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Department of Energy Technology. Annual Progress Report. 1 January - 31 December 1986

Forskningscenter Risø, Roskilde; List, F.

Publication date:
1987

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):
Micheelsen, B., & List, F. (Eds.) (1987). Department of Energy Technology. Annual Progress Report. 1 January - 31 December 1986. (Denmark. Forskningscenter Risoe. Risoe-R; No. 543).

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Department of Energy Technology Annual Progress Report 1 January - 31 December 1986

B. Micheelsen and F. List

Risø-R-543

DEPARTMENT OF ENERGY TECHNOLOGY
ANNUAL PROGRESS REPORT
1 January - 31 December 1986

edited by
B. Micheelsen and F. List

Abstract. The general development of the Department of Energy
Technology at Risø during 1986 is presented, and the activities
within the major subject fields are described in some detail.
Lists of staff and publications are included.

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CONTENTS

1. DEVELOPMENT DURING 1986

1.1. The Department of Energy Technology

The change from nuclear reactor technology towards non-nuclear energy technologies was continued during the year 1986. The Chernobyl accident in the spring 86 gave rise to many activities at Risø and in Denmark, but the work consisted of measurements of fall-out, mitigatory measures, and actions of the authorities, and these activities affected the Energy Technology Department only slightly.

The department still maintains a research and development effort in reactor physics, because this subject field is seen as fundamental to a general understanding of reactor technology, and it is also the basis for reactor physical services for the two research reactors and the fuel work at Risø National Laboratory. Furthermore, the department maintains the educational activity for universities and high schools at the Danish reactor no. 1. At present approximately 13% of the staff of the department are working in these nuclear activities.

The main effort of the Section of Reactor Physics is now simulation of dynamic processes; for that reason it changed its name during the year to the Section of Process Simulation.

The major effort in the Section of Heat Transfer and Combustion was the building and running in of the 2 MW circulating fluid bed. This was used intensively for experiments in the second half of the year.

The differences in salary between industry and state-financed research institutes are today significant for the younger academic and computer staffs. During 1985 the Section of Reactor Physics had an exchange of approximately 30% of the personnel, and this percentage continued in the following year in

the Section of Heat Transfer and Combustion. These exchanges have given problems for competing assignments, and this year especially the completion of the 2 MW circulating fluid bed, and the round the clock shift work for the experiments in the fluid bed, put a heavy burden on the remaining experienced staff.

1.2. Section of Process Simulation

The research and development work of the Section of Process Simulation deals with the modelling of the physics of processes, which can be both static and dynamic. The main areas are now:

- simulation of dynamic processes in industrial plants
- ecological models
- reactor physics

The research within process simulation has the purpose of developing tools that will facilitate the simulation of dynamic processes in industrial plants. The research has been carried out along two lines: Firstly, a software package has been developed that enables the use of a library of submodules, each representing a standard component of an industrial plant (e.g. pumps, valves, etc.). This package now exists both in PC and mainframe versions. Secondly, studies were made to assess the use of AI-techniques in process simulation. Thus, a very simplified model of a power plant was constructed in the object-oriented language Smalltalk. This was done to investigate the advantages obtained by using Smalltalk for constructing user-interfaces for simulators.

As a new activity within process simulation the section is now participating in an ESPRIT project. This involves both the development of a conventionel simulation model of a power plant and a model based on the Multi-level Flow formalism. The latter model creates the data base to be used by an expert system for fault diagnosis in the power plant.

The work on ecological models is centered on the development of the ECCES model system. ECCES contains modules for dispersion of pollutants in the atmosphere, deposition, soil chemistry, and uptake of pollutants in plants. The work during the past year has heen focussed on verification of the soil chemistry model. However, due to changes in staff the work has not progressed entirely as planned. Development of a model for a forest soil system has been delayed and is expected to be carried out in the near future. A cooperation is now established with the National Agency of Environmental Protection, the Air Pollution Laboratory, and the Danish Forest Experiment Station, which jointly carry out measurements of soil chemistry parameters on forest soils, and the model development can now proceed in close connection with the experimental work.

Since verification of models is very important, contacts to experimental groups in other countries have also been established. As a consequence of this a proposal for a joint project between Risø and the Institute of Terrestrial Ecology, UK, has been submitted to the EEC Environmental Protection Programme.

In reactor physics the major development has been the completion of the LWR assembly code LEWARD. LEWARD is based on a number of existing codes which have been combined to a programme complex, which is easy to use. Another activity has been studies in connection with the research reactor DR 3.

The section has participated in the German DEMONA project, which is an experiment concerned with the behaviour of radioactive aerosols in a reactor containment after a large coremelt accident. This work was completed during the past year. The section has also participated in the AKTI programme financed by the Nordic countries. This programme also deals with consequences of reactor accidents. Due to the decreased interest in nuclear power it has now been decided to reduce the activities in the area of reactor accidents and aerosol physics to a very limited participation in the Nordic AKTI programme.

1.3. Heat Transfer and Combustion

Coal combustion and implementation of measurement techniques for combustion and environmental problems have formed the main part of the work during the year.

A 2 MW circulating fluidized bed was built during the first half of the year. The second half of the year has been devoted to an extensive test programme in the fluid bed, performed in close co-operation with the Danish Boiler Manufacturer: Aalborg Boiler.

A laboratory for fundamental combustion research was initiated in 1985, and it is now being built up. A test facility for measurement of single particle combustion parameters has been built, and it is now in the shakedown phase. Furthermore, development of a Laser Doppler system and a TV-Microscope system for measurements of particle velocity and size was pursued.

In the theoretical field two projects on computer modelling of flow phenomena are continuing. In the first a steady-state 3-dimensional turbulent gas-particle flow in a combustion chamber is modelled. The model for the gas flow alone is now in the main part finished. In the second project a computer model has been developed for transient two-phase oil-gas flow in a pipeline. Comparisons between the computer model and experimental data from full-scale operating pipelines have been performed.

The temperature calibration laboratory has calibrated thermometers for both internal and external customers during the year. The amount of work has increased compared to last year.

1.4. Reservoir Group

The development of a 3-dimensional, fully compositional, double permeability reservoir simulator, COSI, has been continued. Code validation has also continued on a number of test examples, using the simulator's black-oil and volatile-oil options, with

good results. The inclusion of the fully compositional routines are nearly completed and improved input- and output routines are under development.

A new computer code for the generation of input for simulators based on mapping of geological data has been developed.

The volatile-oil simulator, ECLIPSE, was used for comparisons with the above-mentioned COSI-code and for further studies of the GORM-field. The simulation study of the TYRA-field, was concluded during the year.

With a view to improved exploration efficiency a project on the modelling of sedimentary basins was funded by the Danish Ministry of Energy. The project involves the Geological Survey of Denmark, the Geological Survey of Greenland, Risø and a number of university institutes. Risø and the Technical University of Denmark are developing a simulator which models the development of a sedimentary basin (sedimentation, erosion and compaction), the temperature history and maturation of source rocks, and the migration and accumulation of hydrocarbons.

The group has continued its participation in the Danish aquifer heat storage project.

1.5. Danish Reactor DR 1

The reactor has been used for educational purposes only. A number of students from technical universities in Denmark and Sweden have carried out experiments at the reactor over periods varying from 2-8 days, and 48 high school classes have carried out one-day experiments.

The reactor has been in operation for almost 30 years. Core samples from the fuel solution have been taken yearly in order to follow the corrosion of the core tank made of stainless steel. Although the content of chromium and nickel has increa-

sed slowly during the years the corrosion is considered to be negligible. Since the reactor has been operated at power levels less than 2 kW, new fuel has never been added to the core.

2. ACTIVITIES OF THE DEPARTMENT

2.1. Esprit Project 96

The Esprit Project 96 is concerned with the development of an Expert System Builder, ESB, which is a tool for use in design of expert systems. This includes creation of general Knowledge Systems (KSs) which may be reused, e.g. KSs containing different fault diagnostic strategies created by a domain expert. The building process also includes facilities for a model editor to help create a model of the actual system from which knowledge about the system may be derived for the KS. The overall idea is to customize ESB elements by filling in knowledge in "shells" which are created at lower layers in the ESB.

To test the means and methods developed in the ESB four prototype sample expert systems (SES) shall be built. The chosen domain is the diagnosis of technical systems (electronic circuits and power plants).

The Energy Technology Department is involved in this work, as subcontractor to the firm Søren T. Lyngsø. One part of the work is to develop a simplified dynamic simulation model of a power plant. Another part is to document and develop a knowledge base for this power plant to be used in fault diagnosis in the simplified power plant.

The power plant is shown in Fig. 1 and consists of a boiler providing superheated steam. Heat for this is supplied by burning
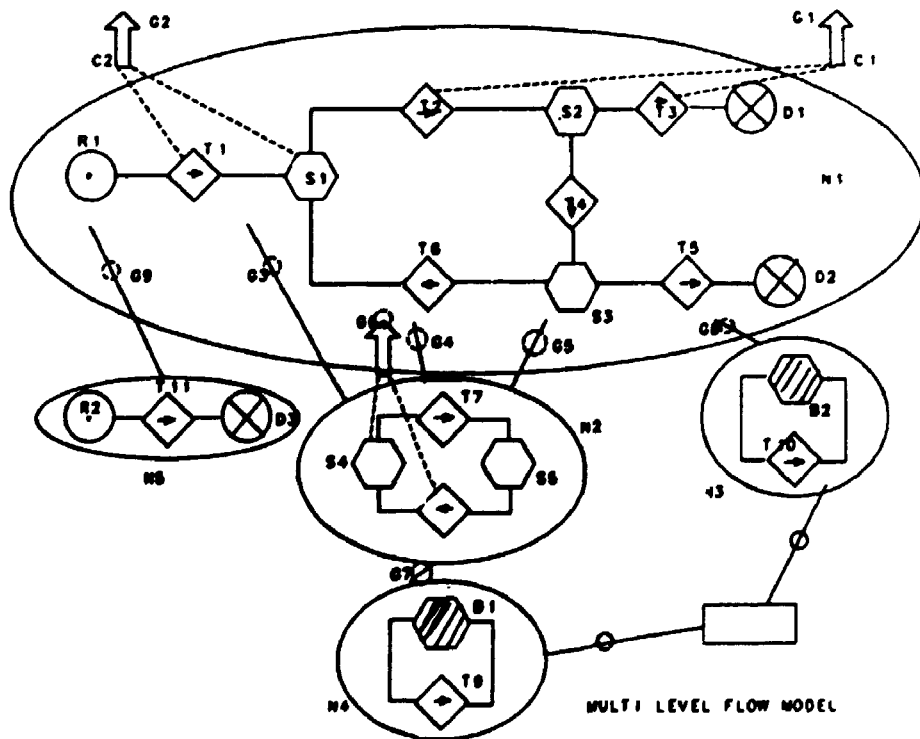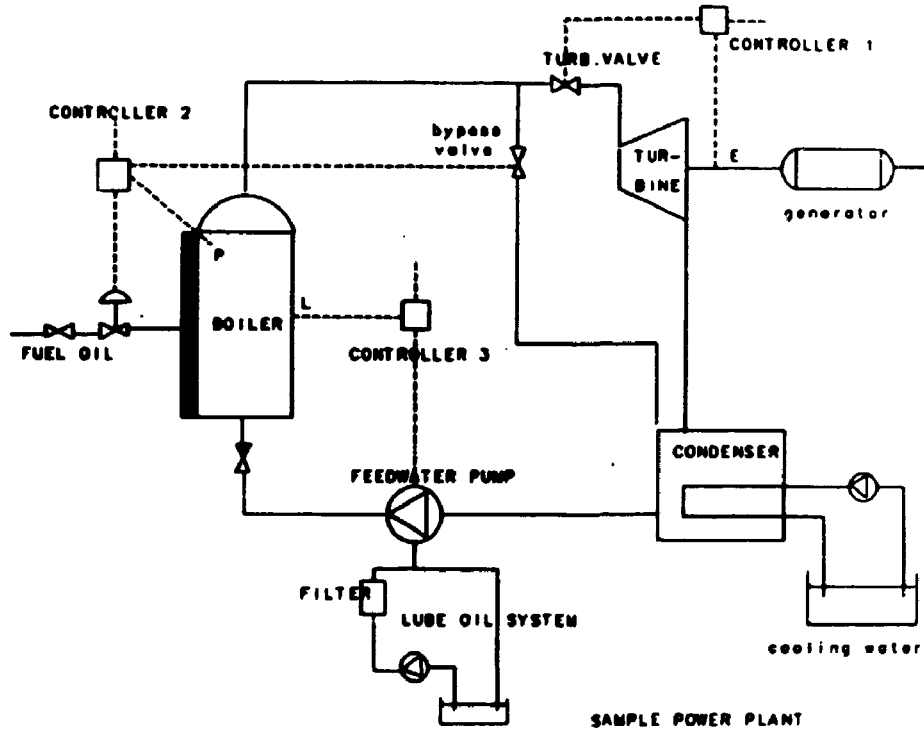
Fig. 1. Esprit model

oil. Steam flow drives a turbine, converting part of the thermal power into mechanical power. The rest of the thermal power is removed by condensing steam. Feedwater is returned to the boiler by a pump. The pump is driven by a motor, lubricated from a lubrication oil circuit. In order to adjust the electrical power produced, steam can be by-passed directly to the condenser, thereby reducing the turbine power.

The model has three controllers: electrical power is controlled by adjusting the turbine valve, pressure is controlled by the supply of oil to the burners, and water level by the speed of the feedwater pump.

It is possible to introduce disturbances or faults in various parts of the model. The expert system communicates with the model through relevant plant parameters assumed to be measured by sensors in the plant giving information about the actual state of the system.

The model is written as a single module to be connected to the general modular simulation system DYSIM.

The model in which the expert knowledge of the power plant is contained in the expert system in order to diagnose faults is a Multilevel Flow Model (LIND, 1984). The basic aim of the MFM methodology is to express in a formal way both the process plant design and the goals for the control system. The formalism describes mass- and energy flow structures, goals and functions of the plant. On the basis of this information a knowledge base is developed.

J.L. Paulsen, N. Larsen

REFERENCE

LIND, M. (1984). Multilevel Flow Modelling of Process Plant for Diagnosis and Control. Risø-M-2357. (Roskilde, Denmark) 26p.

2.2. Implementation of a Small Simulation Model in Smalltalk

In order to evaluate different computer languages for use in simulation, a Tektronix 4404 (later upgraded to a 4405) work-station was purchased. This workstation gives access to the following languages: Fortran, C, Smalltalk, Common Lisp and Prolog. Presently the first 4 languages are available. A small simulation model has been implemented in Fortran, Smalltalk and C. The model is similar to the Esprit project sample power plant. The model exists in Fortran and is running on IBM-com-patible PCs.

Smalltalk is an object-oriented language. This means that generic descriptions of components can be used to describe the same type of components in the model, but with different physical charac-teristics. The Smalltalk language has an easy way to make an in-terface to a model.

The programming of the model started by writing a generic description of a component. In Smalltalk this is called creating a class. The generic description of the actual components was then made as subclasses to the component class. This has the advantage that if there is something all components should be able to do, then the subclasses of components will know how to do this (e.g. all the actual components in the power plant simulator know how to per-form a Runge-Cutta integration based on their own state variab-les).

Smalltalk has facilities for window management and pop-up menues. This has been used for building a user interface. Different pop-up menues can be allocated to different windows, and the choice in one menu can give access to other menues, so that the whole model is run by selecting appropriate menu items with the mouse-buttons, and typing (if necessary) input values from the key-board.

Smalltalk seems to be an ideal language for process simulation as libraries of components can be built and used in different

applications. The problem with Smalltalk is the computational speed for numerical calculations, which are performed in process simulation. In order to assess this problem, the same model was programmed in Fortran and C, the latter having a structure similar to Fortran. The computing time was 10 times shorter in these cases.

Smalltalk is both a programming language and a programming environment. A Smalltalk programmer gets a lot of help from the Smalltalk system. An experienced programmer may quickly develop applications in Smalltalk.

In addition object-oriented languages like Smalltalk lead the programmer to a new way of looking at his processes (maybe a more natural way) which could give a better understanding of how to model the process. The main drawback is the execution speed for numerical calculations.

<div align="right">S. Weber</div>

2.3. Precompiler System for Programming Models in Continuous Simulation

DYSIM 86 is part of a programme system for dynamic simulation of process plants. It is based on a modular concept. In connection with this a simulation tool consisting of two precompilers has been developed. In the precompiler system the modular approach of DYSIM 86 is extended with another level of modularity. The precompiler system produces a FORTRAN 77 code that is compiled and linked to DYSIM 86.

At the first level of this modular approach the precompiler constructs modules, which are programmes modelling a section of a plan. In the module the user can implement models of components by calling submodels from a library. If a library is to be used it must be compiled by the precompiler system.

At the second level of modularity the modules are connected to each other in order to form a model for the entire plant, and they are connected to the run time executive programme. The user defines the connections by writing a source code in a simple syntax. It was not intended to make a simulation language because the elements of standard FORTRAN 77 should be available. The syntax is merely an extension with a few commands.

At run time the executive programme uses a list file with information about the variables used in the modules. The necessary information in the list file is made by the precompiler system. In this way the user always knows that any changes in the module are also made in the list file. Some additional information can be written in the list file using an auxiliary programme.

If the precompiler system identifies an error in syntax in any of the source files it will be indicated. Some kinds of errors can be interactively corrected using the precompiler system directly.

Figure 2 illustrates how the precompiler system uses and produces files.

J. Kofoed

2.4. LEWARD, a Reactor Physics Code for an LWR Fuel Assembly

The LEWARD programme is an LWR fuel assembly code in FORTRAN 77 for neutron and gamma distribution calculations. It unifies a number of existing separate programmes developed at Risø over the years. These programmes were written in ALGOL, and although ALGOL is an excellent computer language, it suffers from the drawback that few other institutions or utilities use it.

It was therefore decided to rewrite some of our basic Reactor Physics programmes in F77, and on the same occasion make them easier to use. The result became the new LEWARD programme which
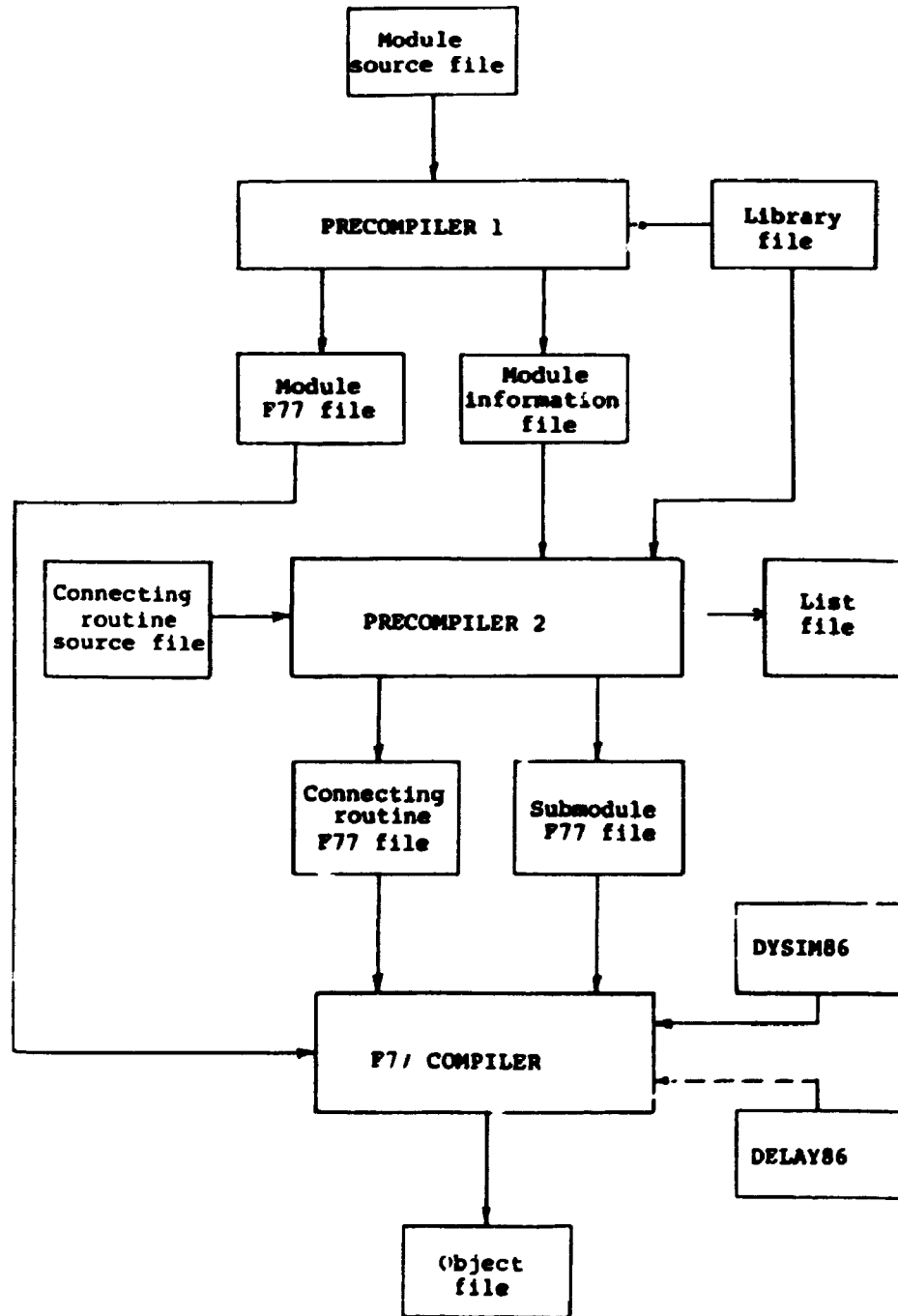
Fig. 2. The precompiler system

is tailored for LWR fuel assembly calculations with a very short
and easily memorized input setup.

LEWARD combined with another programme, NOTAM, (also F77) which
makes whole core neutronic-hydraulic calculations, constitutes
an efficient, easily used BWR core simulator, which is at pre-
sent being tested against the careful measurements reported for
the QUAD CITY reactor.

C.F. Højerup

2.5. Aerosol Physics

In the Nordic AKTI project the phenomena taking place inside
the reactor building in case of a nuclear accident are studied.

In 1986 AKTI was invited to participate in an aerosol physics
code comparison exercise organized by the EEC.

The data for this exercise were supplied from one of the Ger-
man-Swiss DEMONA experiments B3, performed at the model con-
tainment of the Battelle Institut GmbH in Frankfurt.

In the experiment the behaviour in a reactor containment build-
ing of melted fuel, melted structural materials and fission
products was simulated using non-radioactive tin oxide aero-
sols. The injection time was about 45 minutes and the maximum
density obtained was roughly 10 g/m^3 (range of vision below
1 m). After 5 or 6 hours 99.9% of the aerosol material had
settled onto floor and walls under the influence of gravita-
tion and diffusion as shown by the experimental data points.
The significance of this is based on two observations (a) a
reactor containment will remain intact for several days, and
(b) only the fission products suspended in the containment
atmosphere can be released to the environment in case of con-
tainment failure.

The curve in Fig. 3 was calculated with the NAUA code from KfK (Bunz et al., 1983). The data points are reproduced within a factor of 3 to the conservative side, which is satisfactory taking into consideration the complexity of the problem (especially the thermohydraulics).

Most of the other groups taking part in the exercise also used versions of the NAUA code, but a number of other codes were used as well. The results of the exercise will be published in the spring of 1987.
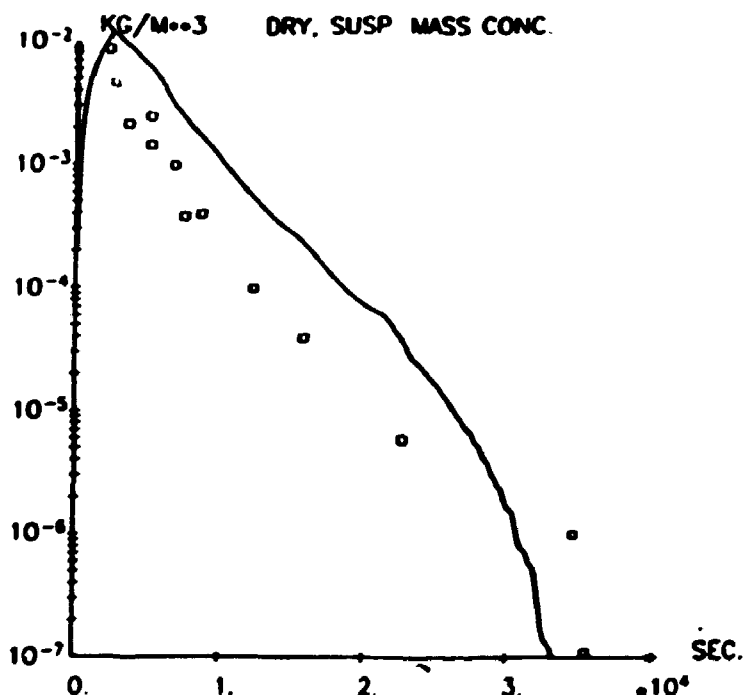
K. Lauridsen, P.B. Fynbo

Fig. 3. Post-test calculation of the DEMONA-B3 experiment. The decrease of the mass density of the tin oxide aerosol was calculated with NAUA and compared with experimental data.

REFERENCE

BUNZ, H., KOYRO, M. and SCHOCK, W. (1983). NAUA Mod 4. A Code for Calculating Aerosol Behaviour in LWR Core Melt Accidents. KfK-3554. 66p.

2.6. Model for the Environmental Impacts of Energy Production

The present version of the program system ECCES/4/2 is able to pred ' environmental impacts of a given energy production scena...o in a given geographical area. In order to illustrate the capacity of the model, scenario simulations have been run (CHRISTENSEN et al. 1985, BRODERSEN et al. 1986). These model runs demonstrated long-term effects of power plant SO_2-emissions on topsoil chemistry and crop-uptake of heavy metals. This further indicated that the key module in the program system was the soil chemistry module.

The soil chemistry module (BRODERSEN, 1984) calculates, on a quasi-equilibrium basis, the chemical changes in soil water and soil matrix upon an input from the atmosphere. In order to validate this module laboratory experiments were performed in which soil samples were extracted with acid rain. The experimental results were simulated by ECCES/VERSION/4/1 (MORTENSEN, 1985; BRODERSEN et al., 1987). Significant discrepancies between model and experimental results necessitated modifications of the soil chemistry module. A major change was the abandoning of starting soil pH as input data for calcareous soils. Alternatively a starting Ca^{++} concentration is now required as input. An example of the experimental and the model results is shown in Fig. 4.

Summarizing, the soil extraction experiments have indicated that: a) pH is simulated fairly accurately, b) Ca is simulated adequately, although dissolution of lime actually appears to occur at a lower rate than simulated, and c) K and Na and especially Mg are only simulated moderately well. In order to improve the model for the former elements it seems imperative to include weathering of soil minerals into the soil chemistry module before this can be used for long-term predictive calculations.

As the soil temperature in the field is subject to significant changes with the season and with depth it can be inferred that chemical equilibrium constants may be affected in a similar way. In ECCES/VERSION/5/1 all equilibrium constants are made

dependent on the soil temperature. Thermodynamic constants are calculated in a special sub-module from "Laurant-expressions". The thermodynamic data was obtained from SKYTTE-JENSEN et al. (1985). Soil temperature input data are incorporated in the standard meteorological data file and was obtained from KRISTENSEN, (1959). An example of the influence of the soil temperature is shown in Fig. 5. In conclusion it can be said that the annual temperature oscillation mostly affects the dissolution of atmospheric CO_2 causing a significant annual oscillation in the HCO_3-concentration. This develops into minor oscillations in the concentration of other ions. On a yearly average basis, however, the temperature oscillation has only slight importance.
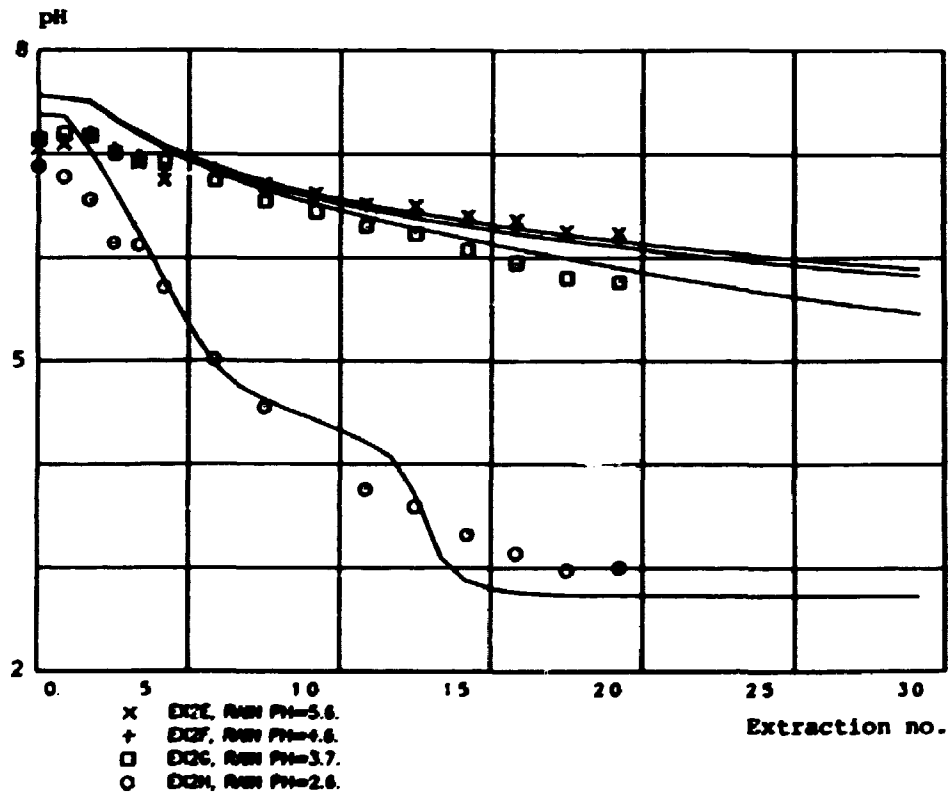
B. Richter Larsen

Fig. 4. The development in soil water pH during 30 consecutive extractions of 5 g soil with 25 ml simulated rain of varying pH.

Points: experimental values. Lines: computer simulation

- 21 -
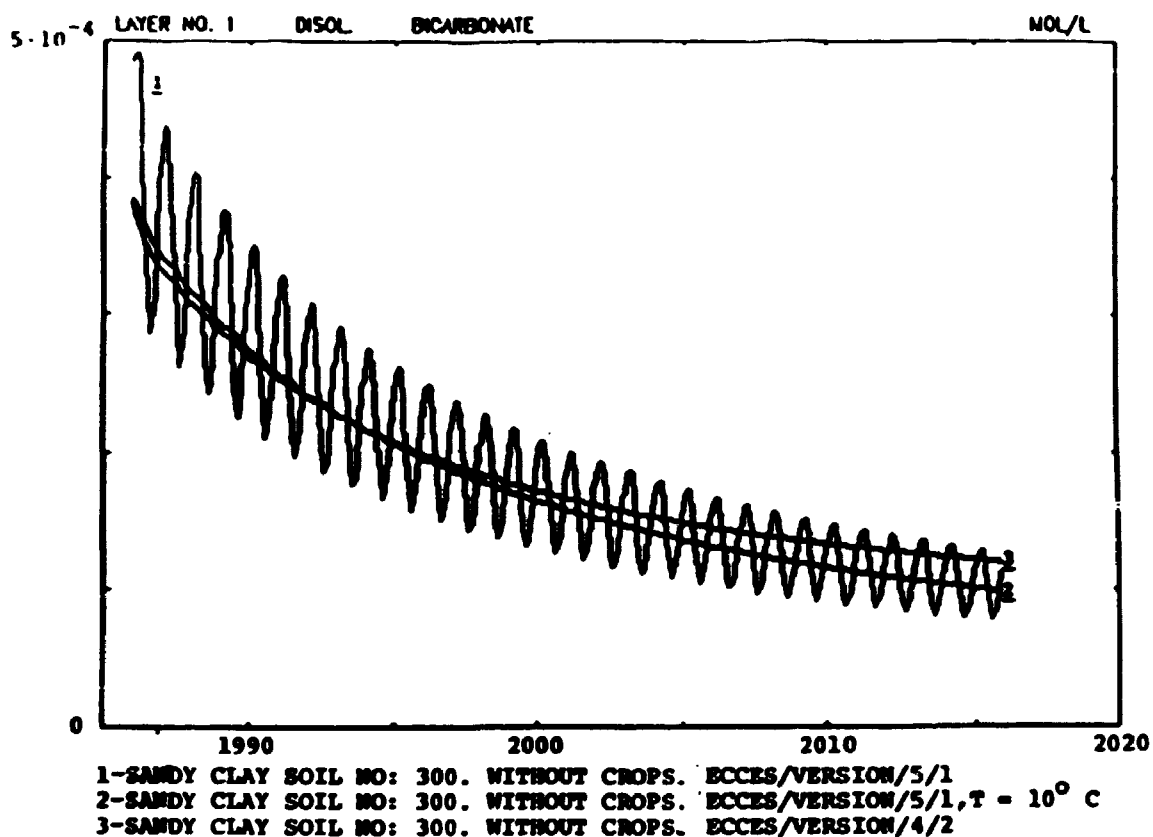
Fig. 5. The development in soil water HCO_3-concentration during
30 years of average "Roskilde conditions".

REFERENCES:

CHRISTENSEN, B. MORTENSEN, P.B. and PETERSEN, T. (1985).
Illustration of the Present Capabilities of the ECCES Program System. Risø-M-2501. (Roskilde, Denmark) 44p.

BRODERSEN, K. LARSEN, B.R. and PETERSEN, T. (1987). Eksperimentel undersøgelse af jordprøve samt udvikling af metode til ekstraktionsforsøg benyttet ved verifikation af ECCES jordbundskemi modeller. (In prep.) (Risø National Laboratory).

BRODERSEN, K., MORTTNSEN, P.B. and PETERSEN, T. (1986). ECCES. A Model for Calculation of Environmental Consequences from Energy Systems Predicting Ion Concentrations and Acidification Effects in Terrestrial Ecosystems. Risø-M-2615. (Roskilde, Denmark) 48p.

BRODERSEN, K. (1984). Water Chemistry in Soil Systems. Risø National Laboratory. Risø-M-2445. (Roskilde, Denmark) 69p.

KRISTENSEN, K.J. (1959). Temperature and Heat Balance of Soil. OIKOS, 10, 103-120.

MORTENSEN, P.B. (1985). Modelberegninger af jordekstraktionsforsøg. Internal report. Risø, ETA. MIL-2-85. (Roskilde, Denmark).

SKYTTE-JENSEN, B. JENSEN, H. and NIELSEN, O.J. (1985). Geochemical Modelling. WHATIF-AQ: A Computer Program for Speciation Calculations. Commission of the European Communities. EUR 10119EN. (Risø National Laboratory, Roskilde) 100p.

2.7. The Temperature Calibration Laboratory

The Temperature Calibration Laboratory was accredited in 1978 by the Danish National Testing Board to carry out certified calibrations of temperature sensors in the -150°C to 1100°C range according to the International Practical Temperature Scale IPTS-68. In 1986 the accreditation was extended to cover calibration of electrical resistance in the range 0 - 1000 Ω and d.c. voltage in the range 0-1.1 V. The standard thermometers, the standard resistors and the voltage standard cells in the Laboratory are traceable to the National Physical Laboratory, England.

The number of calibrations for external customers has increased steadily during the years. In 1986 the Laboratory has performed 182 jobs for external customers and 4 for other Risø departments. In all 586 thermometers ranging from liquid-in-glass models to advanced digital types and 12 thermostats have been calibrated during the year. The calibrations have been made in the temperature region from -145°C to 1100°C which covers the main part of the range accredited.

N.E. Kaiser

2.8. Fundamental Combustion Research

A system for the study of the combustion of single coal partic-
les has been set up in the laboratory as shown on Fig. 6. A
small furnace has been built (1). The gas composition, flow
rate and temperature can be controlled and monitored with an HP
computer and datalogger. The coal particles are inserted through
a cooled feeding probe. After the burning process samples of the
coal particles can be removed with a cooled suction probe (2).
During the burning process, the coal particles can be studied
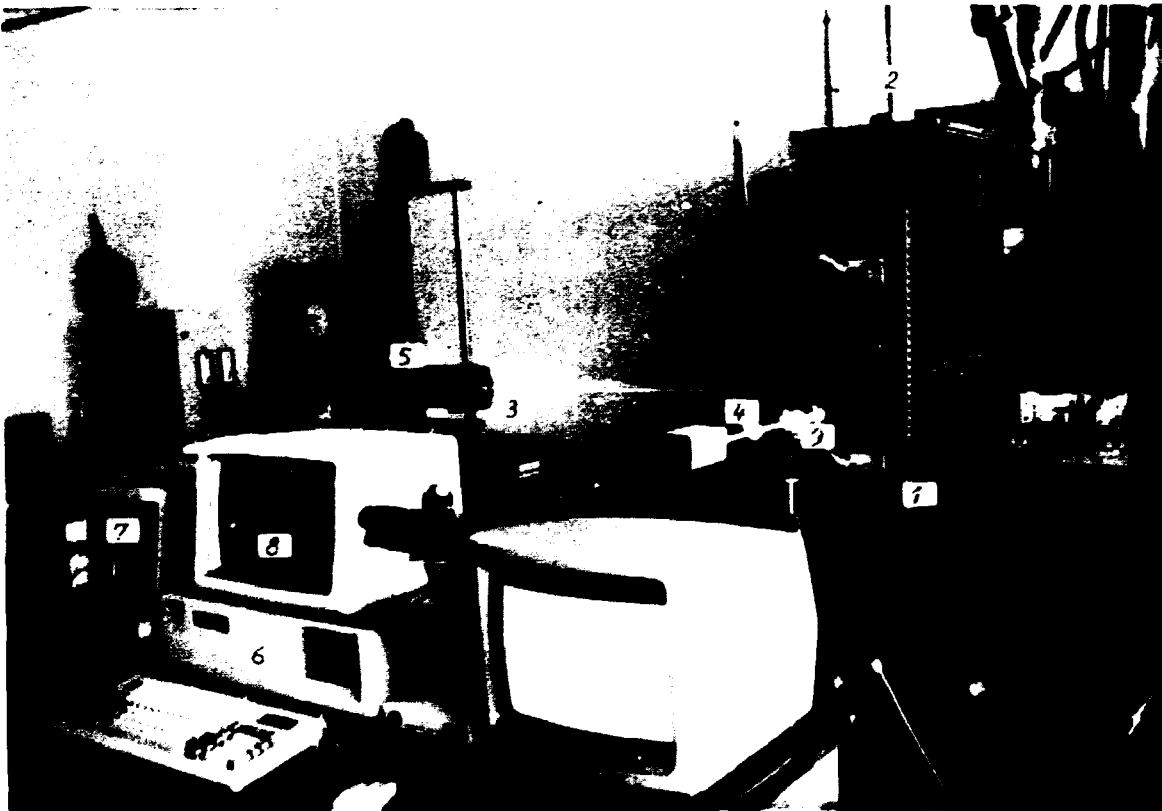through quartz windows with a laser system (3) and a TV-camera
system (4).

Fig. 6. Test facility for the study of single coal particles
burning in a controlled environment

The laser system is a DANTEC LDA for 2-dimensional velocity mea-
surements, with a 3-dimensional traversing system (5). The LDA
measurements are controlled with an IBM-AT computer (6). The
doppler burst from the laser light spread by a coal particle in
the probe volume can be digitized with a LeCroy transient recor-
der (7) and displayed on the IBM-terminal monitor (8). The
samples of burned coal particles can be analyzed with a TV-Mi-
croscope system. The CCD-TV camera is then placed on top of the
microscope (8), the image is digitized and analyzed with GIPS
software to give geometrical features like perimeter, area, com-
pactness and equivalent diameters.

The simultaneous in situ measurements on a single particle with
the laser and the TV-system to give velocity and particle size
is under development. The particles are then backlighted with
a flash and a shadow image is formed in the TV camera by a spe-
cial lens (9) focused on the small laser probe volume. From the
digitized burst the velocity is calculated and from the digiti-
zed TV image of particle geometrical features can be found.

The flash and frame grabbing is triggered by the doppler signal.

P. Gade Nielsen

2.9. Coal Combustion in a Circulating Fluidized Bed

A well-designed circulating fluidized bed combustion system
combines a high fuel flexibility with a low NO_x and SO_x emis-
sion. For that reason the system looks promising for industrial
plants as well as for cogeneration applications.

Our work in this field is done under a contract with the Ministry
of Energy and the Danish boiler manufacturer Aalborg Boilers A/S.

The design of a 2 MW_t circulating fluidized bed combustion test
rig (Fig. 7) was initiated in August 1985 and the first shake
down experiments took place in June 1986. Since then an extensive

test programme has been performed. This programme has included
both steady state performance measurements, and start up and
shut down experiments.
A limited programme was also carried out with limestone addi-
ition and SO_x removal.

The main conclusion up till now is that the fluid bed design
in the main part has satisfied the expectations. The problems
met have in general been related to the convertional equipment
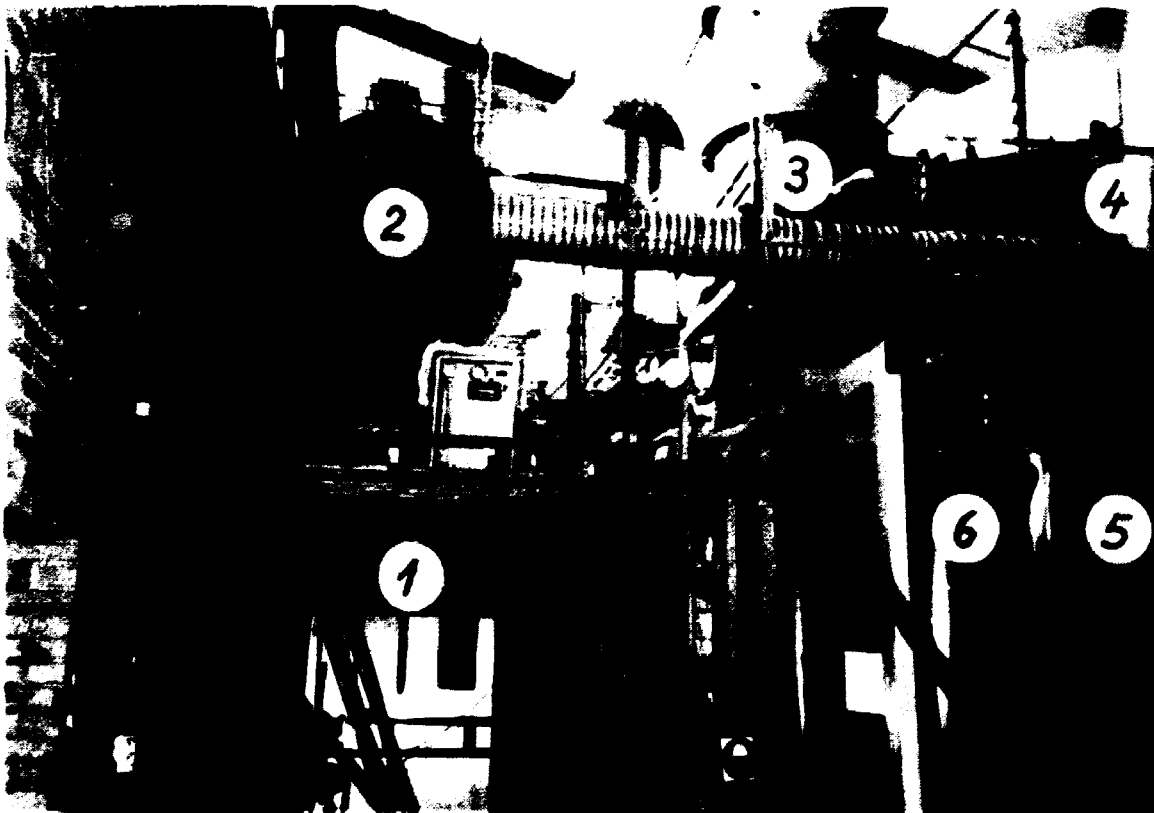(coal handling etc.).

P. Ottosen et al.

Fig. 7. 2 MW circulating fluidized bed. 1 control room, 2 flue
gas cooler, 3 fluidized bed, 4 cyclon, 5 sand, 6 coal.

2.10. Sulphur Dioxide Removal from Flue Gases

Sulphur dioxide can be removed from flue gases by adding lime-
stone. In fluidized bed combustion the limestone can be sup-
plied directly into the combustion zone simultaneously with
the fuel.

In a laboratory test facility 14 different commercially avail-
able qualities of limestone have been tested. The main part was
of Danish origin, but for comparison also two from abroad have
been tested. The four most promising types have been selected
from the laboratory tests. These types have been tested in
Risø's 300-kW atmospheric fluidized bed at real combustion
conditions. Two types of limestone have been tested at the
Danish Boiler Owners Association's test center in Vordingborg
in a 1 MW fluidized bed. Finally, the best type of limestone
has been tested in February 1986 in full scale in a 12 MW bed in
a district heating station located in Skanderborg.

<div align="right">N.E. Kaiser</div>

2.11. Computer Modelling of Steady Three-dimensional Turbulent Gas/Particle Flows

Gas/particle flows are found in many industrial applications
such as cyclone separators, pneumatic transport of powder and
droplet combustion systems. The aim of the present work is to
model the flow and combustion of coal particles with special
reference to conventional furnaces for pulverized coal com-
bustion.

Three main parts of the model can be identified. First, the
turbulent flow of the gas and particles has to be determined.
The second part models the devolatilization and combustion of
volatiles and the combustion of the char residue. Finally,
the thermal radiative heat flux between the gas, particles and
walls of the furnace has to be modelled.

The project is done in cooperation with the Laboratory for Heating and Air-Conditioning at the Technical University of Denmark. The work during the last year has concentrated on the development of their 3-D gasflow model in parallel with a preliminary setup of a particle tracing model. When combined we should be able to simulate nonreacting gas-particle flows. Literature studies of coal devolatilization and char burn-out have been performed in order to facilitate the modelling of the mass exchange, and a radiation model is under development at the Technical University.

P. Astrup

2.12. MULTWO: Compositional Computer Model for Transient Oil/Gas Two-phase Flow

Oil/gas two-phase pipelines are of great technical and economic importance for offshore oil/gas fields, especially as connection lines between a central separation/pumping platform and a number of satellite fields are sharing the platform. Computational tools in the form of computer models may help solve the serious operational and safety problems associated with the use of two-phase pipelines.

In 1984-1985 the first phases of the development of the MULTWO computer model was performed in cooperation with LICconsult Consulting Engineers Ltd. and the Institute for Chemical Engineering of the Technical University of Denmark.

This first development resulted in a code version, which describes the oil/ gas flow in pipelines by a fully integrated calculationa. scheme for time- and position-dependent compositions, volume fractions, velocities, pressure and temperature of the two phases (equal pressure and temperature for gas and oil), and which has detailed submodels for most flow patterns of interest.

The MULTWO code has been tested and further developed by comparison with experimental data from full-scale operating pipelines. Rather encouraging results have been obtained for simulation of severe slugging. With little adjustment regarding the representation of pressure- and surface wave propagation, but without introduction of ad-hoc models, it seems possible for MULTWO to predict with acceptable accuracy whether severe slugging occurs in a pipeline-riser system under given conditions.

It is planned to test the MULTWO model further by comparative calculations with other available data and with laboratory small-scale experiments to be performed in the near future for the purpose.

O. Rathmann

2.13. Porosity and Permeability Mapping

Simulation studies of oil and gas fields require typically more than thousand grid blocks in order to get sufficient resolution for describing the flow mechanisms.

As a part of the set-up of the numerical model each grid block is given a porosity and permeability value. This process is very time-consuming and offers many opportunities for typing errors.

A computer programme for mapping of these parameters has been developed to circumvent the tedious typing and to ensure consistent estimation.

The basic data for the porosity mapping is the interpretations of the log porosities for the wells, whereas the well test analyses and the core measurements constitute the basis for the permeability mapping. Within the space covered by the wells

reasonable estimates can be expected (measured data available),
but at locations outside this space (edge and bottom aquifer)
the estimates cannot rely on measured values.

For each formation a trend function is determined,

$$\phi(z) = A \cdot \exp(B \cdot z)$$

describing the relation between the porosity, ϕ and the depth,
z. The function is fitted to measured log data by a least
square fit, with A and B as regression constants.

The local measured value of the logarithm to the porosity,
$\ln\phi_i$, is described as a function of the trend, $\phi(z)$, and a lo-
cal anomaly, Y_i so that

$$\ln\phi_i = \ln A + Bz_i + Y_i$$

The anomaly is determined for each of N intervals, where the
porosity is measured, as

$$Y_i = \ln\phi_i - (\ln A + Bz_i), \qquad i = 1,\ldots,N.$$

The porosities desired are then mapped by the inverse distance
to the power n method, assuming the logarithm to the estimated
porosity for block k, in the grid, to be equal to the trend
plus a linear combination of the measured anomalies:

$$\ln\phi_k = \sum_{i=1}^{N}\alpha_{ki} \cdot Y_i + \ln A + Bz_k$$

where

$$\sum_{i=1}^{N}\alpha_{ki} = 1$$

as the α's are determined by:

$$\alpha_{ki} = \frac{H_i}{D_{ki}^n} \cdot \frac{1}{\sum\limits_{i=1}^{N} H_i/D_{ki}^n}$$

where D_{ki} is the distance between the midpoint of the kth grid block and the ith measurement point of the total number of the N measured values, and H_i the interval for which the measured porosity is representative.

Near a measurement point the estimated porosity is close to the measured value, and at great distances from these points the estimated porosity is almost equal to the trend value.

The permeability mapping is based on measured permeabilities from core analysis and well tests, and an assumption of a functional relation between permeability and porosity for each formation. This relation is described by a trend function

$$k(\phi) = C \cdot \exp (D \cdot \phi)$$

determined by a least square fit to measured corresponding data for porosity and permeability, with C and D as regression constants.

The locally measured values of the logarithm of the permeabilities (typically test permeabilities) are then described as a function of the trend, based on ϕ-values already determined and a local anomaly calculated in the same manner as for porosities.

Finally, the permeabilities desired are estimated by mapping, using the inverse distance to the power n method, as for porosities, again based on the estimated ϕ-values.

As an example of the output from the mapping programme a contour plot of a porosity distribution for a cell layer is shown in Fig. 8.

The great advantages of the porosity and permeability mapping programme is that changes such as

1) modifications of the grid (refinements, faults)
2) new measurement points or values
3) different number of trend functions

are incorporated immediately into the estimates. The mapping programme ensures futhermore, consistency between porosity and permeability, and the time-consuming typing is sharply reduced.

H. Bagger
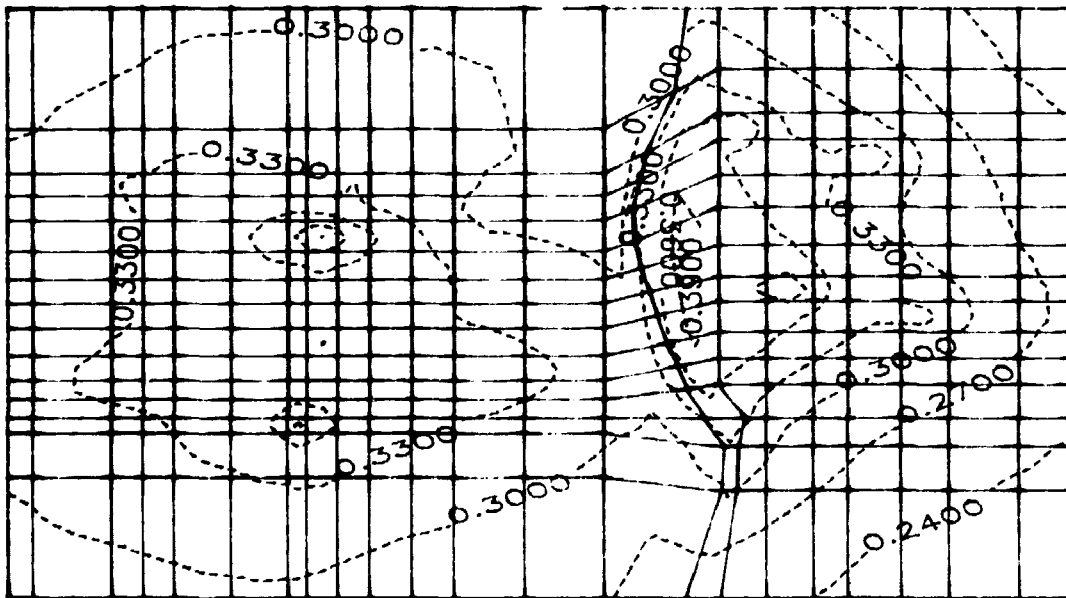

Fig. 8. Porosity distribution for a cell layer generated by the mapping programme.

2.14. Reservoir Simulation

COSI is a 3-dimensional, fully compositional simulator which includes a double-permeability description of the reservoir rock.

A special feature of the COSI simulator is the application of
the integral finite difference method which avoids reference
to a specific coordinate system. As a result, COSI is very
flexible regarding grid cell shape and the way grid cells are
connected. This can be used to reduce the so-called grid orien-
tation effect.

The traditional finite-difference approximation of the convec-
tion term of the mass conservation equation involves five space
points in the two-dimensional case, namely the point or cell
in consideration and its four neighbours in the direction of
the coordinate axes. (The corresponding 3-D approximation is a
7-point formula). It has turned out, however, that the 5-point
scheme performs very poorly for displacement problems involving
unfavourable or even moderate mobility ratios. What happens
is that the displacement front is propagated preferentially
along the coordinate axes. As a result, the predicted perform-
ance depends to an unacceptable extent upon the orientation
of the difference grid. The phenomenon is referred to as the
grid orientation effect.

It is well known that the grid orientation effect can be al-
leviated by use of the 7-point scheme with hexagonal grid
cells or the 9-point scheme where the diagonal cells in the
Cartesian grid are included in the difference operator. (See
f.ex. PRUESS and BODVARSSON (1983) and SHAH (1983)). The fol-
lowing test problem demonstrate that grid orientation can be
eliminated by use of an irregular grid system - at a reduced
cost.

One-eighth of the reservoir under consideration and the "Carte-
sian" grid system used are shown in Fig. 9. All 30 cells, except
the one next to point S, are of equal size with:

$$\Delta x = \Delta y = 400 \text{ ft.}$$

The number of grid cell interfaces is 46. The reservoir section
contains one injection well located in the center of the reser-
voir and two production wells.

One production well is located at the boundary of the reservoir in a direction from the injector which is parallel to the y-direction grid lines. It is denoted the parallel producer. The other one is also located at the boundary of the reservoir but in a direction from the injector which is rotated 45 degrees. It is denoted the diagonal producer.

Ideally, the distance from the injector should be the same for the two producers. This condition cannot be fulfilled exactly, however, when in the same time the producers are to be located in the cell centers and the grid is square. In the present case the distance between the parallel producer and the injector is 7 Δx or 2800 ft while the diagonal producer is 7.071 Δx or 2828 ft from the injector. In other words, the distance from the injector to the diagonal producer is 1% longer than that from the injector to the parallel producer.

Also, ideally the two producers should have identical environmental or drainage areas. Again, this cannot be achieved exactly given the above-mentioned constraints. The angle parallel producer-injector-point S is 23.2 degrees while the angle diagonal producer-injector-point S is 21.8 degrees.

To sum up, the reservoir section is unsymmetric with respect to the line injector-point S, but the difference is small, and it is to be expected that in the case of gas injection, true gas breakthrough times for the two producers will be very close to each other.

The reservoir contains initially undersaturated oil and water. At time zero all three wells are opened. Gas is injected at a rate of 2 MMscf/D while 500 STB/D are produced from each producer. These rates are maintained for 2400 days at which time the calculations are stopped.

The gas-oil ratios produced, as computed by COSI by means of the standard five-point difference scheme are shown in Fig. 10. The results present an excellent illustration of the grid orientation

effect. The gas breakthrough time for the parallel producer is 1050 days while the breakthrough time for the diagonal producer is 1850 days. The difference is 800 days or more than two years. Considering that practically all field scale reservoir simulations made today are carried out with a five-point Cartesian difference scheme this is really something to bear in mind, especially in connection with history matching. Any attempt to correct a mismatch of this size between computed and observed GOR's by modifying the physical reservoir model would be disastrous. The only thing to do is to improve the accuracy of the numerical solution, for example by using an irregular grid.

The grid shown in Fig. 9 was set up. A rough best-eye attempt has been made to align grid cell interfaces perpendicular to expected stream lines. There are a total number of 17 grid cells and 24 grid cell interfaces.

The case referred to in the previous section was repeated with the irregular grid. The resulting gas-oil ratios produced are displayed in Fig. 10. The difference between the two curves is now very small. The grid orientation effect is eliminated. Gas breakthrough is calculated to occur simultaneously after 1600 days.

However, the GOR rise of the "diagonal" producer is slightly delayed. This is consistent with the fact that the "diagonal" producer is farther away from the injector than is the "parallel" producer.

The conclusion is that it is possible to obtain more accurate solutions with fewer grid cells by using irregular, curvi-linear-like grid cells. In particular, wells in field simulations can be treated much more accurately and the above type of grid orientation effects can be alleviated.

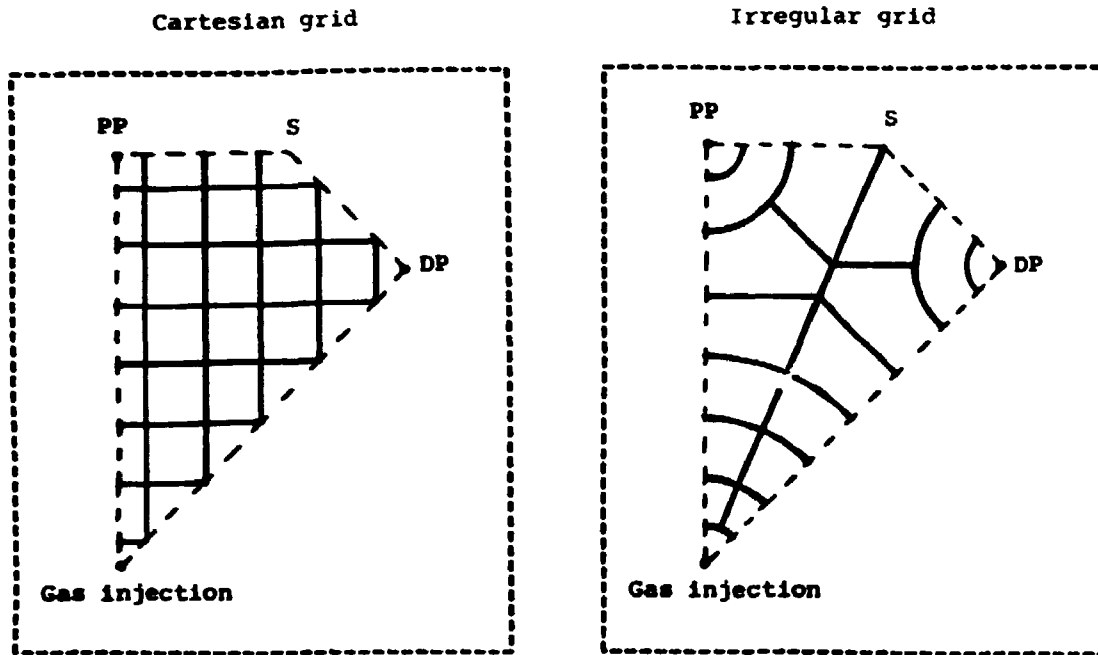The relative computational times for the two cases were as follows

Cartesian grid   Irregular grid

Fig. 9. Reservoir and grid systems applied by COSI

```
——— Parallel producer, PP        ——— "Parallel" producer, PP
----- Diagonal producer, DP      ----- "Diagonal" producer, DP
```
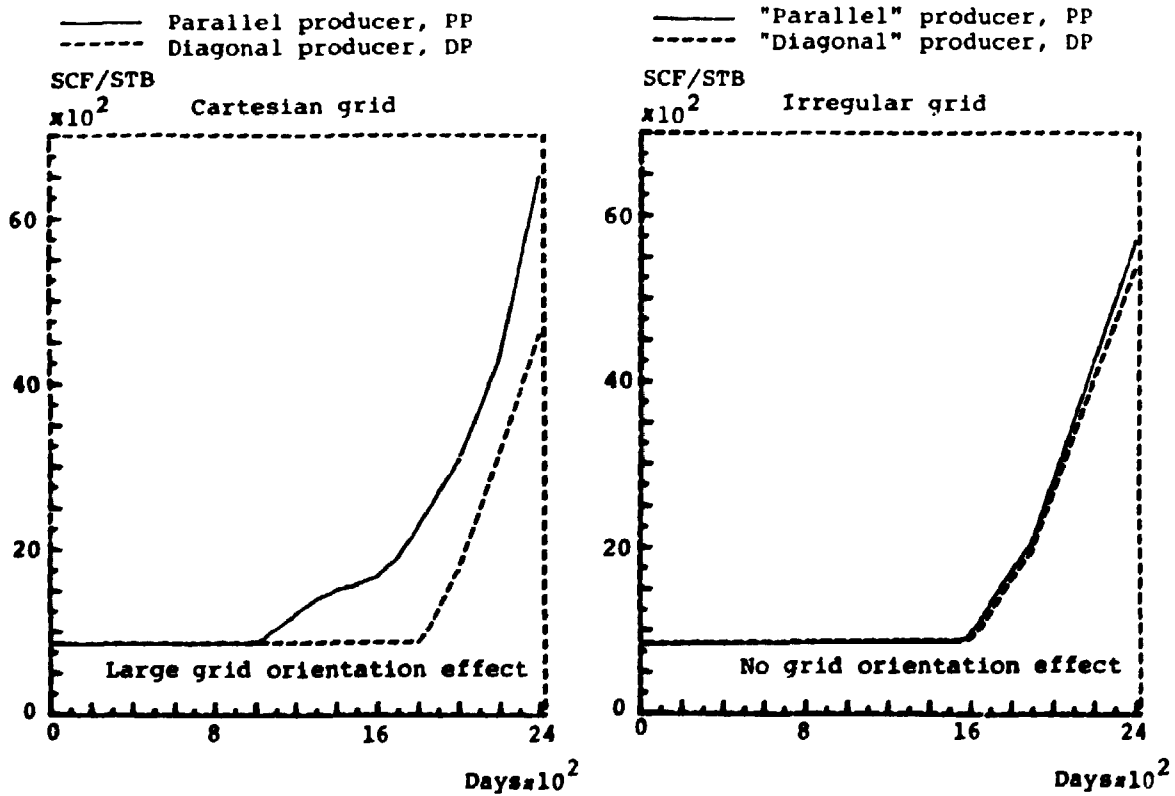

Fig. 10. Produced gas/oil ratios vs. time computed by COSI.

5-point scheme	1
Irregular grid	0.3

N. Bech

REFERENCES:

PRUESS, K. and BODVARSSON, G.S. (1983). A Seven-Point Finite Difference Method for Improved Grid Orientation Performance, in Pattern Steamfloods. SPE 12252. In: Seventh SPE Symposium on Reservoir Simulation, San Francisco, Nov. 16-18, 1983. Pp. 175-184.

SHAH, P.C. (1983). A Nine-Point Finite Difference Operator for Reduction of Grid Orientation Effects. SPE 12251. In: Seventh SPE Symposium on Reservoir Simulation, San Francisco, Nov. 16-18, 1983. Pp. 171-174.

3. PUBLICATIONS

Department of Energy Technology (1986)
Annual Progress Report, 1 January - 31 December 1986. Edited by B. Micheelsen and F. List. Risø-R-538. 45p.

BRODERSEN, K. et al. (1986). ECCES - A Model for Calculation of Environmental Consequences from Energy Systems Predicting Ion Concentrations and Acidification Effects in Terrestrial Ecosystems. Risø-M-2615. (Roskilde, Denmark) 48p.

CHRISTENSEN, P. LA COUR, (1986). Skitse af programpakke til simulering af dynamiske systemer. RP-1-86. (Internal report). (Risø National Laboratory, Roskilde).

CHRISTENSEN, P. LA COUR et al. (1986). DYSIM - A Modular Simulation System for Continuous Dynamic Processes. RP-5-86. (Internal report). (Risø National Laboratory, Roskilde).

CHRISTENSEN, P. LA COUR and LARSEN, N. (1986). Description of a Sample Power Plant Model for Simulation and Expert-System Supervision Purposes. RP-6-86. (Internal report). (Risø National Laboratory, Roskilde).

CHRISTENSEN, P. LA COUR et al. (1986). DYSIM - A Modular Simulation System for Continuous Dynamic Processes. Risø-M-2607. (Roskilde, Denmark) 72p.

FYNBO, P.B. (1986). Input Description for NAUA/5. AER-1-86. (Internal report). (Risø National Laboratory, Roskilde).

FYNBO, P.B. (1986). Modifications Introduced into NAUA. AER-2-86. (Internal report). (Risø National Laboratory, Roskilde).

FYNBO, P.B. (1986). SURRY-1. A Benchmark Recalculated. AER-3-86. (Internal report). (Risø National Laboratory, Roskilde).

FYNBO, P.B. (1986). Nucleation. AER-4-86. (Internal report). (Risø National Laboratory, Roskilde).

HØJERUP, C.F. (1986). LEWARD - A Short Description of a New LWR Assembly Neutronic Code. RP-9-86. (Internal report). (Risø National Laboratory, Roskilde).

HØJERUP, C.F. (1986). Plotflowdiagram. RP-11-86. (Internal report). (Risø National Laboratory, Roskilde).

HØJERUP, C.F. (1986). Comparison of LEWARD with CASMO and RECORD. RP-12-86. Risø-I-263. (Roskilde, Denmark) 26p.

HØJERUP, C.F. (1986). A short Input Preparation Manual for the Programme LEWARD/B. RP-13-86. Risø-I-265. (Roskilde, Denmark) 17p.   .

JENSEN, P.K. (1986). Preliminary Simulations of Transformation Ratios for the Danish Well AARS-1A. Risø-M-2552. (Roskilde, Denmark) 23p.

KOFOED, J. (1986). Development of a Simulator Tool: Description of the Precompiler DYS/PRE1. RP-4-86. (Internal report). (Risø National Laboratory, Roskilde).

KOFOED, J. (1986). Dynamic Simulation of a Power Plant. RP-7-86. (Internal report). (Risø National Laboratory, Roskilde).

LARSEN, A.M. (1986). Forundersøgelse vedrørende AI og simulering. RP-3-86. (Internal report). (Risø National Laboratory, Roskilde).

LIST, F. (1986). Eksperimentelt kursus ved DR 1. Gamma-spektroskopi. (Internal paper). (Risø National Laboratory, Roskilde).

LIST, F. (1986). Eksperimentelt kursus ved DR 1. Reaktorkonstanter. (Internal paper). (Risø National Laboratory, Roskilde).

LIST, F. (1986). Eksperimentelt kursus ved DR 1. Forsøg med neutroner. (Internal paper). (Risø National Laboratory, Roskilde).

MORTENSEN, P.B. (1986). Simulering af $(NH_4)_2SO_4$ tilførsel til landbrugsjord. MIL-1-86. (Internal report). (Risø National Laboratory, Roskilde).

MORTENSEN, P.B. (1986). Data til modelberegninger af skovbundssystemer. MIL-2-86. (Internal report). (Risø National Laboratory, Roskilde).

NONBØL, E. (1986). Flux Calculation for 3 Different LEU Conversion Scenarios Made with the DR 3-Simulator DR 3/SIM. RP-2-86. (Internal report). (Risø National Laboratory, Roskilde).

NONBØL, E. (1986). Development of a Three-dimensional Simulator
    of a DIDO-type Reactor. RP-8-86. (Internal report). (Risø
    National Laboratory, Roskilde).

NONBØL, E. (1986). Recent Reactor Physics Activities in Den-
    mark. RP-10-86. (Internal report). (Risø National Labora-
    tory, Roskilde).

RATHMANN, O. et al. (1986). MULTWO: Compositional Computer Mo-
    del for Transient Oil/Gas Two-phase Flow. Report no.3.
    Risø-M-2556. (Roskilde, Denmark) 55p.

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	Department or group Energy Technology
	Groups own registration number(s)
	Project/contract no.
Pages 42 **Tables** **Illustrations** 10 **References** 38	**ISBN** 87-550-1300-7

Abstract (Max. 2000 char.)

The general development of the Department of Energy Technology
at Risoe during 1986 is presented, and the activities within
the major subject fields are described in some detail.
Lists of staff and publications are included.

Descriptors – INIS:

COAL; COMPUTERIZED SIMULATION; ENVIRONMENTAL IMPACTS; FLUIDIZED-BED
COMBUSTION; HEAT TRANSFER; NATURAL GAS; PETROLEUM; POWER GENERATION;
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