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Physics and Chemistry of Gas Discharges (Further the understanding of discharge physics)

Diagnostics (present the relevant advanced measurements, their capabilities and their foreseeable impact on the subject science)

Aerodynamic Flow Control (Use of plasmas for exerting an aerodynamic force on an airplane's control surfaces)

Combustion and Plasma Chemistry (Use of plasmas for improving emission properties of flames, for ignition and stabilization)

15. SUBJECT TERMS

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Spatio-temporal analysis of a streamer post-discharge by 1D Spontaneous Raman Scattering.

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Nanosecond pulsed discharges are envisaged as a promising new way for ignition or assisted combustion [1,2]. For ignition, these discharges allows the ignition in multiple sites, and the ignition in leaner mixture than conventional spark ignition[3]. The present work investigates the energy deposit within the post-discharge period of a nanosecond streamers thanks to 1D spontaneous Raman scattering.

The pulsed positive corona discharge occurs in air between a point-to-plane gap of 7 mm length. A pulsed high voltage of +25kV is applied with a pulse duration of 30 ns (FWHM) and a repetitive rate of 10 Hz. The pulsed discharge produces "streamer" which, in our case, is a non-branched ionized filament. A radial profile of vibrational distributions and rotational temperatures of the fundamental level of N_2 and O_2 is performed from 1D spontaneous Raman scattering. The Raman scattering is induced by a long pulse Nd:YAG laser[4], and radial profile of this scattering is imaged onto the entrance slit of an imaging spectrograph equipped with an ICCD camera. These radial profiles are measured close to the needle, halfway both electrodes, and near the plane, at different times after the discharges from delay of 150 ns to 10 ms. These data are completed with emission spectra of the streamer.

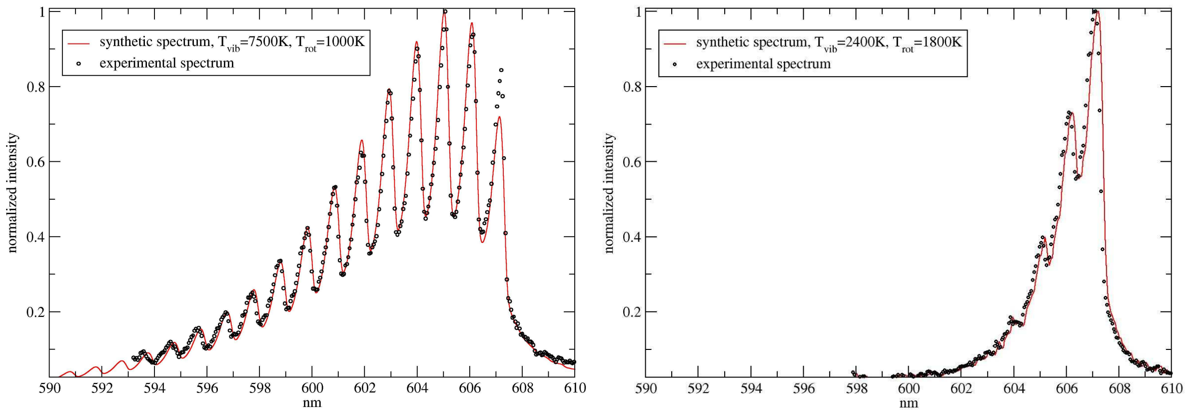

Figure 1 : comparison of synthetic and experimental (average of 2000 shots) spectra of N_2, 150 ns (left) and 50 µs (right)after the discharge

The comparison of the experimental and synthetic spectra (fig 1) provides the radial profiles of the vibrational distribution, rotational temperature and species density at the different times investigated. From these data the pressure in the post-discharge are also deduced.

The results show that high vibrational energy levels are populated and that near the needle high level of rotational temperature (up to 1800 K) are also reached and that strong gas heating near the channel axis leads to the increase of gas pressure and formation of a cylindrical shock wave. These results are interesting to understand the physical processes involved in ignition by nanosecond discharge. The investigation will be completed by results in propane-air and methane-air mixtures.

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2009 Aerospace Thematic Workshop
"Fundamentals of Aerodynamic-Flow and Combustion Control by Plasmas"
Les Houches, Oct. 11-16

POSTER SUBMISSION

Name: RABAT Hervé
Co-authors:JOUSSOT Romain, CAILLAUD Vincent, BAUCHIRE Jean-Marc, HONG Dunpin
Affiliation: GREMI – UMR6606 – CNRS/Université d'Orléans
Poster Title: Investigation of positive discharge patterns of a flexible plasma actuator using an ICCD camera.

Description:

Dielectric barrier discharge plasma actuator is a promising system for aerodynamic control. A plasma ignited onto a surface induces an ionic wind which modifies the boundary layer of an external flow along the surface. The aim of our study is a better understanding of correlations between the plasma pattern and the induced ionic wind as a function of the electrical and design parameters of the actuator.
Thanks to an appropriate optical image recording device, images of the streamers have been recorded during the positive discharge phase. The corresponding current signals have been recorded in the same time. One can observe that one current peak can be related to one streamer formation(Figure 1). From this, the study shows that the plasma length is correlated with the voltage value, the number of streamer branches is linked to the intensity of the current peak and the streamers patterns, for the same electrical parameters, is function of the actuator design (surface material and gap length between the two electrodes).

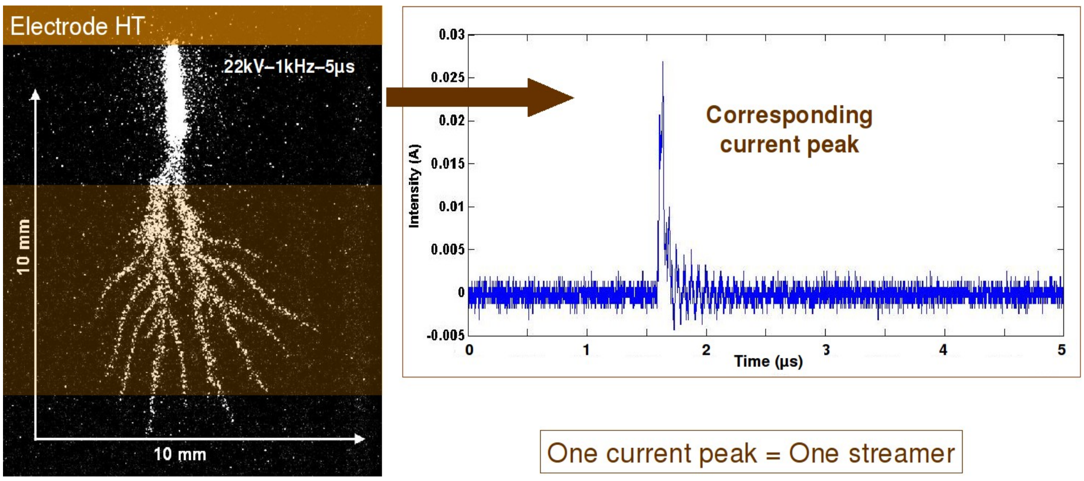

Figure 1 :Lonely streamer picture and corresponding current peak.

Starting, Travelling & Colliding Vortices: Dielectric Barrier Discharge Plasma

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DBD plasma actuators consist of an upper and lower electrode separated by a thin dielectric material as shown in Figure 1. On application of several kilovolts of ac power at kilohertz frequency between these electrodes, local ionization takes place around the upper electrode. This couples momentum to the surrounding fluid to induce a jet flow, which is caused by the movement of plasma ions to and from the dielectric surface. The charge build up on the dielectric surface opposes the charge of the exposed electrode, quenching the emission of the plasma discharge and stopping the plasma from collapsing into an arc. In other words, DBD plasma actuation is a self-limiting process [1].

A combination of flow visualisation and PIV has been used to study DBD plasma actuation in both quiescent air and low-speed flows. Presented in the poster are the effects of asymmetric DBD plasma actuation, which causes a starting vortex [2] propagating along and away from the wall. Opposing plasma actuation from two asymmetric electrodes is also illustrated, which leads to the collision of starting vortices and the formation of a wall normal jet. Furthermore, the application of an inclined DBD plasma actuator over an aerofoil is given [3], showing the formation of streamwise vortices. This enables flow separation control by vortex entrainment and mixing, acting very similarly to vortex generators. A PIV study of sequential plasma actuation generating a spanwise travelling wave in quiescent air is also presented. This is generated through asymmetric actuation of two opposing electrodes. This allows the collection of fluid close to the wall which is moved in the spanwise direction with continuing actuation by neighbouring electrodes. This technique has previously been used for turbulent boundary layer control in water with Lorentz forcing [4], where a skin-friction drag reduction of 30% was observed.

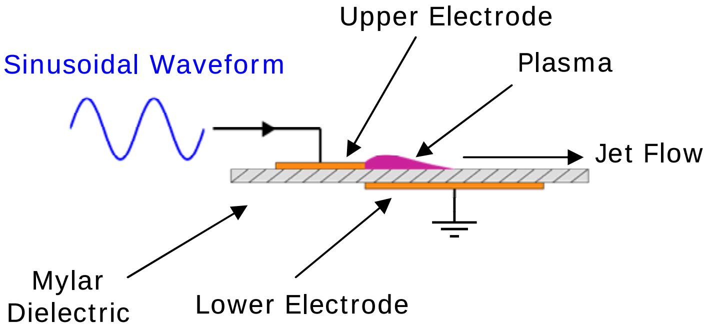

Figure 1. Asymmetric DBD plasma configuration

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Experimental investigations of a simple Dielectric-Barrier Discharge-based flow actuator: characterization and potentialities

Y. Babou, A. E. Kerlo, S. Menyiel, S. Paris

Simple experimental investigations conducted at Von Karman Institute to assess potentialities of dielectric-barrier discharge (DBD)-based flow actuator are reported. Thermodynamic state and electrical characterization of a single DBD-based flow actuator operating in ambient quiescent was performed. The actuator is constituted by two thin alumina foil electrodes asymmetrically displayed on both sides of a dielectric (MACOR) plate (~50 cm^2) and powered by an AC sinus high frequency (~10 kHz) high voltage (~10 kV peak-peak). The lower electrode was encapsulated in a glass substrate. The discharge current (resp. dissipated power) was determined inserting a resistor (resp. a capacitor) in the circuit. The discharge current is constituted of high intensity peaks of few nano-seconds associated to streamers (Fig. 1). The power dissipated by the operating actuator is about 10 W. Thermodynamic state was characterized by means of conventional optical emission spectroscopy technique applied to the measurements of N_2^+ First Negative system emission spectra. Adopting the convenient two temperatures description, vibrational and rotational temperatures where obtained by means of spectra fitting approach. The gas/rotational temperature is at room temperature and vibrational/electronic temperature is at about 2500 K (Fig. 2). Also, the potentialities for subsonic flow control were evaluated by investigating the DBD-based actuator effectiveness to produce thrust, to accelerate the flow and to reduce instability in well-defined configurations. The thrust was gauged in simple manner with commercial balance and was found to be of order of 0.1 g. LDV measurements over a flat plane including a single actuator gave evidence for effective flow acceleration up to 2 m/s for freestream flow velocity of 5 m/s. Hotwire velocity fluctuation measurements behind a cylinder equipped of two actuators suitably designed have pointed out potential prospects to lock instability development.

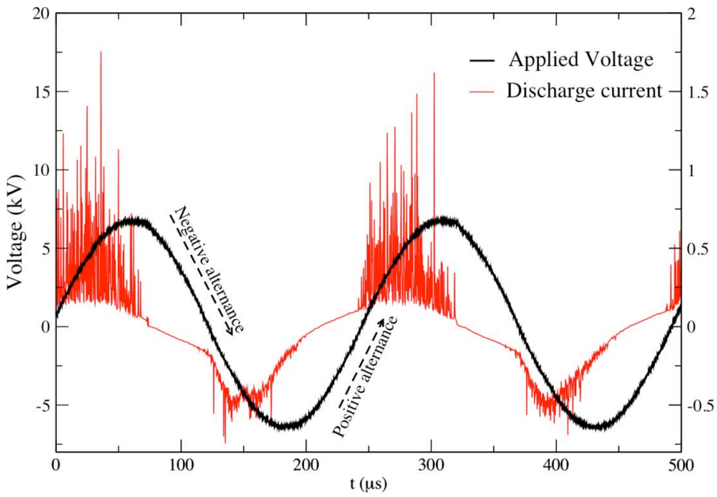

Figure 1: Current and Voltage characteristics in the DBD plasma

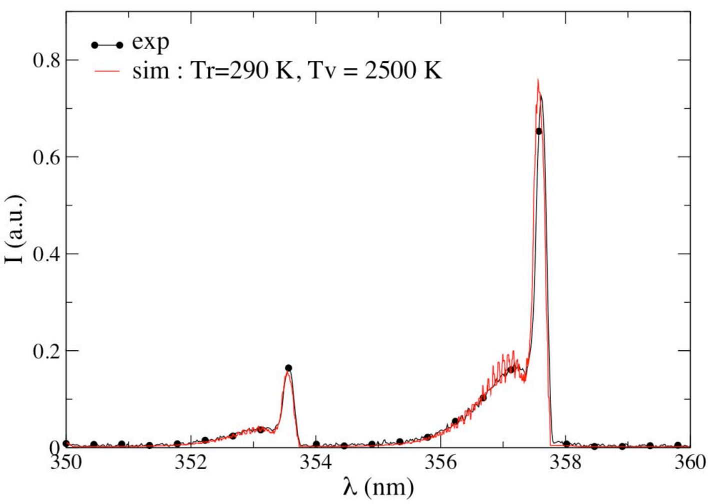

Figure 2: N_2^+ First Negative system emission spectra

Development of a High-Order Transport and Collisional-Radiative Model for Non-Equilibrium Flow Fields

Jean-Luc Cambier, Michael G. Kapper

Air Force Research Laboratory, Edwards AFB, CA

Abstract

Non-equilibrium plasma flows have always been of considerable interest for various applications and have more recently been a particularly promising approach for flow control and manipulation in modern aerodynamics through the use, for example, of pulsed discharges. The study of non-equilibrium plasma is also of key importance in high enthalpy flows such relaxing shock layers and wakes in re-entry flows or hypersonic aerodynamics, stimulation of combustion in hypersonic air-breathing engines, and various designs of electric propulsion systems for satellites. As computer capabilities improve rapidly, the ability to model non-equilibrium plasma conditions with a very high level of detail becomes increasingly feasible. Thus, we have initiated a systematic effort in modeling coupled transport and detailed kinetics of the plasma described by a collisional-radiative (C-R) model, i.e. a non-Boltzmann distribution of the bound electronic states. The poster describes physical models and numerical methods used to this stage and the initial results of validation studies. We have focused initially on atomic plasma (i.e. noble gases, although molecular C-R models are planned as well) to develop and test some key capabilities. At the basic level, the plasma is described by the two-temperature (T_h, T_e), single fluid equations with convection of the population densities of the electronic states. The numerical scheme is conservative and shock-capturing, is based on a 3rd-order version of the MP5 monotonicity-preserving upwind advection scheme [1], and has been thoroughly validated against standard CFD tests[1]. A second-order accurate time stepping using the Adams-Bashforth scheme is found to be a significant advantage over Runge-Kutta time-stepping for parallelization. A special treatment of near-vacuum conditions in the case of fast rarefactions yields an almost perfect agreement with the solution of an exact Riemann solver. The C-R model for Argon is used for validation studies; various numbers of levels and level groupings are considered, with most cases studied using the Vleck [2] and Bultel *et al* [3] schemes for the Atomic State Distribution Function (ASDF). The cross-sections of Drawin [4], Zatsarinny and Bartschat [5] and Deutsch *et al* [6] have been used and compared, and the basic atomic data for level energies, oscillator strengths and radiative transition rates are obtained from the NIST database [7]. The first validation studies concerned the re-examination of shock-tube experiments of ionizing shocks in Ar performed in the 70's by the University of Toronto, as reported by Glass and Liu [8]. This problem was first investigated by one of us [9] but only one-dimensional configurations and a much reduced ASDF could be modeled at the

[1] A version for ideal MHD equations was also developed.

time. Figure 1 shows a typical profile of the heavy particle, electron and excited state temperatures behind the shock, for a steady-state calculation. The avalanche region occurs at the region where rapid convergence of the temperatures occurs, achieving both Boltzmann and approximate Saha equilibrium[2]. However, the most interesting aspects of these experimental results are the coupled oscillations of the shock front and the avalanche region. The current time-accurate simulations (see Figures 2 and 3) are performed in both one and two dimensions, from which the mechanism for coupling between the two fronts by the transfer of electron pressure waves, in a manner reminiscent of the propagation of detonation waves, was clearly discernable. Indeed, the two-dimensional studies revealed a pattern of transverse waves and the formation of induction “cells” which, when properly visualized, can be seen in an artificial “soot” trace, as shown in Figure 4. The agreement between experimental and computational interferogram patterns (see Figure 5) is also very good, providing yet another indication of the accuracy of our computational results. Additional visualization of the traveling shock, ionization front and wave emission and reflections (including movies) will be presented with the poster.

Additional work is proceeding on this basic C-R model; a preliminary radiation transport model will be implemented and theoretical issues such as ASDF truncation will also be discussed. Of similar importance is the development of a non-Maxwellian version of the C-R model, where the Electron Energy Distribution Function (EEDF) is allowed to remain arbitrary. We have focused on the problem of inelastic collisions (excitations and ionizations) and developed a numerical method which guarantees absolute conservation of mass and energy of the coupled ASDF-EEDF during the kinetics of inelastic collisions. A naïve implementation of the kinetics would result in an uncontrolled error in energy conservation, but as seen in Figure 6, in our method it remains bound by numerical round-off errors[3]. The scheme implements detailed balance at a basic level, i.e. both excitations/de-excitations and ionizations/ recombinations are treated consistently using the Klein-Rosseland and Fowler relations, yielding the exact Boltzmann and Saha equilibrium. During the testing of the scheme, some unusual results were observed; for example, the relaxation of an initial Maxwellian EEDF when only excitations and de-excitations are allowed leads to a final distribution that is far from equilibrium and shows discontinuities at values which are multiples of the energy gap. This result was confirmed by independent MCC calculations, the results of which are shown in Figure 7. This behavior is associated with a breakdown of ergodicity in this restricted dynamical system; elastic collisions would prevent its observation. Note that we computed the evolution of the H-function during the relaxation and confirmed that the system entropy increased during the relaxation. A similar situation occurs when ionizations and recombinations only are allowed, although the final, “frozen” distribution takes a different shape. The non-Maxwellian kinetics are currently being augmented with elastic collisions and implemented on a Graphics Processing Unit (GPU) for fast computing; the performance results of this implementation will also be presented. If time permits, preliminary results on non-isotropic EEDF relaxation will also be discussed, as well as the incorporation of radiative processes.

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[2] The deviation from strict Saha equilibrium is due to the radiative cooling, i.e. the uncompensated radiative emission rates.

[3] For all cases studied, the energy was conserved during the relaxation of the coupled EEDF-ASDF up to a relative error of 10^{-13}.

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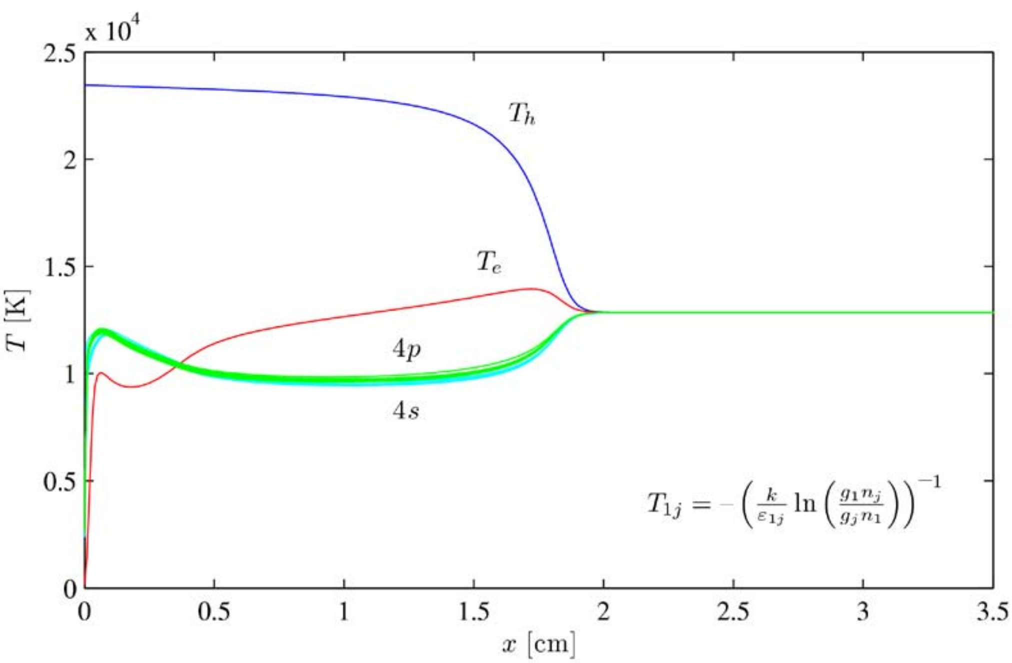


Figure 1: Steady-state profile of temperatures (including excited states) behind ionizing shock front in Ar. Immediately behind the shock is a region of electronic excitation regime, dominated by atom-atom collisions, followed by an ionizing and excitation regime dominated by electron collisions. The rapid ionization avalanche occurs at about 1.7 cm, where all temperatures reach a simultaneous Boltzmann and Saha equilibrium. The partial equilibrium between 4s and 4p levels depends on the rate of transiitons by atomic impact, and has a strong influence on the electron temperature profile immediately behind the shock (parametric studies will be shown).

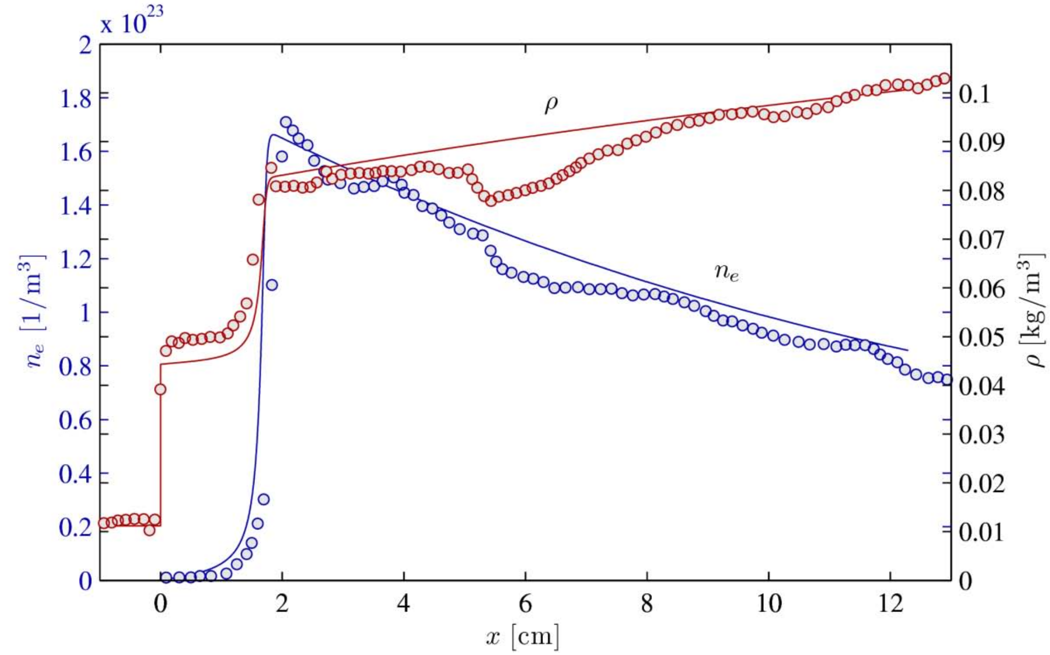


Figure 2: Comparison of experimental (symbols) and computational (lines) profiles of mass density (red) and electron density (blue) for steady 1D computations with radiative rates included. Results include levels 4s, 4p, 5s and 3d; higher levels needed for a correct evaluation of radiative cooling rate. Unsteady 1D computations (not shown here) yield profile fluctuations similar to experimental results, as well as fluctuations of the induction length.

Figure 3: Plot of refractive index of the medium, showing the density fluctuations with high contrast.

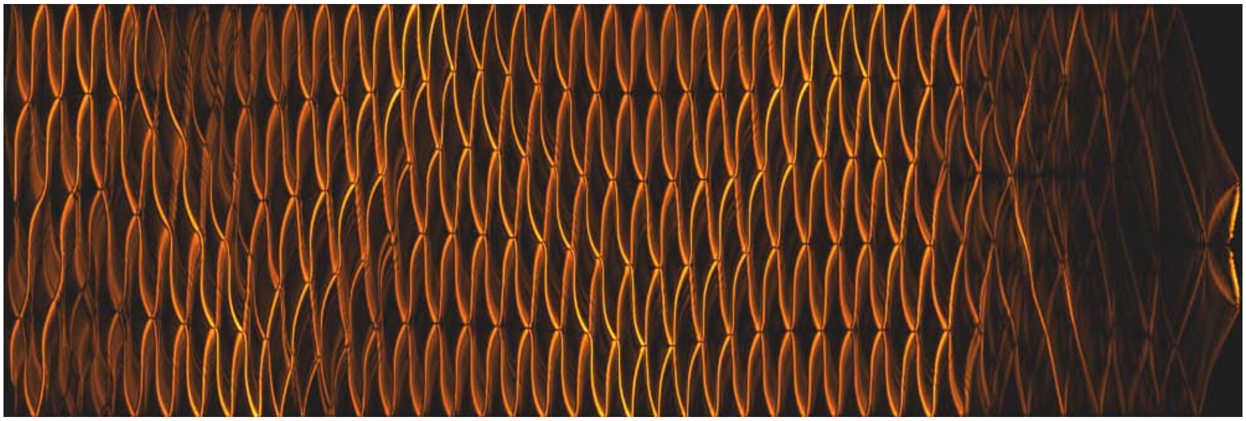


Figure 4: Artificial "soot" traces showing the cellular pattern formed by the locations of peak vorticity; this pattern is entirely similar to experimental traces observed in the propagation of detonations in shock tubes, and is a result of waves coupling the leading shock and reaction fronts.

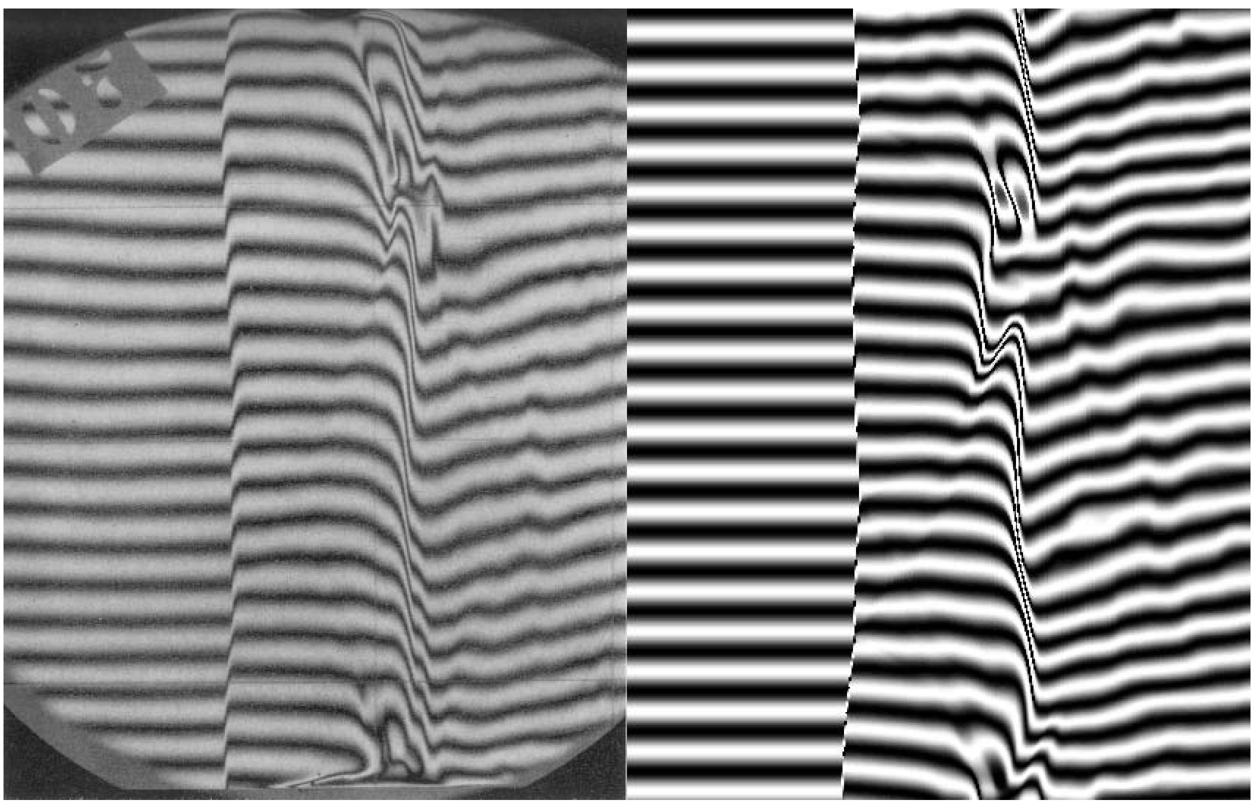


Figure 5: Comparison between experimental (left) and computational (right) interferograms. The slight perturbation of the shock front is clearly visible in both cases. The avalanche region is identified by the second region of fringe shift at the correct average induction length, while the interaction of transverse waves shows as localized perturbations on the avalanche front.

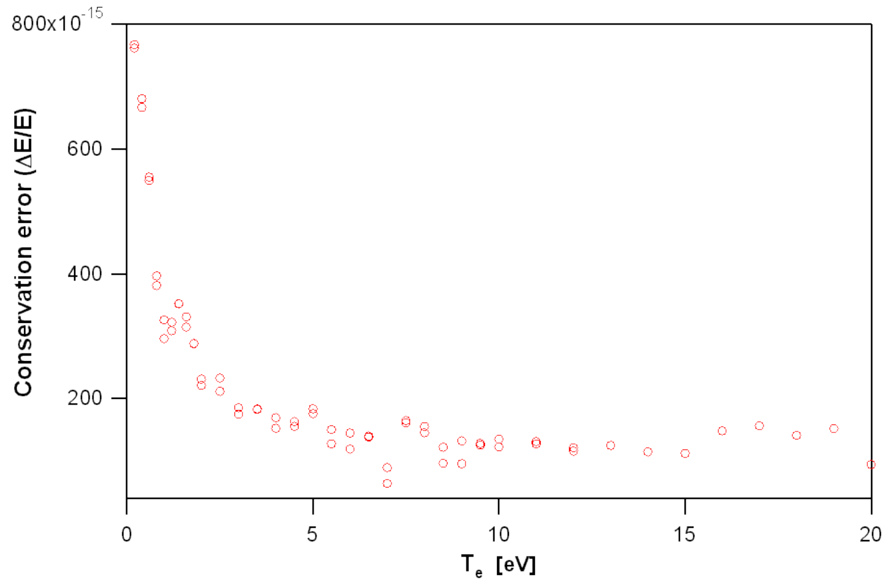


Figure 6: Relative error in energy conservation from non-Maxwellian excitation and de-excitation kinetics as function of initial EEDF temperature. The higher errors at low temperature arise from the lower resolution of the initially Maxwellian EEDF for a fixed energy grid extending to 250 eV. A similar result is obtained for ionization/recombination kinetics.

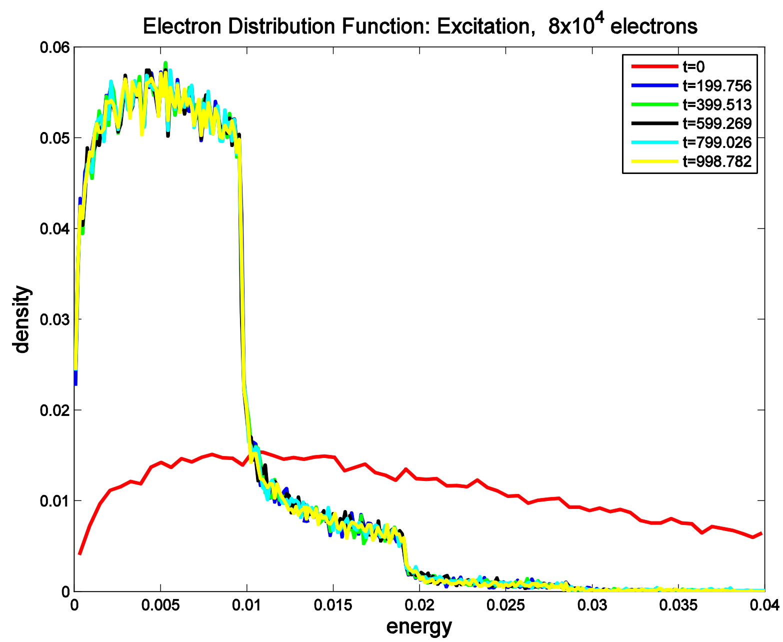


Figure 7: EEDF relaxing from an initially Maxwellian distribution (red curve, t=0) through excitation and de-excitation processes only (two-level atom). Results obtained by a Monte-Carlo Collision (MCC) procedure that is the analogue (satisfying detailed balance) of the energy-conserving discretized solver mentioned in the text. The latter would show the same profiles, without statistical noise (movies of the relaxation process will be shown).

Laboratoire Plasma et Conversion d'Energie

Laplace

Interaction of a nanosecond pulse DBD with a subsonic airflow

Thomas Unfer, Jean-Pierre Boeuf

Introduction

Recent experiments by Starikovskii et al used a surface dielectric barrier discharge driven by a nanosecond voltage pulse generator. Under these conditions, the corona regime that is responsible for the ion wind in sinusoidal regimes is no longer present and the main discharge regime is a streamer regime. This was confirmed by the quasi-zero ion wind measured. However the authors showed that this kind of discharge was able to affect the aerodynamic properties of a flow along the surface and that a detached flow could be reattached when a nanosecond voltage pulse was applied between the electrodes at a repetition rate of a few kHz. One important conclusion of the experiments of Starikovskii et al. is that a large part of the plasma energy is released into gas heating in a short time (less than 1 µs), leading to the formation of a micro shockwave. The purpose of the present work is to better understand and quantify the gas dynamics generated by a nanosecond surface discharge under conditions similar to Starikovskii et al. using a self-consistent model of the discharge and generated gas dynamics. A 2D fluid model of the surface discharge has been coupled with a compressible Navier Stokes description of the gas dynamics. This is a multiscale problem in space and time since time scales from picoseconds to 10s of microseconds and dimensions from a few micrometers to several cm must be resolved. A numerical method specially adapted to cope with the multiscale nature of this problem has been developed. The method is based on asynchronous integration of the fluid transport equations using an asynchronous adaptative mesh refinement and allows to make a good compromise between accuracy and computation time. The effect of the discharge on a flat plate airflow is investigated for different velocities.

Plasma model

$$\frac{\partial n_e}{\partial t}+\vec{\nabla}.\vec{\Gamma_e}=(\alpha-\eta)\left\|\vec{\Gamma_e}\right\|-r_{ep}n_e n_p$$

$$\frac{\partial n_p}{\partial t}+\vec{\nabla}.\vec{\Gamma_p}=\alpha\left\|\vec{\Gamma_e}\right\|-r_{ep}n_e n_p-r_{np}n_n n_p$$

$$\frac{\partial n_n}{\partial t}+\vec{\nabla}.\vec{\Gamma_n}=\eta\left\|\vec{\Gamma_e}\right\|-r_{np}n_n n_p$$

$$\vec{\nabla}.\varepsilon\vec{E}=e\left(n_p-n_e-n_n\right)+\sigma\delta_S$$

$$\vec{\Gamma_e}=\mu_e\left(-n_e\vec{E}-\frac{k_B T_e}{e}\vec{\nabla}n_e\right)+n_e\vec{u}$$

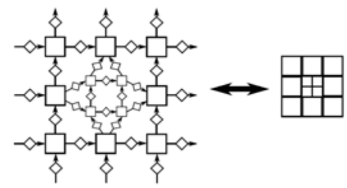
Navier-Stokes equations

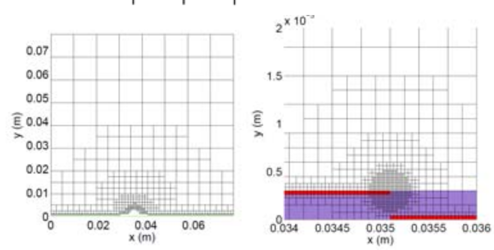
$$\frac{\partial\rho}{\partial t}+\vec{\nabla}.\left(\rho\vec{u}\right)=S=M\left[-(\alpha+\eta)\left\|\vec{\Gamma_e}\right\|+r_{ep}n_e n_p+r_{np}n_n n_p\right]$$

$$\frac{\partial\left(\rho\vec{u}\right)}{\partial t}+\vec{\nabla}.\left(\rho\vec{u}\otimes\vec{u}+pI-\overline{\overline{\tau}}\right)=S\rho\vec{u}+\overline{F_{EHD}}$$

$$\frac{\partial\left(\rho E\right)}{\partial t}+\vec{\nabla}.\left[\left(\rho E+p\right)\vec{u}-\kappa\vec{\nabla}T-\overline{\overline{\tau}}.\vec{u}\right]=S\rho E+\overline{F_{EHD}}.\vec{u}+P_{th}$$

Asynchronous Adaptive Mesh Refinement

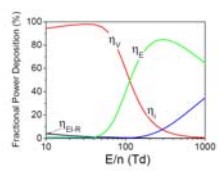




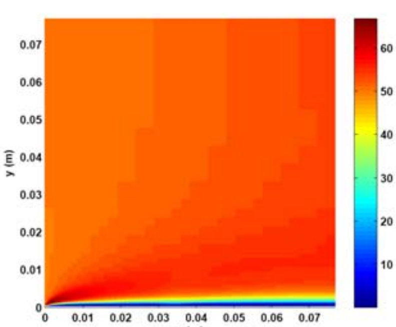
Plasma/Navier-Stokes coupling

$$\overline{F_{EHD}}=e\left(n_e-n_p-n_n\right)\vec{E}-k_B T_p\vec{\nabla}n_p-k_B T_e\vec{\nabla}n_e-k_B T_n\vec{\nabla}n_n$$

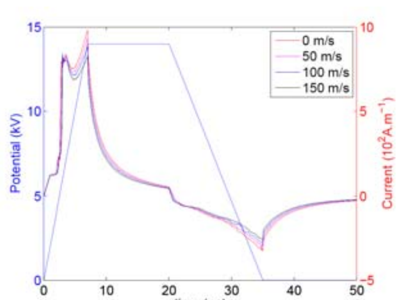
$$P_{th}=\left(P_{el-R}+P_E+P_{VT}\right)+P_{ions}$$



Steady state airflow (50 m/s)



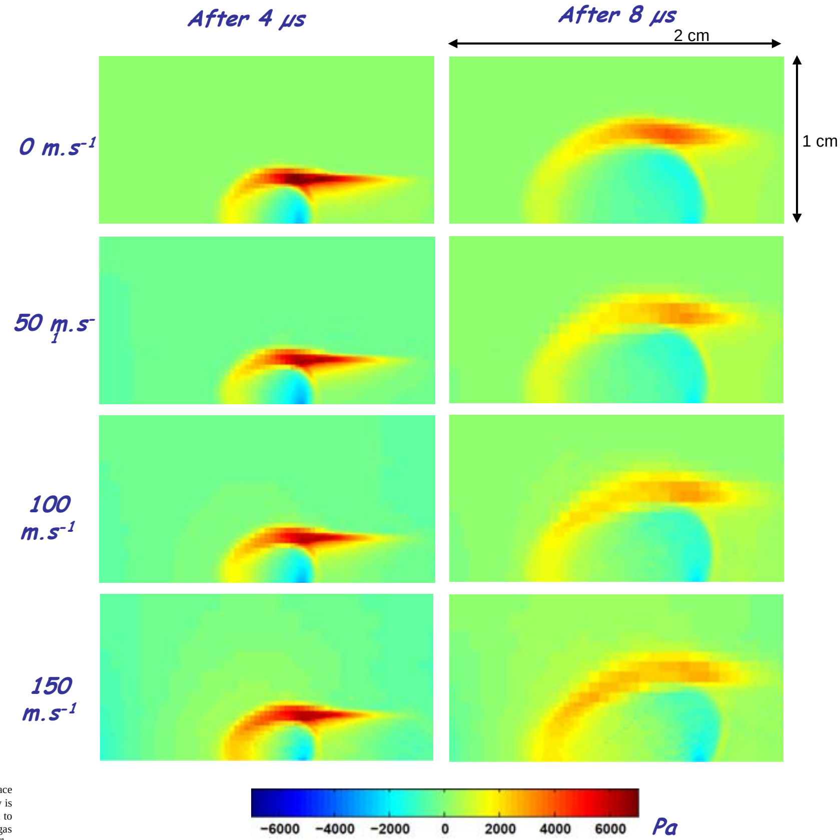
Airflow effect on the discharge



Discharge effect on the airflow: pressure variation (Pa)

After 4 µs

After 8 µs



Conclusion

We have developed a model to describe plasma-flow interaction under conditions of fast energy deposition by a surface discharge plasma, leading to shock wave formation and propagation. The physical coupling between plasma and flow is due to EHD force and gas heating, which are taken into account as source terms in the Navier Stokes equations, and to the change in particle transport and reaction rates due to the variations of the gas density associated with the gas dynamics. In the conditions considered in this paper the dominant aspect of the coupling is due to fast gas heating. The plasma is not significantly affected by the gas dynamics, since, the discharge occurs in the boundary layer where the external flow is quite slow and the gas dynamics induced by the gas heating due to energy deposition by the discharge leads to significant changes of the gas density only after the discharge is extinguished. The developed model used a simplified description of gas heating induced by the discharge. Gas heating is supposed to be due to: ohmic heating by ions (instantaneous), electron elastic collisions and rotational excitation (instantaneous), quenching of excited states (30% of the energy put into electronic excitation of air is supposed to be released instantaneously) and vibration to translation energy transfer (the energy stored into vibrational excitation is supposed to be released into gas heating on a 1 µs time scale). In the near future parametric studies will be conducted to determined which parameters can be optimized to increase the effect of the discharge on the airflow, such as position with respect to the leading edge, applied voltage shape…

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Development of a Mach 5 Nonequilibrium Wind Tunnel

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Walter Lempert, Igor Adamovich, and J. William Rich

The Ohio State University

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Abstract

A supersonic/hypersonic wind tunnel has been developed toward quantifying the effect of vibrational disequilibrium on supersonic / hypersonic flow fields and toward validating / developing reliable theoretical model to predict vibrational disequilibrium in higher Mach number flows.

The tunnel (Fig. 1) uses a high pressure, stabilized glow discharge in its plenum (Fig. 2). The electric discharge system incorporates a high voltage, repetitive, short pulse generator (30 kV, 100 kHz, 10 nanosec-pulse width), which weakly ionizes the test gases (ionization fractions of ~ 10^{-7}). On a separate pair of electrodes, a direct current (d.c.) power supply (up to the power supply voltage of U_{PS}=5 kV) is used to load power into selected internal energy modes of the test gas species (Fig. 3), which was inferred from input electrical power, translational (rotational) temperature measured in emission spectroscopy and a Boltzmann solver.

Figure 4 shows a comparison of a typical NO PLIF image at J=5 (Q1+Q21 branches) in the NO A – X (γ) bands, using a unique pulse-burst laser system (up to 500 kHz pulse repetition rate) developed at OSU NETL, and a Mach number distribution predicted by a 3D compressible Navier-Sokes code with chemical reaction and vibrational non-equilibrium incorporated, showing a good agreement in the stand-off distance and a wake structure behind the cylinder.

Figures 5 show comparisons of baseline case (P_0=350 torr, T=Tv=300 K, top) and vibrationally excited case (T=350 K and Tv=1700 K) with VT relaxer (3% hydrogen in Fig. 5(a) and 0.1% water vapor in Fig. 5(b)). The difference in the bow shock stand-off distances in the temperature distributions predicted by the CFD (Fig. 5(a) and those in Shlieren images (Fig. 5(a)) also show good agreement.

Further measurements are in progress, such as mapping temperature distribution using the NO PLIF and pico-sec rotational and vibrational CARS measurements, to infer the distribution of internal energies in both the tunnel test section expansion and in the shock layer flows. It is planned to adapt the various non-intrusive optical diagnostic systems developed in the present program to make measurements of high enthalpy, high Mach number, short duration test flows in various national facilities in the US.

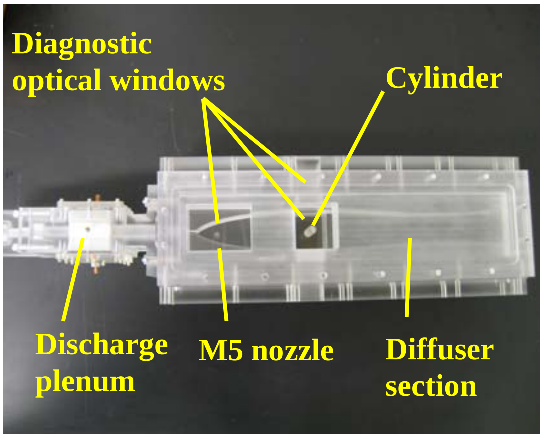


Fig. 1. Side view schematic of M5 wind tunnel assembly. The heights of plenum, throat, and test section are 1 cm, 1.6 mm, and 4.6 cm. The width is 4 cm throughout the tunnel.

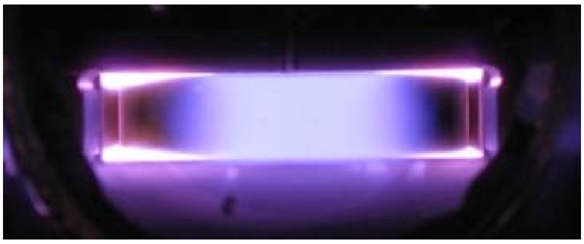


Fig. 2. Photograph of crossed, pulser (vertical direction) - DC sutainer (horizontal direction) discharge in the plenum section at P0=350 torr nitrogen, with the pulse repetition rate of ν=100 kHz and DC power supply voltage of U_{PS}=2 kV.

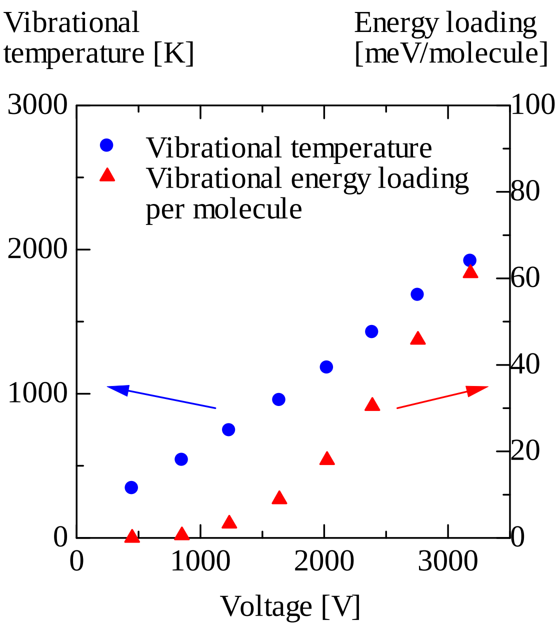


Fig. 3. Nitrogen vibrational temeperature and energy loading per molecule inferred from input power, temperature by emission spectroscopy, and Boltzmann solver.

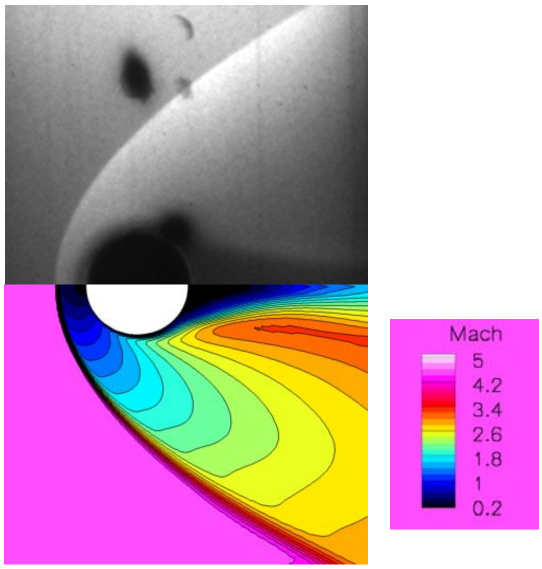
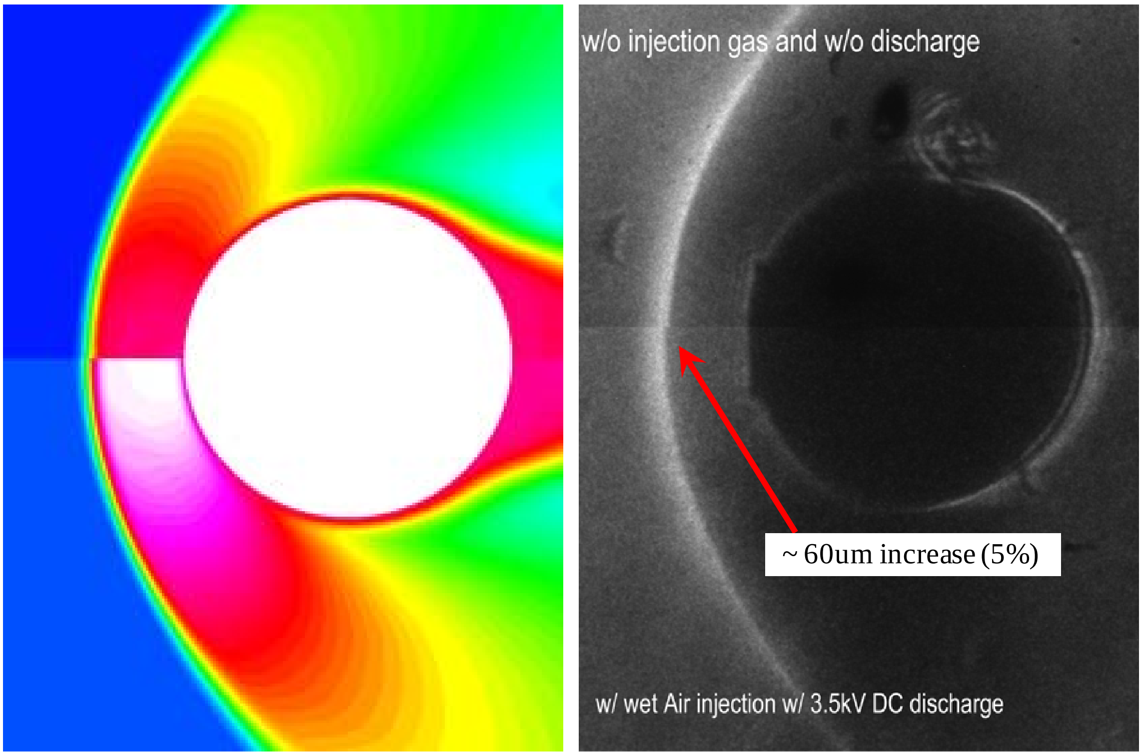


Fig. 4. Comparison of NO PLIF image (top) and Mach number distribution by CFD (bottom) behind a bow shock ahead of 5-mm cylinder in the Mach 5 flow. No discharge.



(a) (b)

Figs. 5. Comparisons of bow shock stand-off distances without VT relaxer (top) and with VT relaxer (bottom) in vibrationally exited M=5 nitrogen flow at T=350 K and Tv=1700 K. (a): Temperature distributions predicted by CFD with VT relaxer of 3% hydrogen. (b): Density gradient distributions measured in the Shlieren method with VT relaxer of 0.1% water vapor.

Abstract for ATW09
J. D. Kelley
18 September 2009

Ongoing development of a phase-space based description of excitation, deexcitation and reaction for small molecules at very high temperatures is presented. Anharmonic vibration and vibrational-rotational coupling are explicitly included, and the approach has been extended into the quasi-bound and continuum regions, allowing dissociation and recombination to be treated. The goal is creation of efficient, few-parameter methods to accurately include nonequilibrium kinetic processes in modeling expanding high-enthalpy flows.

This presentation focuses on atom recombination via third-body collisional stabilization, with N_2 as the model system. The “exact” N_2 potential function $V(r,\theta)$ is approximated as a rotating Morse oscillator potential, because the Morse potential adequately reproduces the behavior of “real” molecules, allowing for dissociation and recombination and the simple relationships among its properties and eigenstates facilitate construction of our model.

Vibrational and rotational motion in diatomic molecules are not separable either classically or quantum mechanically, especially when the internal energy becomes large, approaching the dissociation limit. However, total internal energy and total angular momentum are true constants of the motion classically, and in a complementary way, E and J are good quantum numbers. In the approach here, states of the recombined diatomic are classified by their E and J values, and the product state distribution is obtained consistent with conservation of the total three-body system energy and angular momentum. The relative product state distribution, including bound, quasi-bound and continuum states, is that resulting from the associated volumes in phase space (sometimes called the “prior distribution”). No further assumptions about the interaction potential or collision dynamics are made, although the implications of assuming various dynamical models will be discussed. Connections can be made with experimental results even at this basic level of description, and one can argue that these constrained state densities determine much of the recombination behavior, including temperature dependence, independent of the specific interaction potentials and dynamics.

Discussion of the relationships between the approach and results described here and those from other groups will also be presented.

Assisted Combustion of an Air Kerosene Mixture by Nanosecond Repetitively Pulsed Discharge

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Abstract

A convenient way to reduce NOx emissions in industrial combustion applications is to burn lean perfectly premixed reactants as the thermal formation of nitric oxides is directly linked to the burnt gas temperature. These conditions are generally achieved in swirled lean premixed burners where the rotating flow both enhances the mixing rate between fuel and oxidizer streams and promotes the flame stabilization through the swirl-induced recirculation of hot products near the nozzle. Unfortunately, strong instabilities may occur under these operating conditions and lead to mechanical damages and/or flame extinction. Various solutions have already been proposed to improve and to control flame stabilization in these combustion chambers, from injector design improvements to complex adaptive active control methods. Other ways to improve flame holding or flame ignition is to use high voltage pulses, which can generate active species in air or air/fuel mixture.

In the context of the French program INCA (Initiative for Advanced Combustion), EM2C Laboratory developed a plasma discharges generator and tested it with an air propane burner in lean conditions [1,4], and ONERA Laboratory developed a facility for air/kerosene combustion which allows testing plasma assisted combustion techniques [2].

In a first part, we propose to describe the generator of nanosecond repetitively pulsed discharge (NRPD) used to stabilize a premixed propane/air burner. Different experimental techniques are conducted to demonstrate the possibility to increase the combustion efficiency of the flame in lean conditions.

In a second part, the experimental facility MERCATO, used for testing the combustion of an air/kerosene mixture is presented. The axial flow velocity in the combustion chamber is 70m/s. Test duration is 35 s, allowing a linear decrease of the injected equivalence ratio until the extinction of the flame. This lean extinction limit value is investigated, according to the use of different electrode geometries and discharge voltage values.

The NRPD extends the stability domain of the flame. The repetition rate and the localization of the discharge inside the combustion chamber appear to be keys parameters.

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Electron/molecular cation and atom/diatom reactive collisions relevant for re-entry plasmas and combustion

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The dissociative recombination, the ro-vibrational excitation (de-excitation) and the dissociative excitation of molecular cations:

$$AB^+ + e^- \rightarrow A + B, \quad AB^+ + e^-, \quad A + B^+ + e^-$$

play a major role in the kinetics and in the energy transfer of numerous ionized cold environments – interstellar molecular clouds, planetary atmospheres, combustion flames, plasmas for surface processing and fusion edge plasmas[1].

The measurement of the rate coefficients of these reactive collisions using storage-rings reached a remarkable precision[2], and recently conceived REMPI-based sources allow the ion production in perfectly determined ro-vibrational states. Meanwhile, the *computation* of the rate coefficients is strongly needed, since the measurements correspond to limited ranges of energy and initial states.

We are presently able to describe efficiently the interference between the major mechanisms – direct and indirect – governing the reactive collisions, including in the analysis the contribution of numerous series of valence and Rydberg states of resonant capture, within an approach [3,4] based on the multichannel quantum defect theory (MQDT)[5], taking into account the ro-vibrational structure of the ion and of the neutral system. A recent application of the wave-packet method to the account of the indirect process[6] opens the way to the prediction of branching ratios and to the description of the polyatomic systems.

Our approaches have been applied to several diatomic species for a broad range of energies and target states. H_2 and its isotopes, as benchmark systems, have been extensively studied [4, 7] at low energy, and the numerous Rydberg resonances occurring have been unambiguously assigned. Systematic calculations on NO[8] and, currently, CO, aim to provide rate-coefficients for the modeling of the plasmas formed at the hypersonic entries of spacecrafts in the Earth and March atmospheres respectively.

We are currently working on the modeling of the processes involving ionization channels relying on several ionic cores - dissociative excitation and dissociative recombination into core-excited Rydberg states [9]. Novel systems, like CF[10] and BF are about to be studied, and old ones, like CH and H_2, revisited. We intend to develop our wave-packet method [6] and to apply it to polyatomic systems like HCO and H_3O, highly relevant for the kinetics of the plasma-assisted combustion.

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Kinetics of OH Radicals below Self-Ignition Threshold in Plasma Enhanced Combustion

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An experimental measurements of resolved in time OH density in the nanosecond single filament DBD has been performed for different gas mixtures and different temperatures of he initial gas flow. It has been shown that decay of OH density depends significantly upon initial temperature and gas mixture composition. Preliminary numerical calculations of radical density decay in the discharge afterglow have been made, the difference between the experimentally measured densities and densities obtained while calculating using standard numerical schemes for combustion, is demonstrated.

Experimental Investigation of Gradient Mechanism of Detonation Initiation

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An experimental study of detonation initiation in a stoichiometric propane–oxygen mixture by a high–voltage nanosecond gas discharge was performed in a detonation tube with a single–cell discharge chamber. The discharge study performed in this geometry showed that three modes of discharge development were realized under the experimental conditions: a spark mode with high–temperature channel formation, a streamer mode with non–uniform gas excitation, and a transient mode. Under spark and transient initiation, simultaneous ignition inside the discharge channel occurred, forming a shock wave and leading to a conventional deflagration to detonation transition (DDT) via an adiabatic explosion. The DDT length and time at 1 bar of initial pressure in the square smooth tube with a 20 mm transverse size amounted to 50 mm and 50 μs, respectively. The streamer mode of discharge development at an initial pressure of 1 bar resulted in non–uniform mixture excitation and a successful DDT via a gradient mechanism, which was confirmed by high–speed time resolved ICCD imaging. The gradient mechanism implied a longer DDT time of 150 μs, though under significantly lower initiation energy of 1 J and a short DDT run–up distance of 50 mm.

Control of the energy deposited in a high voltage nanosecond discharge and combustion triggering in $N_2/O_2/C_3H_8$ mixtures at atmospheric pressure

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One growing topic of interest in the plasma and combustion field is car engine ignition by non-equilibrium plasmas. Such kind of discharges could improve the ignition and flame propagation efficiency by promoting the chemical reactivity of the mixture through the creation of a great amount of radicals, instead of heat release only.

In this work, the energy control in a pin to plane corona discharge induced in dry air under nanosecond scale high overvoltage is investigated. The space and time behaviour of the discharge is described by fast CCD imaging coupled to electrical measurements. The energy is modified by changing the voltage and the pulse duration. In previous works, we showed the capability to get a diffuse regime and a streamer regime below 3 bar, and a leader-like regime above [1-2]. In the diffuse regime, the discharge constricts along the pin to plane axis when the energy increases while intensification of the emission can be observed along one or several filaments in the streamer regime. The electrical energy release can be controlled by the pulse duration under a certain limit which is greater for the streamer regime than for the diffuse one. Below this limit, the current pulse ends with the voltage pulse and hundreds of amperes can be achieved in the gap with no control problems. Difficulties appear in the leader-kind regime. When a filament reaches the plane, the current increases at values of hundred to kilo-amperes in a nanosecond scale and does not come back to zero as soon as the voltage pulse ends.

The ignition of $N_2/O_2/C_3H_8$ mixtures by one pulse and the induced flame propagation are studied at 1 bar. By adding propane in the gap, we observed the vanishing of the diffuse regime and its transition into a multi-channel type (figure 1). The filaments become thinner as the ratio of propane increases. The energy is smaller in the multi-channel pattern than in the diffuse one up to a ratio of 8-10% of propane and increases after this limit probably because of heat effects in the filaments. Investigation on the combustion itself shows that it always triggers near the tip with an energy deposited as low as a few millijoules. The evolution of this limit has been investigated according to voltage amplitude. From 45 to 80 kV, it remains near 10 mJ despite differences in the discharge behaviour. Finally we observed the combustion by use of the CCD camera in multi-frame mode (figure 2). It allowed us to prove that the flame begins to propagate within 250 µs after the discharge.

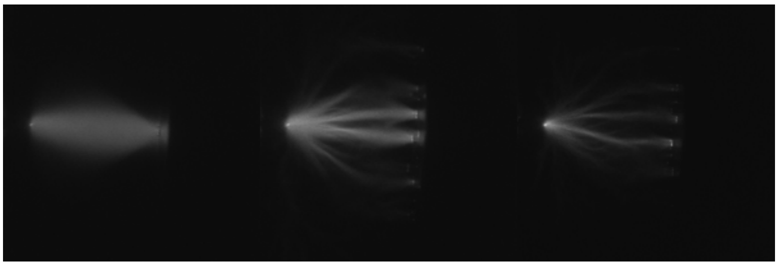

Figure 1 - Discharge spatial behaviour with 0 (left), 4 (centre) and 8 % (right) of propane in dry air at 1 bar.

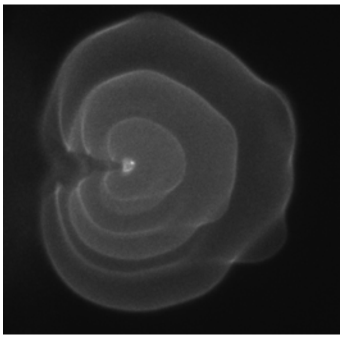

Figure 2 - Combustion triggering near the tip and flame propagation.

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Acknowledgements
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Hydrocarbon dissociation and OH radical production in high pressure plasmas of atmospheric gases with ethane or propane

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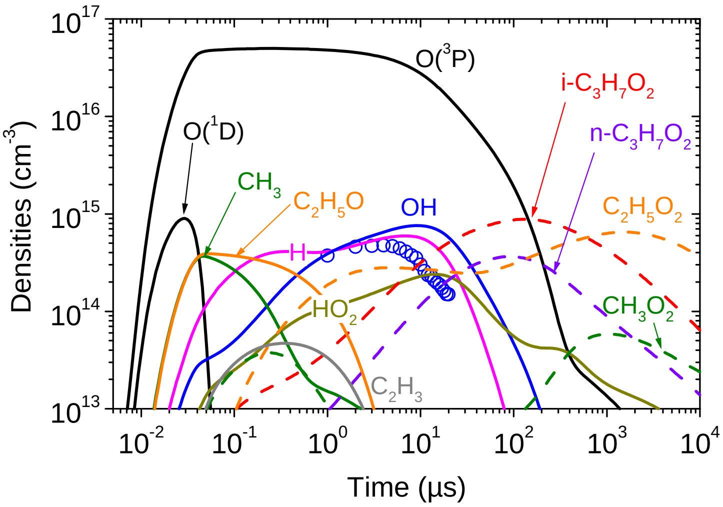
Non-thermal plasmas in N_2/O_2/hydrocarbon mixtures are currently under investigation for combustion triggering and control [1]. Extensive experiments and modelling works are performed in order to understand physical and chemical processes involved. At atmospheric pressure, non-homogeneous (DBD or corona) discharges are widely used in such studies. However a comprehensive kinetic interpretation is not easy to achieve because it requires a self-consistent modelling of both the streamer propagation physics and the strongly reactive chemistry for the gas mixture under consideration. In this work, a pre-ionised (photo-triggered) discharge is used to study the conversion of ethane and propane in nitrogen and N_2/O_2 mixtures at different oxygen concentration values (up to 20 %), and to examine the role of the hydroxyl radical produced by the plasma kinetics. Effect of water vapour added to the mixture (up to 2.3 %) is also examined. Owing to the spatial homogeneity of the plasma, a self-consistent 0D-model is used to determine the main kinetic processes involved in ethane and propane conversion, as well as in OH radical production.

A description of the experimental device (UV510 reactor) and of the model can be found in [2, 3]. The discharge volume is 50 cm^3, with an electrode spacing of 1 cm. The total pressure of the studied mixtures has been fixed to 460 mbar. Ethane or propane is added to N_2/O_2 with a concentration value between 0.02 and 0.55 %. Gas chromatography has been used to follow the removal of the hydrocarbon molecule and the increase of by-products concentrations. A flash lamp synchronised with a gated intensified CCD camera has been implemented on the UV510 reactor in order to measure, in absolute value, the time evolution of the OH density (from 0.5 µs up to 1 ms, time resolution 250 ns) after the current pulse (60 ns duration) through absorption spectroscopy (rotational transitions between the ground X state, v''=0, and the A state, v'=0).

The following figure gives a typical example of results obtained for the hydroxyl radical, for a mixture with 20 % of oxygen and 0.5 % of propane. Symbols correspond to measurements and lines to model predictions for some radicals taken into account in our detailed kinetic scheme.



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Using a repetitively pulsed nanosecond plasma to improve oxidation and ignition processes in methane/air flows

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Control of ignition and combustion processes in aircraft jet engines is of significant importance for their performance and reliability. Reduction in ignition delay time, high altitude flame-holding, flame stability improvement and extension of blow-off limits are some of the key issues which are commonly controlled, with limited success, by systems based on conventional thermal ignition mechanisms (arc discharge …). Alternative mechanisms can also trigger a much more effective ignition mechanism on modifying the chemical reaction kinetics by generating and sustaining large electron number densities, which results in a non-equilibrium excitation of the gas mixture. Better efficiency of population transfer within electronic and vibrational states can then be obtained using pulsed nanosecond discharges which handle weak reduced electric field. Relevant examples, in this regard, are the experimental studies focused of nanosecond pulse duration discharges on various phenomena such as reduction in ignition delay time, flame stabilization, ignition and flame holding. However, the mechanisms of energy transfer between the plasma and the gas medium remain not fully understood. In this frame, experimental data characterizing the thermodynamic and kinetic processes governing this energy transfer are required. More specifically, population distributions of neutral molecules and species composition are key scalar parameters which need to be used as input parameters for the simulation of these mechanisms. Analysing the thermodynamic and kinetic mechanisms of fuel oxidation and ignition by a nanosecond pulsed discharge is then the main objective of the present study.

The probing of the pulsed discharge of a high voltage, nanosecond pulse duration, capacitively coupled discharge sustained in atmospheric premixed methane-air flows was performed using laser diagnostics which enable locally and temporally resolved measurements of temperature and species concentration. Among these diagnostics, coherent anti-Stokes Raman scattering (CARS), laser Thomson scattering (LTS) and planar laser-induced fluorescence (PLIF) were specifically developed and applied to characterize this discharge. CARS was initially used to measure, within the plasma produced in various methane/air mixtures, the population distribution of N_2 in its ground electronic state. Temporal evolution of the rovibrational populations was recorded by delaying the laser shots relative to the discharge pulse (from 10 ns to 1 ms). Experiments were carried out in premixed CH_4/Air flames to study the effect of the nanosecond discharge on plasma ignition and stabilisation of combustion at atmospheric pressure. These results were used to assess the feasibility of single-shot CARS measurements of temperature in order to highlight the thermodynamic and kinetic mechanisms of nanosecond discharges in hydrocarbon/air premixed mixtures. Results show that energy transfer induced by collisions of N_2 with the fuel or its decomposition products considerably increases the thermal heating of neutral molecules at temperature up to 2500 K. Effect of the discharge on the local temperature then leads to the ignition of the CH_4/air mixture for equivalence ratios between 0.7 and 1.3. This work was completed by probing the conversion of the hydrocarbon fuel as well as the kinetic mechanism of recombination of radicals and atoms into neutral molecules such as H_2 and C_2H_2 in situation where no ignition occurs ($\Phi<0.7$ and $\Phi>1.3$). Laser Thomson scattering has been implemented to characterize the electric properties of the discharge such as electron density and electron temperature. Results demonstrate that this nanosecond discharge can be classified in the range of weakly ionized plasmas with a reduced electric field of about 250 indicating a small production of ionized molecules. It is also known that nanosecond discharges can also trigger a much more effective non-thermal ignition mechanism. This non-thermal ignition mechanism implies that not temperature but specific plasma-generated active species -radicals, excited atoms and molecules, charged particles, and so on - stimulate the chain reactions of fuel oxidation leading to the ignition of the fuel–oxidizer mixture. In order to evaluate these effects, the temporal distributions of OH, CH and CH_2O within the discharge were measured using PLIF. All these results allow to demonstrate and to quantify the efficiency of the nanosecond pulsed discharge for the improvement of combustion and ignition processes. They also let foresee new potentialities for application of this new technology on aeronautical injection systems.

Nanosecond Repetitively Pulsed Spark Discharges in Ambient Air

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Abstract

Atmospheric pressure air plasmas have potential applications in biomedical and surface treatment, chemical and biological decontamination, aerodynamic flow control, and combustion. Many of these applications require discharges with high chemical reactivity at low gas temperature, i.e. glow discharges. Others require yet higher levels of chemical reactivity but can tolerate or benefit from significant gas heating, i.e. spark discharges. The Nanosecond Repetitively Pulsed (NRP) method is one means to produce both glow and spark discharges in air at atmospheric pressure. In particular, NRP glow discharges operate at power budgets lower than those of traditional generation methods by several orders of magnitude.

Previously, NRP discharges in atmospheric pressure air were produced at comparatively high temperatures of 750-2000 K [Kruger, *et al.,* Packan, Pai]. In order of increasing applied voltage for given conditions, the three NRP regimes are corona, the glow, and the spark. The glow has low levels of emission, gas heating, electrical conduction current, and a maximum electron density of about 10^{13} cm^{-3} [Pai, *et al.*]. Furthermore, this regime develops through an initial streamer followed by a return wave. In contrast to the glow regime, the spark regime emits strongly, heats the gas by several thousand degrees Kelvin, has tens of amperes of conduction current, and reaches maximum electron number densities of about 10^{15} cm^{-3}. Here we present an investigation of NRP spark discharges at 300 K.

Single-shot imaging of the spark regimes has been performed using intensified ICCD cameras. For the NRP spark regime, single-shot imaging shows that the discharge develops first homogenously, as demonstrated in [Pai], but then disappears towards the electrodes. The discharge channel can take different paths with each applied pulse. Surprisingly, by acquiring single-shot image sequences of a single discharge, it can be seen that the channel can also move during the development of a single spark. The degree of deviation from the inter-electrode axis increases with inter-electrode gap distance.

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Low-energy electron attachment and detachment in vibrationally excited oxygen and oxygen-containing mixtures

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Palm *et al* (2002), Rich *et al* (2004) and Frederickson *et al* (2007) showed experimentally that the vibrational excitation of electron-beam-generated, nonequilibrium O_2:N_2 plasma with CO laser leads to a two orders of magnitude increase in the plasma free electron lifetime. This effect was ascribed to complete mitigation of rapid three-body electron attachment to molecular oxygen due to electron detachment from O_2^- ions in collisions with vibrationally excited molecules. It was mentioned that the mitigation of electron attachment could facilitate the generation and maintenance of nonequilibrium plasma with high electron density and hence could be important to a variety of potential aerodynamic applications of high pressure, low temperature air plasmas.

In this work, three-body electron attachment to O_2 molecules and electron detachment from O_2^- ions have been theoretically studied in vibrationally excited oxygen and O_2-containing mixtures. Assuming that electron attachment and detachment proceed via the formation of vibrationally excited temporary O_2^- ions, the rates of these processes were determined on the basis of the statistical approach for *VV'* and *VT* transfer in collisions between O_2^- ions and O_2 molecules. The calculated attachment and detachment rate constants turned out to agree well with available measurements in unexcited oxygen. This method was used to calculate attachment and detachment rates in vibrationally excited oxygen. It was shown that the effect of vibrational excitation on electron detachment is profound, whereas attachment of low-energy electrons to vibrationally excited O_2 is inefficient. The calculated rate constants were used to simulate the formation and decay of an electron-beam-generated plasma in N_2:O_2 mixtures at elevated vibrational temperatures. The calculations showed that vibrational excitation of molecules leads to orders of magnitude increase in the plasma density and in the plasma lifetime, in agreement with available observations.

Electron-electron collisions in the Boltzmann Equation: energy-conservation

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The knowledge of the electron energy distribution function (eedf) in weakly ionized gases is a fundamental aspect in modeling plasma chemical processes, ranging from gas discharges [1] to re-entry of space vehicles [2]. Inelastic and superelastic collisions of free electrons with neutrals result in large deviations of the eedf from a Maxwellian. In order to reduce the computational effort, the contribution of e-e collisions in electron kinetics is usually neglected or alternatively a Maxwellian distribution is adopted. However, the synergic interaction between electron-electron and superelastic collisions strongly affects the eedf, especially in presence of electronically metastable states [3]. In these conditions the eedf must be calculated by solving the Boltzmann equation. In particular, the P_1 approximation [4], resulting in a Fokker-Planck equation, is commonly used in the case of weak electric field. In the equation, elastic, inelastic and superelastic collisions give a linear contribution, while e-e collisions introduce nonlinear terms. Self-consistent coupling of the kinetics of free electrons and heavy particles makes the global problem non-linear, because the population of atoms in excited states, entering in the e-neutral collisional terms, depends on the eedf, through e-neutrals chemical rates.
The commonly used algorithm to calculate the eedf has been developed by S.D. Rockwood in 1973 [4]. In fact, the method is rather time-consuming in evaluating the nonlinear contribution of e-e collisions. Moreover, conservation of the total electron energy in e-e collisions is formally imposed but not fulfilled when numerical time integration is carried out. In this paper we present an efficient numerical algorithm which takes into account e-e nonlinear terms by using sparse matrices, preserving exactly the total electron energy. These are critical points in self-consistent models, especially in fluid dynamic simulations, where the total energy equation is considered and the Boltzmann equation must be solved many times.
The performance of the Rockwood's and of the present algorithms have been compared, obtaining (for 400 energy groups) a gain in the computation time of a factor 6 when only e-e collisions are considered and a factor 25 when all the processes are considered. The factor increases with the number energy groups. Moreover, the total electron energy is conserved under the required tolerance.

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Large area, atmospheric pressure, non-equilibrium air plasmas.

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Abstract: Atmospheric pressure plasmas have attracted considerable interest in recent years due to their potential in a wide range of applications including biological decontamination [1], plasma assisted combustion [2], and aerodynamic flow control [3]. In many cases the use of air as a working gas is a prerequisite, however, the generation of air plasma at atmospheric pressure proves challenging due to the highly collisional nature associated with high pressure operation combined with an abundance of electronegative oxygen. Under such operating conditions it is typical for instabilities to form on a sub-microsecond timescale. Recent studies have shown that short pulsed excitation is an ideal means of generating diffuse air plasma at atmospheric pressure [4-5]. The short pulse width offers a temporal means of limiting discharge current thus preventing runaway and an undesirable constriction of the discharge.

The focus of this work is to highlight the potential of sub-microsecond pulsed excitation for the generation of large area air plasmas. Experimentally it is shown that short pulsed excitation is capable of generating low temperature, diffuse air plasma over a large area. Several electrode configurations are considered including a parallel plate reactor, a surface discharge, and a coaxial jet structure. In all cases the input power density is on the order of ~W.cm^{-3} yet the instantaneous peak power density can exceed 100kW.cm^{-3}. Such unique operating conditions are only observed under pulsed excitation and have a significant impact upon key plasma properties such as electron density, electron temperature, and species production. To assist in understanding these unique discharges a PIC-fluid hybrid simulation similar to that detailed in ref [6] was employed. The effect of pulse width and pulse rise time upon electron kinetics within the discharge was examined, it was demonstrated that manipulation of the temporal characteristics of each pulse causes a shift in the electron energy distribution function (EEDF). The exciting prospect of EEDF tailoring could have far reaching consequences in many applications and necessitates further research and development in to repetitive pulsed power technology as a viable means of large area air plasma generation.

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Nanosecond surface discharge at high pressures

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Surface nanosecond discharge at elevated pressures has been proposed as a tool to initiate combustion assisted by nonequilibrium plasma at elevated pressures. Preliminary experiments have been carried out; ICCD imaging of the discharge has been obtained for 1-5 atm ambient air.

1. Introduction

Typically, plasma assisted combustion (PAC) experiments are carried out at atmospheric or at decreased gas pressure [1]. Here we propose a system which can lead to ignition under conditions of automotive engines, including HCCI, gas turbines and other high-pressure devices. It is proposed to use surface nanosecond discharge [2] developed for aerodynamic applications in combination with rapid compression machine [3] for quantitative study of PAC initiation at elevated pressures.

2. RCM applications for plasma assisted ignition and combustion

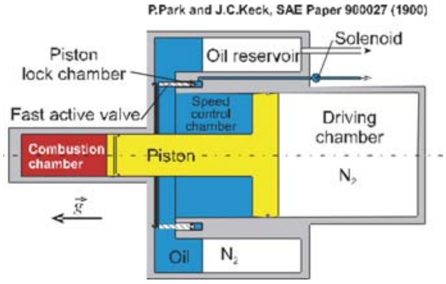

Fig. 1: *Scheme of RCM machine [3].*

Rapid compression machines (RCM, Fig.1) are designed to study the ignition delay time at low temperatures (about 1000 K) and high pressures (tens and hundreds of atm), at the conditions similar to those in internal combustion engine. The only RCM application for artificial (laser stimulated) ignition is known in the literature [4]. If we manage to organize the nonequilibrium plasma between the end plate of the combustion chamber and the piston, or, at least, near the end plate, we will be able do decrease the ignition delay time and to investigate kinetics of plasma assisted ignition at high pressures.

3. High-voltage pulsed discharge at elevated pressure: preliminary experiments

Nanosecond DBD discharge in a special coaxial geometry of electrodes was used to produce a thin layer of quasi-uniform plasma in the vicinity of low-voltage electrode. High voltage pulses of 10-20 kV amplitude, 25 ns duration, 3 ns rise time, positive or negative polarity, and repetitive frequency 40 Hz were used to ignite the discharge in ambient air at pressures 1-5 atm. Emission was registered by LaVision PicoStar ICCD camera (200-800 nm) in nanosecond time scale. ICCD images of nanosecond DBD discharge in ambient air are given by Fig. 1. Gas pressure, voltage amplitude in the cable, and ICCD gate are indicated for each picture. The total energy input in the discharge did not exceed approximately 10 mJ, or 10 % of the energy stored in incident nanosecond pulse.

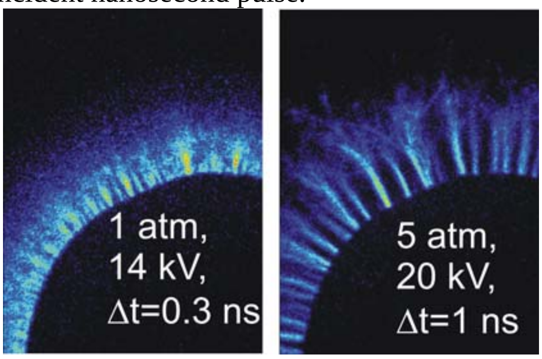

Fig. 2: *ICCD images of nanosecond surface discharge*

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The Challenges and Solutions in Simulation of Plasma Discharge in Reactive Flows: A Multi-Model Multi-Scale Approach

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Simulation of plasma discharge with complex chemistry and flow dynamics is one of the most computationally demanding problems. The application area of plasma chemical processes is expanding at a very fast pace, causing a strong demand for efficient and adequate simulation tools. These modelling tools shall assist in studying the underlying processes on different levels of detail, aid in process parameter optimization and form a good basis for inventing and testing new ideas.

One of the challenges of a realistic simulation of plasma discharge in reactive flows is the sheer complexity of multiple intertwined physical and chemical processes: ionization, dissociation, excitation, recombination, attachment, ion bombardment; convective and diffusive transport, turbulence, thermal effects, gas-phase chemical reactions, heterogeneous reactions on the surface, phase transitions, and electromagnetic wave propagation in conductive media with non-linear properties. The temporal and spatial scales of these processes span many orders of magnitude: from nanoseconds to hours and from Angstrom to meters. Modelling these coupled processes with a fine level of detail and appropriate scale in three dimensions is still out of reach of modern computational resources, and special modelling and simulation approaches are required to meet the challenge.

Another challenge is the imposed interdisciplinarity of the problem. To formulate the problem, we need the expertise in mathematics, theoretical and experimental physics and chemistry, materials science, engineering and other application-specific areas. To solve the problem, we need to bring in the expertise from the fields of numerical algorithms, computational methods, software and middleware engineering, computer architectures, parallel distributed computing, and other relevant branches of computer science. A real progress is only possible when all the domains of expertise meet together and join forces.

A long experience in the field of modelling plasma chemical vapour deposition allowed us to work in most of the key fields listed above. This work resulted in new models and solvers [1,2], new numerical method and parallel algorithm [3], a software architecture [4,5], and load balancing method for heterogeneous distributed computer resources of the Grid [5-7]. Combining different models and tools with a user-friendly interface, data analysis and visualization capabilities, and flexible access to parallel computing resources gave birth to the Virtual Reactor, software that could be considered as a prototype of the virtual laboratory for science and engineering [8,9]. This Virtual Reactor has been extensively used for simulation of various technologies: RF and VHF capacitively and inductively coupled plasma discharges at low and atmospheric pressures, carbon and silicon-based film deposition and nano-particle production, in small-scale (volume of several cubic centimetres to several litres) and very large industrial reactive chambers (several cubic meters volume). This experience has lots in common with the simulation of flow and combustion control by plasma in aerospace applications.

My presentation will describe: (1) the multi-model approach that allows simulation of the sub-processes on the appropriate level of detail and time scale, (2) the coupling strategy that binds together the different models and scales into a consistent simulation, and (3) the inter-disciplinary efforts related to the numerical implementation and parallel simulation on distributed resources of the Grid. All these approaches and solutions are generic: they are applicable in any branch of modelling and simulation of complex physical and chemical processes, not restricted to a particular application.

The multi-model approach is based on splitting the problem into three sub-models: electromagnetic, plasma and reactive flow. Each model is simulated in an appropriate sub-domain of a complete reactor chamber, and mutual influence of the models in overlapping areas is accounted for by iterative exchange of variable fields with adaptive estimation of the required exchange frequency. Such loosely coupled solver technique can gain a tremendous reduction in computational time (several orders of magnitude, depending on the problem size), while preserving the consistency of simulated results. The state-of-the-art modelling approaches in plasma chemical deposition were so far limited to 2D (axisymmetric 3D) and simplified process description in fully coupled simulations. The multi-model approach allowed us to couple a full 3D reactive flow dynamics with detailed 3D electromagnetic wave propagation and 2D axisymmetric capacitively coupled plasma discharge in a plasma chemical vapour deposition reactor. In addition, quantum chemistry simulations were performed to predict reaction rates, surface structure and defects. The approach was validated and used for optimization of existing plasma chemical processes and for development of new technologies [10,11].

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Experimental and Analytical Study of the Interaction of a Weak Shock Wave with an Ionised Gas

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An experimental campaign was carried out to study the interaction of a plasma produced by a dielectric barrier discharge (DBD) and a transonic air flow around a typical airfoil. The flow conditions together with the blade geometry provoke a strong shock to appear on the suction side of the airfoil (see figure 1). The mutual interaction of the DBD with the flow field was studied experimentally in order to determine the influence of the plasma on shock position and strength and of the flow field on the plasma discharge.

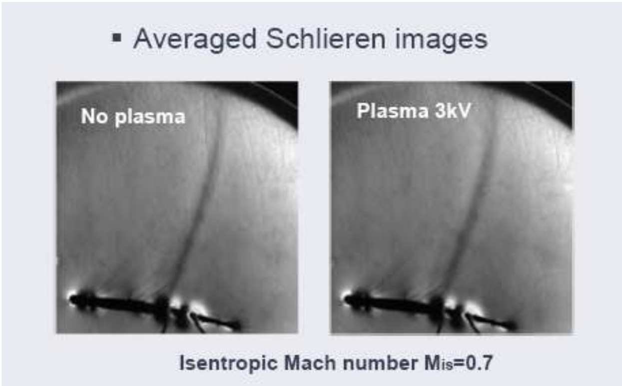

Figure 1: Shock structure over an airfoil equipped with a DBD

Technological advances and understanding of the physics of the interaction open new perspectives in active flow control (sonic boom alleviation) and plasma assisted combustion. A long lifetime surface DBD was developed that can be stabilised in supersonic airflows. Although the interaction between the flow and the plasma showed none or small modification of the shock shape by the plasma (see figure 1), the contrary was more spectacular and the plasma is strongly modified by the airflow. The understanding of these mechanisms will help to design DBDs capable of affecting shocks. (see figure 2)

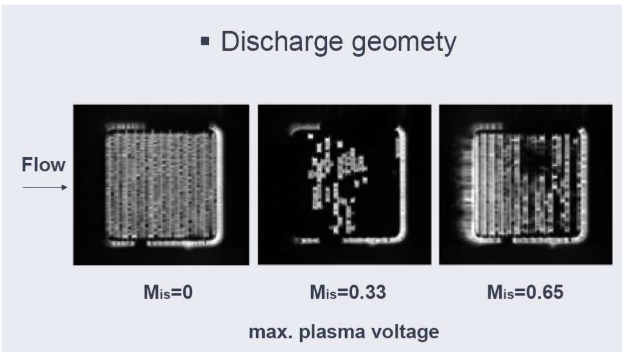

Figure 2: Modification of DBD structure with flow speed on a flat plate (without shock)

An analytical study of a weak shock wave in ionised gas has been conducted in order to clarify and support the experimental study. The mathematical model assumes frozen ionisation over the shock wave and is one dimensional. This model supposes no interaction with a boundary layer and is realised to determine whether shock alleviation is better done in the boundary layer with a DBD system or outside the boundary layer with another system (a corona discharge for example). The governing equations are based on a three-fluid approach. The analytical approach consists in a linearisation of the equations of conservation, which was possible due to the relatively low velocity of the flow under investigation ($M \cong 1$). This approach allowed to explicitly resolve the equation of energy conservation for electrons, which depend only on the electron temperature at this stage. The electron temperature could then be determined explicitly for different electron density (figure 3). This in turn allowed to evaluate the amount of thermal energy transferred to the neutral gas upstream of the shock through the electron gas. To show how this energy affects the shock, the variation of bulk temperature (ΔT_a) due to electron energy transfer is shown in table 1. The increase in bulk gas temperature is dependent on electron density with strong relative variation between lowest and highest electron density, as shown in table 1, however the overall effect of the plasma on the shock wave remains very small.

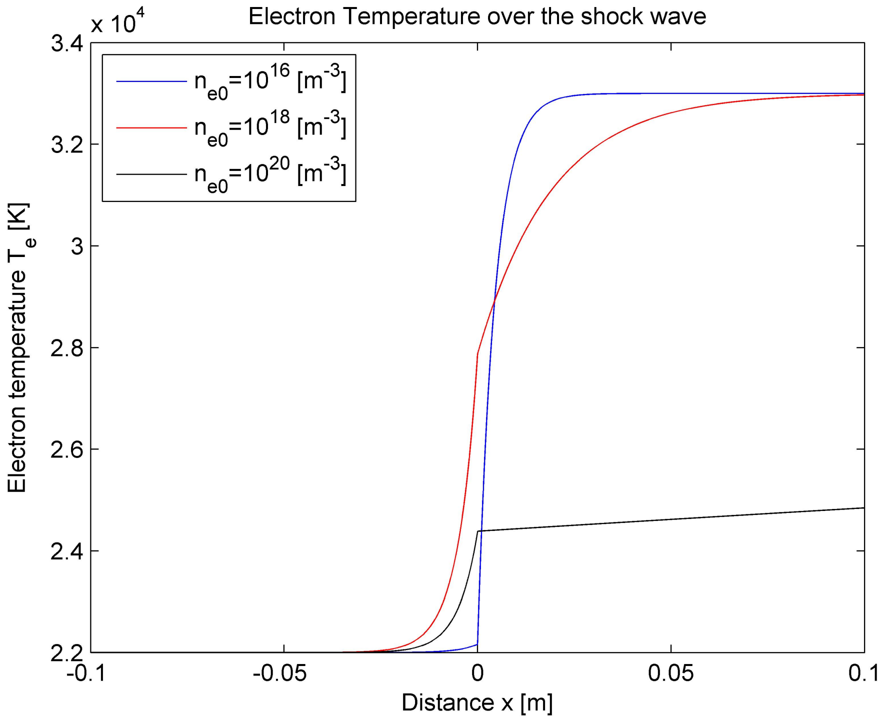

Figure 3: Electron temperature through the shock for different electron densities

Table 1: Temperature increase in the bulk gas

Electron Density	ΔT_a
10^{16} $[el\ m^{-3}]$	6.52 10^{-7} $[K]$
10^{18} $[el\ m^{-3}]$	2.40 10^{-2} $[K]$
10^{20} $[el\ m^{-3}]$	9.72 10^{-2} $[K]$

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Poster Description

Electron temperature and density measurement by mean of a Langmuir probe

S.Goekce, T.N.Eichmann, R.Morgan, P.Leyland and R.Sobbia

An experimental investigation of very high velocity flow (up to 8.5 km/s) generated with the impulse facility X2 at The University of Queensland, Australia, has been conducted. Two flow conditions related to hyperbolic entries in Titan and Mars atmospheres have been used. Titan conditions were investigated using the non-reflected shock tube mode of X2, figure 1, up, and Mars conditions were investigated using the expansion tunnel mode of X2, figure 1, down. The quantities of interest in these experiments were the electron temperature and density, which could be used to validate CFD calculations. To gather quantitative measurements of such quantities, a *Triple Langmuir Probe*, which is suitable for rapidly varying flows, has been manufactured an used successfully. Novel approaches for the computation of the electron density have been developed (referred to as “Unified theory” and “Simple method” in figure 2) and compared with other methods found in literature (referred to as “Triple Probe method” and “Corrected Triple Probe method” in figure 2). Good agreements have been found between all methods validating the new approaches for the cases studied

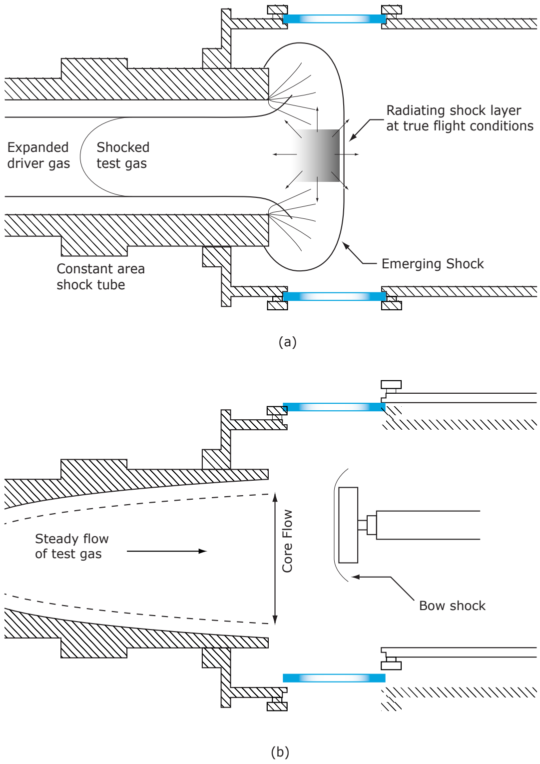
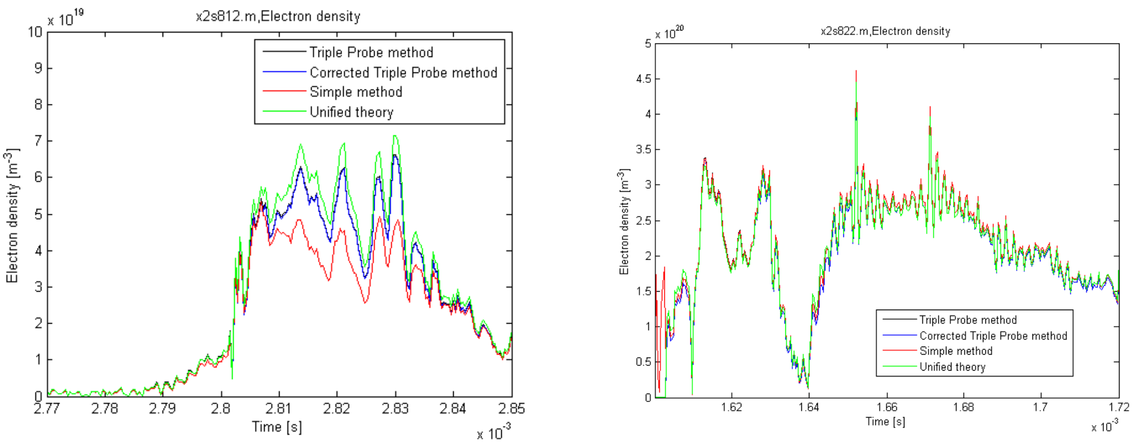


Figure 1: Non reflected shock tube mode (up) and expansion tunnel mode (down) of the X2 facility



(a) *Titan*

(b) *Mars*

Figure 2: a) Electron density computed with all methods, Titan conditions and b) Mars conditions

Energy Coupling to the Plasma in Repetitive Nanosecond Pulse Discharges

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Abstract

A new analytic quasi-one dimensional model of energy coupling to nanosecond pulse discharge plasmas in plane-to-plane geometry has been developed. The use of a one-dimensional approach is based on images on repetitively pulsed nanosecond discharges plasmas in dry air demonstrating that the plasma remains diffuse and uniform on a nanosecond time scale, in a wide range of pressures (Figs. 1).

The two key processes affecting the pulse energy coupled to the plasma and incorporated by the model are (i) nanosecond pulse breakdown and (ii) charge accumulation on dielectric surfaces covering the electrodes. Plasma decay processes, such as electron-ion recombination and electron attachment, are insignificant on the nanosecond time scale. The model provides analytic expressions for the time-dependent electric field and electron density in the plasma (Figs. 2), electric field in the sheath, sheath boundary location, and coupled pulse energy (Fig. 3). The analytic model predictions are in very good agreement with the numerical model of the discharge in drift-diffusion approximation.

The model demonstrates that (i) the energy coupled to the plasma during an individual nanosecond discharge pulse is controlled primarily by the capacitance of the dielectric layers and by the breakdown voltage, and (ii) the pulse energy coupled to the plasma during a burst of nanosecond pulses decreases as a function of the pulse number in the burst. This occurs primarily because of plasma temperature rise and resultant reduction of breakdown voltage, such that the coupled pulse energy varies approximately proportionally to the number density. The energy loading per molecule for the same pulse voltage waveform remains nearly independent of the number density.

Analytic expression for coupled pulse energy scaling with the number density has been incorporated into the air plasma chemistry model, which was validated previously by comparing with atomic oxygen number density measurements in nanosecond pulse discharges. The results of kinetic modeling using the modified air plasma chemistry model are compared with time-resolved temperature measurements in a repetitively pulsed nanosecond discharge in air, by emission spectroscopy and purely rotational CARS, showing good agreement (Fig. 4).

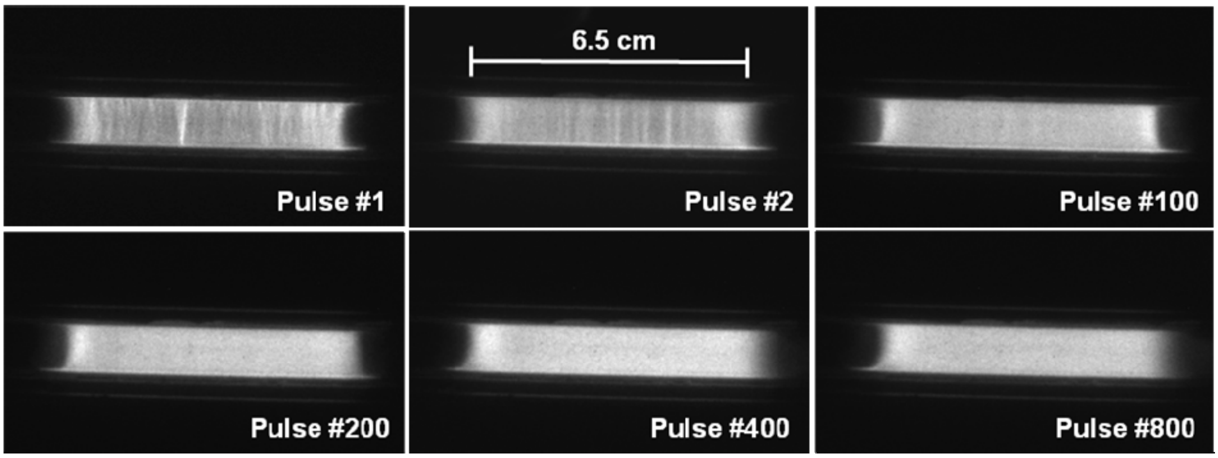
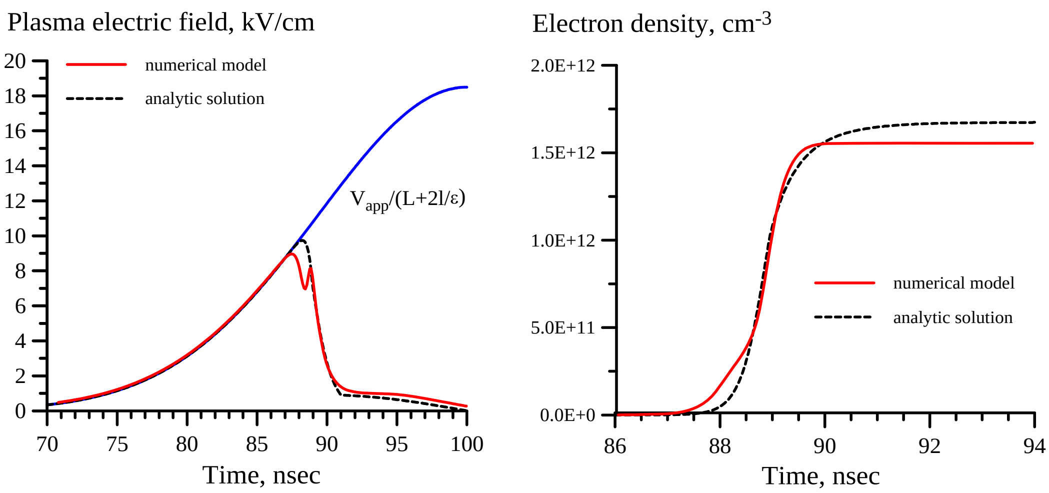


Figure 1. ICCD camera images of a repetitive nanosecond pulse plasma in air flow. P=60 torr, ν=40 kHz (time between consecutive pulses 25 μsec). Camera gate 1 μsec.



Figures 2. Comparison of time-dependent electric field (left) and electron density (right) in the plasma predicted by numerical and analytic discharge models.

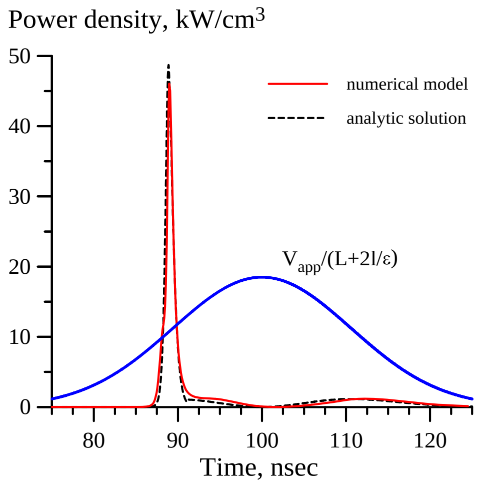


Figure 3. Comparison of time-dependent power density coupled to the plasma during breakdown and post-breakdown predicted by numerical and analytic discharge models. Applied voltage waveform is also shown.

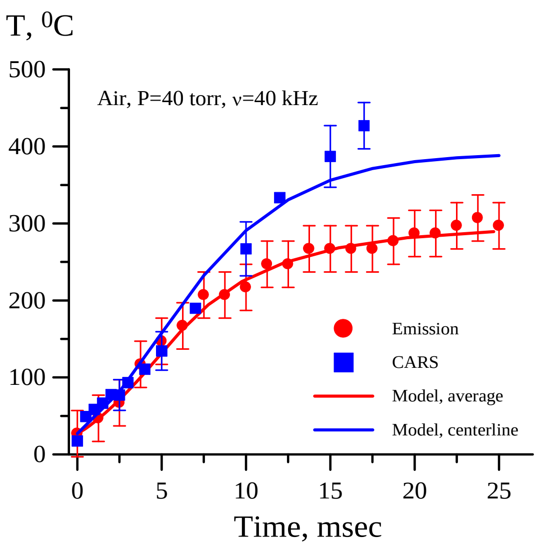


Figure 4. Comparison of experimental spatially averaged (emission) and centerline (CARS) temperatures in a repetitively pulsed nanosecond discharge in air at P=40 torr with the plasma chemistry model prediction.

Investigation of atmospheric pressure air plasma by two-photon laser induced fluorescence

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One of the possibilities to reduce nitric oxides in flames consists in using lean premixed combustion systems. However, these systems tend to be unstable. To solve these problems, it was shown [1] that one can stabilize lean premixed flames by high voltage nanosecond repetitively pulsed discharges (NRPD) [2]. The objective of our study is to determine the kinetic mechanism that leads to flame stabilization. To this end, the density of ground state atomic oxygen has been measured using Two-Photon Laser Induced Fluorescence (TALIF) at 225 nm.

We have applied two-photon absorption laser-induced fluorescence (TALIF) to investigate Nanosecond Repetitively Pulsed Discharges (NRPD) in air at atmospheric pressure, in a pin-to-pin electrode configuration. TALIF measurements have been performed to characterize the formation of atomic oxygen after the discharge pulse. Atomic oxygen is one of the key species in combustion processes and understanding its formation is important to understand the mechanism of plasma-assisted flame ignition and stabilization. Kinetic models suggest that oxygen is produced via a two-step mechanism that involves the dissociative quenching of molecular oxygen by electronically excited nitrogen. In this poster we present measurements of atomic oxygen that support the proposed mechanism.

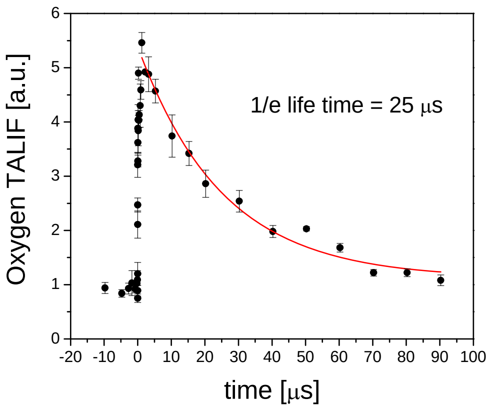

Figure 1. Temporal evolution of the TALIF signal normalized to the squared laser intensity during one discharge cycle.

As an example, one of our measurements concerns the temporal profile of the atomic oxygen, Fig[1]. It shows that the production of atomic oxygen is not dominated by electron-impact dissociation, but rather by a process that begins after the pulse and lasts for about 50 ns. This process is likely to be the dissociative quenching of molecular oxygen by the electronically excited molecular nitrogen produced by the pulse.

References:

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