Preface

Chemically and biologically reacting flows

In any elementary chemistry lab, students intuitively learn that usual reactions proceed faster when the reactants, normally in aqueous solution, are vigorously stirred. The reason is the same than the one by which one stirs coffee and milk to get an homogenous drink: chemistry is about molecules colliding to recombine their atoms into new configurations. And no collision will be possible if the different molecules sit in different parts of a container. It seems obvious that *mixing* together the different components of the reacting fluid will improve the chances of molecular encounters, thus increasing reactivity. And mechanical stirring, i.e. producing irregular motion of the fluid containing the reactants, is an efficient way to mix them.

These apparently simple arguments have been found to be extremely difficult to formalize. The molecular contact needed for chemical reactions occurs at scales many orders of magnitude smaller than the ones at which mechanical energy is injected as stirring. The transfer of energy and inhomogeneities across scales is thus a major ingredient in the mixing process, and it is essentially tied to the very difficult problem of understanding and modelling turbulence. In addition to the complexity of the fluid dynamics, an extra layer of difficulty arises from the nonlinearity inherent to most chemical reactions. As a consequence of all of this, unexpected phenomena can occur. For example, one can find reactions (Epstein, 1995) in which changing the rate at which the solution is stirred can cause a transition from a state in which the concentrations remain stationary to one of periodic or even chaotic concentration oscillations; or

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to crystallization processes that yield sometimes all left-handed and sometimes all right-handed crystals; or to reactions that occur suddenly at random intervals, with mean reaction times depending on stirring. Reaction times can even be longer, not shorter, for increased stirring (Nagypál and Epstein, 1986).

Biological population dynamics can be thought also as a set of complex "chemical reactions" in which organisms, instead of molecules, experience interactions and transformations: biological entities replicate if they find adequate nutrients, predators annihilate preys, and resources are consumed. In addition to occurring in interesting laboratory settings, the interaction of biological dynamics and turbulent flows is an essential ingredient in the life cycle of planktonic organisms (Mann and Lazier, 1991), which are defined as the aquatic living beings unable to completely overcome the ambient ocean currents. Although planktonic species are much larger than molecules, they are also subjected to influences from a huge range of spatial scales, from the microbial ones to the planetary sizes characteristic of the large-scale ocean circulation. As in the case of chemistry, unexpected responses to fluid flow occur which are still far from being fully understood (Martin, 2003; Catalan, 1999; Peters and Marrasé, 2000). Other situations involving reactive fluids in geophysical-scale flows are typical in atmospheric chemistry, or convection in the Earth mantle.

The great complexity of the situations encountered when dealing with biological or chemical interactions under fluid mixing and dispersion has lead some authors to very pessimistic statements: "... *One should expect no general results that describe in all (or most) cases how 'the biology' modifies a spatial pattern that has arisen solely from the dispersal of species ...*". (Powell and Okubo, 1994). In the chemical context, Ottino (1994) states: *"From a theoretical viewpoint, mixing problems appear complex and unwieldy; from an applied viewpoint, it is easy to get lost in the complexities of particular cases without ever seeing the structure of the entire subject. Thus, generally speaking, mixing problems in nature and technology are attacked on a case-by-case basis. Specific experimental results, however, can rarely be extrapolated and there is a pressing need to generate more general results."*

The aim of this book is to contribute to this last request. Without underestimating the diversity and complexity of the situations encountered, we believe that there are some common themes in many of them, which could serve as a guide to find general rules and broad enough methodologies. One of such unifying conceptual frameworks is the paradigm of *chaotic advection* or *Lagrangian chaos* (Aref, 1984, 2002), which allows to transfer to fluid dynamics problems the vast amount of knowledge which has been developed in the study of nonlinear dynamical systems. The power of this approach has been greatly enhanced by recent experimental and theoretical developments in Lagrangian approaches to fluid dynamics in general, and to turbulence in particular (Shraiman and Siggia, 2000; Falkovich et al., 2001), and by the observation of similarities between developed turbulence and low-dimensional chaotic dynamics when considered from the Lagrangian point of view (Bohr et al., 1998, Chap. 8).

The application of dynamical systems concepts to understanding reactions in flows has been developing during the last decade or so, and summaries of the most relevant results have already been compiled for example in the Chaos Focus Issue published by Toroczkai and Tél (2002), and notably, in the very good review by Tél et al. (2005). It is not our intention to repeat here the contents of these works. We noticed instead the need of integrating this recent work into the context of more traditional fluid dynamics and turbulence approaches. Also, the generality of the results is better appreciated after surveying general concepts in chemical, biological, and fluid dynamics. In consequence we have written a significant amount of introductory material on these subjects. We expect that the contents of these first chapters will be useful not only for establishing the adequate framework for the developments in the following ones, but also to provide the interested reader with a compilation of results which are now scattered in different monographs on nonlinear dynamics, fluid mechanics, nonlinear chemistry, and mathematical biology.

Plan of the book

After this introduction, we start (Chapter 1) with a summary of basic facts in fluid dynamics, such as the fundamental equations, the

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http://www.worldscibooks.com/chaos/p471.html

phenomenology and description of turbulence, and the peculiarities of two-dimensional flows. Chapter 2 is devoted to the fundamentals of *dispersion* and *mixing*, i.e. to the mechanisms that move around substances contained in the fluid, eventually homogenizing the different parts. Transport by advection, with a description of the Lagrangian point of view, and molecular, turbulent and anomalous diffusion processes are introduced. Later, advection and diffusion are considered in a sequence of flow-types of increasing complexity: two-dimensional steady, two-dimensional weakly time-dependent, three-dimensional steady, and turbulent. The phenomenon of chaotic advection (Sect. 2.5), one of the unifying themes in the following, is presented, and tools are given for its description. In particular we introduce Lyapunov exponents and a filament, or lamellar, model (Sect. 2.7.1) which turns out to be a powerful tool to analyze mixing and complex reactions in flows. The motion of suspended particles which do not follow exactly the fluid velocity (i.e. inertial particles) is also briefly described.

Chapter 3 is an overview of chemical and biological nonlinear dynamics. The kinetics of several types of reactions –first order, binary, catalytic, oscillatory, etc.– and of ecological interactions –predation, competition, birth and death, etc.– is described, nearly always within the framework of differential equations. The aim of this Chapter is to show that, despite the great variety of mechanisms and processes occurring, a few mathematical structures appear recurrently, and archetypical simplified models can be analyzed to understand whole classes of chemical or biological phenomena. The presence of very different timescales and the associated methodology of *adiabatic elimination* is instrumental in recognizing that.

The rich consequences of adding a diffusive mechanism of transport to chemical or biological activity are described in Chapter 4. Fisher waves and other types of fronts, excitable waves, Turing patterns, and other spatiotemporal phenomena produce striking structures which are observed in chemical and biological media. Understanding them is needed before addressing the additional impact that advection has on these systems.

After these introductory Chapters, we begin in Chapter 5 the study of situations in which reaction, advection, and diffusion act together. We address simplified interactions and flows, which are representative of the different situations previously enumerated. The first case considered is that of a binary reaction occurring sufficiently fast, so that the process becomes limited by the slow diffusive processes which mixes the different chemicals which react. The filament model of Sect. 2.7.1 allows a rather complete description of this situation both in simple and in complex flows. Chapter 6 studies chemical or biological processes which decay, at least locally, to a steady state. The linear regime of such decay can be also understood both in laminar as in turbulent flows, leading to filamental spatial structures with strong intermittency properties. This problem has also implications for the decay of two-dimensional turbulence (Sect. 6.5).

Chapter 7 considers reactions having some kind of autocatalytic behavior, so that one of the components tends to grow fuelled by itself. This is the standard multiplicative reproduction undergone by many biological organisms. Excitable, bistable, and other types of reactions usually have an autocatalytic step, and the impact of flow on these is also discussed here. Oscillations under homogeneous, inhomogeneous and stochastically perturbed situations are considered in Chapter 8.

The spectrum of interesting problems involving active substances in flows is too broad to be fully covered here, and many topics are not touched in this book. The final Chapter 9 summarizes some of the most important ones, giving suggestions for further reading.