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USE OF COMPUTERS IN FERTILIZER PLANT DESIGN  
AND IN OPERATION OF FERTILIZER PLANTS<sup>1/</sup>

by

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SUMMARY

USE OF COMPUTERS IN FERTILIZER PLANT DESIGN  
AND IN OPERATION OF FERTILIZER PLANTS<sup>1/</sup>

by

J. Saetz

Haldor Topsøe  
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Haldor Topsøe has for many years been involved in the use of digital computers for design and operation of ammonia plants and other types of chemical plants. This paper will describe some main features of the work that has been done in this field and the experiences that have been gained.

The development of computer programmes for plant design started about 1958, and since then a large number of programmes has been developed covering such fields as:

- 1) kinetic calculation of a variety of converters and reactors
- 2) calculation of heat and material balances in plants or in parts of plants
- 3) mechanical calculations of piping systems, pressure shells, flanges, etc.
- 4) statistical analysis of kinetic data from our laboratory and other experimental data
- 5) calculation of distillation columns, absorbers, heat exchangers etc.
- 6) thermodynamic calculations including chemical equilibria
- 7) mathematical calculations, especially for optimization and polynomial approximation

These programmes have mainly been used for two purposes:

- a) Design of plants

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- b) Evaluation of plant performance and especially evaluation of the operating performance of catalysts supplied by Haldor Topsøe.

Since 1964 several projects involving the use of computers for optimization, data acquisition and closed-loop control of ammonia plants in Hungary, Poland and Kuwait have also been undertaken.

In this connection a considerable expertise in developing efficient and reliable mathematical models of integrated chemical plants has been developed.

One tool which has proven especially useful in connection with design calculations and overall simulation of integrated plants is the so-called GIPS (General Integrated Programming System) developed by Haldor Topsøe. This highly integrated programming system as well as many other of the working methods which have been developed for simulation and optimization of integrated chemical plants will be described in detail in the paper.

Furthermore, the economic justification for using computers for optimization and on-line control of ammonia plants and similar plants will be dealt with, and some typical figures will be given.

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We regret that some of the pages in the microfiche copy of this report may not be up to the proper legibility standards, even though the best possible copy was used for preparing the master fiche.

## I. INTRODUCTION

The use of digital computers within industry, trade, research, administration etc. has developed and expanded very rapidly since the first commercially available computers were introduced about 1955.

The kind of tasks for which they have been used can mainly be divided into the following three main groups:

1. Administrative data-processing
2. Off-line technical and scientific calculations
3. On-line process control

Of these three groups we mainly will here deal with the two last mentioned areas.

One feature which is very typical for the use of computers within all fields is the extremely rapid technical development towards still more powerful, economic, and reliable computer hardware, - a development which is still opening new possibilities for more economic and efficient applications of the computers.

However, to use computers successfully, efficient hardware is not enough. Another problem - and a very difficult one - is to develop the adequate computer programs: the software. It is mainly with this field we will deal in this paper. It is a field, where very big amounts of work have been done during the latest 10 - 15 years, and still remains to be done.

## II. DEVELOPMENT AND USE OF PROGRAMS FOR PLANT DESIGN

At HALDOR TOPSØE the work with developing programs for technical calculations in connection with design of various types of chemical plants started about 1958. Since then a very big number of programs of this kind has been developed and constantly been adapted to newer calculation methods, new knowledge from laboratory research and operating plants, and to newer generations of still more efficient computers.

These programs could be divided into the following main groups:

1. Calculation of chemical reactors for ammonia synthesis, methanol synthesis, steam reforming of hydrocarbons, water gas conversion, and other reactions. The programs include numerical integration of the reaction rate expressions and calculation of heat transfer, temperature distribution, and pressure drop.
2. Calculation of heat- and material balances in various types of chemical plants or parts of such plants.
3. Calculations for mechanical design of piping systems, pressure shells, and other equipment used in chemical plants.
4. Statistical analysis of kinetic laboratory data. These programs include general type converter calculation programs covering all typical catalytic rate formulas.
5. Calculation of distillation columns, absorbers, heat exchangers, and similar equipment.



6. Thermodynamic calculations, especially for gas mixtures, including calculation of chemical equilibria.
7. Mathematical calculations including matrix operations, polynomial approximation, optimization by respectively pattern search, linear programming or quadratic programming, PERT- analysis etc.

The use of digital computers in connection with the design of fertilizer plants has had a very significant effect on the working methods used and upon the efficiency and accuracy of the work.

The main advantages by using computers for these purposes are:

- a. the possibility quickly to perform much more extensive and accurate process calculations than without using computers makes it possible to evaluate a number of various alternative solutions quite exactly and thereby improve very significantly the possibilities to arrive at a true optimum solution and at the most economic design.
- b. the possibility to update currently the computer programs used for design calculations by taking the latest results from laboratory experiments, pilot-plant runs and actual operations of plants already designed into account ensures, that the design is at any time based upon the latest available knowledge about process performance.
- c. it gives the possibility to ensure, that all process calculations performed within a company are made on the same uniform basis, and that the methods applied are well documented and can be checked at any time. It should, however, be added, that in order to obtain this advantage it is very important, that a good documentation of all programs, that are used, is carried through.

There is no doubt, that the trend during the later years towards design of still bigger and more economic fertilizer plants has to a considerable extent been made possible thanks to the increasing use of computers for design of the plants.

### III. EVALUATION OF CATALYST PERFORMANCE

An important area of application of the programs for calculation of reactors and converters is evaluation of catalyst performance.

Before a catalyst is delivered, the computer is used to evaluate the amount and type of catalyst, which in a given plant will give the best possible operating performance and catalyst life-time.

After the catalysts have been delivered, and the plant in question has come into operation, a regular calculation service is performed for all users of TOPSØE-catalysts, which request such a service.

The purpose of these computer evaluations is to follow the activity of the catalyst during its whole life-time and to determine optimal operating conditions. If the reactor performance is unsatisfactory in one way or another, a computer evaluation may reveal this, long time before it becomes evident at the plant. Thus, conclusions drawn from a computer study could make it possible to take corrective measures at an early time, which could improve the operating economy of the plant significantly.

Furthermore regular computer analysis of the catalyst performance allow prediction with good accuracy of the time when it will become necessary - or economically attractive - to replace catalyst. Accordingly the analysis of the actual performance is often supplemented with a calculation of the performance to be expected, say, one year hence.

In other cases the computer analysis is supplemented with calculations establishing the performance, which can be attained at other operating conditions, which may be under consideration.

A considerable number of the users of TOPSØE-catalysts are using this calculation service. Besides the benefits the users obtain from this, it also has the effect, that a big number of operating data are currently received by us, and this is of considerable help by the current up-dating of the programs which, of course, is very important in order to obtain the best possible and most realistic results.

#### IV. COMPUTER CONTROL OF FERTILIZER PLANTS

HALDOR TOPSØE has ever since 1964 been working with the application of digital computers for on-line control of fertilizer plants. Among the projects, which have been undertaken, can be mentioned:

##### IV.1. Pét - Hungary

The ammonia plant in Pét, Hungary, which was put into operation in 1969, was designed for a nominal capacity of 420 metric tons/day. The plant was constructed by SIM-CHEM Ltd. (Simon-Carves Chemical Engineering Ltd.) of U.K. using technology developed by HALDOR TOPSØE.

The hydrocarbon feedstock for the plant is natural gas, but for short periods naphta may be used. The compressors used are of the reciprocating type.

The hungarian client was just from the very start of this project quite interested in realising some kind of computer-control of this ammonia plant. However, one feared that it would hardly be justified economically to install a relative expensive computer system in the Pét-Plant, which could only be used for controlling this single plant.

Due to these fears a different approach was adopted:

1. On the plant a relatively simple and inexpensive data-logging system - a HONEYWELL type ADRT 1000 data handling system - was installed. This system was able to perform simple data-logging of some 200 measured process variables. Besides printing log-tables, performing alarm monitoring etc., this system is also able to produce a punched tape containing all the measured data.

2. By means of a telex transmission line the measured data from the plant are regularly sent to a computer center, which has been established in Budapest about 100 km away from the plant. For this center a danish GIER-computer has been delivered.

The data from the Pét-plant are with regular intervals fed into this computer, and by means of a comprehensive system of programs, which has been established in cooperation between computer specialists from the "Hungarian Research Institute of Automation" and from HALDOR TOPSØE, the following functions are performed:

2.1. The measured data fed into the computer are checked against errors and inconsistencies arising from instrument or transmission errors.

2.2. A plant performance evaluation is performed. This includes evaluation of important ageing variables as catalyst activity factors, heat-exchanger fouling-factors etc. The results of this are partly used to update the simulation model of the plant, partly to give the operation staff of the plant important informations about the operating status of the plant.

2.3. Optimization of the operation of the plant. The optimization model consists mainly of polynomials that have been developed by performing a large number of calculations on the off-line simulation model of the plant, which has been established by HALDOR TOPSØE. As optimization criterion one can use either:

- a. maximum production rate, taking the bottlenecks limiting this production rate into account,
- b. minimum operating costs at a fixed production rate, or
- c. a combination of a. and b. corresponding to maximum profit from the operation.

After the above mentioned calculations have been performed in the computer center in Budapest, the results are sent back via the telex transmission line to the central control room of the plant in Pét, where the operating staff can, by adjusting a number of set points to the values calculated by the computer, optimize the operation of the plant.

The calculations aiming at optimizing the plant in Pét are only occupying the computer about 1 hour a day in average. The remaining part of the time the computer is used for a considerable number of other tasks of interest for the hungarian chemical industry.

By choosing this solution one has succeeded in obtaining a system, which is economically justified with a very considerable margin.

The computer optimization system has now been in regular operation in about 1½ year and has during this time become more and more appreciated by the operating staff of the Pét plant as a valuable aid in obtaining the best possible operating status of the plant.

A more detailed description of this system is given in ref. 1.

#### IV.2.Z.A.Pulawy II - Poland

The Fertilizer Complex Z.A.Pulawy, which has, during the last 10 years, grown up in Poland, about 120 km south-east of Warsaw, at the Weischel river, is one of the biggest fertilizer complexes in the world. Among other things it includes 8 production lines of ammonia with a total capacity of 3000 metric tons per day. These 8 ammonia units are all based throughout upon HALDOR TOPSØE processes and our firm has been deeply involved in the whole planning, design, construction and putting into operation of this big complex.

The designation Z.A.Pulawy II, which is only a part of the total Pulawy-complex, includes the following units:

- 3 ammonia units with a production capacity of 500 m.t.p.d.each,
- 4 nitric acid units,
- 3 ammonium nitrate units.

This part of the complex was constructed by a consortium consisting of Simon-Carves Ltd. of U.K., VOEST of Austria and HALDOR TOPSØE. This plant was put into operation in 1968.

In this plant a relative small digital computer of the danish type RC 4000 was installed. The task of this computer is to collect data from all the 10 production units of the plant and perform such relatively simple tasks as:

- hourly logging of all measured data (about 700 data are included),
- alarm scanning including about 50 % of the measured data,
- yield balance calculations, normally performed once every 8 hours and giving important production-, consumption- and economy figures for all plant units,
- trend-logging allowing the operator to follow continually any of the signals connected to the system,
- operator communication allowing the operator via his input/output typewriter to request a number of various operations, change of constants etc.

The system has now been in normal operation in about 2½ years and is giving the operating staff of the plant much help in obtaining the informations they need about the operating status of the plant.

#### IV.3.P.I.C. Kuwait

The P.I.C. fertilizer complex in Kuwait includes two 800 metric tons per day ammonia streams and two 700 m.t.p.d. urea streams.

The ammonia units have been designed fully by HALDOR TOPSØE. They are based upon natural gas, released from the Burgan fields, as feedstock, and they use centrifugal-compressors and radial quench converters of the special TOPSØE-design.

In this complex it was decided to install an advanced IBM-1800 system for on-line computer control, which should perform the following main tasks:

For the total complex:

- Data acquisition, with conversion of all the about 600 analog input data connected to the system to correct engineering units, calculation of their short term averages and checking of instrument high and low limits against the instrument reading.
- Alarm scanning of both alarm contacts (about 800 are connected to the system), and of a number of process variables against their appropriate alarm limits with corresponding print-out of alarm messages.
- Trend-logging and/or recapitulation of stored data on operators request.
- Yield reporting of important production and consumption figures every 8 or 24 hours.

For the ammonia plant only:

- Error cross checking of the plant measurements against the material- and heat-balances they must fulfil in order to detect measuring errors and establish a consistent set of measurements.
- Plant performance evaluation including calculation of catalyst ageing factors, heat-exchanger fouling factors, compressor efficiencies, separator efficiencies, pressure drop coefficients etc.
- Over-all plant optimization taking into account the bottlenecks, which limit the production rate of the plant.
- Closed-loop supervisory control by adjusting a number of analog controller set points to their target values calculated by the over-all optimization program and taking local short term variations into account.

The communication between the operators and the computer is realized by means of two Process Operator Consoles, which allow the operator to:

- Select a process variable and have it printed out on the typewriter.
- Request the current value, short term average, high and low alarm limits, target value etc. to be displayed on the console.
- Change the high or low alarm limit of a variable.
- Take the variable in and out of service.
- Suppress the alarm check.
- Request the status of a process contact.
- Select summary reports.

These operator consoles are placed in the control room of the plant. The computer is placed in a room adjacent to the control room.

The plant is at present being put into operation, and the computer system has already during the commissioning period been used successfully for detecting errors during the installation etc.

The computer control system is expected to come in full operation during the autumn of 1971.

This system is described in further details in ref. 2.



## V. SIMULATION AND OPTIMIZATION OF THE OPERATION OF CHEMICAL PLANTS.

The basic problems of optimizing the operation of a chemical plant can be illustrated by fig. 1.:

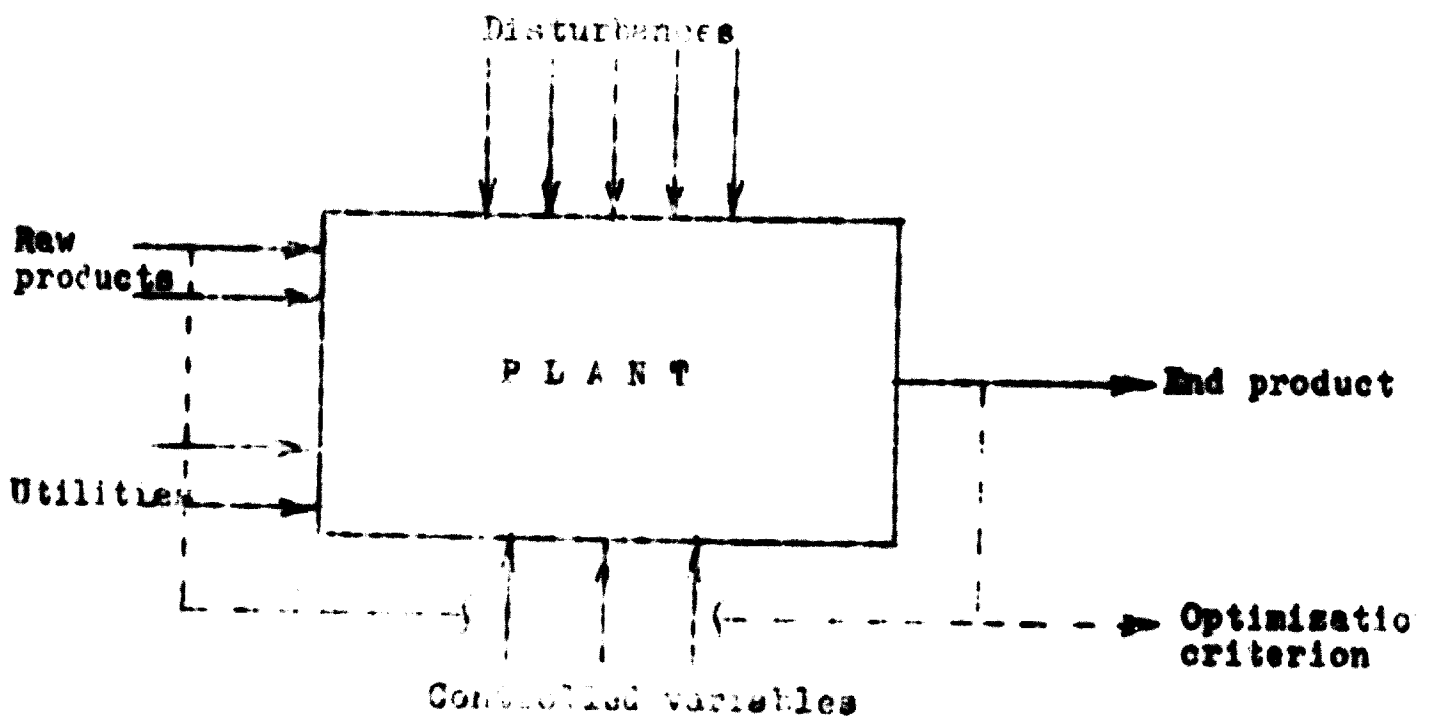


FIG. 1.

The aim of the optimization is to ensure, that one achieves the optimal value of the optimization criterion. A typical optimization criterion is the profit from the operation, i.e. the selling price of the produced amount of end product less the buying price of the consumed amounts of raw products and utilities.

The scope of the on-line optimization is to adjust the controlled variables to obtain this optimal status of the plant at the present status of the disturbances.

The disturbances can be divided into:

1. Short terms disturbances as:
  - variations in raw product compositions,
  - variations in cooling water temperature,
  - variations in ambient temperature,
  - variations in selling price of end product and buying prices of raw products and utilities.
  
2. Long terms disturbances as:
  - catalyst ageing,
  - heat-exchanger fouling.

The controlled variables are a number of important plant parameters selected to ensure optimizing control of the plant.

For an ammonia plant typical controlled variables would be:

- steam-to-carbon ratio,
- fired reformer duty,
- inlet temperatures to shift reactors and ammonia converter,
- purge rate in ammonia synthesis loop,
- H<sub>2</sub> to N<sub>2</sub>-ratio in the synthesis gas.

The allowable variations of the controlled variables will be limited by a number of constraints in order to avoid overloading of plant equipment.

Typical constraints in an ammonia plant could be:

- Maximum reformer tube wall temperature.
- Maximum outlet temperature from secondary reformer.
- Maximum and minimum temperatures in shift converters and methanator.

- Maximum pressure in synthesis loop.
- Maximum load on compressors.
- Maximum pressure and temperature of steam.

To sum up, the scope of the optimization could shortly be described as:

Calculate the set of values of the selected controlled variables, which for a given set of disturbance variables without exceeding the constraints will ensure the optimum value of the selected criterion function.

The most important part of the work needed in order to solve this optimization problem is to develop a reliable and efficient simulation model of the plant.

At HALDOR TOPSØE a very considerable work has been made to develop methods for establishing such simulation models.

The basis for this work has been the design programs, which were described earlier in this paper. However, in order to establish a sufficiently fast simulation model, a considerable work must be done in order to:

1. Link together the programs for each single process unit into a model covering the plant as a whole.
2. Simplifying this over-all model by substituting the quite complicated single design programs with simpler - but sufficiently accurate - polynomial expressions.

In order to solve this problem two integrated programming systems have been developed during the years:

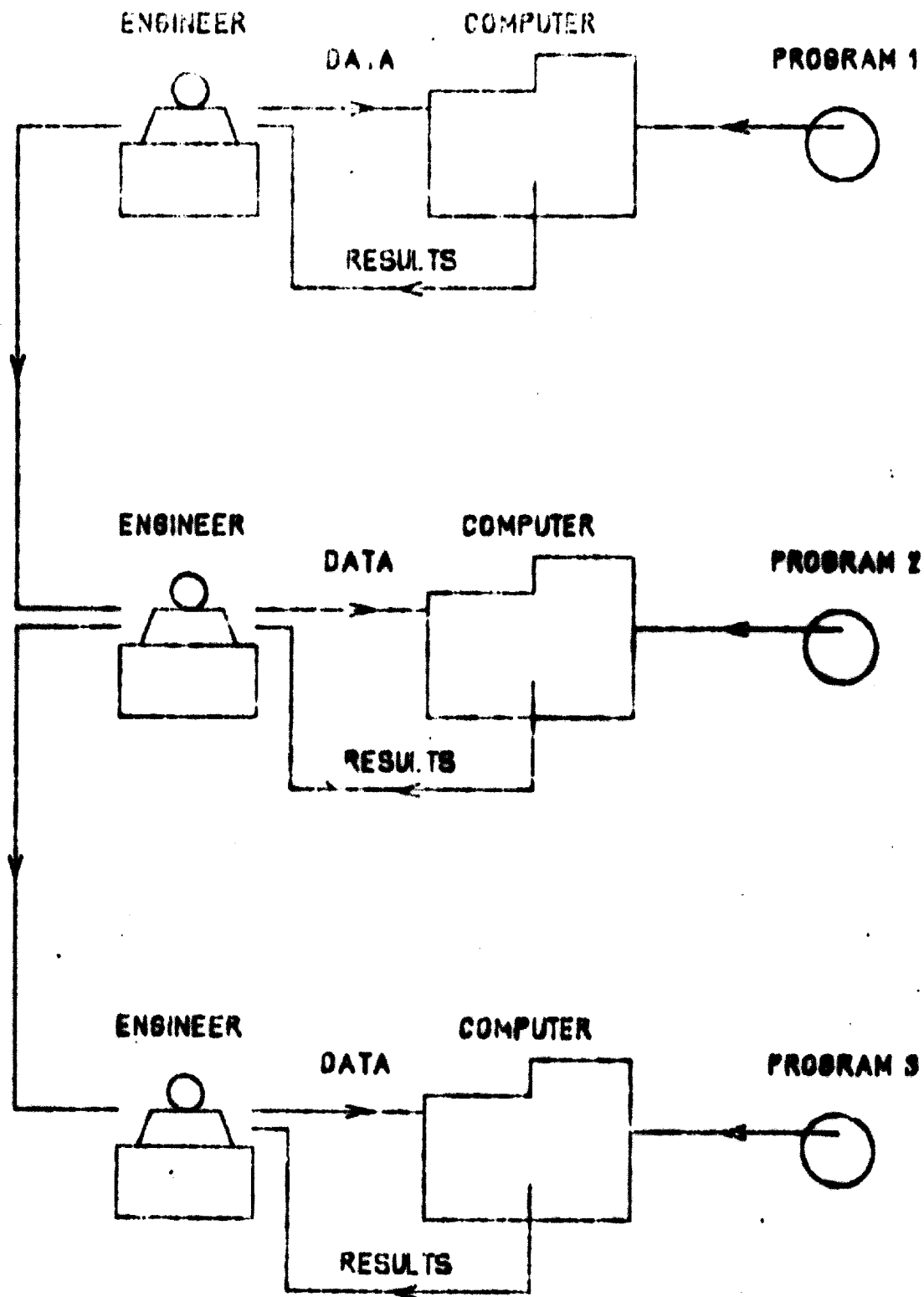
The PLANT-1 system and the GIPS system (GIPS= General Integrated Programming System).

The newest and most advanced of these systems is the GIPS system. This system is very useful, not only for developing simulation models of chemical plants, but also for performing the design of large plants in a more systematic, flexible and integrated way.

The basic philosophy of the system is illustrated by fig.2 and fig. 3.

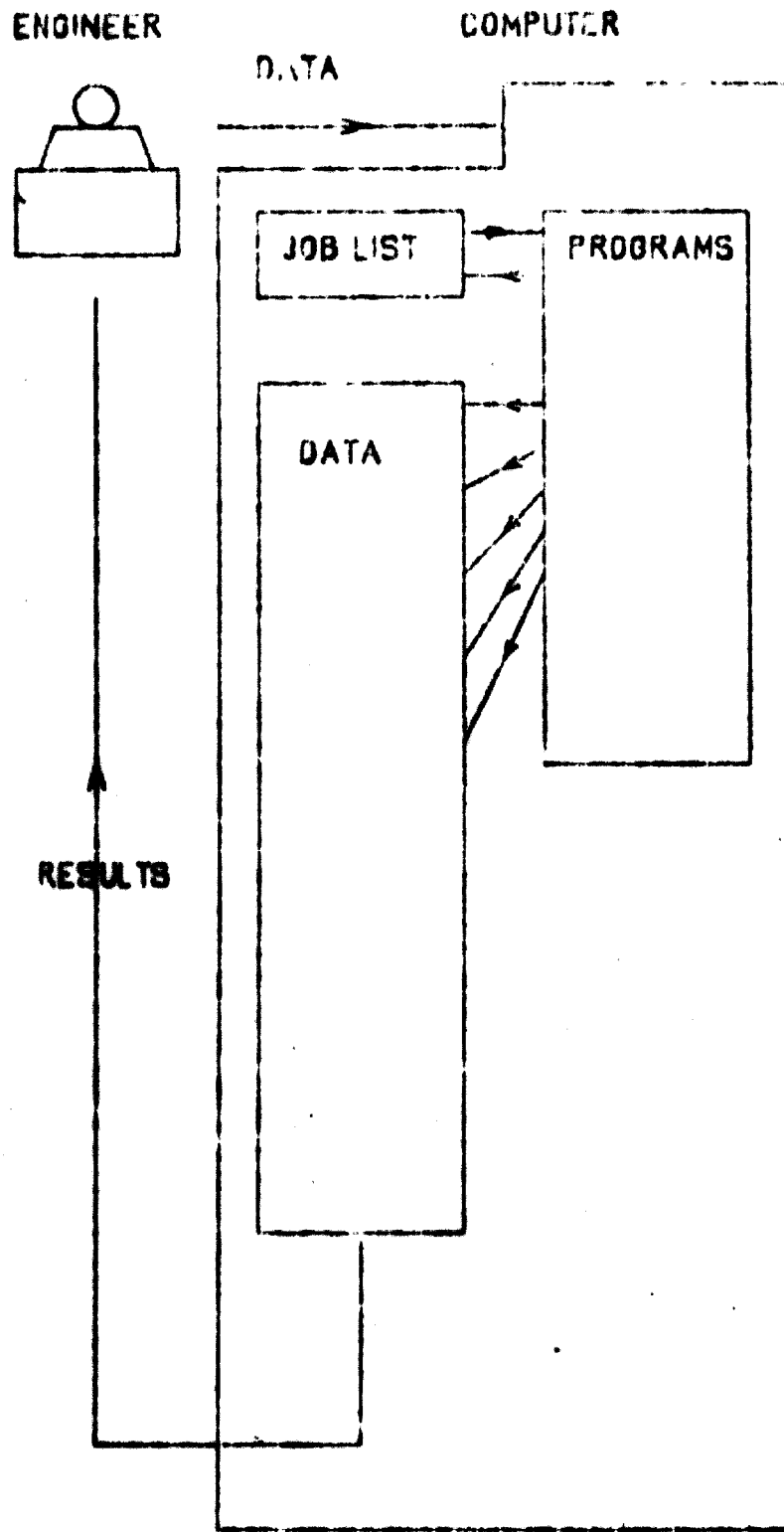
**Fig.2** shows the conventional way of solving a complex calculation problem by performing a number of calculations by means of single independent computer programs. Between each calculation the calculation results must be evaluated and used for defining the input data for the next calculation.

**Fig.3** shows how one can within the GIPS system combine such a number of single calculations into one integrated calculation, where a number of various single programs will exchange data between each other without direct human interference.



CONVENTIONAL DATA PROCESSING

HALDOR TOPSØE	
FIGURE 2	Calc. No. 28433 DR. NO.: 449590



FLEXIBLE PROGRAM CALCULATION

HALDOR TOPSØE	
FIGURE 3	Calc. No. 26434 DR. NO.: 449591

The most important principles inherited in the GIPS system are the following:

1. A fully flexible program structure, which permits the user to build up a calculation for an arbitrary combination of existing programs without assistance from a programmer.
2. An integrated data structure, which makes it possible to transfer data from one program to another during the calculation.
3. Use of data group descriptions -DGD- which are formalized pictures of data groups. A data group is a set of data containing related information.
4. Use of generalized programs for input reading, output printing, message printing and printing of input specifications. The DGD's are mainly used for this purpose.

The main advantages of the system could be summarized as:

1. New and complex calculations can be carried out immediately with use of the programs available within the system.
2. Faster and more efficient programming of new programs, because no programming of input/output is necessary.
3. The machine dependency is greatly reduced by the use of generalized input/output handling.
4. A certain standardization of the programs is achieved. It is hence easier for one programmer to understand a program written by another programmer within the group and it is easier to maintain a survey over all programs available within the system, and to avoid overlapping of, and contradictions between several programmers work.

Further details about the GIPS systems are given in ref.3.

## VI. FEASIBILITY OF COMPUTER CONTROL OF FERTILIZER PLANTS.

One main question discussed very frequently within the fertilizer industry is, if on-line computer control is economically justified at present

We have, at HAILOR TOPSOE, performed an investigation of this question. As a basis for this study we chose, as a typical example, an ammonia plant with a production capacity of 1000 metric tons per day in one stream, based upon natural gas as feedstock, and of the modern type using centrifugal compressors driven by steam turbines.

One thing we especially investigated was the effect of long term variations on the operating performance of such a plant. We assumed, that the most important controlled variables were at the start-up of the plant adjusted to optimal operation. We then calculated how the operating performance at the plant would develop if:

1. The most important controlled variables were kept unchanged at those values, which were the optimal ones just after start-up of the plant.
2. The said controlled variables were adjusted currently to their optimal values calculated by an on-line computer, taking the long term variations (catalyst ageing, heat-exchanger fouling, compressor efficiencies, separator efficiencies, heat losses and gas losses etc.) into account.



The results of this comparison are shown in the table below.

	Per cent of nominal design.	
	Production rate	Relative consumption costs
New plant, optimal operation	105,5	100,0
After 1 year without optimization	101,9	103,0
" " " with "	104,6	102,6
After 2 years without "	98,0	107,0
" " " with "	102,8	105,6

Table I.

The table shows, that after 1 years operation it was, by means of an optimization, possible to increase the production rate with 2,7 % and to decrease the relative consumption costs with 0,4 %.

After 2 years operation the corresponding figures were respectively 4,8 % and 1,4 %.

It might, of course, be possible for clever operators to obtain a part of these improvements by adjusting the controlled variables manually, but there is no doubt, that improvements at least in the order of 1,5 - 2,0 % would, in a typical case, be contributed by using the computer for the optimization.

Furthermore we found, that also other functions of the computer would contribute to improve the operating economy of the plant.

For instance the plant performance evaluation will contribute to ensure, that catalyst exchanges and heat-exchanger cleaning will be performed at the optimal time and with a minimum of down-line of the plant due to improved planning of such operations.

The more advanced monitoring of the plant status, which will be made possible by an on-line computer, will also contribute to reduce the yearly down-time of the plant.

Totally one finds in this study, based upon actual average world market prices of end product, raw products and utilities, the following figures:

	<u>Benefits U.S.\$/year</u>
Increase of production rate: 2,7%	161.000
Decrease of relative production costs: 1,1%	58.000
Decrease of down-time: 70 hours/year	<u>51.000</u>
Total	<u>270.000</u>

Table II.

These tangible benefits should then be balanced against the costs of installing computer control. These are rather difficult to evaluate, because the price range of computer control systems is very large, depending upon how sophisticated systems are chosen.

However, it is found, that a typical average system would to day cost about 350.000 U.S.\$ (including software and engineering), and that the costs per year for such a system, including depreciation, interest, maintenance and operation, would be about 40 - 45% of the total price, thus giving a cost per year of about 150.000 U.S.\$.

Thus it is seen, that the benefits, which could be obtained in such a typical example, will exceed the costs with a very considerable margin.

To this should be added, that this comparison only includes the tangible benefits to be expected. To this one should further add the non-tangible benefits, which are often of considerable importance, when decisions concerning realization of computer control shall be taken.

Further details about this feasibility study are given in ref. 4.

## VII. FUTURE TRENDS, CONCLUSIONS

The future trends concerning the development of the use of digital computers within the fertilizer industry - as well as within other fields - seems mainly to be dominated by two trends.

1. The rapid development, which we have seen during the last 15 years towards cheaper, more efficient and more reliable hardware, still seems to continue and to open up new possibilities for attractive applications of digital computers.

A very interesting feature is the development of small low-cost so-called "mini-computers", by means of which smaller limited tasks can be solved at very low hardware costs. (However, one should not forget, that the mini-computers might in many cases require relatively much programming work, because the available programming systems are less developed than those of the bigger computers).

In the other end of the spectrum one has the development of the big and still more efficient computers, which for inst.

by means of the still more developed use of multi-programming- and time-sharing techniques, can offer a still more attractive ratio between computing power and computing costs.

2. The other trend is the development on the software side towards still more integrated concepts. When talking about the design of fertilizer plants, this trend means a development towards integrating all the various activities: basic process selection and chemical design - basic mechanical design - detailed mechanical design - piping design - instrumentation design - project administration etc., into one common framework, where the use of the computer plays a still more significant role, not least in tying the whole work together, and ensuring a maximum of efficiency and consistency in the work, and that the plant constructed will be really optimal designed.

When talking about operation of fertilizer plants, the trend towards more far reaching integration means, that systems are likely to be realized, which will include as well the direct process-control applications as more administrative tasks, as over-all production planning based upon marketing conditions, inventory control, accounting, planning of maintenance and modification. The core of such more integrated systems would often be an advanced system for management information.

It is likely that such integrated systems will include several computers working together in a so-called "hierarchical" system, which means that the direct on-line tasks might be solved by smaller computers - inst. "mini-computers" - whereas the more general over-all problems might be solved by far bigger computers, and often so, that one single big computer would be used for control and supervision of several plants, thereby ensuring the most economic use of the computer hardware.

One main problem in such complex systems is of course to ensure a satisfactory transmission of the data between the various computers on various levels. This is a field where considerable troubles have been met until now, but where a considerable development also is taking place.

Summing up, there is little doubt, that the development in the use of computers within the fertilizer industry - as within other fields -, which has been so rapid within the last 15 years, will not be less rapid at least within the next 5 - 10 years to follow.

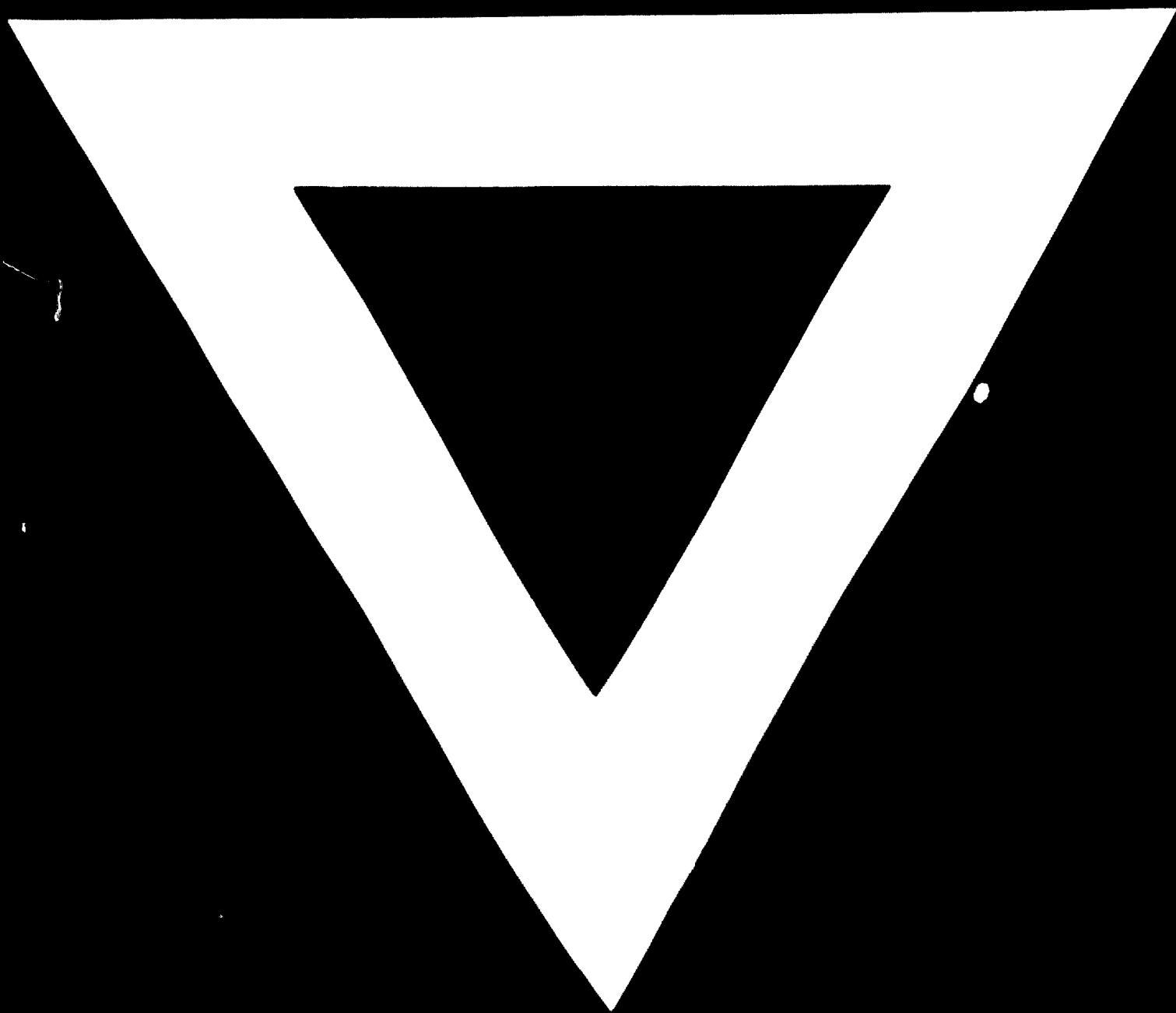
One major problem, which must be solved, is to ensure, that there will be the necessary number of specialists available, who are qualified to solve especially the software-problems involved; these specialists must be able to combine a sufficient knowledge about computer programming with a sufficient knowledge about the technical and economic problems, for which the computers should be used.

So in the years to follow the factor, limiting the speed of development within this field, will not be the capacity of the "electronic brains" as much as that of the human brains.

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