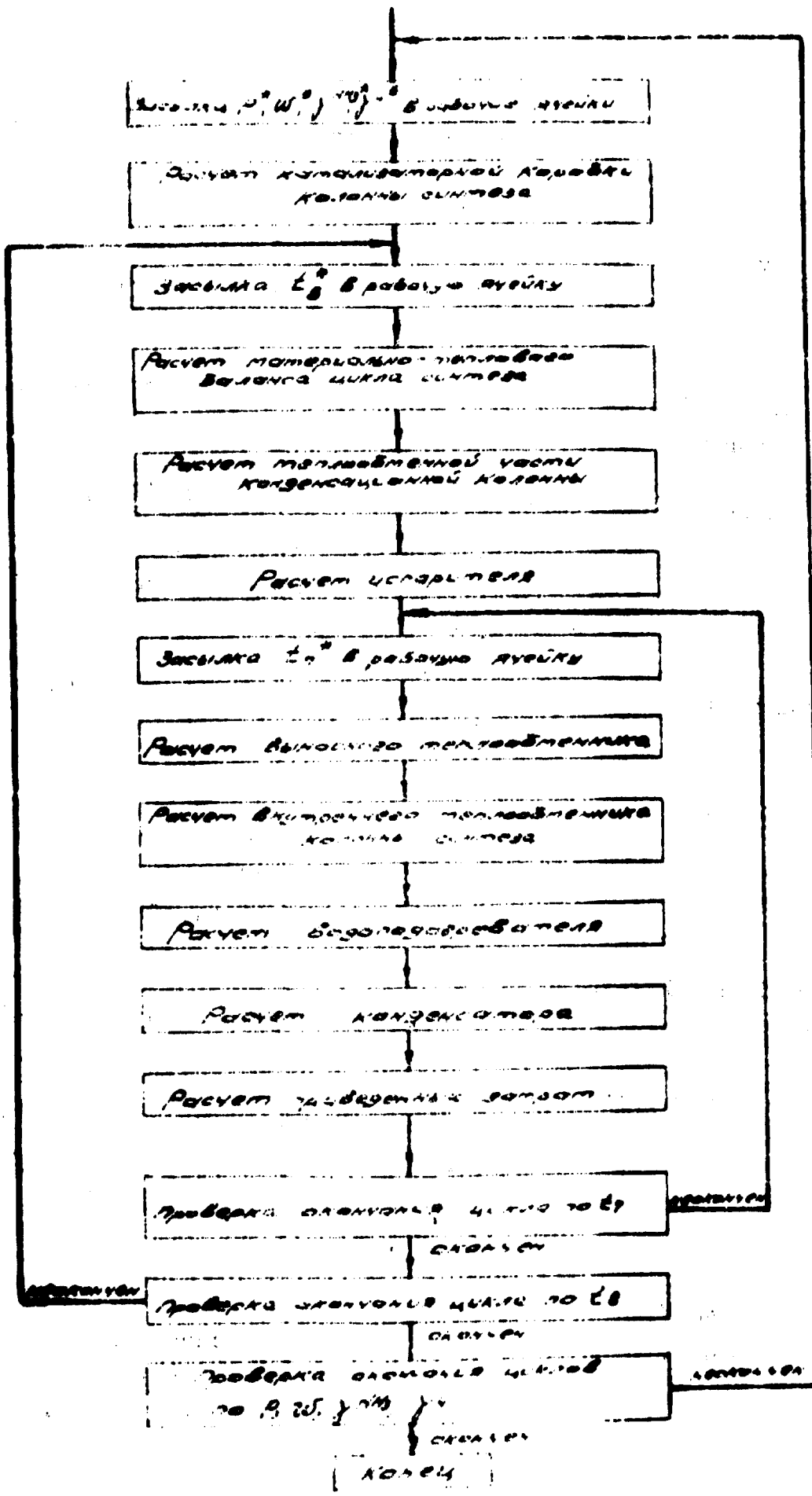


Рис.8. Блок-схема расчета

REFERENCES

1. Tyomkin M, Pizhev V. - JPC, v.3, 871, 1939
2. Smirnov I. - post-graduation paper, Research Institute of Physical Chemistry, Moscow, 1964
3. Sokolinski Y., Krasnoborov N - Theoretical basis of chemical engineering, 551, 1969
4. Sokolinski Y. - "Kinetics and catalysis", 8,878,1968
5. Sokolinski Y. - post-graduation paper, Moscow Institute for Chemical Machine Construction, Moscow, 1964
6. Sokolinski Y. - "Kinetics and catalysis",4,No. 6, 910, 1963
7. Rumjantzev O and others - "Modelling and optimization of catalytic processes Academy of Sciences, Moscow 144,1965
8. Vorotilina Z. and others - "Chemical industry" No. 3,199,1968
9. Vorotilina Z and others - "Chemistry and technology of nitrogen fertilisers", State Institute for Nitrogen Industry, Moscow, Issue 6, 127, 1971
10. Vorotilina Z., Eisenbood M. - "Chemistry and technology of nitrogen fertilisers". State Institute for Nitrogen Industry, Moscow, Issue 6, 153, 1971

11. Mukosei V. - Post-graduation paper State Institute for Nitrogen Industry, Moscow 1968

12. Mukosei V., and others - JPE, 12, 703, 1967

13. Mukosei V. - "Theoretical basis of chemical engineering"1, 936, 1967

14. Mukosei V. - "Theoretical basis of chemical engineering" 2, 286, 1968

15. Rabina P. and other - Chemical industry, No. 5, 1969

16. Kuznetzova O. - Papers of the young specialists conference, State Institute for Nitrogen Industry, Moscoe 1971(in print)

17. Vorotilina Z., Eisenbood M. - "Chemistry and technology of nitrogen fertilisers" Papers of the State Institute for Nitrogen Industry, Moscow, Issue 6, 167, 1971

18. A.P. Colbourn, O.A. Hougen - Ind. Eng. Chem., 11, 1178, 1934

19. Ivanov M. -Chemical Industry,No. 9, 52. 1961

20. T.Stefan,Sitzgs - Ber. Acad. Wiss Wien 1871,68,385,1873

21. Eisenbood M.and others - "Chemistry and technology of nitrogen fertilizers" Papers of the State Institute for Nitrogen Industry Edit. 6, 119, 1971

22. R. Aries, R. Boulitrop - "Rentabilité d'un procede Chimique de l'idee a l'usine, Paris, 1958

23. Mago H., Finneran J.- "Erdöl and Kohle" 1968, v. 21, No. 7

24. Guthrie Kanneth M. - "Chem. Eng." 75, No. 26, 144-146, 148, 1968.

United Nations Industrial Development Organization

ID

Distribution:
LIMITED

ID/WG.93/15 SUMMARY
6 July 1971

ENGLISH
Original: RUSSIAN

Second International Fertilizer Symposium
Kiev, USSR, 1 September - 1 October 1971
New Delhi, India 2 - 13 October 1971
Agenda item III/1f

SUMMARY

LARGE-CAPACITY AMMONIA SYNTHESIS REACTORS AND PLANTS: CONSTRUCTION OF MODELS AND OPTIMIZATION 1/

by

M.B. Lizenbad

State Institute for Nitrogenous Fertilizers
Ministry for Chemical Industry USSR

Mathematical models have been constructed for ammonia synthesis reactors of different types: with internal heat exchange and adiabatic layers. The models take into account the basic processes occurring in the reactor: heat transfer, kinetics of ammonia synthesis, diffusion in the catalyst pores.

The calculation and optimization of technological and constructional parameters for ammonia synthesis reactors of the types mentioned were carried out with the aid of a digital computer. Questions relating to stability and parametric sensitivity were studied for the same types of reactor and methods of estimating ranges and reserves of stability were obtained.

At the same time, calculations were made for an "ideal" reactor with an optimum temperature regime.

By comparing the data for the "ideal" and real reactors, and taking stability into account, it is possible to choose the best ammonia synthesis reactor design

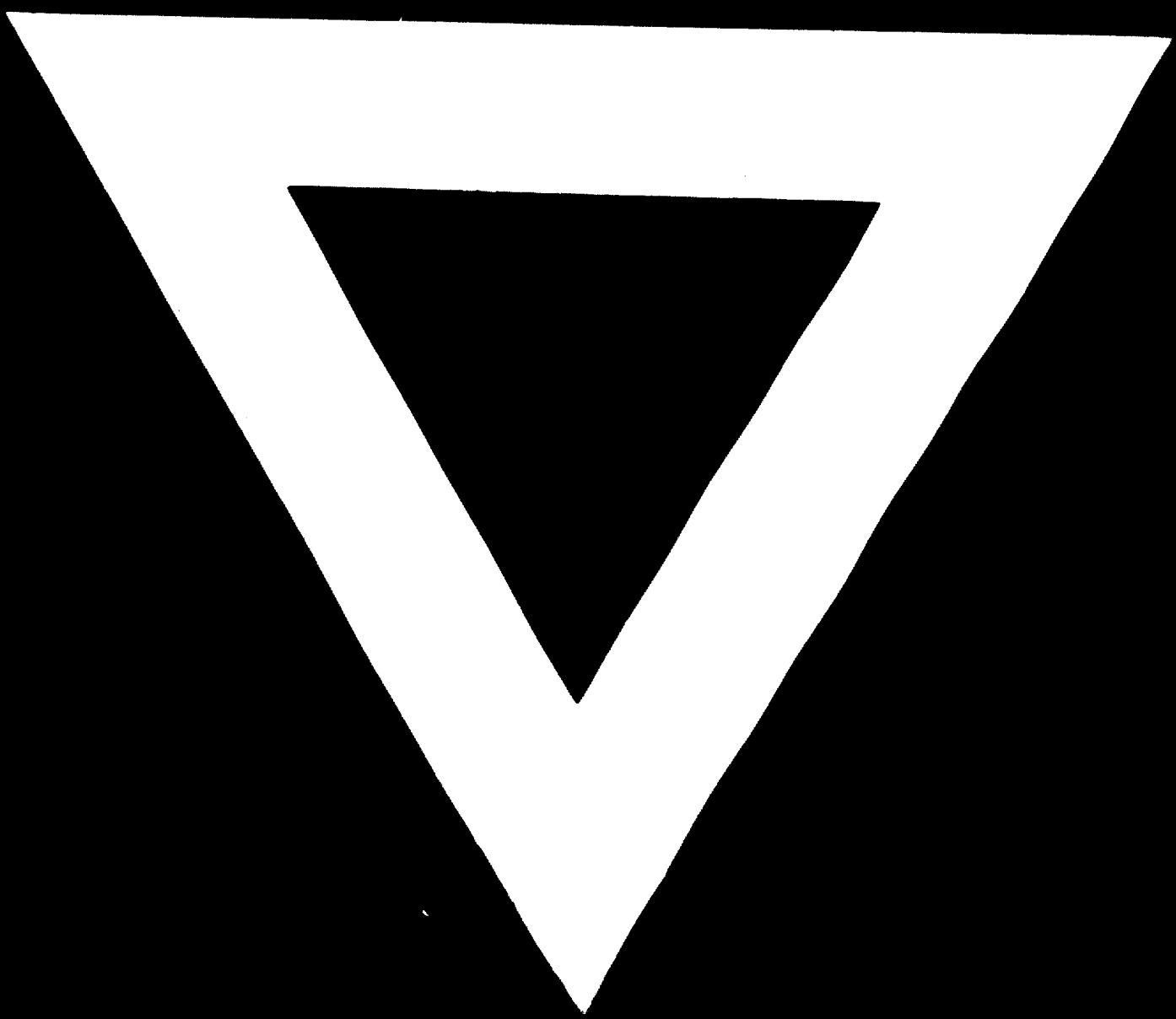
1/ The views and opinions expressed in this paper are those of the author and do not necessarily reflect the views of the secretariat of UNIDO. This document has been reproduced without formal editing.

for large-capacity plants, combining a high rate of operation with reliability.

A mathematical description and programme were worked out for the calculation of consumption of materials and heat and for the heat exchange and condensation apparatus of the ammonia synthesis cycle.

A complex model and calculation programme were prepared for the ammonia synthesis plant. With this programme, the main technological, constructional and economic parameters of a large-capacity plant can be determined.

This model serves as the basis for optimization of the whole ammonia synthesis plant. The optimization criterion adopted criterion adopted is minimum cost per tonne of ammonia.



74.10.2