Fulmer Newsletter

contract research and engineering in materials and process technology

No. 54 January 1985

MATHEMATICAL MODELLING

Mathematics is one of the expanding areas of activity at Fulmer. Over the past few years there has been increasing demand for our exceptional capability to combine engineering and materials technology expertise with mathematical modelling skills. In addition, we have found that we are undertaking an increasing number of projects in which the main emphasis is on the mathematical modelling aspects themselves. This growth reflects a general trend brought about by the increase in the power and availability of computers, and shows a growing awareness of the potential benefits of mathematical modelling and simulation.

ARTICLES ARE INCLUDED IN THIS NEWSLETTER WHICH REVIEW SOME OF OUR WORK AT FULMER IN THE MATHEMATICAL MODELLING FIELD. WE ARE PARTICULARLY EXCITED ABOUT THE ANALYSIS WITH UNCERTAIN QUANTITIES TECHNIQUE, WHICH WE FEEL WILL ALLOW THE INCREASED POWER OF NEW COMPUTER TECHNOLOGY TO BE USED TO GAIN A GREATER DEPTH OF UNDERSTANDING AND INTERPRETATION FROM MATHEMATICAL MODELLING SOLUTIONS.

A mathematical model is an extremely versatile tool which can be used to explore, analyse and design in all branches of technology. A precise definition of what constitutes a mathematical model is difficult to achieve. Nowadays, the concept is inevitably linked with the computer, but there are usually distinct mathematical and computational aspects to a model, and many mathematical modelling exercises are carried out with pen and paper only. The factor which distinguishes mathematical modelling is the interpretation of physical processes and actions in mathematical language, making appropriate and justifiable simplifications along the way. The questions which are required to be answered by modelling need to be clearly identified, as well as the precision to which answers are required. Mathematical and computing skills are then used to produce information, which is interpreted by the modeller to give answers which are expressed in the same physical terms as the original questions.

The benefits of mathematical modelling vary from case to case. They include:

- optimisation of new product designs
- assessment and improvement of existing products and processes
- prediction of performance without costly prototyping.
- prediction of failure without destructive tests
- rapid answering of "what if ...?" questions
- simulation of extended running in compressed timescales
- extension of experimental data where instrumentation is not possible.

At Fulmer, our wide range of expertise and experience allows us to tackle all aspects of a mathematical problem. The only feature which our problems have in common is their diversity, a fact which should be remembered when reading about particular studies and methods in the following pages. We have pride in our ability to adapt to any new problem – perhaps we can solve yours!

FINITE ELEMENT ANALYSIS

The Finite Element Method (FEM) will be familiar to most engineers, and many others, as a method for obtaining solutions to stress and displacement calculations in structural analysis. Although it started life as an adhoc procedure for these calculations, it has now been given a rigorous mathematical foundation, and is used in the numerical solution of a very wide range of problems.

This spectrum of applications is reflected in Fulmer's experience in the use of FEM. Some recent studies include:

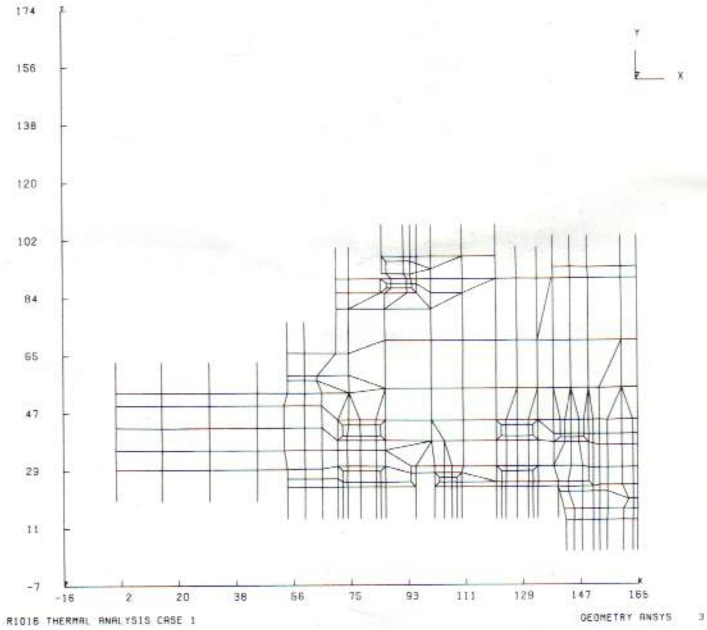
* Design of composite structures using beam elements in an optimised configuration.
* Thermal analysis of double glazing units, involving comparisons of the performance of different "thermal break" materials and of different designs of extruded aluminium frame sections.
* Analysis of ballistic impact data to produce information on the stress and strain patterns in the large deformations in a material following such impacts. This work has involved the treatment of severe mathematical and numerical difficulties inherent in the modelling of large deformations of this type.
* Confirmation of the validity of an approximate method for calculating the shear stiffness of a composite beam with a complex cross-sectional structure.
* Analysis of a reinforced pressurised vessel to choose the best compromise shape for the end cap.

FEM work at Fulmer is carried out at present on large external mainframe computers, using a graphics terminal connected to the telephone network. Each new problem receives detailed consideration to choose which of the many available FEM packages is appropriate. The two packages currently favoured are ANSYS for general purpose work and DYNA2D for highly specialised large deformation impact analysis – this package is on the frontiers of present day computing capabilities. There is also experience of using the C.E.G.B. package, BERSAFE, and of developing new elements for it. As far as possible, output is obtained in computer-generated graphical form. Input can be converted from graphical to numerical form by using a digitiser. At Fulmer, it is possible to draw on mathematical expertise to ensure correct operation of the FEM packages, and on engineering and materials experience to interpret the results.

Other well-established applications of FEM potentially available at Fulmer include:

* Investigation of crack growth in fracture mechanics.
* Study of diffusion in porous media, e.g. the seepage of water through soil.
* Prediction of electrical stress in insulators.
* Calculation of natural frequencies of structures and their response to cyclic or transient disturbance.
* Micro-stress analysis of composite materials.
* Calculation of transport of material in fluid flows.

The field of FEM analysis is a rapidly changing one, driven by new concepts such as the Boundary Element Method and by increases in computer power. An important future development at Fulmer will be the acquisition of an in-house FEM facility, allowing an expansion of the volume of routine work. However, it is envisaged that advanced packages on external computers will always be required for the most specialised applications.



Finite element mesh for thermal analysis of double-glazing

Further Information: Simon Jones
John Denison
Bruce Moxley
Fulmer Research Laboratories

INTERNATIONAL CONFERENCE ON MODELLING UNDER UNCERTAINTY

An international conference on modelling under uncertainty will be held at Fulmer Grange Conference Centre on 17th and 18th April 1986. This conference will provide an interdisciplinary forum for the discussion of methods of analysing uncertain situations.

Further information: Simon Jones
Fulmer Research Laboratories

SEMINARS

Project Planning and Control for Research Managers

2E 500/127 29-30 Apr.'85
2E 500/128 3-4 June '85

The seminar fee is £275 (+ VAT for UK participants) inclusive of accommodation and meals.

Further information from D.G.S. Davies, Fulmer Research Institute Ltd.

AUQ: MODELLING UNDER UNCERTAINTY

Why bother with uncertainty?

Most situations are uncertain, many extremely so. Mathematical modellers, in building their descriptions of processes and systems, need to represent this uncertainty and work out its implications for the decision maker who will use their results. This is equally true whether the problem under study is technical, commercial, economic or scientific. If modellers ignore uncertainty, their results will often mislead, sometimes seriously.

What is AUQ and how does it help you?

AUQ (Analysis with Uncertain Quantities) is a technique developed at Fulmer and unique to us. It enables the modeller to incorporate uncertainties into his specification of the problem and to find out which of them matter. It provides the user with probabilistic information on the quantities of interest to him and reveals the key areas where resources should be deployed to give maximum reduction in uncertainty and in the decision maker's risk.

What is the AUQ view of a problem?

In AUQ, we discuss problems in terms of uncertain quantities (UQs) such as:

- The maximum speed of Concorde
- The total UK market for toothpaste in 1999
- My age at death
- The mass of the earth

and uncertain answers to qualitative questions (uncertain classifications) or (UCs) such as:

- Will any hydrogen be used as an energy vector in the UK in the year 2000?
- Which party will win control at the next election?
- Did Richard murder the princes in the Tower?
- Is lattice diffusion the predominant sintering mechanism in aluminium oxide?

OUR STATE OF KNOWLEDGE ABOUT THE UNCERTAIN SITUATION UNDER DISCUSSION CAN BE EXPRESSED AS A PROBABILITY DISTRIBUTION OVER THE UQs AND UCs. THIS IS THE BAYESIAN VIEW OF UNCERTAINTY AND IS THE VIEW ADOPTED IN AUQ. THE ESSENCE OF AUQ IS THE BUILDING OF A SELF CONSISTENT STATE OF KNOWLEDGE IN WHICH OUR ESTIMATES OF THE QUANTITIES ARE RECONCILED WITH THE KNOWN RELATIONSHIPS BETWEEN THEM.

The AUQ process consists of four steps:

1) MODELLING The quantities and classifications relevant to the problem are identified and the relationships between them are defined, usually in the form of a FORTRAN routine. Relationships in the model may include random processes as well as deterministic ones. Approximate models and rival scenarios can also be used.

2) ESTIMATION The quantities and classifications are expressed as UQs and UCs by assigning probability distributions to them. Many options are available. For example, we might choose to express our knowledge of the yield strength of a given alloy as a normal distribution with expectation 150 MN/m^2 and standard uncertainty 5 MN/m^2. As another example, if we had to estimate the time taken to repair a particular machine, we might choose to give the most likely value, say 1 hour, and a 90% confidence interval, say 0.5 to 3 hours.

   Sometimes the uncertainties in two quantities are related. If average earnings next year are higher than expected then the sales of video recorders are also likely to be higher than expected. AUQ provides facilities for specifying this type of concordance.

3) RECONCILIATION The initial state of knowledge compiled from the estimation process is then constrained to obey the relationships defined in the model. Reconciliation produces a revised probability distribution expressing a state of knowledge consistent with the model.

4) REPORTING In the reporting state the revised state of knowledge is summarised, tabulated and plotted according to the users needs and interests. There will usually be a few key quantities of interest and AUQ will produce probability distributions for these. Just as important is sensitivity information. Suppose that a decision maker is interested in the market for a new product in the U.K. in 1990. This quantity may be highly uncertain. Fashion, prosperity, rival technologies, government regulations and a host of other factors on which it depends can only be specified with great uncertainty. AUQ sensitivity analysis will identify those few key quantities which have the major effect in limiting precision in the sales estimate.

What problems have been tackled so far?

In early trials, a prototype AUQ system was applied to two project appraisal problems. The projects concerned were in the area of process development, one concerned with the production of capital goods and the other with consumer goods manufacture. AUQ proved to be effective in highlighting the key questions determining project viability.

More recently the AUQ system has been used for a major techno-economic forecasting exercise: predicting the use of hydrogen as an energy vector in three European countries to the year 2025. This hydrogen energy model involved over 150 uncertain quantities and classifications. Not surprisingly, many of the predictions for the 21st century were highly uncertain but it was possible to identify the key uncertainties limiting our knowledge of hydrogen usage and to rule out its use in certain application areas.

The latest applications of AUQ has been to a complex military system. This has a large number of uncertainties associated with weather, logistics, human operator problems and computation approximations as well as hardware performance and reliability. AUQ has identified the key uncertainties limiting system performance and the opportunities for its enhancement.

How can you get advice on modelling under uncertainty? David Davies or Simon Jones at Fulmer Research Laboratories will be glad to help.

APPLICATIONS OF MATHEMATICAL MODELLING

Fulmer has applied its mathematical modelling skills to a very wide range of problems, sometimes in close liaison with experimental research and production, and sometimes expanding into wholly new areas. This article gives some idea of the diversity of the work, and draws attention to the areas in which Fulmer has particular expertise.

The majority of the projects mentioned here involved the use of our in-house computing facilities – a Perkin-Elmer minicomputer and numerous microcomputers. For larger problems, bureau mainframe computers are used. In some cases, general-purpose programs are used, but most involved the writing of our own software, which is an integral part of many mathematical modelling studies. An interesting point is that the computer power required for some complex problems can be surprisingly small when they are amenable to mathematical analysis.

The following is a list of some interesting recent studies:–

1. The development and analysis of target training systems using acoustic sensors.
2. Analysis of the thawing and freezing of thermal storage material.
3. Fitting equations to experimental results.
4. Designing (in composite materials) a specialised aircraft component with an exacting mechanical specification.
5. Automatic computer analysis of readings obtained during impact testing of plastics.
6. Search for a relationship between composition and properties of high-temperature alloys.
7. Prediction of future consumption of a commodity from past and present values.
8. Analysis of the transient heating of an electronic device when passing through an oven.
9. Design of filament-wound tubes.
10. Computation of the composition of the product, and other properties, throughout the copolymerisation of a mixture of several monomers.
11. Investigation of cooling-rates during continuous casting of metal.
12. Study of the random packing of powders prior to sintering.
13. Study of the propagation of sound waves in the atmosphere.
14. Modelling of stress waves in rods and other axisymmetric bodies.
15. Optimisation of section shape for an extruded aluminium structure.

The following table shows some of the mathematical techniques used in each of these investigations, and the size of computer required.

	STRESS ANALYSIS	DEFLECTION ANALYSIS	THERMAL ANALYSIS	FINITE DIFFERENCES	OPTIMISATION	POLYNOMIAL FIT	CUBIC-SPLINE FIT	SMOOTHING	MONTE-CARLO SIMULATION	STATISTICAL ANALYSIS	EIGENVECTORS	VECTOR ANALYSIS	DIFFERENTIAL EQUATIONS	INTEGRATION	COORDINATE GEOMETRY	ALGEBRAIC EQUATIONS	MINI COMPUTER	MICRO COMPUTER
1					o					o		o			o	o	*	
2			o	o									o				*	
3						o	o	o									*	*
4	o	o											o	o		o	*	*
5													o					*
6						o		o									*	
7						o	o	o									*	
8			o	o									o					*
9	o	o														o		*
10									o	o	o					o		*
11			o	o									o			o		*
12									o	o					o	o		*
13					o				o			o	o	o	o		*	
14	o																	*
15	o				o											o		*

Further information:
John Denison
Simon Jones
Fulmer Research Laboratories

COMPUTERISED COPOLYMERISATION

Many industrial polymers are produced by copolymerisation of two or more monomers, each contributing to the overall properties and/or functionality of the final product. A uniform distribution of monomers in the chain is sometimes important, particularly in the so-called speciality applications. For example, styrene/butadiene, ethylene/propylene are elastomeric copolymers. Acrylonitrile/butadiene/styrene (ABS) is a high impact terpolymer. Ethylene/vinyl acetate copolymers are used in hot-melt adhesives and emulsion adhesives. A whole family of acrylic copolymers are produced for the paint, cohesive and building industries. Thus a range of properties can be achieved by a simple variation of the monomeric ratio.

When a mixture of two or more monomers (usually liquids or gases) are copolymerised with a free-radical initiator, their rates of addition to the growing polymer chain are governed by their relative reactivities. These are expressed as reactivity ratios r 1, r 2 etc. and depend on the molecular structure of each monomer. In an attempt to quantify the relationship between the molecular structure and monomer reactivity ratios, the so called Q, e scheme was proposed, Q being a measure of resonance and e the polarity of the double bond (each monomer contains at least one carbon to carbon double bond in its structure).

Starting with styrene as a "reference" monomer (the most commonly used monomer in the polymer industries), reactivity ratios have been determined from its copolymerisation rates with other monomers and many such values have been compiled over the years. The mathematical complexity of the system increases rapidly with the number of monomers used. Whilst the reaction of two monomers (binary system) can be easily calculated from the copolymerisation equation, a ternary system involves nine reactions occurring simultaneously and the calculations become very cumbersome. In recent years, with the advent of computers, mathematically minded polymer chemists with assistance from mathematicians and computer experts, have developed copolymerisation programs based on various mathematical models.

Mathematicians and polymer chemists at Fulmer have developed their own suite in BBC Basic, mainly for their own use in various copolymerisation projects. A few examples overleaf illustrate the practical use of the "computerised copolymerisations".

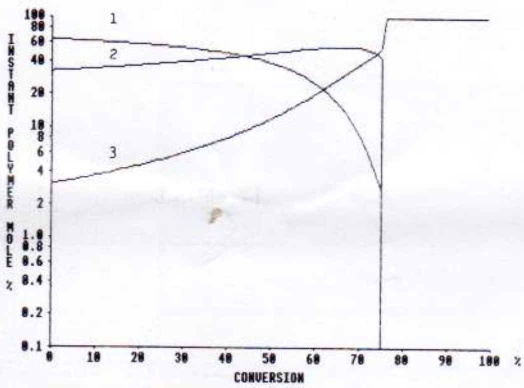
1. Synthesis of Hydrogels

The name hydrogel is applied to a hydrophilic polymer gel plasticized with water. It is used to manufacture soft contact lenses, antimist coatings, medical prostheses, special adhesives etc. HEMA-based copolymers (hydroxy ethyl methacrylate) are usually crosslinked, which makes them dimensionally stable and insoluble in water.

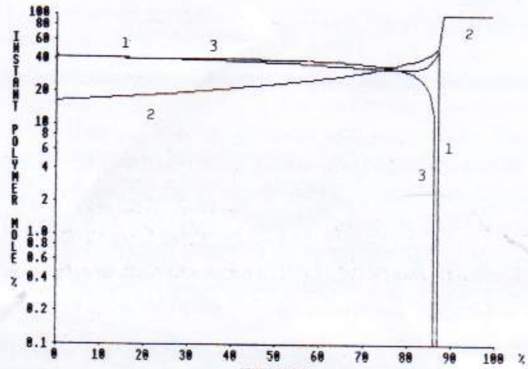
There is a need, however, for a thermoplastic hydrogel without crosslinks, which could be moulded, extruded or cast from solution as a thin film. Instead of crosslinking, the solubility of the copolymer in water can be reduced by copolymerisation with a hydrophobic monomer. A third monomer is usually introduced, which can be a functional monomer for subsequent crosslinking or "curing", or a "bridging" monomer which improves both the reactivity and compatibility of the system (the latter is particularly important for optical clarity).

Using our computer programs, a whole series of terpolymer systems from various commercial monomers can be quickly evaluated, even before any practical work is carried out (cf. below). In half-an-hour the results of computerised "copolymerisation" are known and the most promsing system can be selected.

HYDROGELS



INSTANT POLYMER MOLE %HEMA/MMA/VP TERP



MMA/VP/AA TERP

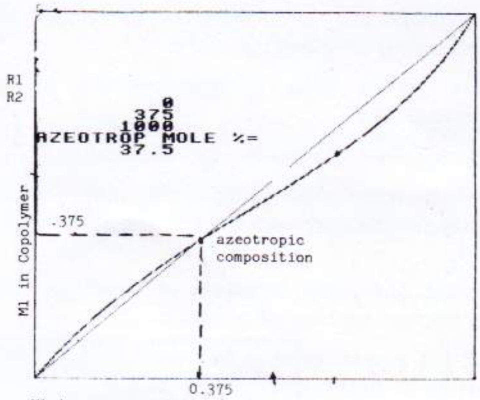
2. Synthese of Polymer Electrolytes

A similar approach has been adopted for selecting suitable monomers for polymer electrolyte synthesis. As it happens in this case the monomer selection is very limited and in order to obtain a uniform copolymer of pre-determined composition the less reactive monomer is then reacted at the ratio calculated from the computer print-out.

3. Synthesis of Piezoelectric Copolymers

The copolymers are made from gaseous monomers under high pressure, in a closed system. Controlled addition technique is not easy with such a system. Therefore, for a uniform copolymerisation, it is necessary to work close to the "azotropic" composition (cf. below). The distribution of monomers along the chain can be calculated.

PIEZOELECTRIC COPOLYMER

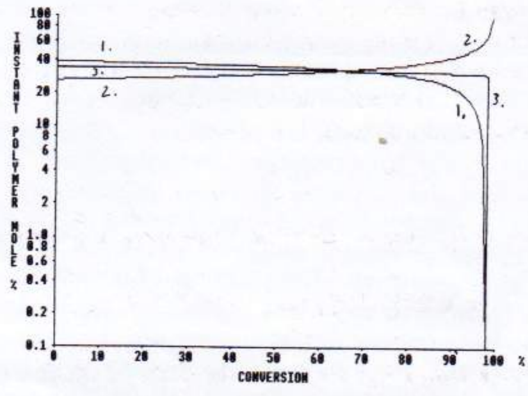


M1 in monomer mixture
Piezoelectric Copolymer P1-2 Inst. Polymer

4. Desalination Membranes

Yarsley Technical Centre developed terpolymers for desalination membranes by reverse osmosis (R.O.). The work was carried out some years ago using a systematic experimental trial and error approach. We have recently applied the computer programs to various systems and it was interesting to note that the best system gave very uniform monomer distribution (cf. diagram).

DESALINATION MEMBRANES



INSTANT POLYMER MOLE %ST/MMA/MAA TERP

CONCLUSIONS

It is our belief based on some experience that the use of computers in polymerisation work has an enormous potential for the future, particularly with the proliferation of cheap micros. Many properties of the copolymers could in future be predicted, such as molecular weight distribution, viscosity, transition temperatures, physical properties etc., even before any practical work is carried out. Our work on copolymerisation has already brought some tangible benefits for the clients, whereby the costs have been slashed by making preliminary computer predictions and thus eliminating unpromising systems.

We offer a consultancy service based on our suite of programs and we would also welcome an exchange of ideas with others working in this new and exciting field.

Further information: Victor Mikucki
Yarsley Technical Centre (Ashtead)

YARSLEY QUALITY ASSURANCE ACCREDITATION SERVICE

Yarsley Technical Centre, listed in the Department of Trade and Industry Directory of Quality Assurance Consultants, have launched a Quality Assurance Registered Firms Scheme which is supported by the Department of Trade and Industry. Accreditation is given to firms which have Quality Managements Systems that conform to the requirements of the relevant part of BS5750. Assessment to meet these requirements is a pre-requisite of any accreditation scheme supported and accepted by Government. The support gained by Yarsley follows the publication of the Government White Paper on Standards, Quality and International Competitiveness, produced by the Department of Trade and Industry in 1982 and forms part of the National Quality Campaign. Further details on the YQAF scheme from Reg Easy Yarsley Technical Centre (Redhill).

WHAT CAN THE BUILDING INDUSTRY LEARN FROM OTHER MANUFACTURING INDUSTRIES?

This was the theme at a recent Association of Building Component Manufacturers (ABCM) Forum for Young Managers. Two members of Yarsley Technical Centre presented papers giving their individual views on the Subject and a precis of their papers is given below. The paper by R. Fryer was placed second by the Committee out of a total of 8 entries, and the one by E. Soja came third. Both authors stress the need for on-site quality control and assurance.

"I consider that there are two major areas in which the building industry can learn from other industries. The first of these relates to quality assurance of building components and materials. The second, is the assessment during construction and completion of structures for their "Fitness for Purpose", especially related to on site supervision of work.

The component manufacturers themselves should follow other industries in respect of quality assurance. It is their responsibility to prove, by testing, that their goods meet specifications; at the present time a few do, but many more should. But more than this, they should ensure that their goods are monitored on a regular basis for quality, and not have just a "one off" series of tests performed. They should insure their product against failure and have on-site investigation to assess the conformity to installation instructions and procedures. On site conditions are very basic, sometimes dirty and not congenial to producing a high standard of workmanship. In these circumstances, it is essential that all phases of construction, are inspected for correct installation and application.

Is it thus, not feasible then, that an organisation be set up within the ABCM the organisation representing all members of ABCM. The organisation would appoint an inspector to each major site, this appointee would be briefed on all the varied components which the building will use. His task would be to observe the delivery, storing, installation and correct functioning on site, and, report any deviations from correct procedure." (R. Fryer)

"One major area where perhaps comparison can be made and lessons learned, is the control of component material input and assembly. The components used, which in their own manufacture may have been subject to some form of control, may then be treated in a haphazard way once they have arrived on site. Apart from problems of storage which can occur, especially with materials arriving too early and with no suitable storage area being provided, the way in which the building components are used can vary from what their manufacturer had intended, and would depend on the builder's experience of the product.

In the manufacturing industries it is assumed that in the production of materials the manufacture is carried out by unskilled labour with Quality Control being carried out by other competent persons. But in the building industry it is the opposite where it is assumed that the builders have an understanding of their materials and will automatically do their own form of Quality Control without external supervision. Prefabricated structures may not be erected correctly and final making good can hide from view, and inspection, many a poorly assembled work. Hence the current disquiet concerning high rise buildings. The final performance of buildings is poorly defined and rarely tested, the end user seldom knows how the building should perform in every way. The original design sets some of the performance characteristic such as sound insulation, thermal insulation, fire resistance or weather tightness of the building, but this is only an expression of intent, the actual in situ performance can be quite different."

(E. Soja)

NEW FACES . . . .

John Gent

John Gent who was with the Van Leer R. & D. laboratories as Senior Scientist at their Hampshire Laboratories has joined the Yarsley Technical Centre at Ashtead. He has been involved with R. & D. and production in the Van Leer Group in both the packaging and insulation fields, working throughout W. Europe and the U.S.A. His recent experiences are in the production of metallised paper, film laminates and fibre drums. Previous experience includes insulation foams having low fire hazard, corrosion resistant linings for steel drums and rotational moulding of large containers. He obtained his degree in Chemistry at Bristol University and then worked on silicones for 2 years at Barry, S. Wales before joining Van Leer.

FULMER RESEARCH INSTITUTE LTD.

Stoke Poges, Slough, SL2 4QD, England.

DIVISIONS

- **Fulmer Research Laboratories Ltd.** (Tel: Fulmer (02816) 2181: Telex 849374)
- **Fulmer Technical Services** (Tel: Fulmer (02816) 2181: Telex 849374)
- **Fulmer Components Ltd.** (Tel: Slough (0753) 35996): Telex 849374)
- **Yarsley Technical Centre Ltd.**
  Trowers Way, Redhill, Surrey RH1 2JN (Tel: Redhill (0737) 65070: Telex 8951511)
  The Street, Ashtead, Surrey KT21 2AB (Tel: Ashtead (03722) 76391: Telex 8951511)

Fulmer Overseas:

Fulmer Research & Development (Singapore) Pte. Ltd.,
520, Balestier Road,
Singapore 1232 Telex 23988

I.D. Conseil, Paris:	776-4201
Fulmer-Skandinavien, Stockholm:	08-755 7773
DJK International Inc, Tokyo:	03 (585) 8131
DJK International Inc. USA:	203 644 8057
OTO Research Cor., Tokyo:	03 (371) 6121
K.J. O'Connor Assoc. Virginia, USA.	703-75-7488