A DIGITAL COMPUTER INSTALLATION FOR CHEMICAL ENGINEERING CALCULATIONS

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PREFACE

Since the publication of my dissertation on converter calculations in 1958 the methods have been programmed for the digital computer GIER. All calculations of ammonia converters carried out in this firm and many related calculations for other reactions are now made on this computer.

The present booklet describes our computer installation and gives some details of interest to people involved in putting up similar computer centers, especially in the chemical engineering field. Other booklets giving our experience in special subjects of this field are being published at the same time:

1. Calculation of Ammonia Converters on an Electronic Digital Computer.
2. Thermodynamic Calculations on an Electronic Digital Computer.
3. A General Calculation Method for Fixed-Bed Catalytic Reactors on a Digital Computer.

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CONTENTS

1. INTRODUCTION

The use of digital computers for chemical engineering calculations raises a number of problems, especially during the period when the installation is built up and the calculation work is gradually transferred from engineers using conventional desk computers and slide rules to the electronic computer with a stored program.

The present booklet describes some of our experience gained during this period of transition.

The computer work started in 1958 using DASK on a hired basis. A new computer, GIER, was bought and installed on the premises in December, 1961. At present, the rewriting of programs from DASK to GIER is nearly finished, and the library of programs for engineering calculations on GIER is increasing steadily.

2. HISTORICAL BACKGROUND

2.1. Manual Calculations.

Before 1958 all engineering calculations in this firm were made by hand using slide rules or desk computing machines. Among the more lengthy of these calculations were:

1. Calculation of ammonia converter performance.
2. Calculation of tubular or autothermal reformers.
3. Calculation of distillation columns.

The author was engaged in calculations of the first type in the period from 1954 to 1958 (see Kjær (1958)). The main part of the calculations is a numerical integration of two or more ordinary, non-linear differential equations. Prior to each calculation a number of thermodynamic data, heat transfer coefficients, etc. must also be evaluated. A typical manual integration takes about 6 hours and gives a single temperature and conversion profile through the converter. Calculation of the optimum profile requires about three profiles. This means that several days are necessary for finding an answer to the expected performance of the converter.

For some converter types the situation is still worse. Boundary conditions are involved in the profiles and 10-20 trials may be necessary before a satisfactory result is obtained.

The use of an automatic electronic computer is highly indicated for calculations of this type and this was actually tried in 1958.

2.2. Use of DASK.

In 1958 the only digital computer of a fairly large size available in this country was DASK. A short description of this computer is given here.

DASK is owned and built by REGNECENTRALEN (Danish Institute for Computing Machinery) a non-profit institute under the Danish Academy of Technical Sciences. It was modelled after the Swedish computer, BESK, in Stockholm but contains many new features. Only one specimen has been built and it was inaugurated in February, 1958.

DASK is of the binary, parallel type. The original version had a ferrite core memory containing 1024 words with 40 binary digits and a magnetic drum with 8192 words. Recently, DASK has also been fitted with a wired core store with 1024 words holding the running system for the ALGOL compiler, a series of magnetic tape stations, and a line printer.

Typical operation speeds for DASK are:

Fixed-point addition:	56	microsec.
Fixed-point multiplication:	360	-
Floating-point multiplication:	1200	-

Floating point operations are programmed as subroutines.

Our use of DASK started in the summer 1958. The author prepared a detailed description of a calculation method for TVA-type ammonia converters, and this proposal was programmed in machine language by Mr. H. J. Aastrup, REGNECENTRALEN. At the same time, another group in this firm, under the direction of Mr. J. H. Hansen and Mr. H. Boeg started programming of distillation column calculations on DASK.

In the period July 1958 to December 1961 a number of technical programs were prepared for DASK and used for routine calculations on a hired basis.

Communication between our firm and the computer center (situated at the opposite end of Copenhagen) was normally by post. In 1959 an automatic typewriter of the Siemens Telex type was installed at our firm and used for preparation of input tapes and writing of results.

A statistical analysis is available for the 8-month period October, 1959 to May, 1960. This is shown in Table 1 below.

Table 1.

Use of DASK, Oct. 1959 - May, 1960

Program	DASK Computer hours					Per cent of time used	Number of calculations	Average computer-time per calculation (hours)
	Oct. Nov.	Dec. Jan.	Febr. Mar.	Apr. May	Total			
Ammonia converters:								
TVA	1.85	1.20	4.00	2.04	9.09	7.6	83	0.11
Quench	0	0	0.19	12.85	13.04	10.9	16	0.82
Fauser	1.36	0.63	0.78	2.67	5.44	4.5	19	0.29
NEC	0.14	0.84	0	0	0.98	0.8	5	0.20
Casale	0	8.33	5.71	6.46	20.50	17.1	27	0.76
Claude	0	0	3.41	0	3.41	2.8	10	0.34
Total of ammonia converters	3.35	11.00	14.09	24.02	52.46	43.77	160	0.33
Other programs:								
General converter	15.17	13.98	5.90	12.82	47.87	40.0	95	0.50
Tubular reformer	0	0	0.72	3.69	4.41	3.7	14	0.32
Distillation	0.80	4.59	2.38	1.50	9.27	7.7	11	0.84
Gasification	0	0	1.71	4.14	5.85	4.9	21	0.28
Total of other programs	15.97	18.57	10.71	22.15	67.40	56.23	141	0.48
Total	19.32	29.57	24.80	46.17	119.86	100.00	301	0.40

2.3. Use of GIER.

The computer GIER was ordered in December, 1959 and installed in our firm in December, 1961. At that time our use of DASK was about 1 hour per day. It was felt that having our own computer would be of great benefit, especially when the engineers using it could have immediate access to the machine. It was also felt that the presence of the computer would have a favorable effect upon those not yet aware of the advantage obtainable from its use. These hopes have been fulfilled to a considerable extent and the computer has been used at a steadily increasing rate.

Table 2 shows the average use of the computer for routine calculations. To this must be added the time for testing of new programs.

Table 3 gives the number of our routine calculations made on both computers until June, 1963.

Table 2.

Use of GIER, January, 1962 - June, 1963.

Period	Average computer time for routine calculations, hours/month
Jan. - March, 1962	6.5
Apr. - June, -	17.2
July - Sept., -	17.1
Oct. - Dec., -	20.5
Jan. - March, 1963	35.9
Apr. - June, -	36.3

Table 3.

Number of Routine Calculations on DASK and GIER.

Period	Computer	Number of Calculations
1958, second half	DASK	20
1959, first -	-	76
1959, second -	-	115
1960, first -	-	314
1960, second -	-	432
1961, first -	-	347
1961, second -	-	291
1962, first -	DASK, GIER	553
1962, second -	- -	866
1963, first -	GIER	1015

3. BASIC FEATURES OF GIER

The computer GIER has been built as the result of a cooperation between the Royal Geodetic Institute and Regnecentralen (Danish Institute for Computing Machinery). The word GIER means Geodetic Institute Electronic Computer, and the prototype was delivered to the Geodetic Institute.

About a dozen copies of the prototype have been manufactured and sold to various firms and institutes in Denmark and abroad.

The logical structure of GIER has been described by Krarup and Svejgaard (1961) and the system and circuit design by Isaksson and Petersen (1961).

3.1. Memory.

The fast memory in GIER is a ferrite core storage with 1024 words each containing 42 bits. Of these 40 are used in normal operations and the two last bits are flag bits used for marking purpose. The computer has built-in floating point operations which interpret the first 10 bits in a word as the 2-exponent and the remaining as the number part.

The slower memory is a magnetic drum with 320 tracks each containing 40 words giving a total of 12800 words. Transfer of one track to or from the drum takes 20 millisec., but it is an essential feature of the computer that normal operations may be carried out simultaneously with the drum transfer, if required. As an example it can be mentioned that calculation of polynomials in several variables and containing many coefficients (several hundreds) may be made with the main part of the coefficients stored permanently on the drum and with transfer of only 40 coefficients at a time simultaneous with calculation using the 40 previous coefficients.

3.2. Command Structure.

A computer word of 42 bits is interpreted either as a full command of 40 bits or two half commands of 20 bits each. One of the remaining bits is used to indicate whether we are dealing with a full command or two half commands, and the other flag bit indicates fixed or floating point operations.

The 20 bits in a half command are used as follows:

Address	10 bits
Basic operation	6 -
Clear accumulator	1 bit
Address is indirect	1 -
Address is relative to actual command	1 -
Address is relative to last subroutine jump	1 -

A full command contains the same 20 bits as above. The remaining 20 bits have the functions:

Counting constant (Automatic address modification)	10 bits
Exchange accumulator and multiplier register	1 bit
Skip next cell	1 -
Direct marking of address	1 -
Indicator part	7 bits

The indicator part is used in connection with a special 10-bit register (the indicator) which is used for storage of information on overflow, sign, zero, and the mark bits. All full commands may be made conditional using the actual situation or the old information stored in the indicator.

The 10-bit address in a command can be used in four different ways:

1. An absolute value in the range from 0 - 1023 (or from - 512 to + 511).
2. A value relative to the actual command.
3. A value relative to the cell from which the last subroutine jump was made.
4. A value relative to the index register. Only one index register is available.

In full commands the value of the counting constant will be added to the core before the command is executed. This gives a fast address modification of special value in connection with matrix operations, polynomial calculations, etc. The last element in a row or a column is normally indicated by means of the flag bits.

3.3. Speed.

Typical operation speeds for GIER are:

	Fixed-point	Floating-point
Addition	50 microsec.	115 microsec.
Multiplication	180 -	165 -
Division	270 -	220 -

Transfer of a block of 40 cells to or from the drum takes 20 millisec., but other operations may be carried out simultaneously with the transfer (but slowed down about 1 millisec. in all).

Use of the counting constant for automatic address modification increases the operation time for a single command with about 9 microsec.

4. PROGRAMMING LANGUAGE

The programming language is a very important factor for the utilization of an electronic computer. We have tried programming in machine language, i.e. a language which specifies directly the commands in each cell of the program, but in recent time we have also started using the ALGOL compiler available to users of the computer.

4.1. Machine Language.

A package of auxiliary programs has been prepared by REGNECENTRALEN for programmers using machine language. Among these programs is a command input program with symbolic addresses. The computer has recently been fitted with an interrupt feature which permits stopping the computer and writing out the contents of the memory.

When the computer was delivered to us in December, 1961, the symbolic input program and the control output program were not available, at least not in their final form. We, therefore, made our own package of input and output programs, largely modelled after the experience gained in the use of DASK, but also containing some new features making it easier to use the computer for a large number of routine calculations. This package of standard input and output programs has been described elsewhere (Kjær (1963)). A short description is given in the following sections.

4.1.1. Core and Drum Layout. The core memory with 1024 cells has been laid out as follows:

Cells 0- 39:	Entries to standard routines, permanent constants, etc.
Cells 40- 799:	Available to the programmer.
Cells 800- 999:	Reserved for input and output routines. When these are not used, the programmer may also use these cells.

Cells 1000-1023:	Storage of secondary information: date, calculation number, page number, line counter, etc.

Layout of the 320 drum tracks is:

Tracks 0- 31:	Storage of standard routines.
Track 32:	Not used.
Tracks 33- 39:	Used by control output for storage of core cells 720-999.
Tracks 40-316:	Available to the programmer.
Tracks 317-319:	Used by cover page routine.

Tracks 0-31 are normally locked to prevent writing here.

4.1.2. Input. The input routine recognizes 6 types of information as read from an 8-channel paper tape:

1. Numbers. These are normally assumed to be floating point numbers. A special action character on the tape will cause them to be interpreted as fixed point numbers.
2. Integer groups. A group of four integers filling one cell (10 bits each).
3. Sedecimal words. 10 digits or letters a-f also filling one cell (4 bits each).
4. Text strings. These are packed with 7 characters per cell (6 bits each).
5. Commands.
6. Action characters. Used for: end of information, change of input address, stop, etc.

4.1.3. Output. The output routine will punch 3 types of data on an 8-channel paper tape:

1. Numbers. These may be floating point numbers, fixed point numbers, or integers with unit in bit 39. A layout giving the integer digits, decimal digits, and significant digits must be specified as well as certain other information.
2. Text strings.
3. Lines. A special routine is available which punches one or more characters giving carriage return and new line and counting the number of lines per page (see below).

4.1.4. Report Editing. Three cells in the core memory are reserved for storage of day, month, and year. They are corrected by the operator every morning. Output from all programs is normally coded to start with a cover page, i.e. a page giving date, file number, calculation number, name of the program, and a variable text explaining the contents of the output. The rest of the output report is divided into pages so that it can be written out on automatic typewriters (Flexowriters) fitted with pin feed and four layers of paper and carbon in endless sheets. Printing of page shift operates automatically when the corresponding output routine is used.

In a computer installation where the programs have been prepared by a small group of programmers, but are used by many other people, it is very important that the output report from a calculation gives a clear picture of the result. We always secure that all input material used in the calculation must be printed again in the output report. This is not only to control that the computer has used the correct figures but also in order to have input and output material together in convenient form in a single report.

It is often necessary to repeat a calculation with the same input data except for a few changes. If the second calculation is made immediately after the first they may be contained in the same output report as Section 1 and Section 2. In the last section we then print only those input data which are different from the material in section 1. This gives a considerable saving in paper and makes the report easier to study.

4.1.5. Control Output. When new programs are tested, it is often necessary to write out the contents of part of the memory. A special routine is available for this purpose permitting output as numbers or as commands. The output is obtained as a continuation of a normal output and contains page shift.

4.2. ALGOL.

4.2.1. ALGOL Compiler. The programming language ALGOL is very useful for technical and scientific calculations. It has been described by Backus et al. (1960, 1963), Dijkstra (1962), and others.

An ALGOL compiler for GIER has been prepared by Naur and coworkers, see Naur (1963). A preliminary version of the compiler was made available to us in September, 1962. It could not handle data stored on the drum and was therefore not used very much. The final version of the compiler was delivered in February, 1963. Since then, nearly all new programs have been written in ALGOL and we have obtained a considerable saving in programming time and testing time.

Rough estimates show, that the size of ALGOL programs is about the double of programs written in machine language. Similarly, their speed may be reduced with a factor 2. This may vary considerably from one program to another.

Programming in machine language is still used in very few cases, especially for programs of a non-numerical nature (e.g. handling and analysis of text strings) or if space requirements or speed makes the use of ALGOL less attractive.

4.2.2. Handling of Arrays. The GIER ALGOL compiler contains special procedures for transfer of arrays (i.e. vectors, matrices, etc.) from the drum to the core and back. This is a necessity because of the small size of the core memory.

4.2.3. Changes in Compiler. We have made a few changes in the compiler in order to have the same conventions for the use of machine language programs and ALGOL programs:

1. A special ALGOL procedure is used for printing the date on the cover page.
2. The character: SPACE has been made a terminator for input numbers.
3. A special version of the compiler is available which will handle very large programs.

5. AUXILIARY EQUIPMENT

5.1. Tape Reader.

The computer is fitted with a FACIT high speed paper tape reader for 500 characters per second. Input is in the 8-channel Flexowriter code with one hole used for parity check and another hole for the single character: carriage return. The remaining 6 holes give 64 combinations in lower case and 64 in upper case. Capital and small letters are used and the list of characters contains the symbols necessary for writing of ALGOL programs.

The tape reader is of the dielectric type and has worked satisfactorily. The reader is easily converted to input of 5-channel tape.

5.2. Punch.

Normal output from the machine is on a FACIT high speed paper tape punch giving 150 characters per second. Output is in the 8-channel Flexowriter code.

This device has worked quite satisfactorily, but some troubles have been met in obtaining a constant spacing of the characters punched, especially in intermittent use. The Flexowriters used for writing out of the output are quite sensitive to small variations in the spacing. The mechanical device feeding the punch with paper tape has also caused troubles.

5.3. Typewriter.

An IBM typewriter is constantly connected to the computer and is used for special purpose input and output. It is not used in routine programs made in machine language. In ALGOL routine programs it writes the message: ready and finished.

The ALGOL compiler uses the typewriter for output of messages with the syntactic and other formal errors detected during the translation.

In testing of machine language programs the typewriter is used for control output.

5.4. Flexowriters.

Three Flexowriters are at present in use in our computer installation. They are not connected to the computer. Normal use is for preparation of input data tapes and writing out of output reports. New programs are also prepared on the Flexowriters.

The performance of the Flexowriters has sometimes been not quite satisfactory with frequent loss of time for repair.

The probability that at least one of the three Flexowriters is out of service due to repair is about 22 per cent.

5.5. Optional Equipment.

Some of the other GIER installations have special equipment. If required, this could be added to our installation. These items are:

A magnetic tape station. This will increase the memory with a factor of about 100.

A line printer printing 10 lines per second instead of 10 characters per second on the flexowriters.

Two further magnetic drums increasing the memory by a factor of 3.

6. OPERATING AND PROGRAMMING STAFF

6.1. Operators.

At present the installation is attended by two operators and two typists. They receive the filled out input specification sheets from the engineering staff. The input is typed on the Flexowriters, verified, and run on the computer. Output is written out on the Flexowriters and delivered back to the engineers.

As long as the daily use of the computer is about 1-2 hours for routine calculations and about the same amount for program testing, this staff of operators and typists should be sufficient for running the installation. Further staff may be required at a later time if more calculations are carried out on the computer. On the other hand, there is a trend in the programs to become more complicated and more powerful so that the same computer time gives increasingly more useful information. It is, therefore, not absolutely certain that an increase in the staff will become necessary.

The operators also carry out a certain amount of programming, especially for programs not involving technical knowledge, or for programs where the technical knowledge has been submitted by other persons, not being able to program themselves.

6.2. Programmers.

Most of the programs available in our installation at present have been made by the author. Two or three other engineers have programmed on a part time basis. Many of these programs are rather complicated and contain a number of standard subroutines, often giving a complete calculation of one type chemical equipment.

Use of the computer for small ad hoc programs prepared by the user himself has not been very popular, but may become so when the knowledge of ALGOL becomes more widespread.

7. COMPUTER RELIABILITY

The operators check the performance of the computer every morning by means of a special test program run at marginal values of the voltages in the computer. No other check on the electronic equipment is made by us. This means, that whenever a fault is observed in the computer, some time will elapse before the maintenance staff from REGNECENTRALEN gets a notice and can come to the site and find the fault. Table 4 below shows the number of hours lost due to machine failure in the first 17 months.

Table 4.

Computer Faults, January 1962, June 1963

Month	Hours lost due to fault in	
	Computer	Punch and Typewriter
1962, 1	21.8	7.6
- , 2	9.9	2.9
- , 3	14.2	0
- , 4	1.4	4.7
- , 5	0	0
- , 6	12.0	2.8
- , 7	12.4	0
- , 8	34.4	2.5
- , 9	0	0.7
- , 10	0.4	0
- , 11	1.0	2.7
- , 12	0	0.6
1963, 1	8.8	0
- , 2	7.5	0
- , 3	11.1	0
- , 4	1.0	0.1
- , 5	7.5	0.3
Total	143.4 hours	24.9 hours
Per cent loss	4.3	0.7

8. SURVEY OF PROGRAMS

A short summary of the programs now in actual use at our installation is given below.

8.1. Ammonia Converter Programs.

These programs calculate the expected performance of ammonia converters of different types. A special booklet is in preparation containing further details about these programs.

The converter types are:

1. TVA-converters. Counter-current cooling in the catalyst bed.
2. NEC-converters. Con-current cooling in the catalyst bed.
3. Casale-converters.
4. Quench-converters.
5. Fauser-Montecatini-converters.
6. Claude-converters (available for DASK only).
7. A general type ammonia converter. The heat exchange terms must be specified by the user.

Minor programs are also available for calculation of separate heat exchangers with ammonia synthesis gas and for calculation of the ammonia equilibrium yield.

8.2. Ammonia Loop Programs.

These programs calculate heat and material balances for ammonia loops with a given production in the converter. They have been made by Mr. J. Saietz.

8.3. Distillation and Absorption Programs.

A general type program for plate-to-plate calculations of distillation columns is available (for DASK only). Minor programs for calculation of ethyl alcohol fractionation, sulfuric acid absorption, etc. are available for GIER.

8.4. General Converter Programs.

These programs perform a numerical integration of the conversion and temperature distribution in a fixed bed catalytic reactor of a general type. A maximum of 16 simultaneous reactions may be used in the programs. The reaction rate constants and the heat exchange terms are input to the programs.

One of these programs also performs an automatic correction for the diffusion restriction in the catalyst particles by a numerical integration of the reaction rate expression and the heat flow inside the particles.

The programs will be described in a special booklet.

8.5. Mathematical Programs.

Typical examples are solution of linear equations and curve fitting for functions of several variables by means of orthogonal polynomials.

8.6. Reformer Programs.

This group comprises a program for heat and material balance for the Topsøe-SBA reforming process and a program for kinetic calculation of a tubular reformer.

8.7. Tape Handling Programs.

A tape correction program is used many times a day in our installation. It first reads a small tape with the corrections and then repunches the error containing tape with simultaneous insertion of the corrections. The present booklet has also been treated on this program.

8.8. Thermodynamic Programs.

A special booklet is in preparation describing some of the formulas used for calculation of thermodynamic properties. Fourth-order polynomials are used for the calculation of enthalpies of formation of ideal gas mixtures.

8.9. Zone Refining Programs.

These programs simulate the zone refining of silicon rods. They have been made by Mr. J. Saietz.

8.10. Demonstration Programs.

These programs are used when the installation is shown to visitors. Among the programs are:

A program which generates up to 28 linear equations in 28 unknowns and solves them. There is no visible output from the program, but the solution can be followed on the loud-speaker which is connected to the sign bit of the result register. Solution time for 28 equations is about 4 seconds.

A program which plays the game: NIM with the visitors. Input and output is via the typewriter and the computer announces whether the visitor has or has not a chance of winning the game. If the visitor looses his chance by making a wrong move this will also be announced by the computer.

A program playing various types of random music.

A program for calculation of prime numbers (by simple division).

Other programs are available which calculate numbers with many digits. Calculation of e = 2.718...... with 2500 digits takes 13.5 min. and pi = 3.1415...... with 2500 digits takes 41 min. The largest number calculated on this computer is the number: $2\uparrow(2\uparrow17)$ which is 2 raised to the power of 2 in the power of 17. It contains 39457 decimal digits. Calculation time is 3 hours starting from unity or 2 hours starting from $2\uparrow(2\uparrow16)$. Another program in this series calculates the number of alcohol isomers for alcohols with N carbon atoms. It has been run up to N = 100. At this point the numbers contain 42 decimal digits.

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