J Eng Math (2006) 56:101–104
DOI 10.1007/s10665-006-9075-9

ORIGINAL PAPER

Thermal explosion: modern developments in modelling, computation and applications

Igor Goldfarb · Rodney Weber

Received: 13 February 2006 / Accepted: 12 July 2006 / Published online: 8 November 2006

Abstract This paper is an introduction to the special issue of the Journal of Engineering Mathematics on the mathematical modelling of the thermal-explosion phenomenon. The issue includes six papers covering a wide range of current studies in the field. This introductory paper is written to bring a description of the phenomenon to readers with a background in mathematical modelling and computational mechanics and without specialization in combustion theory.

Keywords Thermal explosion · Mathematical modelling · Combustion

1 Introduction

This paper is an introduction to the special issue of the Journal of Engineering Mathematics, devoted to modelling of the thermal-explosion phenomenon. The paper represents a broad outline of different, though surely not all, aspects of mathematical modelling of this type of combustion process without the intention of presenting a complete review of the successes in the field. This issue includes six papers covering a wide range of current study in the field. This introductory paper is written to bring a description of the phenomenon to readers with a background in mathematical modelling and computational mechanics and without specialization in combustion theory.

2 Phenomenon

Combustion represents a rapid chemical reaction between substances that is usually accompanied by generation of heat and light in the form of a flame. In most cases, oxygen comprises one of the reactants. The rate of the reaction varies extremely rapidly with temperature. Thus, for example, at room temperature and

I. Goldfarb (✉)
Department of Mathematics, Ben-Gurion University of the Negev, P.O. Box 653, Beer-Sheva 84105, Israel
e-mail: goldfarb@bgu.ac.il

R. Weber
School of Physical, Environmental and Mathematical Sciences UNSW at ADFA, Canberra 2600, Australia
e-mail: rodney.weber@unsw.adfa.edu.au

atmospheric pressure, hydrogen and oxygen hardly react over a period of many years. As the temperature is raised, the reaction rate remains immeasurably small up to some critical value, which depends on the conditions of the specific experiment. At higher temperatures, even those only a few degrees above critical, the combustible mixture reacts very rapidly. The reaction rate is so high that scientists of the 19th century could not study its kinetics in detail. Unlike an ordinary reaction, a combustion reaction is characterized by the existence of a temperature, at which the reaction rate changes suddenly, almost discontinuously. This temperature is referred to as the ignition temperature (or self-ignition temperature).

A combustible material with highly exothermal decomposition potential, when heated, either intentionally or unintentionally (such as in a fire), can produce a thermal explosion or even a detonation, producing a great deal of damage. Thermal explosions are complex events, which couple many chemical and physical processes such as heating, expansion, phase transition, chemical decomposition, heat build-up, thermal runaway and finally heat and momentum transfer. The description of the explosion requires the characterization of the initial material, physical and chemical states, the rate of heating, the rate of decomposition (decomposition kinetics), the changes in the explosive chemical and mechanical properties, the rate of burning, the transfer of explosive energy into thermal and mechanical energy (hydrodynamics), and, finally, the amount of damage (if applicable). Due to the presence of a number of processes with essentially different time scales (characterized by a gap in characteristic times), most of the developed models of the phenomena represent multi-scale problems and their mathematical description can be formulated as singularly perturbed systems of differential equations.

The development of an understanding of and predictive capability for the hazards involved in thermal explosion of energetic materials exposed to high temperatures, such as fires, requires that we understand the fundamental reactions of energetic materials exposed to thermal stimuli. A number of approaches were suggested to quantify the thermal-explosion process under carefully controlled conditions, and to provide a database, which one can use to validate predictive codes and models. The use of the data from experiment is complemented by separate measurements of fundamental reaction kinetics, deflagration behaviour, and thermal and mechanical properties.

3 History's milestones

It seems that no one has been able to conclusively determine when people first began to utilize combustion phenomena. The first known explosive was black powder, which the Chinese were using by the 11th century AD and it is thought that the knowledge of black powder spread from China to the West during the 13th century. It also seems that spontaneous ignition was formally identified by the Chinese in the 2nd century AD [1, Chapter 5].

The early history of the study of combustion is closely related to the history of chemistry and of the molecular theory of matter. Perhaps because fire is spectacular and superficially mysterious, studies of combustion enjoyed prominence in the development of the foundations of chemistry until the end of the 18th century.

The important features of explosions were reported in the middle of the 19th century by Bunsen and van 't Hoff. In 1884 Van't Hoff suggested the prototype of the expression that is well-known today of the rate of a chemical reaction for which he won the first Nobel Prize in Chemistry (1901) "in recognition of the extraordinary services he has rendered by the discovery of the laws of chemical dynamics ...". The existing form $k = A\exp(-E/(RT))$ (here A is a pre-exponential multiplier, E the activation energy of the combustible mixture, R the universal gas constant, T the temperature) of this expression is a result of theoretical considerations of Arrhenius (1889). The formula (called after him) serves nowadays as a basic analytic tool for most of the theoreticians working in the field of combustion theory and closely related fields of chemical engineering. *However, this expression is a source of high nonlinearity in combustion models*.

The development of a rigorous theory of thermal explosions was started in 1926 when Semenov presented the first experimental proof regarding the dependence of the dynamics of the phenomenon on branch-chain reactions (the phosphorus vapour-oxygen reaction). He discovered that an explosion occurs if the partial pressure of O_2 is between two limits (Fig. 1). Simultaneously, he proposed the theoretical model, which is named after him [3, 4]. He showed that explosion occurs when heat release exceeds heat dissipation to the surroundings. Hinshelwood discovered the first and second explosion limits the H_2-O_2 reaction. Semenov and Hinshelwood won the Nobel Prize in Chemistry in 1956: "...for their researches into the mechanism of chemical reactions...". Frank-Kamenetskii [5, Chapters 3, 4] made very important contributions to the analytical analysis of Semenov's model, when he proposed to use a small-temperature approximation [2, Chapters 1, 2]. There was a growing interest in the phenomenon of thermal explosion during the second part of the 20th century, especially thanks to a number of industrial applications of the pure theory. During the last decades we have witnessed the amazing phenomenon of the penetration of the basics of the thermal-explosion ideology (and corresponding models) into scientific fields far removed from combustion theory, for instance, biology, environmental sciences, etc.

4 Special issue

This Special Issue of the *Journal of Engineering Mathematics* contains a set of original manuscripts representing in some sense the state of art of modelling thermal explosions taking place in distinct media. The current progress in studying the field is demonstrated by a number of papers, prepared by groups of experts working in a range of areas where modelling of the phenomenon is important with various applications in engineering sciences, chemical industry, biology, etc. When about a year ago the Editor-in-Chief of the JEM came up with a suggestion to put together such a special issue, the idea was discussed with a number of potential contributors who overwhelmingly supported it. The original submissions have been put through a careful review process resulting in six papers that ultimately make up the issue.

The papers are ordered in alphabetical order according to the first-named author.

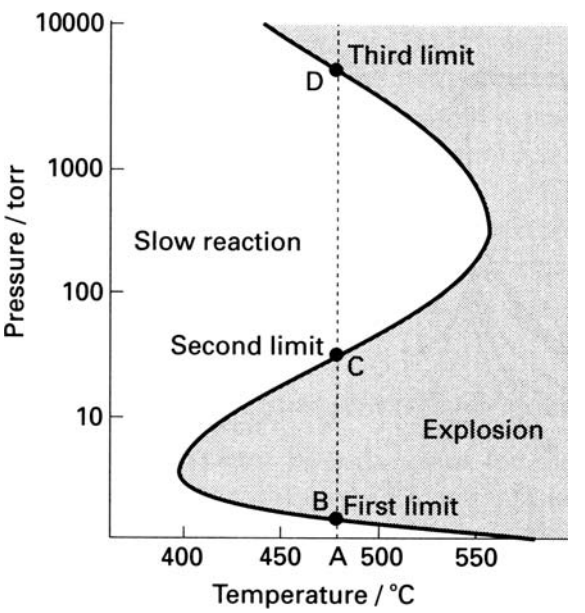

Fig. 1 The explosion limits for a stoichiometric mixture of hydrogen and oxygen [2]

The manuscript by Blythe, Kapila and Short shows clearly how one can make analytic progress with chemistries that are rather more complex and realistic than single-step reactions. The authors obtain very good approximations to crucial values for important parameters such as growth and termination times and the presentation in tabular form is an excellent way of summarizing their results. The contribution by Goldfarb, Gol'dshtein, Greenberg and Zinoviev presents a detailed model of the thermal ignition of gel droplets which occurs via a vapour phase. The result is a valuable addition to the literature on ignition problems that extends the original work of Frank-Kamenetskii and the authors employ their own method of integral manifolds to solve the model. They identify regions of the parameter space where a range of dynamical system behaviours occurs, in particular identifying an interesting route to explosion, which occurs through oscillations over a rather long time.

The paper by Gorelov, Schepakina and Sobolev is devoted to a study of the critical phenomena in autocatalytic combustion models. This work continues a series of their publications on the determination of so-called critical regimes (regimes separating regions of explosive and non-explosive chemical reactions), which are based on a careful investigation of the corresponding mathematical model, representing a singularly perturbed system of differential equations with lumped and distributed parameters. The authors model critical regimes by canards (one-dimensional stable-unstable slow integral manifolds). The geometric approach, in combination with asymptotic and numerical methods, permits to explain the strong parametric sensitivity and obtain asymptotic representations of critical conditions of self-ignition. The contribution by Shah, Brindley, McIntosh and Griffiths continues the very interesting work that the Leeds group has been conducting on the ignition of spherical samples of porous materials, such as lagging insulation. The careful examination of the motion of the ignition front due to external heating and exothermic oxidation is clearly a complicated matter and continues to offer the surprises found in earlier work and corroborated by the other article in this issue on the application of the Method of Lines. The manuscript by Shouman contains an original view on the historical development of one of the numerous aspects of thermal-explosion theory. He shows that the exact solution to the problem, obtained earlier by the author and his colleagues, allows to avoid the approximation proposed by Frank-Kamenetskii and is consistent with the original Semenov formulation. The paper by Weber, Sidhu, Sawade, Mercer and Nelson presents a fresh viewpoint on a recent reactive-hotspot problem (a constant heat source embedded in a concentric volume of reactive material), which has previously been shown to display unexpected behaviour. The authors report on their use of the Method of Lines to corroborate these results. They also describe an application of sensitivity analysis to allow a precise and rigorous determination of criticality in such a dissipative system.

Acknowledgements To recap, the Guest-Editors on behalf of all authors of the Special Issue express their gratitude to Professor Hendrik K. Kuiken. It is our pleasant duty to underline that during our almost a year-and-a-half-long collaboration he demonstrated highly professionalism, excellent work ethics and almost endless patience which made our efforts pleasant, productive and worthwhile. We are especially thankful to the reviewers whose expertise in the field, along with the creative content of their critical comments, helped the authors to improve the level of presentation, and will, as we keenly believe, make the issue a success.

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