The scientific programme REACTOR is based on the study of nonlinear chemical, biochemical and catalytic systems operating far from equilibrium.

The main emphasis will be on the development of fundamental understanding at the molecular level of the processes leading to the formation of spatiotemporal structure and patterns in chemical and biochemical systems.

The project will be developed through a linked series of “strands”:
- spatiotemporal pattern formation and control in novel open reactors;
- nonlinear kinetics of complex chemical and biochemical processes;
- nonlinear processes at interfaces in heterogeneous catalysis and electrochemistry.

The main goals are the development of the fundamental understanding of complex systems and to indicate the longer-term potential for exploitation of their properties to develop new reactors appropriate to such systems. This represents a necessary first step to the future application of such systems, e.g. for new routes to high-value industrial products.

The project will involve both experiment and theory (including computation) and is genuinely interdisciplinary, bringing together chemists, physicists, biologists, mathematicians and engineers to investigate problems ranging from mechanistic chemistry and reactors, combustion and the atmosphere through to biochemistry and physiology.

Participants in the REACTOR programme will have access to significant state-of-the art experimental and theoretical facilities.
**Introduction**

Chemical reactions convert starting reactant molecules into different final products. Generally, this is achieved not in a single molecular rearrangement, but through a series of chemical steps. This sequence is known as the chemical mechanism for the reaction and will involve the formation and subsequent removal of several intermediate species. Commonly, some of these intermediates will be more highly reactive than their parent reactants. The build-up of reactive intermediates may allow the overall rate of formation of the final products to increase – sometimes dramatically – as the reaction progresses. This effect is known as chemical feedback.

Examples of this arise widely in nature. In combustion (where thermal feedback also occurs), free radical species are produced from the original fuel and oxidant mix. In biological systems, enzyme processes frequently lead to autocatalysis. For catalytic systems, the activity of the catalyst may increase as reactant molecules are adsorbed cooperatively onto the active sites. In other situations, the build up of certain intermediate species inhibit the overall reaction, slowing the overall rate until they are subsequently consumed.

A feature of reactions with feedback is that they exhibit nonlinear effects. These may give rise to sustained oscillations in the concentrations of various species – perhaps leading to periodic changes in colour of the reacting mixture – or to sudden changes in rate (ignition or extinction). In unstirred systems, the nonlinearity may give rise to the development of spatial structure – chemical patterns.
Example research topics

Glycolysis in whole yeast cells
The concentrations of several key metabolites are known to oscillate during glycolysis. This feature has been observed recently in living yeast cells. The transition to oscillation occurs in all cells simultaneously, indicating some strong coupling within the system. A nonlinear analysis of the response of the system to perturbations of various species concentrations allows detailed questions about the underlying mechanism driving the oscillations to be answered.

Dynamics of excitable media
“Excitable” or “active” media occur widely in biological systems. Waves of “excitation” are used for signal transmission or for synchronising reaction events. Important examples of excitable media include cardiac muscle and neuronal tissue. Methods for studying biological systems in vivo are developing, but in many cases it is possible to determine generic features by investigating model systems such as chemical analogue systems. The Belousov-Zhabotinsky (BZ) reaction is widely used in this respect. Several groups in the REACTOR programme have experience of such studies both in experiment and modelling. Recently, certain “universal relationships” underlying the dynamics of “spiral wave” structures (thought to be important in the onset of ventricular fibrillation, for instance) have been proposed and tested. The influence of electric and magnetic fields on wave propagation in these systems is one of the features being investigated.

Nonlinearity in combustion
Ignition, extinction and quenching are important “nonlinear responses” in combustion. Flames show spatial and temporal instabilities such as the development of “cellular”, “pulsating” and “spiral flames” all of which can be detrimental to combustion efficiency in commercial burners. The development of new flame extinguishants is also of great concern following the ban on halons. Oscillatory burning also occurs in the processes of “self-propagating high-temperature synthesis” which is used in the manufacture of several refractory materials.

Control of chaotic systems
Systems with feedback frequently show oscillatory responses and in many cases these can develop into so-called “chaotic” behaviour. The properties of a chaotic system can be exploited using the idea of “chaos control”. Using very small perturbations to the operating conditions, a chaotic state can be tuned into oscillations of any desired period. Recently,
groups within the REACTOR programme have shown that the chaotic combustion of carbon monoxide can be controlled and a steady periodic combustion obtained. In other situations, changing from one controlled state to another can vary the selectivity of a reaction between two different products. In all these cases, the information required to control the system is obtained from the experimental behaviour and does not require any knowledge of the underlying chemical or physical mechanisms involved in the reaction.

Control of pH
pH regulation is vital in many biochemical processes which are catalysed by either H⁺ or OH⁻ ions. The mechanism and dynamic responses of several pH oscillators have been characterised by several groups in the REACTOR programme. Methods are currently under development for establishing stationary pH patterns in different reactor types. pH changes can be coupled to the swelling of polymer gels to provide mechanical work. pH reactions also form the basis of recently designed “chemical electronic components”.

Surfaces and interfaces
Reactions at surfaces underpin the majority of major industrial chemical processes through heterogeneous catalysis. Nonlinear features arise at the most fundamental level through several mechanisms, including adsorbate-induced reconstructions of the surface atoms (typically studied on single crystals under “clean conditions” and at low pressure) or thermal coupling (typical for reactions at high pressure on composite catalysts). Various groups in the REACTOR programme are addressing issues such as the “pressure gap” between laboratory and industrial conditions. Electrochemical systems have reaction at a surface exposed to an electrolyte. Pattern-formation in these systems is being studied by imaging techniques under development at the Fritz-Haber Institute in Berlin and chaos in electrode arrays is featured in work in Debrecen and Würzburg.
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REACTOR activities

Exchange visit grants

The REACTOR programme supports a number of exchange visits between laboratories in different countries to allow joint experimental or theoretical work.

Two different types of exchange are offered:

- Short exchange visits
- Long exchange visits

Short visits are typically appropriate for senior researchers and of up to one week in duration.

Long visits offer support to assist junior researchers such as graduate students or postdoctoral workers without a permanent position at their home institution spend a period of up to one month in another laboratory.

Approximately 20 exchange visits are expected to be supported in each year of the programme.

Applications are invited at regular intervals and should involve at least one contributing country.

Workshops

The Steering Committee organises International Meetings which will be held about once a year. The first meeting is planned for January 2001 in Palermo, Sicily. The second meeting is planned for Leeds, United Kingdom, in September 2001. In addition, workshops and a Theme School are expected to be organised on specific aspects of the REACTOR programme. The Steering Committee invites proposals from potential organisers on topics with a clear connection to the scientific goals of the REACTOR programme.

Even shell patterns can be modelled from reaction-diffusion equations. © S.K. Scott, University of Leeds
Professor Steve Scott (Chairman)  
*University of Leeds*  
*School of Chemistry*  
Leeds LS2 9JT  
United Kingdom  
Tel: +44 113 233 6463  
Fax: +44 113 233 6565  
E-mail: s.k.scott@chem.leeds.ac.uk  
Web: www.chem.leeds.ac.uk/People/SKS/ef_reactor

Professor John Merkin  
*University of Leeds*  
*Dept of Applied Mathematics*  
Leeds LS2 9JT  
United Kingdom  
Tel: +44 113 233 5108  
Fax: +44 113 242 9925  
E-mail: amjhm@amsta.leeds.ac.uk

Professor Zoltan Noszticzius  
*Budapest University of Technology and Economics*  
*Dept of Chemical Physics*  
1521 Budapest  
Hungary  
Tel: +36 1 463 1341  
Fax: +36 1 463 1896  
E-mail: noszti@phy.bme.hu  
noszti@phyndi.fke.bme.hu (for long messages)

Dr. Lars Folke Olsen  
*Odense University*  
*SDU Institute of Biochemistry and Molecular Biology*  
Physical Biochemistry Group  
Forskerparken 10  
5250 Odense M  
Denmark  
Tel: +45 63 15 71 72  
Fax: +45 65 93 23 09  
E-mail: lfo@dou.dk

Professor F.W. Schneider  
*Universität Würzburg*  
*Institut für Physikalische Chemie*  
Am Hubland  
97074 Würzburg  
Germany  
Tel: +49 3188 86300  
Fax: +49 3188 86302  
E-mail: fws@phys-chemie.uni-wuerzburg.de

Dr. Maria Liria Turco Liveri  
*Università di Palermo*  
*Dpto di Chimica Fisica*  
*Fnte delle Scienze*  
Parco d’Orleans II  
90128 Palermo  
Italy  
Tel: +39 091 596 702  
Fax: +39 091 590 015  
E-mail: tliveri@unipa.it  
cavasino@unipa.it

Dr. Svenje Mehler  
*ESF Scientific Secretary*

Ms. Pat Cosgrove  
*ESF Administrator*  
*European Science Foundation*  
1 quai Lezay-Marnésia  
67080 Strasbourg Cedex  
France  
WWW Home Page:  
http://www.esf.org  
Tel: +33 (0)3 88 76 71 06  
Fax: +33 (0)3 88 37 05 32  
E-mail: pcosgrove@esf.org

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Cover picture:  
Propagating oxidation waves in a  
membrane reactor.  
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