PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A
MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

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Preface

All the papers in this issue are concerned with fundamental aspects of combustion theory. Combustion science finds many practical applications in developments leading, for example, to improvements in the efficiency and performance of combustion systems, reductions in emissions of noxious pollutants, and the minimization of explosion and fire hazards during the transport, storage and use of combustible substances. Many of these papers discuss topics in the general area of hazards due to explosions and fires. All of them describe time-dependent combustion processes. The 11 papers are grouped together under four headings: Initiation of Explosions, Deflagrations, Detonations, and Combustion of Solids.

The first section contains papers by Blythe, Lee & Higgins, McIntosh and Oran & Khokhlov. All four discuss the role of pressure waves in initiating an explosion. Blythe considers a reactive gas mixture in a closed vessel. A classical analysis treats the mixture as homogeneous and leads to the conclusion that an explosion will not occur if the rate of heat loss exceeds a critical value. Blythe shows that a pressure disturbance can result in an explosion when the homogeneous system is subcritical and that the mechanism involves reactive amplification of the pressure wave. In the paper by Lee & Higgins the pressure disturbance is a blast wave. If this is sufficiently strong it will lead to to an almost instantaneous, direct initiation of detonation in an explosive gas mixture. The question posed is: what is the minimum blast wave energy required for direct initiation? The paper presents a critical assessment in which simple models and data from experiments and numerical simulations are reviewed with emphasis on one-dimensional situations. It is concluded that a direct initiation criterion must take account of blast wave amplification due to coupling with energy release and that the formation of localized hot spots due to wave interactions may also be important. In his paper McIntosh continues to explore the theme of pressure waves interacting with premixed combustion fronts. However, in this case, the interaction does not necessarily lead to an explosion. The treatment is one dimensional and the paper seeks to bring together and contrast results from a number of different situations including cases of acoustic and steep-fronted pressure waves interacting with low speed flames. For example, a steep pressure rise can lead to rapid flame acceleration, whereas a sufficiently large steep drop causes extinction. The relevance of the work to interactions with turbulent flames is discussed. Finally in this group, Oran & Khokhlov investigate the interaction between shock waves and laminar flames and describe the sequence of events leading to a deflagration-to-detonation transition (DDT).

Their work differs from that of the earlier papers in this issue in two respects: the flow field under investigation is two rather than one dimensional, and the equations solved in their numerical simulations are the full Navier–Stokes equations including molecular transport terms. Note, however, that McIntosh does include molecular transport processes in some of his cases. Oran & Khokhlov consider initially cylindrical laminar flames that are distorted by the incident shock–flame interaction. Subsequently, secondary and later shocks and rarefactions continue to disturb the flame and generate vorticity, which soon gives the flame a quasi-turbulent structure.

Wave interactions outside this flame region generate hot spots whose enhanced reaction rate leads to transition to detonation. Laminar flame structures are found to be resilient and to survive throughout this process. Multidimensionality and molecular transport effects are both features of the DDT events described here.

Laminar and turbulent deflagrations are discussed in the second group of papers, which are written by Dold & Crighton, Bradley and Cant. In the first of these contributions Dold & Crighton discuss the influence of flame curvature on laminar flame propagation and stability. Differences between the diffusivities of heat and a lean reactant are known either to stabilize or destabilize flames, depending on the Lewis number of the deficient reactant. This behaviour is associated with a monotonic relationship between flame speed and curvature. Classical analysis shows that if the relevant Lewis number is sufficiently small the governing equation describes an anti-diffusive instability. Dold & Crighton study the influence of non-monotonic curvature-dependent flame propagation on flame instabilities and find a wide range of new phenomena. In his paper, Bradley analyses the effects of hydrodynamic flame instabilities on the development of accidental explosions in initially quiescent combustible premixtures. In a large-scale event the developing flame instabilities cause wrinkling and acceleration of the flame. By using established linear stability theory it is found that instabilities develop at large scales and cascade to progressively smaller scales until they are stabilized by thermodiffusive effects. A fractal analysis then leads to a prediction of the mean flame speed after a critical Peclet number has been reached. The final paper in the group, by Cant, describes direct numerical simulations of turbulent deflagrations in which all of the wide range of chemical and turbulence length- and time-scales are fully resolved. The paper presents the formulation of the problem, the simplifications introduced, the numerical discretization scheme for efficient parallelization and some sample results. The relevance of these essentially model-free predictions to the improvement of current turbulent combustion models is discussed.

The third of these topics is analysed in two papers: one by Clarke & Nikiforakis, and the other by Short, Kapila & Quirk. Clarke & Nikiforakis show that molecular diffusion generally plays a negligible part in the propagation of high-speed planar combustion waves. This perspective leads to a classical gas dynamic description in terms of discontinuous combustion waves, which may be either detonation waves, travelling supersonically, or subsonic deflagrations. Whereas the classical description relies on empirical information to specify the speed of these waves, Clarke & Nikiforakis present a self-contained rational theory from which both the flow and the wave speed can be predicted. The analysis is illustrated in terms of the role of the transient weak detonations in the formation of a strong detonation wave. Short *et al*. use numerical simulation to explore the mechanisms leading to pulsating instabilities of detonation waves. They solve one-dimensional, time-dependent flow equations, again in the absence of molecular diffusion terms, and consider a three-step, chain-branching combustion reaction. Using these calculations they explain the hydrodynamic mechanisms leading to the regular and irregular instabilities that have been observed experimentally.

The final two papers in this issue are concerned with combustion of solid materials. The processes involved in these situations are particularly complex and only partly understood. Flows, which involve two or three phases, are often turbulent, radiation heat transfer is often important, and reaction mechanisms and rates are

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not well established. In their contribution Lowe & Clarke analyse the combustion of solid propellant materials that burn rapidly and release large quantities of chemical energy and so are suitable for use in rocket motors and in ballistic weapons. Numerical simulations of internal ballistics are presented in which the ignition and combustion processes are modelled via averaged one-dimensional, two-phase flow equations for a mixture of solid particles and a compressible reactive gas mixture, subject to a one- or two-step chemical reaction. Predictions are compared with available experimental data. In the final paper Nelson & Brindley model the combustion of polymer materials. A nonlinear dynamical systems model is developed to gain insight into the flammability of polymeric materials. The configuration considered is that of the cone calorimeter, which is used for flammability tests. The authors conclude that their technique can be used to identify the types of fire-retardants that will be most effective at decreasing the flammability of a given material.

The editors would like to add as a historical note that the incentive for compiling the papers presented in this issue can be traced back to 1997. It was in April of that year when a number of distinguished colleagues who work in the field of combustion gathered in Cambridge to present an overview of the latest advances and research directions for the next century, of their specialized area. A wide range of topics was covered, from turbulent diffusion flames and detonations to polymer and solid propellant combustion. Some of the presentations found their way into this issue, albeit not necessarily under the same title. The lecturers and the titles of their talks are listed on p. 3486.

The 70th birthday of Professor J. F. Clarke was celebrated in 1997. To mark his contribution to mathematical combustion, a special theme of the meeting was research carried out by his past and present colleagues; many of his accomplished students, as well as more recent postdoctoral researchers, gave presentations. Many of the lectures referred to work related to what is known as 'Clarke's equation':

$$\frac{\partial}{\partial t^2}\left(\frac{\partial T^{(1)}}{\partial t} - \gamma \exp T^{(1)}\right) - \frac{\partial}{\partial \psi^2}\left(\frac{\partial T^{(1)}}{\partial t} - \exp T^{(1)}\right) = 0.$$

These addressed the impact of the equation on detonation theory, the numerical and (Newtonian) asymptotic ways to solve it and, of course, the various areas in which it has found applications, from detonation initiation to wall heating problems.

The editors thank the lecturers at that conference and particularly those who have contributed to this issue. Our thanks extend to everybody who helped with organizing the conference at the Department of Chemistry, and in particular Yvonne Rose. Many thanks also to Professor D. G. Crighton for his support and for hosting the conference dinner at St John's College.

K. N. C. Bray
N. Nikiforakis

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A group photo of the lecturers at the 'Combustion Science at the End of the Millennium' meeting, held at the University of Cambridge, April 1997. Top row from left to right: G. I. Barenblatt, M. Short, D. S. Stewart, P. A. Blythe, J. Brindley, A. C. McIntosh, D. G. Crighton, R. Klein, J. S. H. Lee, J. B. Moss. Middle row from left to right: C. A. Lowe, R. S. Cant, G. O. Thomas, A. K. Kapila, Y. Rose, N. Nikiforakis, D. Bradley, N. Peters, P. Clavin, D. R. Kassoy. Bottom row from left to right: E. S. Oran, K. N. C. Bray, A. Linan, J. W. Dold, F. A. Williams, J. D. Buckmaster, J. F. Clarke, E. F. Toro, N. Riley.

'Combustion Science at the End of the Millennium' meeting 1997: a list of oral presentations

Professor G. I. Barenblatt (Cambridge & Berkeley) Scaling laws for developed turbulent flows with applications to combustion.

Professor P. A. Blythe (Lehigh) Wall heating, ignition and the Clarke equation.

Professor D. Bradley (Leeds) Instabilities and burning velocities in large-scale explosions.

Professor K. N. C. Bray (Cambridge, UK) Theoretical models of premixed turbulent combustion.

Professor J. Brindley (Leeds) Polymer combustion.

Professor J. D. Buckmaster (Illinois) Déjà vu, leading edge—two illustrations of how mathematical modeling can illuminate combustion physics.

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Dr R. S. Cant (Cambridge, UK) Direct numerical simulation of turbulent flames.

Professor J. F. Clarke (Cranfield) Remarks on diffusionless combustion in gases.

Professor P. Clavin (CNRS) Recent theoretical advances in dynamics of gaseous detonations.

Professor D. G. Crighton (Cambridge, UK) Newtonian asymptotics for combustion.

Professor J. W. Dold (UMIST) Non-monotonic curvature-dependent propagation of a front.

Professor P. Gray (Cambridge, UK) Thermal explosions in chemistry.

Professor A. K. Kapila (Rensselaer) Detonations provoked by gradients.

Professor D. R. Kassoy (Colorado) Revisiting 'combustion' stability in solid rocket motors: the dynamics of acoustically generated vorticity.

Professor R. Klein (Wuppertal) Numerical issues arising in DDT simulations.

Professor J. H. S. Lee (McGill) Detonation initiation.

Professor A. Linan (Madrid) The anchoring of diffusion flames in the near wake of the fuel injector.

Dr C. Lowe (Cranfield) CFD modelling of solid propellant ignition.

Professor J. B. Moss (Cranfield) Combustion modelling for the aircraft gas turbine.

Dr A. C. McIntosh (Leeds) Time delays and oscillations in combustion.

Dr N. Nikiforakis (Cambridge, UK) Evolution of nonlinear combustion-driven waves.

Dr E. S. Oran (NRL) Theoretical and computational aspects of DDT.

Professor N. Peters (RWTH) Direct numerical simulation of the eikonal equation for flame propagation in turbulent flow fields.

Professor N. Riley (UEA) Free convection over a burning sphere.

Dr M. Short (Illinois) On the role of Clarke's equation in detonation theory.

Professor D. S. Stewart (Illinois) The dynamics of multi-dimensional detonation.

Dr G. O. Thomas (Aberystwyth) Continuing challenges to the understanding of transition to detonation.

Professor E. F. Toro (MMU) On numerical methods for combustion-driven flows.

Professor F. J. Weinberg (Imperial) Electrical aspects of combustion at the end of the millennium.

Professor F. A. Williams (UCSD) Evolution of asymptotic analyses of flames.