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.

Nonlinear Chemistry in Complex Reactors: models and experiments (REACTOR)

An ESF scientific programme

The project will be developed through a linked series of "strands":

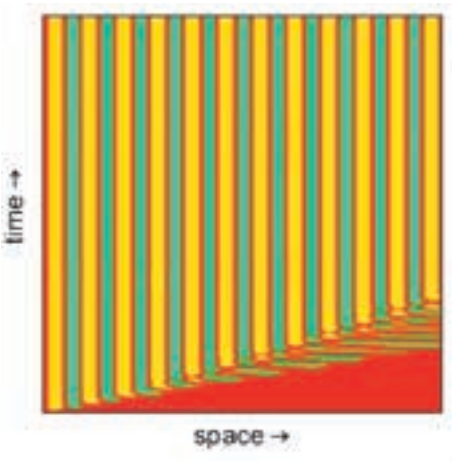
- *spatiotemporal pattern formation and control in novel open reactors;*
- *nonlinear kinetics of complex chemical and biochemical processes;*
- *nonlinear processes at interfaces in heterogeneous catalysis and electrochemistry.*

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.

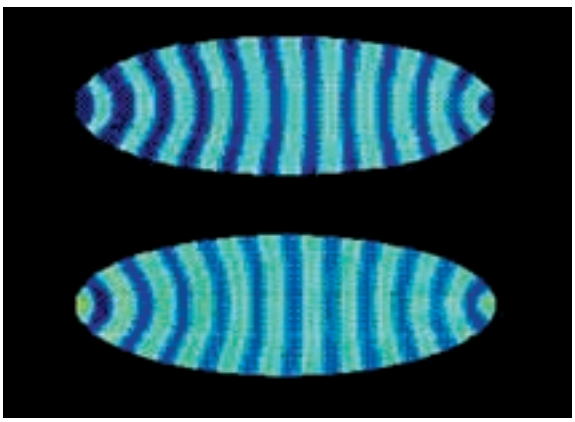
The European Science Foundation acts as a catalyst for the development of science by bringing together leading scientists and funding agencies to debate, plan and implement pan-European initiatives.



Flow Distributed Oscillations: the formation of a steady spatial pattern in an oscillating chemical reaction in a plug-flow reactor.

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*.



Computer simulation of "Turing" structures for reaction-diffusion in a 3D elliptical region showing the development of striped "segmentation patterns".

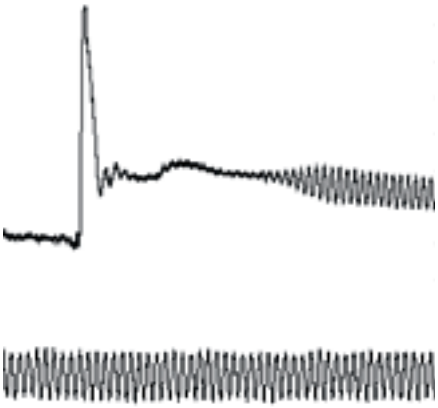
Examples of this arise widely in nature. In combustion (where *thermal feedback* also occurs), free radical species are produced from the original fuel and oxidant mix. In biological systems, enzyme processes frequently lead to autocatalysis. For catalytic systems, the activity of the catalyst may increase 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.



Large amplitude damped and small amplitude undamped oscillations in NADH fluorescence accompanying glycolysis in yeast cells.
© S. Danø and P.G. Sørensen, Copenhagen

Dynamics of excitable media

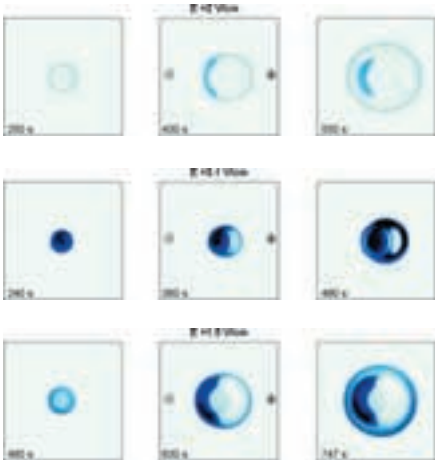
"Excitable" or "active" media occur widely in biological systems. Waves of "excitation" are used for signal transmission or for synchronising reaction events. Important examples of excitable media include cardiac muscle and neuronal tissue. Methods for studying biological systems *in vivo* are developing, 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,

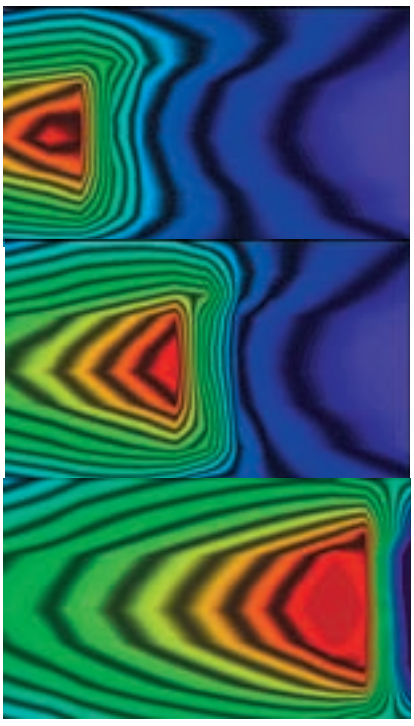


The effect of an imposed electric field on wave propagation in the iodate-arsenite reaction.
© H. Sevcikova, Prague, Institute of Chemical Technology

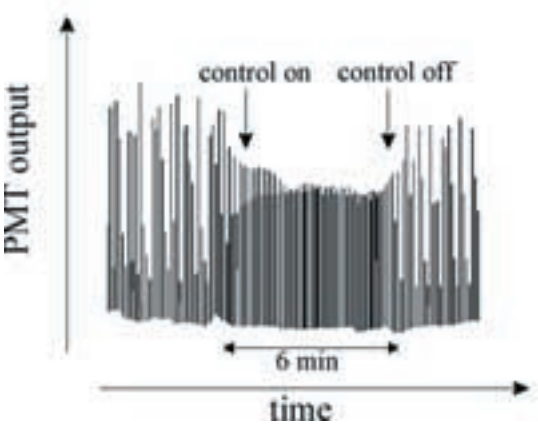
groups within the REACTOR programme have shown that the chaotic combustion of carbon monoxide can be controlled and a steady periodic combustion obtained. In other situations, changing from one controlled state to another can vary the selectivity of a reaction between two different products. In all these 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

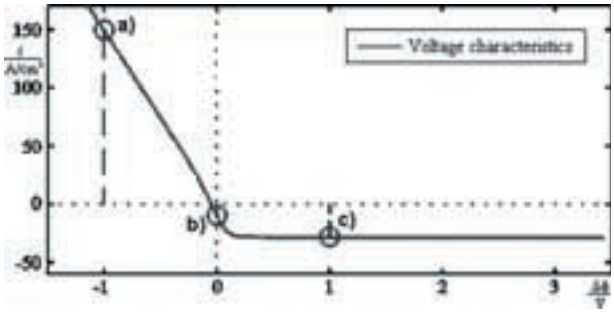
pH regulation is vital in many biochemical processes which are catalysed by either H^+ or OH^- ions. The mechanism and dynamic responses of several pH oscillators have been characterised by several groups in the REACTOR programme. Methods are currently under development for establishing stationary pH 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".



The development of temperature distribution within a honeycomb catalytic reactor. © J. Lindner, Prague Institute of Chemical Technology



Control of chaotic combustion in the CO + O_2 reaction in a flow reactor: control is achieved through small amplitude perturbations of the feed of the O_2 supply. When control is ceased, the system returns to its aperiodic oscillation. © M. Davies, University of Leeds



Voltage-current "characteristics" for a chemical diode. © J. Lindner, Prague Institute of Chemical Technology

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

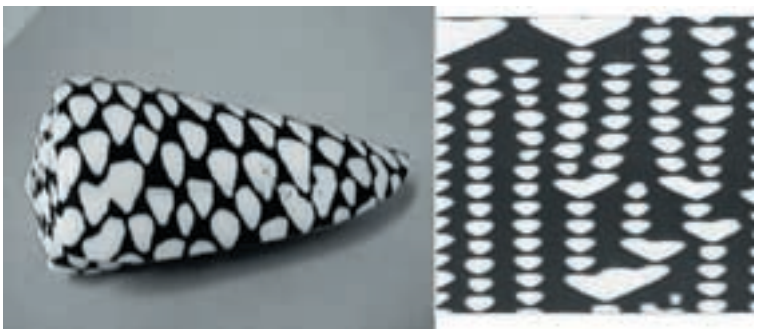
The REACTOR programme supports a number of exchange visits between laboratories in different countries to allow joint experimental or theoretical work.

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.



Even shell patterns can be modelled from reaction-diffusion equations.
© S.K. Scott, University of Leeds

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.

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For the latest information on this programme consult the REACTOR home pages:
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Cover picture:
Propagating oxidation waves in a membrane reactor.
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