SFB 606 – a German research initiative on unsteady combustion

Henning Bockhorn, Jochen Fröhlich, Rainer Suntz

Institute for Chemical Technology, University of Karlsruhe, 76128 Karlsruhe, Germany

1 Introduction

Combustion is and for the foreseeable future will be the major source for the production of mechanical and electrical energy. Currently, more than 90% of primary energy are generated through combustion [1]. According to the World Energy Council the energy demand will increase by 65% until 2020. Against this background it is of primordial interest to make economic use of the available resources while at the same time minimizing the impact of pollution and other detriments. New concepts are being developed to cope with this situation. Direct injection for spark ignition- and Diesel-engines is supposed to yield better efficiency and reduced emissions. For stationary and mobile gas turbines LPP (lean-premixed pre-vaporized) and RQL (rich-quenchlean) operation modes are developed and investigated, to name but two types of applications.

Ubiquitously, unsteady phenomena are encountered in combustion. In some cases, as with reciprocating engines, they are an inherent design feature of the process. In other cases, as illustrated by the example of a gas turbine, they are related to dysfunctions. Lean conditions, e.g., chosen to reduce emissions like NO_X, make flames substantially more susceptible to combustion instabilities such as the thermo-acoustic resonance which in the limit can even destroy the device. Although unsteady processes of reaction, heat- and mass transfer, change of phase, etc., and their intricate coupling through unsteady velocity, temperature, and/or pressure are critical items in a large variety of energy conversion applications, these are to date still not fully understood. Furthermore, design procedures in industry are often based on steady considerations with only scarce coverage of unsteady phenomena. Unsteady phenomena are inherently more complex than steady ones and represent a substantial challenge to the analyst. To match this demand and contribute to the knowledge on unsteady combustion a research initiative was initiated at the University of Karlsruhe, Germany, as a so-called "Sonderforschungsbereich" (SFB). This research constitution is a long-term funding instrument of the German Research Foundation (DFG) for interdisciplinary research dedicated to a particular subject with a duration of up to twelve years.

SFB 606 is operational since spring 2002. Its full title is "Unsteady Combustion: Transport phenomena, Chemical Reactions, Technical Systems" and it assembles various groups from the Universities of Karlsruhe and Stuttgart, DLR Stuttgart, and Forschungzentrum Karlsruhe (FZK). The purpose of the present paper is to report on the objectives and goals of this SFB. As the start up time of research projects, in particular of experimental nature, is relatively large, no conclusive results can be expected at this stage. A few spotlights will illustrate the ongoing research, notwithstanding due publication of the material at a later stage. The second and third author of this paper are project leaders while the first author is additionally the initiator and coordinator of SFB 606. They have undertaken the task of editing on behalf of their colleagues, but it goes without saying that the contents of this report is based on the concerted effort of the entire consortium. For lack of space citations have been almost completely avoided here. Further detailed information on all projects is available in the publications of the www.sfb606.uniunder members and karlsruhe.de. This site is continuously updated and the participants of SFB 606 will be happy to interact with other researchers of the community.

2 Themes and Structure

Table 1 provides an overview over the different projects comprising SFB 606. It covers the first funding period of three years. Hence, investigations are conceived so as to be continued, complemented and enlarged during subsequent periods.

The structure of research activities, created during the conception phase of the SFB, distinguishes between elementary processes (label A), composite processes (label B), and technical applications of full complexity (label C). It is the vision of the participants that a fundamental understanding of unsteady processes, particularly on the elementary and composite level, will contribute to a better understanding of the full processes which may then be exploited to optimize the latter in a desired way. Therefore, the focus of the SFB is not to develop or optimize a particular device, experimental technique or numerical tool, but to provide understanding of a large variety of unsteady combustion and combustion-related phenomena. This understanding is to be condensed into models which can then be

employed on the next level of complexity. The diversity of unsteady phenomena considered in this research programme offers the possibility of mutual stimulation and transfer of experimental, numerical or modelling procedures to configurations for which they have not been employed yet.

Apart from the level of complexity mentioned above, the research activities in SFB 606 can be grouped around subjects of common characteristics. Three such clusters have been created so far as visualized in Table 1. In the following we use this structure to organize the presentation. It should however be stressed that many other points of contact between individual projects exist resulting from common experimental or numerical procedures or the transfer of the results.

3 Mixture Formation, Ignition, Flame Propagation

Combustion starts with the creation of the combustible. For engines with direct injection (DI) this involves an intricate coupling between the dynamics of the injected liquid, its interaction with the gas in the combustion chamber, evaporation at the liquid's surface, mixture formation, and ignition of the reactive mixture. Figure 1, as an example, illustrates the self-structuring of the spray jet upon injection. In many cases additional complication arises through a partial interaction of the spray with a solid wall of the combustion chamber. While by itself local ignition and quenching is an unsteady process, for a reciprocating engine the whole operation is also unsteady on a larger time scale. The group of projects labelled 'Cluster 2' in Table 1 is concerned with themes around this process. One focus is the relatively recent concept of DI spark ignition- and Diesel- engines.



Figure 1: A laser-light sheet visualizes a fuel jet from a multi hole nozzle at 200 bar (courtesy A. Nauwerk).

On the elementary level, Project A3 investigates the ignition of a jet under different conditions by experimental methods. Project B5 is concerned with spray ignition. The interaction between fluid dynamics, change of phase, and chemical kinetics is studied numerically using different one- and two-dimensional models. These are validated through corresponding experiments. In project B4, the interaction of a liquid jet with a wall is investigated experimentally in order to study the modifications to its characteristics generated through the impact. A corresponding result is shown in

Figure 2 showing that the fuel spray in fact hits the piston before ignition. Particularly relevant for ignition and propagation of flames is the turbulence of the fuelgas-mixture. An important phenomenon, still not sufficiently understood, is the generation of turbulence by the propagating flame itself through heat release and the resulting expansion of the gas. This is the subject of Project A9. In project B2, the interaction of a nonadiabatic flame with a cold wall is studied. This investigation is carried out in an one-stroke engine providing detailed control of the initial turbulence and full visual access to the chamber. Figure 3 reveals the deceleration of a flame towards the cold sidewalls of a combustion chamber. In project C3, finally, a realistic engine is employed for most of the investigations to study the full process. Here, the focus is on the appropriate guidance of the injected fuel towards the location of the spark ignition (see Figure 2).



Figure 2: Spray-wall interaction in a one-cylinder research engine 33° C.A. before ignition. Visualization by Mie scattering of the spray droplets, averaged over 20 events (courtesy J. Pfeil).



Figure 3: Flame-wall interaction in a single-stroke engine with low turbulence level. The picture shows the flame front in a methane-nitrogen-oxygen mixture $(\lambda=1.3)$ 32ms after ignition (courtesy M. Hunzinger).

4 Unsteady Kinetics, Ignition of Hydro-Carbons, Pollutant Formation

Another group of projects (Cluster 1) is of somewhat more fundamental nature than the one described before. It is concerned with reaction kinetics in the broadest sense for unsteady conditions. These are frequently characterized by highly variable concentration, temperature, and pressure. As a consequence, nonequilibrium effects may prevail and govern the reaction process. Different reaction channels can become active depending on pressure, temperature and history of the process as illustrated in Figure 4. Such data are

particularly relevant for ignition and quenching processes and not sufficiently available so far. In Project A1, non-equilibrium effects are investigated for the alcoxy-system ($C_nH_{2n+1}O$) by shock-tube experiments. These investigations are of special concern in the understanding of engine knock. Project A2 focuses on the ignition of complete real fuels. Data on the kinetics of the thermal decomposition of cyclo-alcane and aromatis during this process are relevant for a large variety of configurations and the basis for adequate modelling. They will subsequently be used by several other projects in the consortium. Another issue where detailed knowledge about the reaction kinetics is indispensable is the formation of pollutants such as NO_x. The inhomogeneous composition of the mixture in a DI engine provides a particular situation in this respect. Project A4 aims to clarify whether these kinetics are already sufficiently well understood for an adequate modelling. Furthermore, the impact of unsteady pressure and temperature is to be elucidated. In recent years, particular relevance is attributed to soot formation and legislation is becoming stricter and stricter on this matter. This issue is investigated in projects B1 and C4. The former is devoted to the soot formation in unsteady, non-adiabatic flames. Figure 5 shows a result form a simultaneous measurement of different quantities characterizing the formation of soot my means of the RAYLIX technique [4]. In Project C4, experiments are performed on soot formation under the conditions of a full-scale DI engine.



Figure 4: Energy dependence of reaction channels of the C_2 - H_5 -O-System [2].



Figure 5: Simulataneous measurement of two- dimensional maps of soot volume fraction f_V , mean particle

radii r_m and particle number density N_V for a turbulent flame (time resolution 100ns).

5 Numerical Modelling of Flames, Combustion Instabilities

The third cluster is organized around flame propagation and unsteady effects generated by perturbations of a reference state. This can take place on the elementary level of the flame but also on the level of an entire system for which combustion instabilities in a burner are an example. In the later case, a complex interaction between fluid mechanics, mixing, reaction and largescale compressibility effects is observed. In Project A5, the flame itself is the subject of interest, in particular its response to unsteady fluctuations in composition. Experimental data will be obtained from LIF and Raman spectroscopy. Numerical modelling is performed by means of the level set approach while the reaction mechanism is reduced with the ILDM technique. Preliminary work has shown that perturbations with frequency in the range of 10 ... 1000 Hz may substantially change the inner structure of the flame. The ILDM approach allows to control the representation of chemical time scales accordingly to secure adequate modelling. Data on the response of flames to unsteady perturbations are highly relevant for combustion instabilities. An example is the thermo-acoustic instability where the Rayleigh criterion relates ignition times depending on chemical and fluid mechanical properties of the flow to pressure time scales. This instability is a prototype for complex unsteady behaviour in combustion. It furthermore is of high economical and ecological relevance as it prevents burners from being run in certain parameter ranges where they might be more efficient or les pollutive.



Figure 6: Frequency spectrum of a hot-wire signal obtained in the cold flow after the burner exit with and without swirl [3].

Project C1, provides experimental data on piloted, swirl stabilized premixed flames. Apart from their own wealth, they will be used for comparison and validation in the related numerical projects. In the present funding period, most of the work is performed on cold flows. The reason simply is that many central issues to be addressed already appear without combustion and can hence adequately be investigated under these conditions. This is illustrated by Figure 6 showing such a fluid mechanical instability in the cold flow at the exit of a movable-block burner into the ambient. Without swirl, characterized by the swirl numbers S or $S_{0,theo}$, the flow is steady, while with swirl it is highly unsteady with a well-defined peak in the frequency spectrum.



Figure 7: Iso-surface of the pressure in a swirling annular jet obtained by LES for $Re= 163\ 000$ and swirl number S= 0.9, flow from upper right to lower left (courtesy M. García-Villalba).



Figure 8: URANS computation of an unsteady lifted diffusion flame in a swirl burner with S=0.8 using a presumed-joint-PDF model. Left: sample of phaseaveraged temperature, right: phase shift of periodic temperature oscillations in degrees. Vertical coordinate is along the burner axis, horizontal coordinate is radial, lengths in mm (courtesy B. Noll).

Project A6 focuses on fluid mechanical phenomena in the vicinity of the nozzle outlet by means of Large Eddy Simulation (LES). Figure 7 displays a computational result for one of the configurations experimentally investigated in Project C1 showing a spiral instability of the flow. Instabilities of the fluid flow can trigger unsteadiness of the total reaction rate which in turn may launch the thermo-acoustic instability. To assess the sensitivity of the systems with respect to such fluctuations, not only the resonance but also the damping characteristics of the burner need to be known. This issue is investigated in Project A7 by means of LES. Computations for the entire burner with reactions and with the full geometric complexity including secondary streams, etc., require a higher level of modelling in order to keep the problem tractable. In Project B6, devoted to such simulations, unsteady RANS is therefore selected as the computational approach. Figure 8 shows such a computation for a swirl burner. The right picture displays the phase shift of the temperature oscillations, a quantity which is pertinent for the thermo-acoustic instability via the Rayleigh criterion.

6 Experimental and Numerical Techniques

Apart from the interactions between projects in each cluster numerous points of contact exist across these groups. The kinetic data obtained in the respective projects, the basis for subsequent e.g., is combustionmodelling projects. in several other are exchanged Experimental techniques between different researchers such as the RAYLIX method. Also, devices as lasers and cameras are used in common. In particular, a high-speed camera was purchased recently and will be shared by several projects. Also, the numerical projects in different clusters exchange numerical and modelling strategies. An example is given by the reaction modelling in Cluster 2 which will be transferred to projects in Cluster 3. A particular feature of SFB 606 is the close interaction of experimental and numerical work. This is also supported by additional activities not within the SFB but associated to it at the different institutions. In the future, the character of the projects is supposed to gradually move from fundamental ones (label A) to more applied ones (label C).

6 Dissemination

The results of SFB 606 are published in papers and conferences according to the usual standards. Regular seminars open to the public are organized and a workshop on results achieved during the first funding period will take place in September 2004 (see specific announcement). SFB 606 is also able to host top-level foreign researchers for short and mid-term collaborative projects. The most recent grant, e.g., was delivered to G.I. Sivashinsky from Tel Aviv University for a one-month stay at the University of Karlsruhe.

Acknowledgements

The authors like to thank all colleagues in SFB 606 for their cooperation and stimulating discussions. The German Research Foundation (DFG) is acknowledged for the substantial support dedicated to this research.

References

[1] International Energy Agency, *Key Word Energy Statistics*, Paris (2003).

[2] H. Hippler, B. Viskolcz, Addition complex formation vs. direct abstraction in the $OH+C_2H_4$ reaction, Phys. Chem. Chem. Phys. **2**, 3591 (2000).

[3] M. Lohrmann, H. Büchner, *Periodische Störungen im turbulenten Strömungsfeld eines Vormisch-Drallbrenners*, Chemie-Ingenieur Technik **72**, 512-515 (2000) [4] H. Bockhorn, H. Geitlinger, B. Jungfleisch, Th. Lehre, A. Schön, Th. Streibel, R. Suntz: *Progress in Characterization of Soot Formation by Optical Methods,* Phys. Chem. Chem. Phys., 4, 3780 (2002)

	Α	В	С
Cluster 1 Unsteady kinetics, ignition of hydrocarbons, pollutants	 A1: Non-equilibrium effects in chemical reactions Exp H. Hippler A2: Elementary kinetics for the ignition of hydrocarbons Exp H. Hippler, P. Frank A4: Coupling of NO-formati on and unsteady flame propagation Exp T. Dreier, H. Hippler 	 B1: Soot formation in non-adiabatic, unsteady flames in laminar and turbulent flow focussing on flame-wall interaction Exp. H. Bockhorn 	C4: Soot formation in DI engines Exp R. Suntz, U. Spicher
Cluster 2 Mixture Formation, Ignition, Flame propagation	 A3: Auto-ignition of unsteady jets Exp, Num H. Bockhorn, W. Breitung, U. Maas A9: Experimental investigation of lame-induced turbulence in un- steady flame propagation Exp, Num N. Zarzalis, R. Suntz 	 B2: Non-adiabatic flames in the presence of cold walls and inhomogeneous mixtures Exp. U. Spicher B4: Spray-wall interaction in unsteady flow Exp K. Dullenkopf, U. Spicher B5: Auto-ignition of fuel jets in hot gas flow Exp, Num R. Koch, U. Maas 	C3: Mixture Formation in DI spark- ignition engines Exp U. Spicher
Cluster 3 Numerical modelling of flames, Combustion instabilities	 A5: Experimtents and hierarchical Modelling of flames with periodic perturbations Exp, Num A. Claas, U. Maas, W. Stricker A6: LES of the oscillating flow in burner configurations with piloted premixed flames Num J. Fröhlich, W. Rodi A7: Investigation of the resonance characteristics of an exper- imental combustion chamber of Helmholtz- resonator type Num F. Magagnato, M. Gabi, H. Büchner 	B6: Numerical simulation of periodically excited turbulent combustion in real systems Num B. Noll, M. Aigner	C1: Experimental investigation of oscillatory tendencies in piloted premixed flames Exp. H. Büchner

Table 1: Overview over the different projects comprising SFB 606 during the first funding period. The labels A,B,C distinguish between more fundamental projects, projects concerned with interactions of different phenomena, and investigations of full systems, respectively. The original title is translated to English here. The labels "Exp" and "Num" indicate whether preferentially experimental or numerical methods are applied, or both. The third item provides the names of the project leaders.