AAEC/PR44-D

AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS

NUCLEAR SCIENCE AND TECHNOLOGY BRANCH REPORT 1977

DIVISIONAL RESEARCH

December 1977

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<u>PREFACE</u>

The Nuclear Science and Technology Branch Report is an annual technical report dealing with work done in a twelve month period ending on September 30th of each year.

The report is issued in several volumes, each recording the technical effort within broad areas of responsibility as follows:

AAEC/PR44-P   Power and Energy Program
AAEC/PR44-U   Uranium Fuel Cycle Program
AAEC/PR44-N   Nuclear Science and Applications Program
AAEC/PR44-D   Divisional Research
AAEC/PR44-S   Site Management Program

The contributions to each report are made by Research Divisions, Research Sections, and Site Management Departments where appropriate. Wherever possible the names of staff responsible for each project are indicated.

K.H. TATE
Controller, Site Information Services

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INTRODUCTION

This report describes progress in independent research work which has been carried out on the initiative of the Division Chief or Leader of a Research Section and which is considered to be necessary for or relevant to that Division's responsibilities and capabilities. For this work the Division Chief or Section Leader is responsible directly to the Head, Nuclear Science and Technology Branch. A nominal 10 per cent of the Branch research effort can be made available for this work.

1. PHYSICS DIVISION

1.1 Neutron Moisture Meter Investigations (D.B. McCulloch, D.J. Wilson, J.A. Daniel)

Neutron moisture meters [IAEA, Vienna 1970 - Neutron moisture gauges. Technical Report Series No.112] have been widely used for many years in varied disciplines for *in situ* determinations of free water content in soil strata. Although the principles are simple, interpretation of field measurements has not generally been fully satisfactory. It appears that the problem of interpretation may largely be attributable to (i) the use of very simplified neutron diffusion theory calculations which do not take adequate account of the finite size and geometrical details of calibration experiments compared with field conditions, and (ii) the neglect of possible effects on neutron count rates of reflections from materials outside the calibration drums.

Since there was a requirement for soil moisture determinations in connection with Rum Jungle environmental studies, and a general solution to the problem would be of widespread interest and benefit, the Division began development of a suitable calculational model and a small series of carefully controlled calibration experiments.

1.2 Deep Ocean Currents and the Disposal of Radioactive Waste into the Ocean (J.R. Harries)

The conditions in the deep oceans in the vicinity of Australia are being studied to identify local problems associated with ocean disposal of radioactive waste by other countries. Most of the problems are not unique to radioactive waste, but are common to any material added to the ocean whether intentionally by disposal operations, or unintentionally *via* rivers. The deep ocean circulation patterns are being estimated from the published data. There are, however, considerable uncertainties about the variability and timescale of the flow. The distribution of naturally occurring radioactive and stable tracers in the ocean shows that the transport of ocean pollution depends strongly on both the nature of the elements and the chemical species present.

1.3 Thorium Analysis by Neutron Activation and Gamma Spectrometry (G. Durance, D.B. McCulloch)

Neutron capture in ^{232}Th leads to the production of ^{233}Pa, whose β-decay with 27.0 day half-life to ^{233}U is accompanied by emission of a 311.8 keV γ-ray. By suitable choice of irradiation and cooling times, this γ-ray can be rendered relatively free from interference by other γ-rays emitted from typical activated geochemical samples, including ores

with significant uranium content. A thorium analysis technique based on this process would offer substantial advantages over delayed neutron activation or proton induced X-ray emission.

Preliminary experiments to investigate the potential of the method for routine quantitative assay of thorium in mineral ore samples appear promising. Samples made up from specially prepared $ThO_2/CaCO_3$ mixtures with thorium content ranging from 1 to 2000 $\mu g\ g^{-1}$ suggest that an accuracy of about 3 per cent may be possible above ~ 15 $\mu g\ g^{-1}$ with a detection threshold of ~ 5 $\mu g\ g^{-1}$.

1.4 Interactive Computing Methods (B.E. Clancy)

In many scientific computing installations, a substantial number of jobs submitted are small FORTRAN compile, link and run jobs, designed to test out new ideas or to perform relatively straightforward calculations. Even when conceptually simple, these jobs are not free from programming mistakes, and the job may need to be revised and resubmitted several times before the 'sucessful-definitive' run is made. Monitoring the execution of these runs and modifying program and/or data between runs are often best done in one interactive session at a computer terminal. Machine manufacturers have provided systems - such as the IBM TSO system - to allow this to be done.

Designed to support many users simultaneously, the TSO system makes large demands on computer core storage and has not been implemented at the Research Establishment. To provide most of these facilities to a single user at one time, an interactive program package - COMFORT - has been developed to run under the normal operating system to which COMFORT looks like an ordinary batch job.

The heart of COMFORT is the control segment which interacts with the user allowing him to enter, edit and modify his FORTRAN program and data as well as to save or recover his program held in a disk library. When appropriate, this control program activates a FORTRAN compiler and then passes control to the user's compiled program. A comprehensive set of subroutines and functions is available to the control segment, and linkage to these from the user's program is made at compilation time. A complete error monitor is available and, when necessary, this will regain control from the user's program and return to the control segment without aborting the user's session at the terminal.

1.5 Inverse Reaction Problem (E.J. Clayton, D.W. Lang, J.L. Cook)

A standard method of obtaining information about a two-body force involves the measurement of scattering cross sections. It is known that the scattering alone does not define the radial dependence of the force. The situation resembles that of X-ray diffraction analysis of crystal structure, where the pattern of scattered photons conveys the information about molecular structure. In the case of scattered particles, the scattering cross section angular distribution is divided into partial angular momentum states and the partial wave amplitudes are expressed in terms of phase shift. Each phase shift defines a whole class of phase-equivalent potentials and an attempt is made to define the properties of this class.

The problem of finding all equivalent potentials was reduced to that of finding all orthogonal matrices that transform non-interacting wave functions into interacting ones. All such matrices must have the same leading column and the construction of these has been demonstrated. These are to be tested by computer studies of reconstructed measured phase shifts from the defined class of potentials.

To apply these methods to measured data, the pion-nucleon system is being examined using new data. The class of non-local potentials in the seven most prominent angular momentum states are to be evaluated, and transformations between phase equivalent potentials are to be investigated.

1.6 Publications

Reports

Clancy, B.E. [1977] – SUPERFIT – An Interactive Program for Function Evaluation and Least Squares Fitting. AAEC/E408.

Clayton, E.J. & Derrick, C.H.* [1977] – A Numerical Solution of Wave Equations for Real or Complex Eigenvalues. Aust. J. Phys., 30 : 1. (*Univ. of Sydney).

Clayton, E.J., Cook, J.L. & Rose, E.K. [1977] – Application of the Inverse Scattering Problem to Low Energy Pion-Nucleon Scattering. Aust. J. Phys., (in press).

2. CHEMICAL TECHNOLOGY

2.1 Analytical Chemistry Research (T.M. Florence, G.E. Batley, P. Pakalns, P.S. Rendell)

Development of new and improved methods of chemical analysis is essential to the provision of a modern analytical chemistry service. Research in this area is carried out in order to anticipate requests for chemical analyses and to solve special analytical problems.

The Effect of Surfactants on the Determination of Metals in Waters
(P. Pakalns)

The presence of surfactants in domestic and industrial waste waters can lead to interferences in standard methods of analysis for trace concentrations of certain anions and cations. Methods for the analysis of aluminium, iron and sulphate have been examined to assess the magnitude of these interferences. A range of surfactants including cationic, anionic and non-ionic detergents, formulated detergents, sodium tripolyphosphate, sodium pyrophosphate and the detergent additive, nitrilotriacetic acid (NTA), has been investigated.

Aluminium in water was determined using the eriochrome cyanine R, ferroin-orthophenanthroline and chrome azurol S methods. Cationic, anionic and non-ionic detergents at concentrations up to 2, 100 and 1000 mg ℓ^{-1}, respectively, did not interfere. Sodium tripolyphosphate interfered badly above 1 mg ℓ^{-1}, and therefore interference by formulated detergents containing tripolyphosphate was serious. Concentrations of NTA, soap and sodium pyrophosphate had to be below 0.5, 10 and 20 mg ℓ^{-1},

respectively, to limit the error to 5 per cent. It should be possible to determine aluminium satisfactorily by all three spectro-photometric methods in polluted natural waters because the concentration of detergents seldom exceeds 0.5 mg ℓ^{-1}. Unless raw effluent is released into natural water streams, tripolyphosphate will be con-verted to phosphate, and anionic detergents will be degraded by 90 per cent after the effluent has been treated in an activated sludge treat-ment plant.

Soluble iron was determined using the phenanthroline, tripyridine and biquinoline methods. The tripyridine method is superior to the other two methods for the determination of iron in the presence of up to 1000 mg ℓ^{-1} of various surfactants, but not up to 100 mg ℓ^{-1} of non-ionic detergent. In the phenanthroline method, sodium tripolyphosphate interfered above 2 mg ℓ^{-1}, but the biquinoline method can be used to determine iron in the presence of 50 mg ℓ^{-1} of sodium tripolyphosphate.

Surfactants were investigated for their effect on the turbidimetric and titrimetric determination of sulphate in water. In the turbidi-metric method, cationic and non-ionic detergents at concentrations of up to 1000 and 20 mg ℓ^{-1}, respectively, did not interfere, but the anionic detergent concentration had to be below 0.5 mg ℓ^{-1}. Sodium tripoly-phosphate interfered above 5 mg ℓ^{-1}, but NTA could be present up to 500 mg ℓ^{-1}. The titrimetric method can tolerate higher concentrations of surfactants and is recommended for sulphate determinations in solutions containing anionic and non-ionic detergents, tripolyphosphate and soap. With the latter method, interference by metals can be removed by passing the acidified solution through a cation-exchange column.

Speciation of Heavy Metals in Sediments
(G.E. Batley, P.S. Rendell)

A knowledge of the distribution or partitioning of metal species between different sediment components is important in studies of heavy metal transport and of toxicity to aquatic life in river and estuarine systems. One means of investigating this distribution has been the use of selective chemical extractants. A range of extractants for the selective dissolution of metal species, has been examined to determine their suitability for inclusion in selective extraction schemes.

Studies of metal extraction from aerobic sediments have shown that many accepted reagents are in fact non-selective, with metal extraction dependent more on the experimental conditions than on the sediment phases present. As currently used, extraction speciation schemes can only provide general information about metal availability. Adequate interpretation in terms of actual geochemical phases present is not possible. A more detailed study of selected extractants is continuing, in order to establish their potential applications and to enable mean-ingful interpretations of previous work in this field.

Determination of Trace Metals by Gas Chromatography –
Research Contract

The aim of this research contract with Dr S. Dilli, Department of Analytical Chemistry, University of New South Wales (AAEC Liaison Officer Dr T.M. Florence) is to investigate the volatility of organo-metallic complexes in terms of the separation and determination of

metals by gas chromatography.

The project has continued on a broadening front over the past year. The work with vanadium proved to be invaluable for the purpose of consolidating the fundamental aspects of the project and showed that vanadium(III) β-diketonates have the necessary properties of volatility, thermal stability and chromatographic behaviour. Despite the tendency to oxidation in solution, an analytical method has been proposed for vanadium based on the vanadium(III) chelate of the ligand 1,1,1,2,2-pentafluoro-6,6-dimethylheptane-3,5-dione. An advantage with this ligand is that its oxovanadium(IV) chelate is also suitable for chromatography with the possibility, therefore, of effecting a separation and distinction between V(III) and V(IV) species.

Parallel studies with various tetradentate Schiff bases have demonstrated the volatility, thermal stability and satisfactory gas chromatographic behaviour of their oxovanadium(IV) chelates. An analytical procedure has been presented recently whereby vanadium, copper and nickel can be determined simultaneously in petroleum products. Relevant to this work was the finding that, for compounds and hence ligands containing fluorine, detection limits of about 5 picograms are possible for these elements when using the electron-capture detector. With unfluorinated ligands, the detection of the chelates was so poor that the flame ionisation detector was preferred.

A further study which is well in progress concerns the effects of substitution in β-diketones, $R-CO.CH_2.CO-R'$, in which R or R' is an aromatic moiety. Chromatographic properties appear, in this extensive series, to follow closely the intrinsic volatility of the individual chelates.

Some preliminary work has begun with uranium compounds. It is expected that this work will continue in the ensuing year.

2.2 Non-aqueous Reactions of Heavy Metal Fluorides - Research Contract

The aim of research under contract to the Department of Inorganic Chemistry, University of Melbourne, Dr T. O'Donnell (AAEC Liaison Officer Mr R.N. Whittem) is to study redox relationships and the nature of species and reactions of heavy metals in anhydrous hydrogen fluoride.

Research during this year centred largely on spectroscopic studies in anhydrous hydrogen fluoride (HF). Previous work had demonstrated for the first time the feasibility of studying the electronic spectra of heavy metal cations in normal oxidation states, dissolved in HF. This work has been extended to studies of cations in unusually low or high oxidation states, e.g. vanadium(II), chromium(II), silver(II) and manganese(IV).

Uranyl fluoride was found to dissolve readily in solutions of arsenic pentafluoride in HF and this provided a spectrum for the UO_2^{2+} cation showing much greater resolution than is obtained in aqueous spectra.

Raman spectra for molybdenum hexafluoride and tungsten hexafluoride

in anhydrous HF, much better than those previously published, have been obtained. New spectral studies have been carried out on UO_2^{2+}, fluorosulphates and sulphates in this acidic solvent.

Systems studied by anodic voltammetry in hydrogen fluoride included Co^{2+} and CrF_6^{3-}.

Details of a crystal structure for $PuOF_4$, a compound made for the first time using facilities at Lucas Heights, have been published.

In 1976, during sabbatical leave at the Lawrence Berkeley Laboratory, University of California, Dr O'Donnell carried out spectral studies on HF solutions containing uranium in oxidation states (III), (IV), (V) and (VI). This was derived directly from the Melbourne work of 1975. The Berkeley studies have already been extended to analogous ones of neptunium. Work on plutonium is to follow.

This contract was completed in June 1977 and the final contract report is being prepared.

2.3 Structural Chemistry (J.C. Taylor, A.B. Waugh)

The structural chemistry of uranium halides and other compounds of interest in the nuclear fuel cycle is being determined and related to their physical and chemical properties.

Equipment and Facilities

A Debye-Scherrer powder camera has been modified to carry out low temperature studies down to 77 K. A stream of liquid nitrogen passes in and out of the camera through copper tubes, which are staggered at different angles to the X-ray beam so that both forward and back reflections can be obtained without the tubes blocking out part of the diffraction pattern. Moisture-sensitive samples are contained in Lindemann tubes. Some samples already examined include $MoOCl_4$ and UBr_5 while the hexafluorides of molybdenum, tungsten and uranium are to be examined shortly.

A second Debye-Scherrer camera has been modified to give an effective radius of 1.8 times that of the unmodified camera. This, together with the use of longer wavelengths to CrK_α, and improved resolution, is expected to assist greatly in the indexing of powder samples.

Modification of the 6HB powder diffractometer to a high resolution diffractometer with a 120° monochromator take-off angle, by Engineering Services Department, should be completed early in 1978. This will greatly extend the precision of the neutron profile technique at Lucas Heights, permitting structures to be studied which are 3 or 4 times more complex than those permitted by the present elastic diffraction arrangement.

The fine focus copper X-ray tube for use with the Guinier-Simon camera has arrived and will enable better data to be obtained on high temperature studies of the actinide halides.

New Computer Programs and Data Bank

A bank of theoretical neutron powder pattern data has been commenced, initially for MX_5-type structures, using published crystal structure data to allow ready identification of the structure-type of new phases.

A computer program has been developed in collaboration with the Applied Mathematics and Computing Division (Dr G.W. Cox, M. Johnson* [*Vacation Student]), to identify the polyhedron type in crystal structures. Data for various ideal polyhedron types are stored in the form of solid angles subtended by the surrounding atoms at the central metal atom. A given polyhedron is then compared with all the possible types for that particular coordination number. Matching of observed and theoretical solid angles is being done by a least squares fit. The best polyhedron is the one with the lowest least squares residual. The program has been tested on a range of uranium halide structures and shows, for example, that the polyhedra in UF_4 are best described by square antiprisms and not dodecahedra.

Crystal Structures

α- and β-UF₅

A recent X-ray study by Ryan et al. [Acta Cryst., B32 : 3311, 1976] found a slightly different structure for β-UF$_5$ than that proposed by Zachariasen, in that one of the seven coordinated fluorine atoms in the Zachariasen model is moved above the pentagonal ring to give an 8-coordinate structure. A sample of β-UF$_5$ has been prepared and neutron diffraction patterns are presently being collected between 77 and 398 K, where the β-phase transforms to α-UF$_5$. The α-UF$_5$ phase, whose fluorine positions have not yet been directly measured, will also be studied.

MoOCl₄

Neutron diffraction patterns have been collected at 77 and 293 K. The structural analysis is still in progress.

ReCl₆

X-ray powder patterns have shown this to be a new MX_6 type not isostructural with UCl_6 or WCl_6. As the pattern is complex, attempts are being made to grow a single crystal in a Lindemann tube. The compound has to be carefully treated as it melts at 29°C.

UBr₅

The neutron powder pattern data bank has shown that UBr$_5$ is not of the α-PaBr$_5$ type, as proposed by Brown et al. [Acta Cryst., B25 : 178, 1969], but instead is of the WSCl$_4$, β-UCl$_5$ type. Refinement by the profile-fitting technique shows the structure to consist of U_2Br_{10} dimers, the anions being arranged in a simple hexagonal close-packed manner.

Phases Formed in Heat Treatment of Canadian Chrysotile Asbestos

(J.C. Taylor, W.I. Stuart, P.M. Kelly*, A. Jostsons*
(*Materials Division))

It is accepted in the literature that when chrysotile is heated to 750°C or above, forsterite and silica are produced, the latter phase being assumed amorphous, as only forsterite diffraction lines are seen. Enstatite has been observed above 1000°C, and has been assumed to be formed by the reaction of forsterite with silica:

$$Mg_2SiO_4 + SiO_2 \rightarrow 2 MgSiO_3 \quad .$$
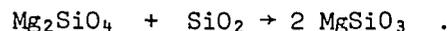
Guinier photographs were taken of Canadian chrysotile samples heated to various temperatures between 25 and 1100°C and showed the forsterite pattern developing between 750 and 1100°C with the lines becoming strong and sharp at 1100°C. However, enstatite was observed between 850 and 1000°C, but in contrast to the forsterite, the enstatite lines were broad, especially at 850°C, and even at 1100°C. At no stage were silica lines observed. This suggested the possible alternative mechanism for the decomposition of chrysotile,

$$Mg_3Si_2O_5(OH)_4 \rightarrow MgSiO_3 + Mg_2SiO_4 + 2H_2O \quad ,$$

$$\text{chrysotile} \quad \text{enstatite} \quad \text{forsterite}$$
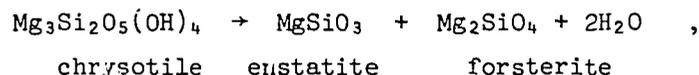
and threw doubts on the silica theory.

Electron diffraction pictures of the heated fibres showed regions of forsterite and enstatite, but no silica. The enstatite was observed to be faulted, with a streaked reciprocal lattice, explaining the diffuse enstatite pattern. The electron diffraction pictures thus confirmed the doubts as to the reliability of the literature data raised by the X-ray work.

2.4 Publications

Papers

Cheetham, A.K.* & Taylor, J.C. [1977] – Profile Analysis of Powder Neutron Diffraction Data: Its Scope, Limitations and Applications in Solid State Chemistry. J. Solid State Chem., 21 : 253. (*Chemical Crystallography Lab., Oxford Univ.).

Flynn, W.W. [1977] – A Solvent Extraction Method for the Spectrophotometric Determination of Sulphate. Anal. Chim. Acta., 90 : 343.

Levy, J.H., Taylor, J.C. & Wilson, P.W. [1977] – The Structures of Fluorides XVII. Neutron Diffraction Study of Alpha-Uranium Oxide Tetrafluoride. J. Inorg. Nucl. Chem., (in press).

Levy, J.H., Taylor, J.C. & Wilson, P.W. [1977] – The Crystal Structure of Uranium Pentabromide by Powder Neutron Diffraction. J. Inorg. Nucl. Chem., (in press).

Pakalns, P. & Farrar, Y.J. [1976] – Effect of Fats, Mineral Oils and Creosote on the Extraction-Atomic Absorption Determination of Copper, Iron, Lead and Manganese in Water. Water Res., 10 : 1027

Pakalns, P. & Farrar, Y.J. [1977] – Effect of Surfactants on the Determination of Aluminium in Water. Water Res., 11 : 387.

Conference and Lecture Papers

Ekstrom, A. [1977] – The Chemistry and Chemical Technology of the
        Actinide Elements. A Series of Six Lectures to the Department
        of Chemistry, James Cook University, Townsville, 8–12th
        August.

Ekstrom, A. [1977] – Energy Resources and Demand Between Now and 1984.
        RACI Meeting, Townsville, 7th August.

Pakalns, P., Batley, G.E. & Cameron, A.J.* [1977] – The Effect of Sur-
        factants on the Concentration of Trace Amounts of Copper,
        Nickel, Manganese, Zinc, Cadmium, Cobalt and Lead from Natural
        Waters on Chelex-100. Fourth Australian Symposium on Analytical
        Chemistry, Brisbane, 29th August-2nd September. (*NSW Institute
        of Technology).

Rendell, P.S. [1977] – Speciation of Heavy Metals in River Sediments.
        NSW Institute of Technology, School of Chemical and Earth
        Sciences, 23rd August.

Rendell, P.S., Batley, G.E. & Cameron, A.J.* [1977] – An Assessment of
        Schemes for Speciation of Heavy Metals in River Sediments.
        Fourth Australian Symposium on Analytical Chemistry, Brisbane,
        29th August-2nd September. (*NSW Institute of Technology).

3. MATERIALS DIVISION

3.1 Heat Transfer in Reactor Fuel Materials (W.J. Buykx)

Laser Thermal Diffusivity Apparatus

The apparatus was successfully tested to 900°C. The only problem
was the failure of the recrystallised alumina furnace tube to maintain
vacuum. The furnace is being rebuilt with a mullite furnace tube, so
that measurements in non-oxidising atmospheres can be made if required.

The bandwidth of the amplifier used in the apparatus was found to
be inadequate. An error of about 10 per cent occurs in the measurement
of high thermal diffusivity materials such as Armco iron. However, for
low thermal diffusivity materials, such as UO_{2+x}, SiO_2 or ZrO_2, the
distortion is small and the error in the measured value is only 1-2 per
cent.

Thermal Conductivity of Non-Stoichiometric UO_2

It was reported previously that the thermal conductivity of UO_{2+x}
decreases with increasing excess oxygen content, and that the cooling
rate used in the fabrication of the material has a marked effect on the
microstructure, which also affects the thermal conductivity. Compo-
sitions ranging from stoichiometric UO_2 to $UO_{2.10}$ have been investi-
gated. The cooling rate in the temperature interval 600-200°C is
considered to determine the microstructure of the UO_{2+x} specimens. Four
different cooling rates have now been investigated.

At a 'FAST' cooling rate (averaging an estimated 1400°C/h over the
temperature interval 600-200°C) the microstructure consisted of inter-
connecting needle-shaped U_4O_9 particles embedded in the UO_2 matrix.
Both the U_4O_9 precipitate and the UO_2 matrix are continuous. This is
called the 'penetration' type microstructure. The agreement between the

measured thermal conductivity, relative to UO_2, and the thermal conductivity calculated from the theoretical penetration model is good.

At a 'SLOW' cooling rate ($11°C/h$, $600-200°C$) the microstructure is characterised by massive equiaxed lumps of U_4O_9 precipitate at the UO_2 grain corners. These lumps increase in size with increasing O/U ratio, but remain isolated from one another. This is known as the 'variable dispersion' type microstructure. The experimental values of thermal conductivity were far below those calculated from the theoretical variable dispersion model. However, these specimens were extensively microcracked. When this system of microcracks was regarded as a third phase of zero thermal conductivity, and incorporated in the theoretical model in quantitative terms, the agreement between theory and experiment was good.

At a 'MEDIUM SLOW' cooling rate ($70°C/h$, $600-200°C$) specimens with a low O/U ratio (up to O/U = 2.05) show both the massive U_4O_9 precipitate which fits the variable dispersion description, and the U_4O_9 needle precipitate which fits the penetration model. At higher O/U ratios only the variable dispersion type structure remains. Microcracks also appear increasingly with increasing O/U ratio. The thermal conductivity of these specimens is close to that of the SLOW cooled specimens.

At a 'MEDIUM FAST' cooling rate ($800°C/h$, $600-200°C$) specimens with a low O/U ratio show only the needle-shaped U_4O_9 precipitate, but at higher O/U ratios (2.08, 2.10) there is also some massive U_4O_9 precipitate at UO_2 grain corners, as in the variable dispersion type microstructure. The relative thermal conductivity decreases with increasing O/U ratio, but unlike all the other cooling rates, the rate of decrease is slower over the composition range $2.04 < O/U < 2.06$, than on either side of this range. In the only previous study of this kind on UO_{2+x}, a similar hump in the curve of k_{rel} vs O/U was reported. In other two-phase systems it is a fairly common occurrence, and microcracking is often reported. Work is in progress to explain these results in terms of the theoretical penetration and variable dispersion models, or perhaps a combination of both.

Thermal Diffusivity of $UO_2-Gd_2O_3$

The effect of the addition of Gd_2O_3 (up to 15 mol %) on the thermal diffusivity of UO_2 was investigated and, for comparison, the thermal diffusivities of Gd_2O_3 and the compound $UO_2.3Gd_2O_3$ were also measured. The specimens were prepared by co-precipitation followed by cold pressing and sintering for 2 h at $1700°C$ in H_2.

The thermal diffusivity of UO_2 was found to decrease very rapidly with increasing Gd_2O_3 content. At 4 mol % Gd_2O_3, the observed value relative to UO_2 was 0.67, and at 15 mol % it was only 0.46. The thermal diffusivities of $UO_2.3Gd_2O_3$ and of Gd_2O_3 were about the same, *viz.* 0.52 of the value for UO_2. Metallographic examination revealed much more porosity and extensive cracking, particularly at 8 and 15 mol % Gd_2O_3, and this probably exaggerates the decrease in thermal diffusivity. A new set of specimens is being prepared to check these findings.

Thermal Diffusivity of Transition Toughened Zirconia

Transition toughened zirconia (TTZ) is an interesting, strong and tough material developed over the last few years by CSIRO's Division of Tribophysics. It is made by heat treating (ageing) partially CaO-stabilised zirconia to form small domains of metastable tetragonal ZrO_2 in a matrix of fully stabilised cubic zirconia.

In a small joint project on the thermal conductivity of zirconia, CSIRO will provide well characterised specimens of pure monoclinic ZrO_2, partially stabilised zirconia compositions, including TTZ, and fully stabilised cubic zirconia (CSZ). For the first phase of this project, two samples of CSZ (15 and 20% CaO), one specimen of correctly aged TTZ and one specimen of over-aged TTZ were provided. The thermal diffusivity of correctly aged TTZ was found to be 49 per cent higher than that of CSZ (15% CaO). For over-aged TTZ this value had dropped slightly to 45 per cent above CSZ (15% CaO). The thermal diffusivity of CSZ (20% CaO) is 16 per cent higher than that of CSZ (15% CaO).

CSIRO is preparing more specimens for this project.

3.2 Fabrication Methods for Nuclear and Special Materials
(N.W.D. Chrimes, A. Ridal, S.W. Spain, S.E. Rowling, R.V. Gardner)

Fabrication of Maraging Steel

Investigation of fabrication methods for commercial maraging steels continued. These studies were mainly concerned with extrusion techniques. A number of extrusions were produced and tooling design and lubrication methods were examined. Improvement was noted when the die entry angle was changed and a number of glass lubricants gave good results. The best lubricant used to date is a low melting point glass containing potassium, lead and silica. The compounds were melted, cooled, crushed, sized to pass through a 100 mesh sieve and suspended in distilled water. The suspension is brushed onto the billets before heating to extrusion temperature. Combination of the changed die entry angle with this lubricant improved the extrusion operation.

Electron Beam Welding

A smaller welding chamber 500 mm x 200 mm diameter was constructed and commissioned. The chamber is evacuated using a 150 mm diffusion pump backed by the rotary pump of the main chamber. The chamber is being set up to produce circumferential welds on small tubular components. Some advantages are:

- Reduced evacuation time.
- Easier access to the electron gun for dismantling and cleaning.
- Allows welding of radioactive or toxic materials.

A new electron gun was built to examine the effect of gun geometry. The material used was AISI 310 steel - chosen because of its oxidation resistance and non-magnetic properties. The variables being investigated include:

- Anode tube diameter and length.
- Grid plate orifice diameter.
- Grid to anode distance.

This work is continuing.

3.3 Electron Microscopy Techniques (R.G. Blake, A. Jostsons, P.M. Kelly, J.G. Napier, R.B. Warren)

The aim of this project is to develop new techniques to support the two main areas of work with the transmission electron microscope - radiation damage (Power & Energy Program) and high strength steels (Uranium Fuel Cycle). Progress has been made in the following areas:

(i) The interpretation of electron microscope images which is largely based on the analysis of images *via* the two-beam dynamical theory of electron diffraction. Over the years we have either developed or adapted a large number of computer programs devoted to this task. During the past year these have been edited and prepared for publication as an AAEC/E report.

(ii) There are two important parameters in the two-beam dynamical theory of electron diffraction:
(a) the extinction distance, and
(b) the anomalous absorption coefficient.
In the past, these parameters have been evaluated from theoretical considerations and, because of experimental diffi-culties, tests of these predictions have been few. This has been rectified by the development of a simple and relatively accurate experimental technique which uses convergent beam electron diffraction patterns obtained with a commercial scanning transmission electron microscope. The experimental work was done on copper which has been studied in greater depth than other metals. The results obtained had sufficient sensitivity to permit critical distinctions to be made between various theoretical approaches. The results have been accepted for publication.

(iii) A study of the electron optical parameters of the scanning transmission electron microscope (STEM) has been made in greater depth. The dependence of the size of the electron probe on lens parameters has been studied by a variety of techniques, involving both direct and indirect measurements. From this work a better understanding has evolved of the optimum operating modes for diverse problems in materials science. The capability of the STEM instrument to obtain diffraction patterns from areas below 20 nm in diameter has proved to be most useful.

(iv) The design of a low cost electronic accessory which, when coupled to a scanning electron microscope, will give automatic measurements of the usual parameters in quantitative metallo-graphy. The logic circuits have been tested and proved by

simulation of typical cases on the IBM360 computer. Construction of the prototype unit has commenced. Scanning electron microscopes are ideally suited to quantitative metallography. There are several commercial instruments available for measuring volume fractions of phases and the number and size distribution of the particles of each phase, but these instruments are highly expensive.

3.4 Materials Division

Positron Annihilation in Defected Solids
(J.T.A. Pollock)

The study of defects in solids using the angular correlation of positron-electron annihilation photons has continued at a low level.

The effect of rolling deformation on the angular correlation characteristics of high purity Ni has been investigated. A 14 per cent increase in the annihilation peak height parameter (APHP) was measured prior to saturation at about 45 per cent deformation. Since rolling of Ni introduces vacancies as well as dislocations, measurements were repeated after annealing at 280°C for 2.5 h. This treatment removes the vacancies but leaves the dislocation structure unchanged. The APHP in annealed samples was found to be only 11 per cent higher than for undeformed Ni. This result implies that the trapping cross section of a vacancy in Ni for a positron is greater than that for a dislocation. Estimates of the dislocation densities present were made using the annihilation data. Values in the range 9×10^9 to 10^{12} cm^{-2} were calculated for the deformation range 5 to 50 per cent. These values are in reasonable agreement with transmission electron microscopy (TEM) measurements, which were complicated by the formation of dislocation cell networks at low levels of deformation.

A study of neutron irradiation damage in high purity Al was completed. This work was complemented by TEM measurements which showed that damage took the form of voids which increased in size and number with fluence. The final results confirm that, despite a 50 per cent increase in APHP, saturation did not occur with increasing fluence up to 3.4×10^{26} neutrons m^{-2}. This behaviour contrasts with that of cold rolled Ni, which is typical of vacancy and dislocation defects. The absence of saturation at fluence levels where large voids (diameter > 50 nm) were present suggested that positronium (a short lived positron-electron bound state) might be present. An experiment was designed and carried out in a 1.2 T magnetic field to detect the presence of positronium. No positive evidence was found.

Publications

Pollock, J.T.A. & Jostsons, A. [1976] – Positron Annihilation in Neutron Irradiated Aluminium. Proceedings of Metals Technology Conference, Sydney, 23rd–27th August, 14-2-1.

4.   ENGINEERING RESEARCH DIVISION

    4.1 Solar Energy (I.F. Mayer, N. Reed, A.K. Ozolins)

    The TERRESSOL project (Total Energy Requirements of a RESidence or
other small energy consuming unit from SOLar energy) in Engineering
Research Division has the dual aims of providing first-hand knowledge of
the problems and possibilities of solar energy while, at the same time,
developing technology to help meet a national energy need. This tech-
nology would most likely be utilised first by isolated consumers in
remote regions where energy costs are highest, but cost reductions
resulting from this experience together with rising costs of conven-
tional energy forms might encourage use in more closely settled regions;
the potential contribution to Australia's energy needs would then be
quite substantial.

    A principal energy supply for a residence must be in the form of
electricity (for lighting, motors, television, etc.). Because photo-
voltaic devices seem likely to remain far too expensive, it is necessary
to devise methods for collecting solar energy at a temperature high
enough to permit conversion to electricity with adequate efficiency.
The research component of the TERRESSOL project has, to date, concen-
trated on this problem.

    A fundamental decision was made to achieve the necessary high
temperatures by optical concentration - the necessary sun-tracking
components being isolated from the effects of wind, rain, hail, dust,
etc., by a transparent enclosure. This decision was made because

    (a) the ratio of direct to global solar radiation is high in
         Australia, particularly in the regions where TERRESSOL tech-
         nology would first be applied;

    (b) concentration of solar radiation before its conversion to heat
         avoids the high costs that are associated with heat transfer
         and transport apparatus when only low heat fluxes are available;

    (c) the large areas of material needed to gather the low solar
         flux can then be made of very lightweight low-cost substances
         (e.g. metallised polyester film) since only photons, not
         fluids, have to be handled by them, provided they are isolated
         from wind, etc., by a transparent enclosure;

    (d) the use of lightweight environmentally isolated concentrating
         devices should result also in savings in the weight and cost
         of their support structures, tracking mounts and drive mechanisms,
         and in the energy consumed in tracking; and

    (e) the alternative method of achieving high temperatures (i.e. by
         reducing heat losses by means of selective surfaces, vacuum
         insulation, etc.) is already being studied extensively by
         other groups in Australia and elsewhere.

    Subsequently it was learned that a somewhat similar concept (viz. a
lightweight, flat reflector in a transparent enclosure) is being studied
by Boeing Engineering Corporation in the USA for a possible heliostat

design for the power tower proposal. Some results from the Boeing work should be applicable to the TERRESSOL project.

In the experimental program, the tracking mount was completed and commissioned with the large ($\sim$ one metre diameter) plastic Fresnel lens, obtained earlier, mounted on it. The energy distribution in the focal region of the lens has been measured, using the thermistor bolometer developed last year. Some improvements to the bolometer have resulted, and considerable experience has been acquired in the operation of a sun-tracking and concentrating device, and in radiometry at high concentration levels (several thousand suns) without the need to purchase commercial instrumentation. This has been consistent with an interim policy of minimising additional equipment purchases for the solar project. This policy has not been unduly limiting in the early learning phase of the project, but undoubtedly future progress would be faster with a more normal equipment purchasing policy.

The experimental work outlined above was carried out in temporary quarters in a rather unsatisfactory location. This situation will shortly be remedied with the provision of more suitable accommodation on the roof of the Engineering Research Building (centre wing, office roof), at present in the design and procurement phase.

In parallel with the experimental work, studies were made of alternative concentrator concepts based on spherical mirrors. (Experiments last year showed that it should be possible to manufacture light-weight low-cost curved mirrors of high quality using metallised polyester film.) In one concept studied, a reflective surface of revolution in the focal region of a spherical mirror deflected rays from various zones of the mirror into a stationary target zone. In one variant of this concept both mirror and deflector would track the sun, while in another, only the deflector would move. A computer program was written to calculate the necessary shape of the deflector. Results showed that the deflector would be rather too long or too wide (depending on mirror aperture) for a promising concentrator configuration.

The concentrator concept currently favoured has some similarities to (but more differences from) the power tower configuration. Several spherical mirrors, each in its own transparent enclosure on the roof of the residence, will concentrate the sun's rays onto a common target region, from whence the light will be channelled to the residence basement *via* a light guide. Present efforts are directed towards analysing the optimum number and size of mirrors, and planning development of the light guide.

In addition to the research just outlined, the technical literature is monitored for developments relative to other elements of the complete TERRESSOL system. The first of these is the diurnal storage system which at present is seen as a tank of melting/solidifying salt in the residence basement, 'charged' daily by the solar energy conducted to the basement in the manner described. During prolonged solar 'outages', or periods of low insolation, the tank would be maintained in its minimum charge state by burning a chemical fuel - probably heating oil initially and possibly locally produced electrolytic hydrogen at a later stage when even this small use of oil becomes too expensive (approximately 10

per cent of the annual energy consumption would come from this back-up energy storage). Several R&D programs overseas are developing molten salt phase change energy storage systems.

Another area of the literature being monitored deals with the development of heat pipes. These will be used in the TERRESSOL system to transfer high grade heat from the molten salt tank to usage points, i.e. cooking facilities, the alternator prime mover, and possibly the heat storage tank of a vehicle (e.g. private motor car) in the garage (see below).

A third area of the literature which is being monitored deals with the development of external combustion engines as alternatives to the present automobile engine. Stirling, Rankine and Brayton cycle engines are being developed overseas because they promise much lower pollution, equal or better fuel economy, and less specific fuel requirements than the spark ignition internal combustion engine. These developments are extremely important for the TERRESSOL project which must have a low cost, highly reliable, externally heated engine capable of rapid response to varying loads, for the conversion of high grade heat to electricity. Furthermore, a vehicle with an externally heated engine could use a tank of molten salt, rather than fuel, as its on-board energy storage. Published studies indicate that such a heat-storage vehicle would offer more than an electric-battery car. The existence of vehicles of this type would enable solar energy to make a contribution to the most difficult energy supply problem, i.e. energy for transportation. For this to be done in a TERRESSOL residence it would be necessary for the salt mixture in the basement tank to have a slightly higher melting temperature than that in the vehicle's tank to permit rapid heat transfer (*via* heat pipe) from one tank to the other (eutectic salt mixtures with constant melting/freezing points are used in these phase change heat storage concepts).

The final element of the TERRESSOL scheme, i.e. use of heat rejected in the conversion to electricity for building heating/cooling and domestic water heating, will use technology that is also under development elsewhere. Again the literature on these subjects is being monitored.

5. ISOTOPE DIVISION

    5.1 Kinetics of Radiolytic Reactions (D.F. Sangster)

    The spectra and reaction rate constants of the transient species produced when N-vinyl pyrrolidone solutions are irradiated have been established over a range of concentrations. This is giving a better insight into the radiation polymerisation reactions of this monomer.

    Further data have been collected on the rates of reaction of a series of substituted phenyl boronic acids with hydroxyl radicals. Analogues of these compounds are used in neutron radiation therapy of brain tumours and it is hoped to provide information relating to the role of the radiolytic products in treatment.

    Using a high resolution grating spectrometer the fine structure of the ultra violet emission from irradiated water vapour has been obtained. The decay characteristics of three transition levels which can

be characterised unequivocally have been measured. Measurements of
quenching rates in the visible region have shown evidence of trans-
lationally 'hot' hydrogen atoms.

Apparatus has been assembled for studying electron trapping and
tunnelling in alkane and alcohol glasses at low temperatures.

It is 'known that crystalline choline chloride decomposes under
irradiation with a G value of several thousand, indicating a chain
reaction. Studies have shown that concentrated aqueous solutions
exhibit similarly high yields and it is hoped to elucidate the detailed
reaction steps.

5.2 Optical Transitions of Transient Free Radicals (N.A. McAskill, D.F. Sangster)

The electronic spectra of the benzyl radical have been extensively
studied over the last 25 years. The main absorption peaks in the ultra
violet region are due to transitions from the ground state of the radical
to two different excited states, designated 2^2A_2 and 4^2B_2. Early workers
failed to observe the latter transition and it was not until 1966 that
this intense peak at 258 nm was observed; however, no agreement could
be reached as to its intensity relative to the 2^2A_2 band at 307 and 318
nm.

An important contribution to the controversy which surrounds the
spectrum of the benzyl radical has been made by submitting benzyl com-
pounds to pulse radiolysis using the 1.3 MeV Van de Graaff electron
accelerator. These experiments showed that the intensity of the 4^2B_2
transition at 258 nm decreased with increasing solute concentration
while the intensity of the other band increased as expected. We can now
explain why some workers failed to observe the 258 nm peak and why no
agreement could be reached as to the relative intensity of the two
absorption bands. It is thought that the population of radicals in the
sub-levels of the ground state from which the 4^2B_2 transitions take
place is affected by a concentration dependent interaction or associa-
tion process involving the solute molecules.

5.3 Publications

Papers

Davison, A. & Sangster, D.F. [1976] – Gamma Radiation Induced Carboxy-
lation of Pyrrolidine. Aust. J. Chem., 29 : 2603.
Davison, A. & Sangster, D.F. [1977] – The Isomeric Distribution of Amino
Acids Produced in γ-Radiolytic Carboxylation of Amines. Aust.
J. Chem., 30 : 807.
McAskill, N.A. & Sangster, D.F. [1977] – Ultra Violet Absorption Spectra
of the Benzyl Radical Formed During Pulse Radiolysis. Aust.
J. Chem., 30 : 2107.

Conference Papers

Cooper, R., Grieser, F. (University of Melbourne) & Sangster, D.F.
[1976] – Excitation Processes in Electron Irradiated Rare
Gases and Rare Gas – Iodine Mixtures. 8th AINSE Radiation
Chemistry Conference, Lucas Heights, November.

Sangster, D.F. [1976] – Possible Alcohol Multimers Involved in Electron
         Solvation. 8th AINSE Radiation Chemistry Conference, Lucas
         Heights, November.
Brown, B.J., Fitch, P.G. (Macquarie University) & Sangster, D.F.
         [1976] – Electron Inductive Effects in the Radiolysis of
         Substituted Phenylboronic Acid Solutions. 8th AINSE Radiation
         Chemistry Conference, Lucas Heights, November.
Irvin, J.A., Quickenden, T.I. (University of WA) & Sangster, D.F.
         [1976] – Electronically Excited Species Produced by the Pulse
         Radiolysis of Water Vapour. 8th AINSE Radiation Chemistry
         Conference, Lucas Heights, November.
Lynn, J.E., Senogles, E. (James Cook University) & Sangster, D.F.
         [1976] – Pulse Radiolysis of N-Vinyl Pyrrolidone. 8th AINSE
         Radiation Chemistry Conference, Lucas Heights, November.
Sangster, D.F. [1977] – Pulse Radiolysis – An Investigational Tool.
         Ions and Radicals in Growth and Development. Royal Australian
         Chemical Institute Symposium, Warburton, Victoria, August.

6.   INSTRUMENTATION AND CONTROL DIVISION

6.1   Electronic Circuit Development (H.J. Fraser, V.E. Church, G.C. Watt)

A 'band gap' voltage reference was developed for portable E.H.T.
power supply applications. This circuit consumes only 4×10^{-6} A from
a nominal 4 V supply and is stable to 15 parts per million per degree
temperature change.

The group has started a familiarisation study of the COSMAC micro-
processor. This study is directed initially to controlling the
technetium-99 production plant and to a longer term development of
portable field instruments (particularly multichannel gamma ray spectrum
analysers) for use such as environmental analysis in the field.

A design study of forced commutated silicon controlled rectifier
three-phase inverters has commenced and a prototype is under construction.
If this design is successful it will be better suited to experimental
work than the load commutated design already in laboratory use.

Some development work has been done on a simple fluorimeter to
support work done by R. Matthews on a chemical dosimeter for the 10-1000
rad range. The feasibility of this project should be known within the
next quarter.

6.2   Computer Hardware (P. Ellis)

Owing to staffing difficulties and the heavy service commitment on
the group, little time was available for research activities. However,
an investigation was made of the various microprocessor systems avail-
able on the market, with a view to standardisation. The conceptual
design for an improved communication link for the Site computer system
was initiated. The proposal employs Synchronous Data Link Control
(SDLC) techniques with a microprocessor based remote station. This
system offers an exceedingly low 'drop out' rate and low cost.

6.3 <u>Techniques for Reliability Analysis</u> (E.R. Corran, H.H. Witt,
     T.J. Moss)

A computer program package has been developed to estimate the
reliability of high integrity systems such as reactor protection systems.
Some parts of these programs have been derived and adopted from codes
used elsewhere, but the backbone of the package, a code to identify the
groups of system components responsible for system failures, has been
developed locally after experiencing problems of computer time and
space with overseas codes, which appear unable to cope with systems of
practical complexity. Further development of the package is concen-
trated on making it easier to use, eliminating opportunities for intro-
ducing error, and optimising the methods of recording and reporting the
results.

Work to review the design approach of the reactor protection system
has led to the identification of principles relating to good documen-
tation, communication between different groups and minimising the time
and effort involved in design and assessment. The compromise between
these needs is difficult to establish, but principles adopted at Lucas
Heights for modification and alteration of reactor installation are in
general agreement with our proposals.

<u>Conference Paper</u>

Corran, E.R. [1976] – An Approach to the Design of Nuclear Plant Pro-
         tection Systems. Statistical Society of Australia, Symposium
         on Reliability – Theory and Practice, Sydney, November.

6.4 <u>Dynamic Analysis Development</u> (C.P. Gilbert, P.C. Miskelly)

In addition to the work on two-phase flow mentioned in a contribu-
tion to the current Power and Energy Progress Report, techniques for the
solution of partial differential equations have been further explored in
the development of a physiological model. Since only one differencing
operation is required, this model is able to exploit the maximum operating
speeds of the patchable logic and mode switching circuits.

Table look-up procedures have been developed for use in problems
involving compressible flow and studies of bearing dynamics.

Further progress has been made with the transfer of the HIFAR
simulator from the obsolescent 231R analogue computer to the hybrid
computer.

7.   <u>HEALTH PHYSICS RESEARCH SECTION</u>

7.1 <u>Acoustic Sounder Meteorological Studies</u> (G.H. Clark,
     E.O.K. Bendun)

The evolution of the atmospheric mixing layer and onset of the sea
breeze are two clearly identifiable features detectable by the acoustic
sounder. In both cases, other experimental studies have shown that the
elevated acoustic echoes are associated with stable temperature inversion
layers which effectively limit vertical dispersion of atmospheric pollu-
tants.

An acoustic sounder has been operating continuously at Lucas Heights since October 1975. On 134 mornings, a rising mixing layer was clearly observed. The rate of rise of the layer was less than 4 metres/minute in 75 per cent of the observations and for 97 per cent of the cases the ascension rate was less than 7 metres/minute. Usually the acoustic sounder cannot detect the full daytime development of the mixing layer because of the intrinsic insensitivity of the technique. Only on four days did a detectable low level (< 920 metres) layer persist throughout the day. In 85 per cent of the cases the echo disappeared within four hours of its initial observation. The statistics of the atmospheric mixing layer will be important input parameters to the atmospheric transport and dispersion codes associated with the new reactor study.

Likewise, statistics on the sea breeze are important for the afternoon atmospheric dispersion processes. Although, in general, sea breeze wind speeds are higher after the passage of the front, at Lucas Heights the average speed rises by less than 1 m s^{-1} to 2.7 m s^{-1}, with an average maximum gust of 7.4 m s^{-1}. The 86 sea breeze days at Lucas Heights also showed a time lag between the appearance of the characteristic acoustic sounder pattern and surface wind changes, a feature also observed in wind profiles at other locations in the Sydney region. On 93 per cent of the days the height of the mesoscale subsidence inversion associated with the sea breeze was less than 800 metres.

During September a balloon-borne atmospheric boundary layer profiling system was taken to Mt Isa, Queensland, for a collaborative research program with Mt Isa Mines Limited. The purpose was to measure profiles of wet and dry bulb temperatures and wind speeds and directions to altitudes of near 600 metres above the ground. These meteorological data are then to be compared with the facsimile records from an acoustic sounder operating nearby.

The AAEC has developed a pattern recognition scheme for interpretation of the acoustic sounder facsimile records. Previously most data analysed using the scheme have been collected in a coastal environment. Mt Isa offers a suitable continental climate for observing contrasting meteorological influences indicated on the acoustic sounder records. These studies will aid the ultimate calibration of the acoustic sounder in terms of quantitative meteorological parameters.

7.2 Diet of *Mogurnda mogurnda* in the Polluted Finniss River
(R.A. Jeffree, N.J. Williams)

The omnivorous freshwater gudgeon *Mogurnda mogurnda* is being investigated for change in composition of its diet with severity of pollution of the Finniss River (Northern Territory) which receives drainage from the Rum Jungle area via the East Branch. *Mogurnda mogurnda* occurs abundantly throughout the Finniss River. Collections taken during the dry season from shallow sites in broad zones known from a previous study to be either polluted or unpolluted, showed that of 39 mutually exclusive categories of foods which were consumed, 19 occurred widely and often enough for statistical comparison of the zones. Adjustments were made for the effect of size of fish on diet for each food separately, and for the effects of time since the end of the wet season, habitat structure, and presence of other fishes. The collections

from the unpolluted zone were used to define the relaticnships.

Hierarchical agglomerative analysis yielded dendrograms which separated the polluted from the unpolluted collections when foods were divided between those obtaining dissolved oxygen with no intervening gas film, and atmospheric or bubble breathers.

Beginning with the set of 19 foods, individual foods were successively eliminated to yield a set of 14 foods from which a dendrogram more clearly separating the collections from the two zones was derived. This reduced set of 14 foods may be regarded as a package of indicator species in the diet. A single iteration was performed using the dendrogram as an 'improved' or *de novo* classification of the polluted and unpolluted collections; this interpretation was supported by known local conditions observed at the times of collecting the fish originally. New dendrograms clearly distinguished the *de novo* groups of collections. Collections from Florence Creek, a perennial unpolluted tributary stream fell within the *de novo* unpolluted group.

Discriminant function analysis was used to quantify the contributions made by the types of food towards predicting polluted/unpolluted differentiation along a linear scale. The statistical significance of the discrimination was very much greater for the *de novo* division of collections than for the initial division. For the *de novo* classification of polluted and unpolluted collections, Ephemeroptera, Gerridae and Dytiscidae discriminated well by their greater abundance in the unpolluted collections. Insect pupa and Copepoda discriminated well by their greater abundance in the polluted collections. Discriminant function analysis was also used to obtain sets of foods which discriminated between the *de novo* polluted and unpolluted groups of collections at different stages through the dry season. Ephemeroptera and Chironomidae were important predictors of pollution throughout the dry season, with Copepoda and Cladocera increasing in importance as predictors as the dry season progressed.

The polluted and unpolluted zones of the Finniss River are characterised by the relative abundance of dietary components. Both individual taxonomic and broad physiological categories reflect this zoning.

The wide variety of foods consumed, the lack of differentiation in dietary pattern between zones when only foods occurring in the East Branch were used, and the change through the dry season in the indicator-value of certain foods (some foods remaining predictive, others changing in predictiveness), are all arguments supporting the interpretation that differences in behaviour of the *Mogurnda mogurnda* resulting from pollutant stress are at most a minor factor in the zonal differences in diets.

The results of this study – the collections for which were not taken with this study in mind – suggest that *Mogurnda mogurnda* or other species which consume a wide variety of foods can be used as samplers of available foods so that overall patterns of faunal and habitat differences can be detected.

8. APPLIED MATHEMATICS AND COMPUTING DIVISION

   8.1 Introduction and Summary

   The Applied Mathematics and Computing Division has four divisional
research projects: approximation techniques in numerical analysis,
distributed computer networks, interactive computing and graphical
representation, and computer operating system design and optimisation.

   A joint collaborative effort between the Applied Mathematics and
Computing Division and the University of Tokyo has resulted in a highly
efficient implementation of the new general purpose programming language
PASCAL for IBM360 and IBM370 computers. This implementation, containing
excellent run-time diagnostic facilities, is particularly suited to
university and research use. At the time of writing, over forty requests
for the version developed at the Commission have been received from
Australian and overseas establishments.

   The Interdisk project, to give alternative access to the central
computer's disk storage, is well advanced. A test module has been
developed and proved, circuit diagrams are being drawn, and the neces-
sary printed circuit boards for the final version are being laid out.
It is hoped to begin full-scale testing of Interdisk later this year.

   The Datercom terminal communication system has been extended to
give fuller support to display terminals. Features have also been added
to allow a later, more general, network communication. Network diag-
nostic programs have been developed and enhanced.

   Mathematical modelling has clarified the nature of the diffusion of
inflammatory products near lung artery branch point lesions. Windowing
techniques for using limited capacity dynamic display screens in computer-
aided circuit design are being developed.

   Considerable work has been done, with the cooperation of the
Metropolitan Water Sewerage and Drainage Board (MWS&DB), in developing
program portability across the various IBM360 and IBM370 operating
systems. This experience will be important in any upgrading of the
central computing facility.

   8.2 Approximation Techniques in Numerical Analysis

      Mass Transfer Between Tissue and Blood in Arteries
                      (M.R. Davidson)

   In a report written in 1975, Dr A.D. Tucker and his co-w.   ·'s
traced the development of a lesion across the tip (apex) of the
flow divider of a 600 μm diameter artery of the rat lung. The lesion
develops as a result of tissue breakdown from the outer aspect of the
artery wall initiated by the proximity of an inflammatory lymph node.
As a result of the formation of a cleft through the wall, interchange
between tissue fluid and blood occurs.

   A theoretical study has led to the development of a simplified
model of the diffusion of inflammatory products to account for the
localisation of the lesion. Prior to the formation of the cleft,

diffusion is controlled by wall permeability which is known to depend on wall shear stress. It is proposed that the variation in wall shear and hence permeability near the apex is an important localising factor in the formation of the lesion. Later, when the artery wall is broken, diffusion is enhanced by the local blood flow and the absence of the wall barrier. Diffusion calculations have been made to predict the increase in the flux of inflammatory products resulting from the breaking of the wall. These calculations have particular relevance to a proposal by Tucker that the wall gap permits the injection into the blood of antibodies from the lymph node, thereby providing an economical and rapid defence to infective invasion.

Specific detailed calculations were performed to analyse flow near a high curvature stagnation point. Particular body geometries, the parabola and hyberbola, were considered. The results indicate that, although the local skin friction decreases initially as the curvature increases from zero, the overall trend is for skin friction to increase with increasing curvature.

Natural Convection in a Box
(M.R. Davidson)

Numerical calculations of natural convection in a box involving finite difference approximations to the flow and temperature equations in three dimensions are being made. Particular care must be taken in the choice of approximation and in the treatment of boundary conditions. Preliminary calculations have prompted a study of possible difference schemes which, for the method used, numerically conserve heat and energy when the boundary conditions are correctly treated.

Least Squares Pre-processor for BMDX85
(A.P. Browne (Vacation Student), J.M. Barry)

A program for performing non-linear least squares analysis, BMDX85, using a Gauss-Newton method, has associated with it a pre-processor to perform function differentiation and to generate FORTRAN subroutines for differentiation.

The BMDX85 pre-processor was modified in this period to allow correct use of error functions. The program was extended to allow users to express their non-linear model in terms of simpler sub-expressions. This will greatly assist users to test new formulations.

Rotating Compressible Flow
(G.W. Peady)

Work proceeded on the solution of the problem of flow in rotating compressible fluids using finite elements but the solution has not been obtained. Several changes were made to the solution techniques but none so far have proved successful.

8.3 Distributed Computer Networks

Interdisk Developments
(J.M. Tobias, D.J. Richardson)

Considerable progress has been made towards attaching the PDP11/03

computer to the disk storage control units. The logic needed to handle the data transfers to the 11/03 core from the disk controllers, and *vice versa*, has been established and circuit diagrams have been drawn.

The three-word data path between the PDP11/03 and PDP11/45 is being utilised more heavily than expected, and software conventions have been established to enable each computer to read and write the other computer's memory. Such conventions will be replaced in the final model by an inter-memory window between the PDP11/45 and the PDP11/03, similar to the window currently operational between the PDP11/45 and the PDP11/40.

Facilities to enable Interdisk to operate with both IBM360 and IBM370 control units have been incorporated in the design.

Perhaps the most significant development has been the completion of a simplified 'test bed' module that enables approximately half the full range of disk control commands to be executed. This module enables commands such as seek, set-file-mask, reserve, release and sense, to be executed.

The PDP11/03 was connected to the two control units and this module and the line protocols were extensively tested. A control program was written for the PDP11/03 that enabled the commands to be tested in succession and in any order.

Owing to the ability of this program to signal overlapped seeks, it was possible to have all ten disks, from both control units, continually performing seeks with the IBM360 continuing with normal processing.

A great deal has been learned from the development of this module as regards conventions and timing requirements. Several changes have been made to the design of the final prototype as a result of this experience.

Printed circuit boards for the final version are now being laid out by the Digital Systems Group. It is pleasing that no major problems have been encountered during the design phase, and it is felt that the interface holds a great deal of potential for the network as a whole.

Enhancements to Dataway Diagnostics
(J.M. Tobias)

Several new features have been incorporated into the Dataway diagnostic program. A version was written to run on a VT11 display without the use of a teletype. This enables the diagnostics to be used on the Physics Division batch station via the GT40 graphics terminal.

Four additional diagnostics were added, and several options were extended. For example, speed of transfer is now selectable from the front panel switch register of the computer, and the amount of data involved in the transfer has been doubled.

The diagnostics have proved useful in diagnosing faults in control and interface units of the Centrifuge Enrichment Development and Physics Division batch stations, the Noise Analysis Laboratory, the PDP11/40 and PDP11/45 in the computer room, and the Neutron Physics computer system.

The Dataway Terminal Communication System
(P.L. Sanger)

Modifications were made to the DATERCOM system to

- include some new mathematical functions in ACL mode;
- provide lower case to upper case input translation;
- reduce polling overheads;
- implement a new error correction strategy for the SMUT system;
- include checksums with blocks of data transferred with ACL Load and Save requests;
- allow the control/P character to terminate conveniently non-ACL mode activity;
- allow ACL programs to be saved in and loaded from a private library;
- support password validation from the modem terminal;
- give an 8K limit for ACL work space;   and
- allow the Backspace character on Teleray display terminals to be used to delete input characters.

Changes were also made to allow DATERCOM to be used to call up variable Dataway addresses using the non-ACL mode $nXYZ type command, and this will allow terminals to communicate with software to be developed for other network computers.

PDP11/03 Program Development
(J.M. Tobias)

Several programs were written both for stand alone use and for inter-communication with the PDP11/45 computer.

A version of FOCAL was implemented on the PDP11/03 computer, involving modification of a PDP11/40 computer version. This programming tool is now used by AINSE on its PDP11/03 computer.

8.4 Interactive Computing and Graphical Representation

Computer-aided Circuit Design
(J.M. Tobias)

Although it has been established that the GT40 graphics screen of the satellite computer is very restrictive as to the amount of data that can conveniently be displayed at any one time, methods are being investigated to overcome some of these difficulties.

One task is that of making the screen a 'window' into a much larger drafting board (nine times the screen size). With the use of the light pen and function keys, it is possible to 'move' the window around the board, and so view various sections of the drawing under composition.

The main problem with this approach is that of displaying elements that fall across a window edge. At present, elements are only displayed if their initial drawing position is within the window.

With the use of the light pen, the circuit designer can correct, delete, rotate, move and replace circuit elements, as well as save and

restore completed diagrams.

8.5 Computer Operating System Design and Optimisation

IBM370 Operating System Experience
(G.W. Cox)

The MWS&DB relies heavily on the AAEC-developed AEMOVE utility program which now operates successfully on their IBM370/158 computer under the SVS (single virtual storage) operating systems. The more advanced MVS (multiple virtual storage) operating system has been under test for some time now at the MWS&DB, and some changes in AEMOVE have been required for successful operation in this environment. Collaboration with the MWS&DB has enabled the areas requiring change to be identified, and has enabled the Commission to gain considerable experience with the IBM370 operating systems SVS and MVS.

Such experience is important in enabling us to keep abreast of some of IBM's latest developments in operating system technology, and will prove most valuable in assessing future computing requirements for the Commission.

Operating System Command Languages
(C.B. Mason)

Continuation of a research project commenced at the UKAEA Culham Laboratories led to the preparation of a paper on recent developments in operating system command languages. This was presented at a Seminar on Programming Language Systems held at the Australian National University in February 1977. Research on this topic is continuing with greater liaison with overseas research groups. Particular attention will be paid to the possibilities of a generalised command language for the Commission's distributed computer network.

PASCAL Language and Compilers
(C.B. Mason)

As part of a growing interest in the PASCAL programming language at the Commission, further efforts were made to develop the PASCALJ (Janus) Compiler, developed at the University of Colorado, as an exercise in program portability. Much more work needs to be done before this aspect of the compiler can be realised.

The PASCALJ compiler is written in PASCAL and has proved a good test vehicle for the implementation of the PASCAL-8000 compiler, origin- ally obtained from Japan.

Development of a New PASCAL Compiler
(G.W. Cox, J.M. Tobias)

PASCAL is a general purpose programming language proposed and defined by Professor N. Wirth, Zurich, about 1970. Its principal emphases are the provision of ample data structuring facilities as well as making available sophisticated control structures suitable for 'structured programming'.

A great deal of interest has been expressed in PASCAL by computing communities around the world, and it is heavily used by universities as a tool for the teaching of computer science. Unlike FORTRAN, COBOL and other more popular scientific and business languages, PASCAL has not had the support of the major computer manufacturers; for this reason, commercial organisations have been slow to appreciate its advantages and to seek to use it.

PASCAL was originally implemented on CDC computers, and more recently, subsets of the language have been implemented on other computers. There have been several attempts to develop a PASCAL compiler that executes on IBM360/370 computer systems; however, all of these have either failed to implement the language as originally defined, or have provided poor operational characteristics.

After collaboration with Tokyo University, an IBM360/370 PASCAL compiler has been developed that not only fully implements the PASCAL language, but also provides many powerful extensions. Further, its performance is eminently suited to a production environment. The present system evolved from a compiler developed at the University of Tokyo that executed on a HITAC computer - a machine not unlike an IBM370. This compiler was adapted for IBM operating systems and has been heavily modified and extended within the AAEC, and all restrictions of the original compiler have been removed. The result is an elegant and efficient software system that, for the first time, enables IBM users to gain access to the sophisticated programming facilities provided by the PASCAL language.

Two versions have been developed. The first is a load-and-go system that produces object code in an internal form. The second system produces IBM linkage-editor compatible object decks, and these can therefore be linked together with externally compiled PASCAL, FORTRAN and Assembler routines.

Completely new run-time support has been developed for both systems, and these have been written completely in IBM assembler language. The run-time systems load and initialise compiled code, perform I/O, and generally control and assist the execution of the code produced by the high-level PASCAL program, remove any local files that were opened, and give post-mortem dumps of variables if execution is terminating owing to an erroneous condition.

The compiler source (itself written in PASCAL) was also heavily modified. The compiler size was substantially reduced, and the code optimised in several areas. Several new language features have been incorporated, and code-producing areas of the compiler were completely rewritten for the linkage-editor version. The fact that the compiler is written in PASCAL makes the whole process of compiler modification and testing far less cumbersome than if another language were involved.

The PASCAL system is currently operational at the Research Establishment. Extensive testing is being performed under the operating systems SVS and MVS on IBM370/158 computers at the MWS&DB.

Many organisations and universities in England, USA, and other parts of Australia have requested copies of the system. It is being

distributed to organisations that will use it for non-profit purposes, and a small distribution fee is being charged.

An extensive compaign to encourage computer users on Site to write programs in PASCAL will be initiated.

8.6 Publications

Reports

Sanger, P.L. [1977] – Terminal Facilities Provided by the DATERCOM
System. AAEC/E409.

Conference Papers

Mason, C.B. [1977] – Operating System Command Languages – Some Recent
Developments. Presented at a Seminar on Programming Language
Systems, ANU, 24–25th February.

Tobias, J.M. [1976] – INTERDISK – An Interface for Dual PDP/11, IBM360
Computer Access to IBM360 Disk Storage. Presented at a
Colloquium on Microprocessor Systems, Sydney University, 15–
16th November.