Commission of the European Communities

Needs for strategic R&D in support of improved energy efficiency in the processing industries

Views of research experts

Report

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energy

Needs for strategic R&D in support of improved energy efficiency in the processing industries

Views of research experts

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MANAGEMENT SUMMARY

In Stage 1 of this survey 23 industrial organisations representing the 8 major energy-intensive sectors of the process industries were interviewed to ascertain their views on priority areas for strategic R&D which could lead to improved energy efficiency in the process industries. Several fields emerged as having widespread industrial interest in the possibility of international collaborative research with CEC support.

In Stage 2 further interviews have been conducted with 42 leading experts, mostly in universities and research institutes, who are at the forefront of research in the priority fields identified in Stage 1; a list of these experts is given in Appendix B of this report. Through these interviews it has been possible to define more precisely what pre-competitive research needs to be done in each of these fields, what the main application areas and energy efficiency benefits are likely to be, and what the strength of Europe's current research position is in these fields compared to other parts of the world.

In all the areas surveyed there are many opportunities for strategic R&D which is likely to lead to improved energy efficiency and consequential pollution abatement in the process industries. The principal needs and opportunities highlighted by the experts are summarised below.

Chemical reactors

* Novel reactors with lower energy consumption than conventional reactors.

* Improved models for hydrocarbon cracking furnaces and multi-phase reactors to facilitate design and operation for maximum energy efficiency per tonne of product.

Low energy separation processes

* Selective adsorption

  - Development and design of novel adsorbents for specific applications.

  - Novel configurations for truly continuous adsorption.

  - Improved engineering models for equipment design.

* Melt crystallization

  - Improved scientific understanding of crystal nucleation, growth and purification kinetics.

  - Engineering models for equipment design and exploration of new equipment concepts.

* Supercritical extraction

  - Better prediction of phase equilibria for mixtures in the critical region.

  - Mass transfer models for equipment design.

* Liquid-liquid extraction

  - Better design and scale-up methods and adaptive control schemes for column contactors.

Furnaces, kilns and ovens

* Advanced 3-D modelling of fluid dynamics, heat and mass transfer and chemical reactions.

* Development and testing of novel equipment concepts.

Dryers

* Novel process and equipment concepts.

* Better drying kinetics and engineering models for improved dryer design.

Process intensification

* Intensified evaporators and reactors.

Advanced 3-D flow modelling

* More comparison of model predictions with laboratory and field experiments.

* Improvements in grid generation techniques, visual presentation of predictions, turbulence modelling and particle/fluid interaction modelling.

Dynamic simulation of complex systems

* Improved computing strategies and optimal trajectory calculation methods.

* Better thermodynamic property prediction methods for highly non-ideal mixtures.

* Dynamic modelling of interaction of compressors, turbines and pumps with each other and with other components of large process plant systems

Simulation of batch systems

* Methodologies for batch process synthesis, extending energy and process integration concepts to batch processes and evaluating trade-offs between energy integration, plant utilization and flexibility.

* Batch process dynamic simulator.

* Design criteria for thermal utility systems using a single heat transfer medium for heating and cooling.

Expert systems for process control and production management

* Evaluation of rule-based closed loop expert systems for a wider range of plant and processes.

* Improvements to current types of system, eg incorporation of real time, methods for validating sensor inputs, and assessing situations in the face of uncertainty.

* Systems comprising tunable, user-friendly combination of a process model, a control model and a heuristic model.

Advanced on-line sensors

* Small, rugged, non-invasive sensors based on laser, ultrasonic, microwave or nuclear techniques, especially for measurements of chemical composition and/or particle size distribution in hostile environments.

* Improved film sensors or flow injection analysis sensors for chemical composition measurements.

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INTRODUCTION

The process industries, excluding steel, account for about 50% of industrial energy usage in the EEC. The largest of these in terms of energy consumption is chemicals, followed by non-metallic minerals, food and drink, paper and printing, non-ferrous metals and textiles. The distribution of energy consumption by industrial sector in the EEC member states in 1984 is shown in Table 1.

The EEC is anxious to help these industries improve the efficiency with which they use energy. The purpose of the present study is to ascertain what strategic R&D needs to be done in support of this objective. Since energy consumption and pollution are frequently linked, the implications for pollution abatement are also considered.

The study is being conducted in two stages. In Stage I the views of industry on strategic R&D needs were sought. The result of that exercise was a set of recommended areas for in-depth discussion with research experts, reproduced here as Table 2.

In Stage II a further series of interviews has been conducted with leading researchers, primarily from Universities and Research Institutes, who are acknowledged experts in the priority topics listed in Table 2. The objectives of Stage II were to define more precisely what research needs to be done on these topics, what the main areas of application and energy efficiency benefits are likely to be, and what the strength of Europe's current research position is in these fields compared to other parts of the world. This document is the report on Stage II.

The method adopted for the survey was as follows:

- a letter (reproduced as Appendix A) was sent to the researcher concerned. This letter set the scene for the subsequent visit.

- a visit was made to the expert and a discussion was held based on the letter.

- a record was made of the discussion and the record agreed between those concerned.

Appendix B presents a complete list of the experts consulted. A reference code is given for each, which allows the origin of comments cited in the report to be identified.

CHEMICAL REACTORS

In the chemical industries the heart of every process is the reactor. Substantial improvements in the energy efficiency of the overall process can be made by improving product yield and selectivity in the reactor, or by reducing the temperature or pressure at which the reactor is required to operate. A common way of achieving such improvements is the development of improved catalysts, which is already a priority theme in another CEC programme and will not be considered further here. However, significant improvements to energy efficiency are also possible through the development of novel types of reactor or refinements of existing types. It is this theme of novel or improved reactors with which we are concerned here. Attention is focussed primarily on continuous chemical reactors, because it is the continuously operated bulk chemical plants which are the largest consumers of energy in the chemicals industry.

Europe has a strong research tradition in chemical reaction engineering and its expertise is at least the equal of that in other parts of the world. There is no shortage of ideas among leading European researchers, most of whom have strong links with the chemical industry.

The following ideas were put forward for novel chemical reactors.

a) Chemical reactors with simultaneous reaction and separation of the desired product, eg by selective adsorption, membrane separation or distillation (2A, 2K, 2P, 2V). This would enable equilibrium - limited reactions to be driven to completion in a single pass, thereby avoiding recirculation of unreacted feed materials. The concept has been demonstrated on a small pilot plant scale for methanol synthesis (2V); a techno-economic comparison with the conventional process showed a 75% reduction in circulation energy, a 50% reduction in cooling water requirement, a 25% increase in steam produced for export and a 5-10% reduction in raw materials consumption per tonne of product. Other potential applications are ammonia synthesis (overall energy saving of 5-10 tonnes of natural gas per 100 tonnes of ammonia) and consecutive processes where immediate removal of the desired product can prevent loss by further reaction (eg maleic anhydride production).

b) Novel reactors which permit the concentration of reactants to be increased substantially, thereby reducing the energy demand for separations and recycling (2V, 2k). An example would be partial oxidation reactors, where the oxygen concentration has to be kept well below the stoichiometric limit to avoid the risk of an explosion. Elimination of ethylene recycle on a 100,000 tonnes per year ethylene oxide plant would save energy worth £2.5 million per year (2V). It was suggested that one way of achieving this would be to have a pure hydrocarbon feed and supply the oxygen on a solid catalytic carrier which would be circulated for external reoxidation (2k).

c) Low pressure drop monolithic catalytic reactors for chemical process reactions, particularly for operations involving large amounts of recycle (2A). This type of reactor is used for emission control on car exhausts, where low pressure drop is essential to avoid impairing engine efficiency, but it has not yet been applied on the large scale in the process industries. Compared to packed bed catalytic reactors, monolithic reactors have a much lower pressure drop per unit reactor volume but may require a greater reactor volume to achieve the same conversion. The net saving in pressure drop is typically in the range 20% to 50%. In addition to operations involving a large recycle of unreacted feed, the concept is also potentially applicable to after-burners on waste incinerators, eg for destruction of PCBs.

d) Photo-reactors use light instead of heat as their energy source. Compared to conventional reactors, they can offer very high selectivity and increased yield together with substantial energy savings through operation at ambient temperatures (2A). However, the need to use glass in their construction limits them to reactions carried out at moderate pressures, and another expert thought that they would not become economic until there is a drastic change in the price of electricity relative to fossil fuels (2P). Potential applications include removal of NOx from exhaust gases, photo-polymerisation, photo-oxidation for selective synthesis of high-value organics and destruction of low levels of organic pollutants in water.

The most likely route to improvement of convential types of reactor was felt to be development of improved mathematical models. These would permit more precise optimisation of design and improved simulation of existing reactors. On large throughput energy-intensive reactors, even marginal improvements in efficiency can yield substantial energy savings. The areas where the greatest gains were thought to be possible are as follows.

a) Hydrocarbon cracking furnaces (2K, 2W). Here the need is to integrate advanced furnace simulation models with advanced cracking reaction models. The objective would be greater selectivity for the desired product through optimal tailoring of the heat flux profile.

b) Multi-phase reactors (2P, 2W, 2V, 2X, 2e, 2k). The principal need is for improved understanding of the hydrodynamics of multi-phase reactors, particularly the prediction of interfacial area. Multi-phase reactors include trickle bed reactors, sparged or agitated bubble reactors, 3-phase fluid bed reactors, spray reactors and liquid-liquid reactors.

The experts interviewed generally had good links with the chemicals industry. There is informal contact between several of them but not structured coordination. Coordination between industry and universities or research institutes was seen as the most effective way of achieving major goals, eg pilot-scale development of novel chemical reactor concepts or the development of advanced simulation models in areas such as cracking furnaces and multi-phase reactors. Consistent and coordinated CEC support could be very important in facilitating such cooperation through reducing the financial risk to industry.

LOW-ENERGY SEPARATION PROCESSES

Selective Adsorption

Selective adsorption is an energy-efficient alternative to distillation for separation of gases and light hydrocarbons, breaking azeotropes, separating isomers and other close boiling liquids and recovery of alcohols from dilute aqueous solutions. Compared to distillation, energy savings are in the range 30%-90% for such applications. Other uses of selective adsorption are for the removal of toxic chemicals and other pollutants from aqueous and air streams, and the recovery of solvents and vapours.

Selective adsorption is an area where there has been intense research and development activity in the USA and Japan in recent years and these countries currently enjoy a lead over Europe in commercial applications. However, Europe has some good centres for adsorption research and is starting to catch up.

Most of the experts interviewed thought that the most important pre-competitive research goal is a methodology for designing new adsorbents for specific applications (2A, 2K, 2N, 2b, 2e). This will require:

- improved prediction of multi-component adsorption equilibria and kinetics from single-component data;

- improved knowledge of the relation between effective transport properties and adsorbent structure;

- improved understanding of adsorption forces.

Advances in these areas would aid tailoring the selectivity of adsorbent materials to the needs of the process by controlling their structure and their chemical composition. New adsorbent forms are also expected to be developed, for example adsorbing fibres (2K) and adsorbing membranes (2A).

Current adsorption processes are usually semi-batch in nature, with two or more adsorbent beds in series going through successive cycles of adsorption and regeneration. This leads to high capital cost, high adsorbent inventory and complexity in operation. Attempts to develop a truly continuous adsorption process in the past have involved continuous transport of solids between adsorption and regeneration vessels, with severe problems of adsorbent attrition and breakage. A truly continuous adsorption process which did not involve with fixed beds of solids or solids transport between vessels would be very welcome (2A). Such a process might conceivably follow the development of tubular adsorption membranes. Alternatively, if advanced adsorbents could be made more resistant to attrition and breakage, fluidised and moving bed processes for continuous adsorption would become practicable (2A).

The cost of modern highly selective, high capacity adsorbents such as molecular sieves tends to be very high and this can adversely affect the economics of selective adsorption. Application of the process would be aided greatly if new high selectivity, high capacity adsorbents could be developed from low cost raw materials (2A, 2N, 2b).

The design of fixed bed adsorbers still tends to be fairly empirical, reflecting the uncertainties in current engineering models. Improved models are required for regeneration kinetics (2A, 2R), multi-component non-isothermal adsorption (2A, 2b) and rapid cycling pressure swing adsorption processes (2A, 2e). Also mentioned were the complete lack of models for moving bed adsorbers (2b) and the importance of accurate modelling of the fluid flow distribution in both adsorbers and regenerators (2D).

There are a substantial number of university groups engaged in adsorption research in Europe and European chemical companies are increasingly active. However, there is no structured collaboration between researchers in what ought to be a multi-disciplinary effort and CEC support could be instrumental in achieving this. The need at present is seen to be mainly for bench-scale and small pilot scale research. Hence, since the resources available are likely to be limited they would be better spent on supporting a number of comparatively modest projects rather than, for example, building a large and expensive pilot plant. Researchers in adsorption have a particular need for advanced instrumentation, eg for in-situ measurements of chemical composition and surface phenomena; it was noted that such instrumentation can be very expensive.

Melt Crystallization

Melt crystallization is an energy-efficient way of separating and purifying organic compounds having melting points between -50°C and +200°C. The energy consumed is an order of magnitude lower than for distillation, due to the latent heat of fusion being much lower than that of evaporation and much less reflux being required. Typical applications could be the separation and purification of dinitrotoluene, fatty acids, maleic acid, adipic acid, phenols and naphthols. Purification of raw materials for the polymer industry is economically promising. Melt crystallization is ecologically beneficial compared to crystallization from solution because there is no waste liquor for disposal. However, its industrial applications have been hampered by high capital costs and poor equipment reliability; also, lack of basic knowledge means that equipment suppliers have had to use an empirical approach to design for new applications, sometimes with disappointing results.

Research in melt crystallization in the EEC countries is centred in the Netherlands and Germany. Elsewhere in Europe, the Swiss firm Sulzer has established a leading commercial position. There is comparatively little work in the USA, but in recent years Japan has become very active in this area with four research centres and four major industrial organisations well supported financially and materially. Europe currently has the largest number of industrial applications of melt crystallization, but considering the Japanese effort this could well change in the future.

The development of good engineering models of the process, based on scientific understanding of the phenomena involved, would greatly improve the reliability with which melt crystallization equipment can be designed and scaled up. There is a particular need for better understanding of the influence of system chemistry on crystal nucleation and growth kinetics, and of sweating and recrystallization (2S, 2T). Progress is hampered by lack of a crystal size measurement technique which can make rapid in situ size measurements (typically 200 micron crystals in a 20-30% slurry). It would also be very helpful if solid-liquid phase diagrams could now be predicted theoretically in the way that vapour liquid-equilibria are predicted (2T).

One disadvantage of melt crystallization is that if the mixture to be separated is a eutectic system, the yield of pure compound is limited. For example, if the mixture comprises materials A and B, melt crystallization will give pure A plus an A/B eutectic, which limits the yield of A. Ideas are needed for separating the A/B eutectic (2T).

Supercritical Extraction

This is a separation process which was invented in Europe and found its first industrial application here (the extraction of caffeine from coffee using supercritical carbon dioxide). While there is still a certain amount of research going on in Europe, in recent years a much bigger effort has been mounted in the USA and Japan and these countries are now more advanced than Europe in several aspects.

In comparison with Liquid-Liquid Extraction, using a supercritical fluid has advantages for both regeneration of the solvent and increased rate of mass transfer. In the region of the critical point of the solvent, both temperature and pressure have a significant effect on the solubility of species in the solvent, so that small changes in temperature and/or pressure can change solubilities by a factor of 100 or even 1000. Thus, the solvent can easily be regenerated by letting down the pressure by a small amount, and if this is done in stages a selective deposition of different solutes can be achieved. High mass transfer rates between the phases are achieved because a supercritical fluid has a low viscosity (close to that of a gas) and a high mass diffusivity (between those for a gas and a liquid). The main disadvantage of supercritical extraction compared to liquid-liquid extraction is the pressures used which are high enough to make the construction of large equipment expensive.

Commercial applications to date include the extraction of caffeine from coffee beans with supercritical carbon dioxide, increasing the recovery of crude oil from porous rocks with supercritical carbon dioxide or nitrogen, and extraction of lube oil extract from vacuum distillation residues with a supercritical light hydrocarbon.

Improved energy efficiency is not the usual reason for development of a supercritical extraction process, although it may sometimes be an added benefit. For the chemicals industry the main attraction is the very high selectivity the process can achieve in the separation of solutes from complex mixtures. It is particularly suitable for the separation of large molecular weight, heat-sensitive materials for which distillation would have to be under vacuum. The use of non-toxic carbon dioxide is a strong attraction for the food and biotechnology industries.

The most important research need is for <u>better methods of predicting phase equilibria for mixtures near the critical point of the solvent</u> (2K, 2M, 2R, 2f). This is crucial to process conception, development and design and at present virtually all new advances in this area originate in the USA. Work is also needed on improving our understanding of the action of "<u>entrainers</u>" (additional components, usually with volatility intermediate between that of the extractant gas and the material to be extracted, which improve the dissolving power of the gas) (2R). Finally, there is an urgent need for the development and experimental testing of <u>mass transfer models</u> for the most common phase contacting devices used with supercritical solvents (2K, 2R); this information is needed for contacting equipment design and scale-up, and currently it is not known whether it is possible to use extensions of conventional approaches or whether a completely new approach is required.

<u>Liquid-liquid Extraction</u>

Liquid-liquid extraction is a well established process for selective separation of solutes from liquid mixtures. The mixture is contacted with an immiscible solvent in which the desired solute preferentially dissolves, and then in a separate vessel the solvent and the extracted solute are separated by distillation and the solvent returned for re-use. If there is a large difference in volatility between the solute and solvent this distillation will be easy and the overall process may require less energy than the alternative of a batch distillation operation or a sequence of continuous distillation columns. However, capital costs may be higher, equipment design methods are less well established and an expensive solvent may have to be used. The main applications to date have been for selective extraction of aromatics in oil refineries, extraction of high molecular weight materials in the fine chemicals industry and separation of fission products in nuclear fuel reprocessing. The food and biotechnology industries are showing considerable interest for extraction of heat-sensitive materials.

Europe has a strong research tradition in liquid-liquid extraction. Both Japan and the United States are thought to be behind Europe in this area, where we maintain a significant competitive advantage (2J).

Two principal research needs were identified. These were adaptive control systems for liquid-liquid extraction columns and improved methods of design and scale-up based on bench scale characterisation tests (2J). In both cases the fundamental pre-competitive research requirements are similar. These are;

- better understanding of the fundamental physics of mass transfer, droplet breakup and droplet coalescence;

- better understanding of the role of surface impurities in bench-scale characterisation tests;

- development of models for the hydrodynamics of mechanically agitated contactors to allow scale-up from bench tests to full-scale equipment;

- practical selection techniques for solvents based on thermodynamic models of phase equilibria.

It was noted that the proposed work on column hydrodynamics is likely to require advanced flow modelling computer programs and advanced optical sensor techniques for measurements in two-phase liquid-liquid mixtures.

The main beneficiaries of this research were thought likely to be the fine chemicals and pharmaceuticals industries. Greater certainty in equipment design and scale-up, better simulation models and adaptive controllers for multi-product plants would speed up the penetration of liquid-liquid extraction technology in these industries. Energy savings could result if it replaced vacuum distillation. There could also be pollution abatement benefits through the use of liquid-liquid extraction for the purification of effluents.

FURNACES, KILNS AND OVENS

Equipment such as glass-making furnaces, brick-making kilns, cement kilns and baking ovens are very energy-intensive. A common theme which emerged from discussions with several experts was that more energy-efficient designs could be anticipated from the appropriate use of advanced flow modelling techniques to examine alternative process and furnace configurations (2D, 2X, 2a, 2d). The models should be 3-dimensional and should include fluid dynamics, heat and mass transfer and chemical reaction models where appropriate. It will be particularly important to compare their predictions with good quality experimental data obtained either on pilot plants or full-scale plants. Advanced laser diagnostic techniques are likely to be required for obtaining such data. If successful models can be developed, this would facilitate the answering of "what if" questions and would enable computer-aided exploration of novel energy-saving equipment and operational concepts.

Other research needs mentioned by individual experts were:

- development of improved methods of preheating glass furnace raw materials using waste heat from the furnace exhaust gases (2X, 2a);

- development of an expert system for glass furnace control (2a);

- improvements to the design of cement kiln cyclone preheaters to reduce the fan power required (2Q): (NB This is already the subject of two projects within the CEC Energy Conservation Programme).

- exploration of new energy-saving baking oven concepts (2U). (NB This could require the use of advanced flow modelling [Stage I, Interview 1P]).

Energy savings in the region of 18% for glass-making furnaces and 25% for baking ovens were quoted as predictions of what could be achieved by new designs based on improved fundamental understanding and modelling.

DRYERS

Drying accounts for at least 10% of the energy consumption of the chemicals industry (2m). It also accounts for a substantial amount of energy usage in the other process industries considered in this survey. Europe currently has a leading position in drying research, but there is increasing activity in North America and Japan.

About 90% of current industrial dryers are of the convection type, using hot air as the drying medium. The greatest source of energy inefficiency is the wasted heat in the exhaust air. There would be significant energy savings by using superheated steam as the drying medium in a total recycle system (2R). Such dryers would also have environmental advantages through reduced emissions and good fire and explosion protection. However, they could not be used for heat-sensitive products because of the high dew point of superheated steam; this would severely restrict their use in the food industry, but there could still be wide areas of application in other process industries. A commercial dryer of this type has been developed in Sweden for drying forest products. Research in this area is planned at the University of Karlsruhe.

Contact drying can offer energy reductions over convection drying, through eliminating the exhaust air. Vacuum contact dryers with closed loops are also more contained and environmentally secure. Research into equipment design has advanced considerably in this area over recent years and it is now more a matter of applying this knowledge in industry (2R). However, contact dryers usually have a higher capital cost than convection dryers because of the relatively low heat transfer coefficient between the heating surface and the moist material. Novel equipment concepts which overcome this problem would make contact drying more economically attractive and hence contribute to improved energy efficiency. One such concept is the vacuum fluid bed dryer containing immersed heating coils, which has been proved on the bench scale but now requires pilot scale testing (2g).

There is still a considerable need for improved models of conventional types of convection dryer such as spray dryers, rotary dryers and pneumatic conveying dryers (2m). Better models will allow dryer designers and users to explore a wider variety of options, leading to plant which is closer to the optimum from an energy efficiency and capital cost viewpoint and which has a reduced risk of failure (2R, 2m). Better models will also lead to improved control of dryers (2m).

CEC support would benefit all the highlighted areas of research. For research involving the development of new equipment concepts it would reduce the risk to industrial companies involved. For research on dryer modelling and control, CEC support could lead to a more coordinated programme of work, thereby avoiding duplication and shortening the timescale for achieving results.

PROCESS INTENSIFICATION

Process intensification is the name given to miniaturisation of chemical plant in order to reduce capital costs, save space and, in certain cases, reduce inventories of hazardous materials. The resulting equipment is usually radically different to conventional equipment, so implementing it outside the laboratory may have considerable risks attached at first. This has hindered application of the technology.

Two areas were identified as having the potential for improving process industry energy efficiency. The first of these is intensified evaporators. A centrifugal evaporator has been invented which is like a conventional falling film evaporator turned on its side with the heat exchange plates spinning about a central axis. Dilute feed is introduced at the centre of each plate and is flung outwards by the centrifugal force, evaporating as it goes, with the concentrated liquor being collected at the rim. Since the centrifugal force can be many times the acceleration due to gravity, the liquid film can be much thinner than in a conventional falling film evaporator, leading to a much higher heat transfer coefficient (2E). Exploitation of this improved heat transfer performance could typically lead to a doubling of the number of effects in a given temperature interval for a multi-effect evaporator, or a halving of the pressure increase required over the compressor in a vapour compression evaporator. Some fundamental work has been done on fluid dynamics and evaporation from thin films on spinning discs, but much more work is needed along these lines to optimise the design. The time is now also right for construction of a small pilot unit (2E).

The second area is innovative intensified reactors. As examples, one of the experts proposed intensified smelting reactors for sulphidic minerals using pure oxygen or oxygen-enriched air, and plasma processing reactors for the treatment of recycled dust or metallurgical residues or for primary smelting operations (2i). These intensified reactors would operate at much higher temperatures than conventional reactors, thereby achieving high reaction and heat transfer rates. In turn, these would permit high feed rates and very short residence times with reduced complexity, improved energy efficiency, improved environmental characteristics and reduced capital cost. Mathematical and physical modelling of these complex intensified processes is urgently needed.

Europe has been the pioneer in developing process intensification concepts for the chemical industry, but there is now a real danger that the first commercial applications will occur elsewhere. European industry is generally unwilling to fund the development of radical new equipment without substantial help from external funding agencies such as the CEC. Such help is essential to get over the "activation energy barrier" (2E). In the metallurgical field, innovative processes appear not from Europe, USA or Japan but from relatively small countries with highly advanced primary metals industries, eg Finland, Canada and Australia (2i).

ADVANCED FLOW MODELLING

A number of areas have been identified in this study as being likely to benefit from advanced flow modelling using the methods of computational fluid dynamics. In general, these are high temperature processes with fluid flow patterns which are likely to be both turbulent and highly complex. Examples include intensified reactors, furnaces, kilns and ovens. Improvements in all of these systems relative to performance, fuel economy and environmental impact depend on increasingly detailed understanding of the interplay between the complex fluid flows, heat and mass transfer and chemical reaction. Accordingly, several experts in advanced flow modelling were consulted to discover what research is needed for computational fluid dynamics codes to be applied successfully and with confidence to these types of equipment.

The main needs were seen to be the following:

- improved grid generation techniques to facilitate modelling of complex geometries (2C);

- comparison of model predictions with field or laboratory measurements;

- improved visual presentation of predictions to facilitate comparison with experimental data (2C);

- multi-grid solvers to speed up solution procedures (20, 2j);

- more advanced modelling of fluid turbulence (20, 2D);

- more advanced modelling of the interaction of particles with turbulent flows and with containing walls, and particle behaviour at high particle concentrations (20, 2j).

The advanced flow models must be coupled with advanced process models and, in many cases, advanced combustion models (2W). Powerful computers are needed for carrying out the model calculations and advanced laser diagnostics techniques are usually required for the acquisition of realistic experimental data on operating plant. The benefits from such work would arise in two main ways (2C);

- through enabling designers to answer "what if" questions which could lead to improved designs and facilitate the development of novel equipment concepts;

- through helping to solve operating plant problems which may be having a deleterious effect on energy efficiency and environmental control.

It was estimated by one expert that application of successful models to the afore-mentioned equipment could result in energy savings of 20% - 30% in many cases together with reduced levels of NOx and particulates in exhaust gases. (2d).

This area of research is likely to advance rapidly over the next decade due to rapid increases in computing power and rapid advances in the non-invasive instrumentation required for experimental data acquisition. There is considerable European activity in advanced flow modelling at the moment but it is poorly coordinated and there is very little work published on process industry applications other than combustion (2C). There is a major computational fluid dynamics effort in the United States but it appears to be directed largely at aerospace problems. Japan is starting to get active in this area and an important feature of the Japanese work is their better visual presentation of model predictions. Europe has the opportunity to gain a world lead in the application of computational fluid dynamics to process engineering problems, but this will only be achieved if there is a sustained and coordinated attack on the problems by several centres acting in collaboration. Consistent and coordinated CEC support would be extremely valuable in securing this collaboration.

DYNAMIC SIMULATION OF COMPLEX PROCESSES

Considerable advances have been made in the past decade in the development of computer programs for steady state simulation of complete processes and dynamic simulation of single plant items. With the rapidly increasing availability of cheap computing power, industry can see benefits in extending the range of dynamic simulation to groups of plant items and even complete processes.

Dynamic process simulation will improve energy efficiency by the following means:

- defining optimal control schemes to maintain a process at the desired set point;

- defining optimal trajectories for control variables in discontinuous processes, or for moving as efficiently as possible from one optimal steady state to another following a change in a continuous process, eg a change in feedstock;

- training operators in the most efficient handling of critical situations such as alarms, breakdowns and emergency shutdowns.

A case study was quoted in which the time required for a plant in a oil refinery to reach steady state after a change in crude feedstock was reduced from thirty hours to two hours by application of an optimal control scheme developed using a dynamic simulation package (2G). Dynamic simulation can also result in pollution abatement through reduced production of off-specification material while the plant is being restored to the optimal steady state or moved from one optimal steady state to another.

Some research needs which were identified in order to achieve these goals were as follows:

a) Improved computing strategies for reducing computing time, including use of parallel computing techniques. This will permit more complex processes to be simulated at reasonable cost and more realistic models of distributed systems such as tubular reactors and adsorber beds to be used (2G, 2f).

b) Methods for calculating the optimal trajectory of a system between two steady states (including start-up and shut-down), taking account of the practical constraints such as product quality, equipment limitations and safety (2C, 2G, 2Y).

c) Improved mathematical techniques for optimisation, expecially for handling large sets of equations involving both integer and continous variables as well as discontinuities and a large number of non-linear constraints (2G, 2Y).

d) Better thermodynamic property prediction methods for highly non-ideal mixtures, eg solutions of polymers, electrolytes and polar gases. At present there is considerable uncertainty surrounding these predictions and this will lead to corresponding uncertainties and errors in the dynamic process simulation predictions (2f).

e) Dynamic modelling of the interaction of compressors, turbines and pumps with each other and with other system components, eg vessels, pipelines, etc (2c). This is a neglected but potentially important area of control system design. A good dynamic model would be of value in sizing system components, staff training (awareness of system response) and accident prevention ("what happens if" simulation). The current approach to these problems is to be conservative, which often leads to over-sized plant operating at part-load far from the point of maximum efficiency.

Europe is currently at least the equal of the USA and is ahead of Japan in the field of dynamic process simulation (2G). European university research in this area tends to be well supported by industry, which regards it as an important field. Certain of the university teams have developed proprietary dynamic simulation packages which are being sold commercially. This accelerates the penetration of the techniques into industry but it introduces an element of competition between the university teams which could hinder efforts to achieve an international coordinated collaboration unless several teams agreed to work together to develop a common product. This would appear to be advantageous in the case of the smaller teams and CEC support could help promote it.

SIMULATION OF BATCH SYSTEMS

Batch operations account for about 20% of energy use in the chemicals industry. Some of this will be in comparatively large single-product plants such as those for bulk polymer production. The remainder will be in what can be broadly classified as the fine chemicals sector.

The fine chemicals sector is currently the fastest growing part of the chemicals industry in Europe. It consists mainly of small multi-product plants producing comparatively low tonnages of high added-value materials. The keynote is flexibility, with the same plant probably being required to produce several different chemicals during the course of the year. Energy is a much smaller proportion of the manufacturing cost than is the case for large, continuously operated bulk chemical plants, so energy efficiency tends to be neglected in fine chemicals manufacturing.

Research attention at present is focussed mainly on optimising production schedules and developing optimal control schemes for individual plant units, eg reactors, distillation columns etc. In itself this will probably have a beneficial effect on energy efficiency through improving plant utilisation and shortening heating times. However, more can undoubtedly be done.

The research needs identified by the experts interviewed are summarised below.

a) Extension of the concepts of energy and process integration (pinch technology), which have been fully developed for continuous processes, to batch processes (2I, 2n). This will require a new analysis taking full account of variation of process conditions with time, and also a new methodology for evaluating trade-offs between energy integration, plant utilisation and flexibility. The benefits in energy terms would probably be greatest on bulk batch plants producing relatively large quantities of low-added product such as edible oils and bulk polymers (2n).

b) A methodology for synthesis of new batch processes, where energy efficiency will be one of the factors taken into account systematically.

c) A batch process simulator based on experimentally verified dynamic models of individual plant items (2c). Ideally this should be linked to production scheduling algorithms for optimisation of equipment utilisation, and to expert systems for process and equipment selection and design. This would allow a much more rapid assessment of process and plant design alternatives from the energy efficiency viewpoint and would also facilitate the development of energy-efficient optimal control schemes.

d) Development of design criteria for thermal utility supply systems using a single heat transfer medium for both heating and cooling duties (21). The great majority of batch processes are carried out in the temperature range -50°C to 104°C. Conventional thermal utility systems use steam, water and chilled ethylene glycol, frequently in sequence on the same vessel. This leads to cross contamination of utilities, unavailability of coolants during a heating cycle (which is a potential process hazard) and far from optimal control. The latter factor leads to an inability to produce uniform batches in the least possible time, which has an adverse impact on batch yields, equipment utilisation and hence energy efficiency. The use of a single heat transfer medium which spans the range of temperature for a given processing application has been proposed as a solution to this problem, but there are many unanswered questions about how such a utility system should be designed (21).

At present Europe is ahead of the rest of the world in process integration and batch scheduling optimisation. The USA is ahead of Europe in batch plant simulation but Europe is catching up.

Batch process simulation is a relatively new field in which activity is growing rapidly due to the rapidly increasing industrial interest in fine chemicals manufacturing. A structured collaboration between industry and universities or research institutes, and between specialists in different aspects of the problem, would be very beneficial and CEC support could be instrumental in achieving this.

EXPERT SYSTEMS FOR PROCESS CONTROL AND PRODUCTION MANAGEMENT

There is considerable interest at present in expert systems for process control following the successful development of such a system for controlling a cement kiln (2B). This system was developed originally to provide real-time, closed loop, supervisory control of a large cement kiln. In the absence of an adequate process model, a fuzzy logic type approach was used to capture the empirical knowledge of good operators in sets of rules. These rules use observations of factors such as kiln temperature and exhaust gas oxygen content to make appropriate adjustments to the fuel and feed rate controller set points. The basic idea was to try to achieve 100% of the time the quality of operation provided by the best operators. The system has been an outstanding success and has led to substantial energy savings, improved product quality and a reduction in NOx in the exhaust gas.

There is now considerable interest in evaluation of rule-based closed loop expert systems for a wider range of plant and processors and this was recommended as a research priority (2B). The areas suggested included glass furnaces, blast furnaces, chemical plant and oil refineries.

A second priority is the incorporation of realtime into rule-based expert systems in order to extend the approach into intelligent plant monitoring. This would be based around rule-based trend analysis so that progress towards an upset condition could be detected and appropriate action taken before an alarm situation is reached. The ability to project plant performance on the basis of trend analysis could also be very useful for planning and scheduling of operations, including plant maintenance (2B, 2K, 2o).

Another research need is the development of methods for validating sensor inputs and assessing situations in the face of uncertainty, eg unreliable or missing sensor inputs (2K). There is currently a fashion for producing software which uses parallel processing to mimic the inter-connections of the human brain and developments in this field may provide a better framework for problem solving in the face of uncertainty (2o).

So far we have been talking about rule-based expert systems which aim to capture the empirical knowledge of the best plant operators. A more ambitious objective, which should ultimately yield greater savings, would be to try to construct an expert system containing the deeper knowledge which an experienced process engineer would use if he were operating the plant. It is common experience that when the operation in taken over by process engineers, for example when the operators go on strike, significant improvements in plant efficiency and performance occur. This arises because the process engineers use a much deeper knowledge of physics, chemistry and engineering, usually encapsulated in a mental model of the plant, to guide their reasoning and actions. The conventional "expert systems" approach, whether rule-based or frame-based, is incapable of representing knowledge of this depth and complexity and the simplistic inference procedures currently in use cannot cope realistically with the compromises and decisions which have to be made. Long range R&D should focus on devising ways to solve this problem (2F). This is an area where the USA is currently much more active than Europe. The principal need at present is that there should be good communication between researchers in the field in order to avoid duplication of effort and to aid cross-fertilization of ideas. Only when the basic concepts have emerged will there be a need for a structured coordination of effort to speed up their practical development and implementation; that is the stage at which CEC support would be most useful (2F).

As an intermediate objective between the rule-based systems of today and the potential deep knowledge-based systems of the long-term future, it was suggested that the separate disciplines of process engineering and control engineering should be brought together to develop user-friendly, tunable controllers or operator decision support systems based on a combination of process models, control models and heuristic models (2F). This was viewed with some scepticism by the protagonists of rule-based systems, and clearly the role of mathematical models in expert systems for process control is a controversial subject. One expert felt that the way forward could be to develop process models based on qualitative or symbolic physics, in which quantitative relationships are replaced by qualitative trends and mathematical logic is replaced by causal reasoning (2o). This qualitative expert physics approach was felt to be more compatible with expert systems. Optimisation algorithms will also need to be developed in the same way.

ADVANCED ON-LINE SENSORS

In Stage 1 of this study a general consensus was found among industrial companies that sensor development has lagged seriously behind control theory development. The consequence is that implementation of advanced control strategies, which could improve energy efficiency significantly, is hampered by lack of adequate sensors to make the on-line measurements needed by such control systems. It was also stated repeatedly that on-line sensors must be accurate, reliable, rugged and reasonably cheap. Therefore, in Stage 2 a number of experts in sensor development have been interviewed.

Most of the sensor needs identified by industry referred in one way or another to on-line measurement of the composition of process streams, particularly in hot, dirty, hostile or multi-phase environments. In such environments non-invasive instrumentation would be advantageous and a number of interesting possibilities were proposed by the experts. Some examples are given below.

- Optical techniques have been used successfully for some time for laboratory measurements on 2-phase flows, eg mass flow rate of dispersed phase, particle/droplet concentration and size distribution. The advent of laser diodes, avalanche photo-detectors and optical fibres offer the potential for low cost, quite rugged and physically small equipment which will be much more appropriate to process plant (2H, 20, 2Q). Advanced image processing software may also help (2h). There is a particular need for research on ways of measuring particle size distribution in dispersions with a high particle concentration (20).

- Within the nuclear industry there have been significant developments in the use of ultrasonic techniques for measurements in process plant (2H). Reliable non-invasive measurements of temperature, level, liquid-liquid and liquid-solid interfaces have all been achieved using ultrasonic techniques.

- The new technique of process acoustic monitoring involves mounting a sonic transducer on the outside of the process vessel, listening to the operating plant; by appropriate processing of the received signals the current state of the process may be inferred. Potential applications include the monitoring of mixing, drying and grinding processes as well as plant condition monitoring in plant with moving parts (2H).

- The nuclear industry has also pioneered the use of gamma ray, X-ray and neutron techniques for non-invasive measurements of the chemical composition of process streams. These techniques are thought to have considerable potential in non-nuclear situations (2H).

- Advances in semi-conductor devices have led to a significant reduction in the price of microwave components, thus offering the possibility of microwave-based instrumentation at an acceptable market price (2H). Microwave techniques are believed to have considerable potential for measuring the concentration of liquid water or water vapour in dusty or dirty environments.

Another area where there is considerable research interest at present is film sensors for chemicals composition measurements on industrial process streams (2Z). These rely on the process stream component of interest changing the chemical state of a substance laid down as a film on the sensor. These sensors must be placed in the process stream and hence may not be suitable for dirty or aggressive environments, but if this is not a problem they can exhibit high selectivity for concentration measurements of individual components in a mixture. The main research needs are seen to be;

- improved materials giving better selectivity, repeatability and durability

- improved sensor construction techniques

- improved understanding of chemical reactions on sensors and improved analysis of the signals which they generate.

A further technique which is being explored for continuous chemical composition measurement process stream is flow injection analysis (2f). In this technique a very small sample flow is continuously withdrawn from the process stream and injected into a small flow of reagent which passes through a tiny coiled tube. At the tube outlet the extent of reaction, which is proportional to the active species concentration in the sample, is determined by colorimetric, electrochemical or thermal means. Simultaneous analysis for several components is feasible. The main research needs are improved sample preparation and injection techniques, making the system more rugged, tackling a wider range of applications and testing over extended periods on full-scale plants.

In all of these areas international collaboration with consistent and coordinated CEC support was seen to be potentially very valuable. Partnerships must be formed between researchers, industrial companies possessing the plants on which the instruments can be tested and instrument manufacturers. International collaboration with CEC support would allow a range of techniques and applications to be developed simultaneously, and at the same time rugged plant versions of the sensors could be engineered and tested. This would speed up practical implementation in industry.

CONCLUSIONS

In all the areas surveyed there are many opportunities for strategic R&D which is likely to lead to improved energy efficiency and consequential pollution abatement in the process industries. The principal needs and opportunities highlighted by the experts are listed below.

1. CHEMICAL REACTORS

a) Novel reactors with simultaneous reaction and separation of the desired product, thereby enabling equilibrium - limited reactions to be driven to completion in a single pass or consecutive reactions to be stopped at the desired product.

b) Novel reactors which permit the concentration of reactants to be increased substantially, thereby reducing the energy demand for separations and recycling.

c) Novel catalytic reactors with low pressure drop, thereby reducing compression costs particularly in recycle systems.

d) Photochemical reactors.

e) Improved models for hydrocarbon cracking furnaces and multi-phase reactors, thereby facilitating design and operation for maximum yield of desired product and maximum energy efficiency.

2. LOW ENERGY SEPARATION PROCESSES

2.1 Selective adsorption

a) A methodology for designing new adsorbents for specific applications. This will require:

* improved prediction of multi-component adsorption equilibria and kinetics from single-component data;

* improved knowledge of the relation between effective transport properties and adsorbent structure;

* improved understanding of adsorption forces.

b) Development of new adsorbents, particularly from low cost raw materials.

c) A truly continuous adsorption process without fixed beds of solids or solids transport between vessels.

d) Development of advanced adsorbents in a more rugged form for use in fluidised or moving beds without attrition or breakage.

e) Improved engineering models for regeneration, rapid cycling PSA processes and multi-component, non-isothermal adsorption.

Potential applications of selective adsorption include recovery of alcohols from dilute aqueous solutions; breaking azeotropes, separating isomers and other close boiling liquids; replacement of cryogenic processes for bulk separation of gases and recovery of inert gases; removal of toxic chemicals and other pollutants from aqueous and air streams; recovery of solvents and vapours. Compared to distillation, energy savings are in the range 30 to 90%.

2.2 Melt crystallization

a) Improved fundamental understanding of crystal nucleation and growth kinetics, sweating and recrystallization.

b) Engineering models of melt crystallizers.

c) Combination of melt crystallization with other separation processes for complete separation of eutectic systems.

d) Theorectical prediction of solid-liquid phase diagrams.

Attainment of these goals will enable design and optimisation of melt crystallization processes to proceed rapidly. Melt crystallization is applicable to separation and purification of materials having melting points between - 50°C and + 200°C. The energy consumed is an order of magnitude lower than for distillation. Melt crystallization is ecologically beneficial compared to crystallization from solution because there is no waste liquor for disposal. Japan is putting in a big R&D effort in this area.

2.3 Supercritical extraction

a) Better prediction of phase equilibria for mixtures near the critical point.

b) Better understanding of the effect of entrainers on volatility and selectivity.

c) Mass transfer models for common contacting devices with supercritical solvents.

The present poor state of knowledge in these areas is a significant barrier to exploitation of this process. Potential applications include food processing, recovery of alcohols and other water-soluble organics from aqueous solutions, and selective separation of very narrow fractions from complex mixtures. Energy requirement is much less than for distillation but capital cost is usually higher. Europe lags behind the USA.

2.4 Liquid-liquid extraction

a) Better design and scale-up methods for column contactors based on bench scale characterisation tests.

b) Adaptive control systems for column contactors on multi-product plants.

Liquid-liquid extraction can have higher selectivity and a lower energy requirement than distillation for some separations in the fine chemicals and pharmaceuticals industries. It may also be useful in certain circumstances for liquid effluent purification.

3. FURNACES, KILNS AND OVENS

a) Development and experimental checking of advanced 3-D models of aerodynamics, heat and mass transfer and chemical reactions. Such models would facilitate the answering of "what if?" question and would enable computer-aided exploration of novel equipment and operational concepts.

b) Development of methods of preheating glass furnace raw materials using waste heat from the furnace exhaust gases.

c) Improvements to the design of cement kiln cyclone preheaters to reduce the fan power required.

d) Pilot-scale testing of novel energy-saving baking oven concepts.

4. DRYERS

a) Drying in superheated steam with total recycle.

b) Novel types of contact dyer with substantially reduced capital cost per unit of throughput.

c) Better experimental techniques and kinetic models for characterising drying properties of materials, thereby facilitating design for maximum energy efficiency and product quality.

d) Better models for common types of dryer to facilitate optimal design and operation.

5. PROCESS INTENSIFICATION

a) Intensified evaporators with much higher heat transfer coefficients than conventional equipment.

b) Intensified reactors with much higher reaction rates, much higher heat fluxes and much shorter residence times than conventional equipment.

6. ADVANCED 3-D FLOW MODELLING

Several of the topics listed above would benefit from advanced 3-D modelling of fluid flows coupled with heat and mass transfer, chemical reactions and, in some cases, dispersed phase transport. The following developments in advanced 3-D flow modelling were identified as desirable by the experts to enable it to be applied successfully to these topics:

a) More comparison of model predictions with laboratory and field experiments.

b) Improved grid generation techniques to facilitate modelling of complex geometries.

c) Improved turbulence modelling.

d) Improved modelling of the interaction of particles with turbulent flows and with walls, and of particle behaviour at high concentrations.

e) Improved visual presentation of predictions to facilitate comparison with experimental data.

7. DYNAMIC SIMULATION OF COMPLEX SYSTEMS

a) Improved computing strategies for reducing computing time, including use of parallel computing techniques. This will permit more complex processes to be simulated at reasonable cost and more realistic models of distributed systems such as tubular reactors and adsorber beds to be used.

b) Methods for calculating the optimal trajectory of a system between two steady states (including start-up and shut-down), taking account of practical constraints such as product quality, equipment limitations and safety.

c) Improved mathematical techniques for optimisation.

d) Better thermodynamic property prediction methods for highly non-ideal mixtures, eg solutions of polymers, electrolytes and polar gases, thereby improving quality of simulations.

e) Dynamic modelling of the interaction of compressors, turbines and pumps with each other and with other system components, eg vessels, pipelines etc.

8. SIMULATION OF BATCH SYSTEMS

a) Extension of energy and process integration concepts to batch processes.

b) A methodology for evaluating trade-offs between energy integration, plant utilization and flexibility.

c) A methodology for synthesis of new batch processes.

d) A general purpose batch process simulator based on experimentally verified dynamic unit operation models.

e) Design criteria for thermal utility systems using a single heat transfer medium for both heating and cooling duties in order to facilitate optimal plant operation.

9. EXPERT SYSTEMS FOR PROCESS CONTROL AND PRODUCTION MANAGEMENT

a) Evaluation of rule-based closed loop expert systems for a wider range of plant and processes.

b) Methods for validating sensor inputs and assessing situations in the face of uncertainty, eg unreliable or missing sensor input.

c) Incorporation of real time into expert systems, eg for trend analysis, projection of plant performance, planning and sequencing of operations.

d) Development and evaluation of expert systems based on a tunable, user-friendly representation of process model, control model and heuristic model.

10. ADVANCED ON-LINE SENSORS

a) Small, rugged, laser instrumentation for industrial measurements on two-phase flows, eg mass flow rate of dispersed phase, particle/droplet concentration and size distribution, particularly in concentrated dispersions.

b) Small, rugged sensors based on ultrasonic or microwave techniques for non-invasive industrial process measurements in hostile environments.

c) Nuclear techniques for chemical composition measurements on industrial process streams.

d) Film sensors for chemical composition measurements on industrial process streams:

* improved materials giving better selectivity, repeatability and durability

* improved sensor construction techniques

* improved understanding of chemical reactions on sensors and improved analysis of the signals which they generate.

e) Rugged flow injection analysis sensor systems for chemical composition measurement on industrial process streams.

TABLE 1

Distribution of Energy Consumption in Industry

EUR-10 in 1984 (Eurostat provisional data)

INDUSTRIAL SECTOR	FINAL ENERGY CONSUMPTION TOE x 10^6	%
Steel	48	25.3
Chemicals	35	18.4
Non-metallic minerals (Cement, ceramics, glass, etc)	21.6	11.4
Food and drink	15	7.9
Paper and printing	9.3	4.9
Non-ferrous metals	7	3.8
Textiles	6.4	3.4
Metal manufacture	18.6	9.8
Others and adjustments	29	15.2
	190.2	100.0

TABLE 2

Recommended areas for investigation in Stage 2

Although the areas listed below have been recommended on the basis of potential energy efficiency benefits, it should be noted that advances in these areas will usually also lead to pollution abatement benefits.

1. Alternative or improved unit operations and reaction routes, including advanced flow modelling where appropriate*

    a) Chemical reactors, including electrochemical processes and multi-phase systems
    b) Low-energy separation techniques, eg gas adsorption, melt crystallization, liquid-liquid and supercritical extraction
    c) Glass-making furnaces, cement kilns, brick-making kilns, baking ovens and dryers
    d) Process intensification

2. Energy and process systems models

    a) Dynamic simulation of complex systems, including development of control strategies
    b) Simulation of batch systems, including energy and process integration

3. Sensors, instrumentation and control

    a) Expert systems for process control and production management

    b) Advanced on-line sensors for:

        - measuring composition of process streams
        - measurement in multi-phase flows, eg mass flow rate, concentration and size of particles and drops
        - measurements in difficult environments
        - plant condition monitoring

NB

(i) Heat exchangers, heat pumps and combustion are not included in this Table since they are important energy conservation topics in their own right and consequently are the subjects of separate surveys under the CEC Energy Conservation Programme. Membrane separations, catalysts and biochemical processes are not included because they are covered under other CEC Programmes.

(ii) Advanced flow modelling topics have been grouped together with alternative or improved unit operations and reaction routes because the areas where advanced flow modelling could lead to the greatest energy efficiency improvements are either reactors or unit operations.

APPENDIX A

Letter Sent to Research Experts

Dear ....

The Process Engineering Research Centre at Harwell Laboratory has been asked to conduct a survey of certain process industries research needs on behalf of the Commission of the European Communities. A letter from the European Commission is enclosed in confirmation of this. The intent is to assess the present position of, and future requirement for, strategic R&D in support of efficient use of energy and its implications for pollution abatement in the process industries within Europe; that is, precompetitive R&D which will come to fruition over a period of 5 - 10 years and may then have some impact on the process industries.

In the first stage of this survey discussions were held with 16 leading industrial companies from various member states of the EEC, 4 European industry federations and three research institutions. Following these discussions certain topics have been selected as being of the highest priority and these are listed in the attached Table.

In the second stage of the survey discussions will be held with leading researchers in each of these topics in order to define the most important research needs in each areas more precisely. The research would be expected to have a high degree of novelty and the results would be expected to be general and to bear ona variety of products and processes. The survey will lead to a position paper which will be presented to the CEC at the end of 1987. Information for the paper will be gathered in a series of interviews and we would like to invite you to participate since you are an acknowledged expert in at least one of the priority topics as listed in the Table. If you agree, a researcher from Harwell will visit you for a discussion. A record of the discussion will be submitted to you for editing, and may subsequently be included as an Appendix to the position paper. Any parts of the discussion which you would not want included in the Appendix will be kept confidential.

The aim of the interview will be to obtain an overview of the needs and possibilities in your speciality as you see them. The following questions are posed as a framework for the discussion:

1. From the viewpoint of improving the energy efficiency of the process industries, what are the most important research needs in the priority topic(s) listed in the Table in which you are an expert?

2. If these research goals are achieved, what would be the main areas of application and what energy efficiency benefits and associated pollution abatement benefits would become possible?

3. Which aspects of R&D within your topic(s) are most likely to advance rapidly over the next decade?

4. What manpower and facilities does Europe possess for R&D in your topic(s)? Are there important gaps which should be filled? What are competitors (eg Japan or the USA) doing in these areas?

5. Which of these areas of R&D within Europe would benefit most from International cooperation with consistent and co-ordinated CEC support of strategic research?

6. What practical benefits would arise from this support? What resources would be needed to achieve these benefits?

7. Would you be interested in participated in in international linked research actions with Community support for cost sharing projects in your topic(s)? Please note that this letter in no commits the Commission to conclude a contract.

We understand that, of the topics listed in the Table, your principal area of expertise is ......

A member of the Harwell staff will contact you by telephone in the next few days to arrange a visit at some mutually convenient time.

Yours sincerely

David Reay
Manager, Process Engineering Research Centre

enc Letter from Dr Strub

cc

PS the Commission of the European Communities is sending you under separate cover some additional information on its activities in energy conservation.

COMMISSION
OF THE
EUROPEAN COMMUNITIES

DIRECTORATE-GENERAL
FOR SCIENCE, RESEARCH
AND DEVELOPMENT
JOINT RESEARCH CENTRE

XII-E

0 6 7

Brussels 7 January 1987

TO WHOM IT MAY CONCERN

The UK Atomic Energy Authority (UKAEA) Research Establishment at Harwell is carrying out for the European Communities a study on the state of the art of strategic R & D in support of efficient use of energy and its implications for pollution abatement in the process industries. As a result an inventory will be made to report what needs to be done in R & D in this field.

On the basis of this study the Commission's services intend to examine the interest in, and the opportunity for, carrying out such R & D work in an international joint venture, with Community support afforded to participating research organisations.

The purpose of this letter is to inform you about the UKAEA study and to seek your co-operation in its execution.

A. STRUB
Director
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TABLE (Attached to Letter)

Recommended areas for investigation in Stage 2*

Although the areas listed below have been recommended on the basis of potential energy efficiency benefits, it should be noted that advances in these areas will usually also lead to pollution abatement benefits.

1. Alternative or improved unit operations and reaction routes, including advanced flow modelling where appropriate

   a) Chemical reactors, including electrochemical processes and multi-phase systems
   b) Low-energy separation techniques, eg gas adsorption, melt crystallization, liquid-liquid and supercritical extraction
   c) Glass-making furnaces, cement kilns, brick-making kilns, baking ovens and dryers
   d) Process intensification

2. Energy and process systems models

   a) Dynamic simulation of complex systems, including development of control strategies
   b) Simulation of batch systems, including energy and process integration

3. Sensors, instrumentation and control

   a) Expert systems for process control and production management

   b) Advanced on-line sensors for:

      - measuring composition of process streams
      - measurement in multi-phase flows, eg mass flow rate, concentration and size of particles and drops
      - measurements in difficult environments
      - plant condition monitoring

* Heat exchangers, heat pumps and combustion are not included in this Table since they are subjects of separate surveys under the CEC Energy Conservation programme. Membrane separations, catalysts and biochemical processes are not included because they are covered under other CEC Programmes.

APPENDIX B

Experts interviewed during the course of the survey are referenced in the main text as follows:

Reference	Expert
2A	Dr B D Crittenden, University of Bath (UK)
2B	Mr D W Haspel, Sira Limited (UK)
2C	Prof P Hutchinson, Cranfield Institute of Technology (UK)
2D	Dr G L Quarini, Harwell Laboratory (UK)
2E	Dr C Ramshaw, Imperial Chemical Industries (UK)
2F	Dr J W Ponton, University of Edinburgh (UK)
2G	Prof R W H Sargent, Imperial College of Science and Technology (UK)
2H	Dr R D Watkins, Harwell Laboratory (UK)
2I	Prof B Linnhoff, University of Manchester Institute of Science and Technology (UK)
2J	Prof H Angelino, Institut du Genie Chimique, Toulouse (F)
2K	M A Rojey, Institute Français du Petrole (F)
2L	Prof P Le Goff, INPL,. Nancy (F)
2M	Prof M Perrut, INPL, Nancy (F)
2N	Prof Tondeur, INPL, Nancy (F)
2O	Prof Dr F Durst, University of Erlangen-Nurnberg (D)
2P	Prof Dr Ing H Hoffmann, University of Erlangen-Nurnberg (D)
2Q	Dr Ing A Scheuer, Forschungsinstitut der Zementindustrie, Dusseldorf (D)
2R	Prof Dr Ing E U Schlünder, University of Karlsruhe (D)
2S	Dr Ing J Ulrich, University of Bremen (D)
2T	Dr G J Arkenbout, TNO (NL)
2U	Ir P Sluimer, TNO (NL)
2V	Prof K R Westerterp, Twente University (NL)
2W	Prof Froment, University of Gent (B)
2X	Prof R Jottrand, Université Libre de Bruxelles (B)
2Y	Prof B Kalitventzeff, University of Liege (B)
2Z	Dr Massi Mauri, Eniricerche, Monte Rotondo (I)
2a	Dr Ing Toninato, Stazione Sperimentale dei Vetro, Murano, Venezia (I)
2b	Prof E Costa, Universidad Complutense, Madrid (SP)
2c	Prof L Puigjaner, Universidad Politechnica di Catalunia, Barcelona (SP)
2d	Prof D F G Durao, Insituto Superior Tecnico, Lisbon (P)
2e	Prof A E Rodrigues, University of Porto (P)
2f	Prof A Fredenslund, Technical University of Denmark (DK)
2g	Dr A Sorensen, Technical Universty of Denmark (DK)
2h	Prof A J Karabelas, University of Thessaloniki (GR)
2i	Prof A Kontopoulos, National Technical University of Athens (GR)
2j	Prof N Markatos, National Technical University of Athens (GR)
2k	Prof C G Vayenas, University of Patras (GR)
2l	Dr N Murphy, University College Dublin (I)
2m	Mr R E Bahu, Harwell Laboratory (UK)
2n	Mr I C Kemp, Harwell Laboratory (UK)
2o	Dr F Jakob, CGE, Marcoussis (F)
2p	Ir JK A Knobbout, TNO (NL)

European Communities — Commission

EUR 11920 — Needs for strategic R&D in support of improved energy efficiency in the processing industries —
Views of research experts

D. Reay, P. A. Pilavachi

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Interviews have been conducted, in universities and research institutes, with 42 leading experts who are at the forefront of research in the priority fields identified. Through these interviews, it has been possible to define more precisely what pre-competitive research needs to be done in each of these fields, what the main application areas and energy efficiency benefits are likely to be, and what the strength of Europe's current research position is in these fields compared to other parts of the world.

In all the areas surveyed there are many opportunities for strategic R&D which is likely to lead to improved energy efficiency and consequential pollution abatement in the processing industries.

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