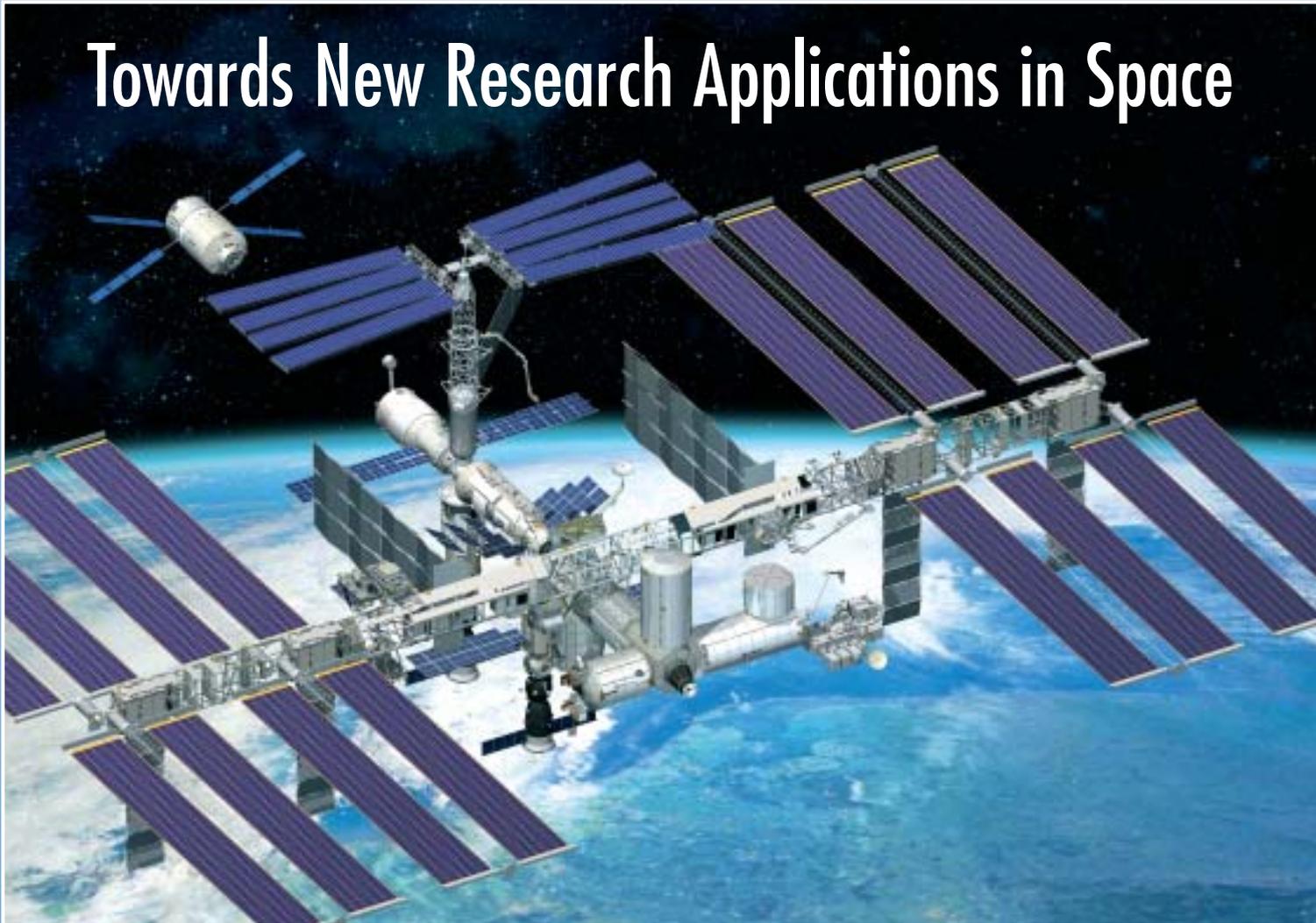




Topical Teams in the Life & Physical Sciences

Towards New Research Applications in Space



Instabilities in Lean Gas-Phase Combustion

Lean burning is the burning of fuel-air mixtures with less than the chemically-balanced (stoichiometric) mixture. It produces a significant increase in fuel efficiency and reduction in pollution. However, the limits and control of lean burning are still not well understood. This is the motivation behind the study of instabilities in lean gas-phase combustion under microgravity conditions via direct numerical simulations and comparison of the results with experimental data. The goal is to gain fundamental insights in order to identify and understand the intrinsic chemical and fluid dynamical mechanisms responsible for these instabilities. The potential of this microgravity combustion research includes the development of technology that would reduce pollution and fire and explosion hazards, improve hazardous waste incineration and increase efficiency of the conversion of chemical energy to electric power or motive force. The results from this fundamental research will thus benefit chemical engineering and power generation. Its wide range of applications in industry includes lean-burning car engines.

1. Motivation for Research

The design of efficient, low-pollution combustion engines and the assessment of fire and explosion hazards in, for example, chemical plants and mine shafts require a profound knowledge of the behaviour of lean premixed-gas flames, i.e. those near extinction or stability limits. Under these conditions, the flames are highly sensitive to disturbances such as buoyancy-induced turbulent flow. Microgravity is thus a suitable environment for investigating these

phenomena (Ronney, 1999; Eigenbrod et al., 1997). Owing to the absence of buoyant convection, which on Earth generates convection and strongly influences the reaction zone, other transport mechanisms, such as Lewis-number effects or radiation, can be investigated in detail. To elucidate these questions, microgravity experiments within the mix of theoretical and numerical studies are indispensable. Experiments are typically performed in a combustion chamber containing a quiescent, premixed lean-gas mixture with a reactant of small Lewis number. A point ignition leads to a flame that rapidly breaks up into cells. In some cases, steady spherical flame balls that are not supported by any source of reactants or sink of products in their centres. The conceptual importance of such a configuration resides in the possibility of investigating flammability limits. In general, these limits depend to a very large extent on the experiment hardware, whereas the flame-ball experiment may provide a limit that is practically device-independent.

2. Examples

Figure 1 (first frame) shows a candle lit in Earth gravity. The flame quickly forms a teardrop shape caused by the hot air rising and cold fresh air flowing in behind to keep it burning. However, this airflow also obscures many of the fundamental processes that we aim to understand in order to control combustion for heating, fire-safety and pollution. In the microgravity environment of an orbiting spacecraft or a drop tower, gravitational effects are eliminated and many combustion processes are slowed down. The last three frames of Fig. 1 show that, when the capsule is

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dropped to create microgravity, the teardrop shape relaxes towards a sphere. Moreover, the candle flame, like many others, produces an unsteady 'flicker' at 1 g, whereas in microgravity this flicker is eliminated. Hence the study of flames becomes much easier.

Figure 2 shows the results from a high-resolution direct numerical simulation of a premixed lean hydrogen-air flame in microgravity (Gerlinger et al., 2000). Temperature isosurfaces are shown at different instants in order to highlight the 3-D instabilities induced by local perturbations. An open question for the behaviour of spherical flames is the pattern formation when they split into cells. Figure 2 shows that the initial pentagonal structure first grows continuously and then splits at the five preferred locations triggered by the initial perturbation. Gradual splittings then create a pentagon of five balls; these do not change positions or shape for a long time.

Figure 3 shows the results from numerical simulation of the interaction of a spherical flame structure in a premixed lean mixture with an adiabatic wall under microgravity conditions (Roussel et al., 2003; 2004). The figure shows the temperature (left), the chemical reaction rate (middle) and the adaptive grid used in the numerical computation (right) at different times. The reaction rate gradually decreases when the flame reaches the wall. At later times, the front curvature is modified through



Fig. 1. A candle in the microgravity of a drop tower. The teardrop shape of 1 g (first frame) relaxes towards a sphere.

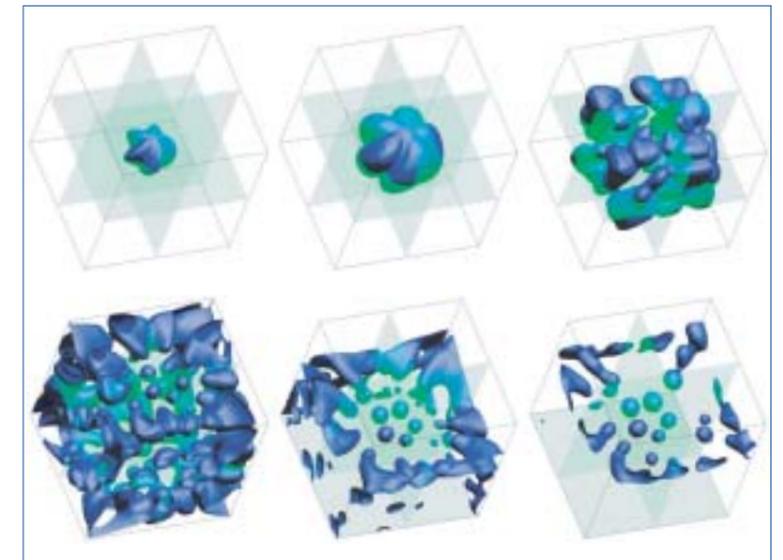


Fig. 2. Instabilities of spherical flame structures. High-resolution direct numerical simulation showing temperature isosurfaces. (Gerlinger et al., 2000).

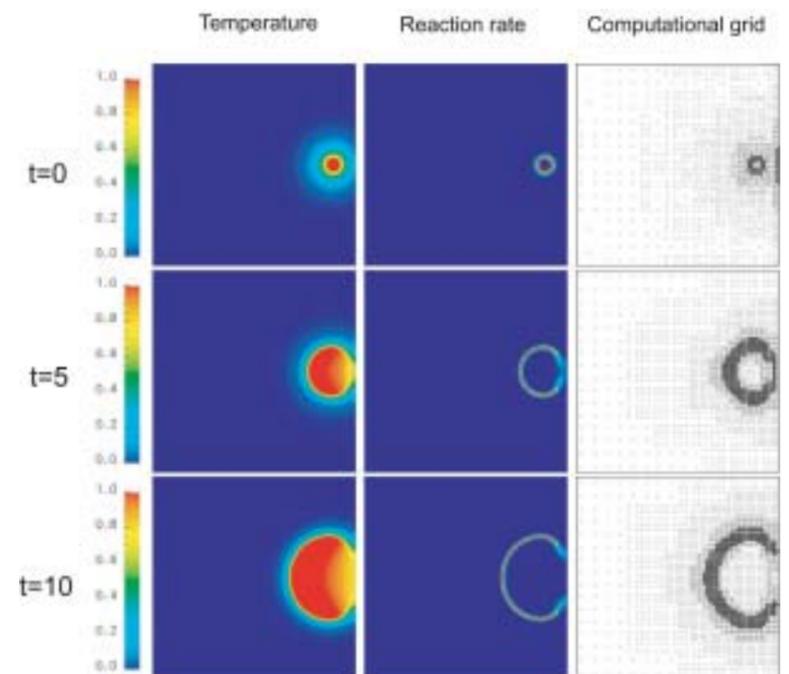


Fig. 3. Interaction of a flame ball with an adiabatic wall at low Lewis number (Roussel et al., 2003; 2004).

tangential diffusion. This phenomenon has similarities to capillarity effects in fluid mechanics.

3. Expected Results, Space Experiments and Future Impact

The objective of the research group is to study the transient behaviour of lean gas-phase combustion under microgravity conditions, including ignition-extinction phenomena of reactive mixtures, by means of numerical simulations and experiments. The participating teams have complementary knowledge to address the different questions. Applications in the context of homogeneous combustion are the main consideration. The behaviour of spherical flames is studied in order to gain fundamental insights into the flammability behaviour of premixed gas flames near their extinction limits. The project is based on the strong interplay between theoretical predictions using asymptotic stability theory, numerical simulations with different level of complexity and experiments under microgravity conditions. The following projects are therefore being pursued:

- development of 3-D computer codes for direct numerical simulation of flame instabilities in lean mixtures;
- development and validation of complex reaction mechanisms for lean mixtures;
- development of the mixture generation and homogenisation system through the definition of studies and preparatory experimental projects;

Microgravity offers the potential for major gains in our knowledge of combustion.

- development of ignition devices and the combustion chamber design;
- development of laser diagnostics to meet the experimental requirements.

3.1 Relevance for Microgravity

Gravitational forces on Earth hamper the combustion and conversion of chemical matter in many different ways such that experiments provide no fundamental insights. As exothermic chemical reactions intrinsically involve production of high temperatures, the density changes and thereby triggers buoyant motion, which vastly complicates the execution and interpretation of experiments. Furthermore, the effects of buoyancy are strongest in the highest temperature regions, where the chemical reactions take place. Buoyancy causes these reaction zones (where our understanding is most limited) to collapse into very thin sheet-like regions, unresolvable by existing techniques such as laser diagnostics, under normal gravity conditions. Additional complications arise from the onset of turbulent convection being triggered by buoyant motion. This yields unsteadiness at a wide range of temporal and spatial scales. Finally, buoyancy causes particles and drops to settle, inhibiting studies of heterogeneous reactions important to catalysts, incineration and power-generation technologies. The effects of buoyancy thus seriously limit our ability to conduct the experiments needed to advance our understanding of chemical reactions in technical devices and, in particular, to conduct experiments that can be directly compared to numerical simulations.

Microgravity offers the potential for major

gains in knowledge of combustion: it allows experimenters to establish controllable conditions for the precise examination of accepted but unverified theories, and to develop fresh insights into elementary phenomena that are hidden in ground-based combustion processes.

4. Roadmap

4.1 Direct Numerical Simulations with Simple Chemistry

The transient behaviour of premixed gases will be studied by direct numerical simulation of flame structures under microgravity conditions. The numerical code is a fully parallel implementation on massively parallel computers with 256 processors. The developed code is the only available tool to perform simulations of such large-scale microgravity problems (Gerlinger et al., 2000). Issues being addressed include the modelling of the ignition source and the resulting number of spherical flames produced for a given ignition source. Whether and to what extent the predictions of the stability limits of 3-D flame structures based on asymptotic analyses agree with the numerical simulations and experiments will also be investigated. The influence of complex chemistry on the evolution of the flame balls and their stability properties will be checked.

The influence of the Lewis number for mixtures of different species is another point of research. The open question is whether and how the lowest Lewis number present in the mixtures determines the behaviour of the evolution of the spherical flame structure. The interaction of spherical flame structures with each other and the walls will be simulated using a volume-penalisation

These new techniques can be used for combustion research in drop towers, on parabolic flights and aboard the International Space Station.

method that has to be implemented in the 3-D computer code. Also clarified will be the link between flame balls with turbulent combustion, and simulations that study the response of the flame structures to vortical structures and homogeneous isotropic turbulent flow fields.

4.2 Numerical Simulations with Complex Chemistry

For the numerical simulation of lean flames with complex chemistry, 1-D spherically symmetric flames involving methane, H^2CO and other mechanisms are being considered. Different radiation models are incorporated, such as the optically-thin model and a narrow band model. This allows the study of the near-limit structure of lean flames and will yield information concerning the ignition, ignition limits and burning velocity. The 1-D code works with the optically-thin radiation model, which considers only heat loss due to emission of radiation from the gas; work needs to be done to add the narrow band model, which includes absorption and re-emission of radiation. After, different detailed chemistry studies are being performed. The code will be subsequently extended to 2-D axisymmetric spherical flames to investigate the flame stability with respect to curvature-induced perturbations and to the formation of cellular structures (the local extinction effects).

4.3 Experiments and Exchange of Data

The proposed experiments aim to obtain basic data for comparison with the numerical

models of lean premixed gaseous flames discussed above. Microgravity conditions are essential, as otherwise laminar propagating lean flames are strongly affected by buoyancy driven by natural convection. Besides this, the facility will enable the lean flammability limits and flame propagation velocities of gaseous pre-mixtures to be measured. For methane/air mixtures, these values have been proved to be leaner than under terrestrial conditions. This part of the project will be performed in close collaboration with the ESA Microgravity Applications Project (MAP) combustion project on 'Combustion Properties of Partially Premixed Spray Systems' (CPS). Particularly interesting here is the development of advanced laser diagnostics for inflight application on the CPS project (Triebel, 1998). Current methods are 2-D laser-induced emission (LIE) techniques like laser-induced fluorescence (LIF), particle image velocimetry (PIV), and Rayleigh- and Mie Scattering for temporally- and spatially-resolved measurements of species concentrations and temperature fields (König et al., 1998). Enhancements towards 3-D diagnostics through tomographic spectroscopy will be developed to a prototype status where applicable. The reaction zones of spherical flames can then be investigated. For gaseous fuels considered in the MAP project, OH and CH are the most interesting species. There are two important points to note with the application of high-resolution LIF techniques:

- the time-resolved, 2-D spatial resolution close to the diffraction limit will allow characterisation of the interaction mechanisms between flames and vortices;
- the developments will commonly apply to combustion research in drop towers,

parabolic flights and the International Space Station. Synergy effects to and from new terrestrial applications are foreseeable.

References

- Eigenbrod, Ch., König, J. & Triebel, W. (1997). Recent Developments and Applications of the Combustion Diagnostics at Bremen Drop Tower. *Proc. 4th Int. Microgravity Combustion Workshop, NASA Conference Publication 10194*, Cleveland, 317.
- Gerlinger, W., Schneider, K. & Bockhorn, K. (2000). Numerical Simulation of Three-Dimensional Instabilities of Spherical Flame Structures. *Proc. Combust. Inst.* **28**, 793-799.
- König, J., Eigenbrod, Ch., Bolik, T., Rath, H.J., Gerber, D., Müller, D. & Triebel, W. (1998). Observation of Two Stage Autoignition of n-Heptane Fuel-Spheres by LIF of Formaldehyde. *27th. Symp. (Int.) on Combustion*, The Combustion Institute, Boulder, Colorado, USA.
- Ronney, P.D. (1999). A Perspective on the Role of Microgravity in Combustion Research. *Combust. Flame* **116**, 317.
- Roussel, O., Schneider, K., Tsigulin, A. & Bockhorn, H. (2003). A Conservative Fully Adaptive Multiresolution Algorithm for Parabolic Conservation Laws. *J. Comput. Phys.* **188**(2), 493-523.
- Roussel O. and Schneider K. (2004). Numerical Study of Spherical Flame Structures Interacting with Adiabatic Walls using an Adaptive Multiresolution Scheme. *Combustion Theory and Modelling*, submitted.
- Triebel, W. (1998). Laser Diagnostics of Combustion Processes under Short-Term Microgravity Conditions. *Space Forum* **4**, 121.

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