Fundamental Mechanisms, Predictive Modeling, and Novel Aerospace Applications of Plasma Assisted Combustion

AFOSR
MURI Kick off meeting

The Ohio State University

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Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

Drexel Group: Main Tasks

Thrust 1. Experimental studies of nonequilibrium air-fuel plasma kinetics using advanced non-intrusive diagnostics

Task 1: Low-to-Moderate (T=300-800 K) temperature, spatial and time-dependent radical species concentration and temperature measurements in nanosecond pulse plasmas in a variety of fuel-air mixtures pressures (P=0.5-5 atm), and equivalence ratios

Task 4: Moderate-to-high (T=800 – 1800 K) temperature PAC oxidation kinetics in Discharge Shock Tube Facility at pressures up to 10 bar

Task 5: PAC oxidation and combustion initiation at high pressure, high temperature conditions

Thrust 2. Kinetic model development and validation

Task 8: Development and validation of a predictive kinetic model of non-equilibrium plasma fuel oxidation and ignition

Task 9: Mechanism Reduction and Dynamic Multi-time Scale Modeling of Detailed Plasma-Flame Chemistry

Thrust 3. Experimental and modeling studies of fundamental nonequilibrium discharge processes

Task 10: Characterization and Modeling of Nsec Pulsed Plasma Discharges

Thrust 4. Studies of diffusion and transport of active species in representative two-dimensional reacting flow geometries

Task 13: Ignition and flameholding in high-speed non-premixed flows

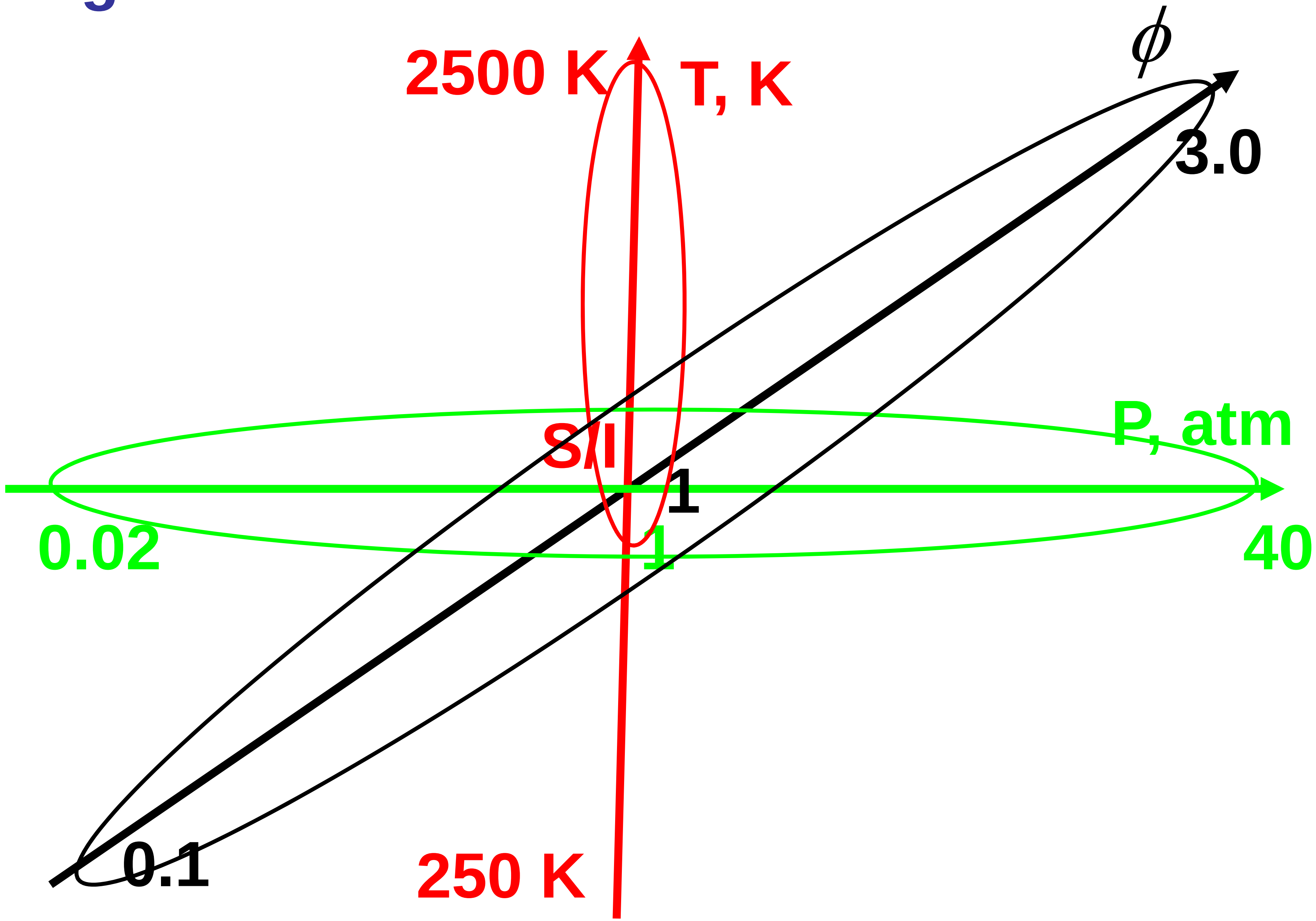
Task 14: High Fidelity Modeling of Plasma Assisted Combustion in Complex Flow Environments

Drexel Group: International Collaboration

International Collaborators

Svetlana Starikovskaya (Ecole Pol) – Thrust 1
Alexander Rakitin (NEQLab) – Thrust 1
Boris Potapkin (KIAE) – Thrust 2
Alexander Konnov (VUB) – Thrust 2
Nickolay Aleksandrov (MIPT) – Thrust 3
Sergey Pancheshnyi (Univ Toulouse) – Thrust 3
Sergey Leonov (IVTAN) – Thrust 4

Range of Parameters – Combustion Kinetics



Problems of Plasma-Chemical Models

Availability and accuracy of data on electron collision cross sections

\+ H_2 CH_4 C_2H_6 C_3H_8

? C_4H_{10} C_5H_{12} …

Availability and accuracy of chemical models below self-ignition point

\+ H_2

? CH_4 C_2H_6 C_3H_8 C_4H_{10} C_5H_{12} …

Availability and accuracy of physical and chemical models for non-equilibrium conditions

\+ Radical’s mechanism

? Ionic chain mechanism

? Energy chain mechanism

Models for Low-Temperature Plasma Assisted Combustion

Starikovskii et al.,

Plasma Physics Reports, 2000 (26) 701

$O_2 + e^- + M \rightarrow O_2^- + M$

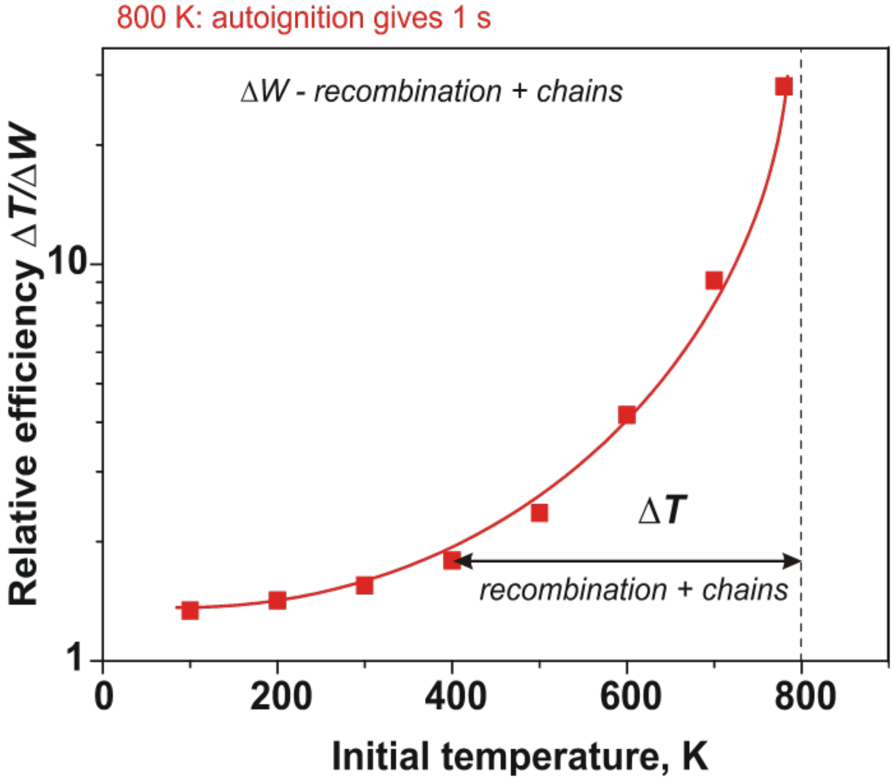
$H_2 + O_2^- \rightarrow OH^- + OH$

$OH + H_2 \rightarrow H_2O + H$

$OH^- + H \rightarrow H_2O + e^-$

$H + O_2 + M \rightarrow HO_2 + M$

$OH^- + HO_2 \rightarrow H_2O + O_2 + e^-$



Starikovskii,

Chemical Physics Reports, 2003 (11) 1

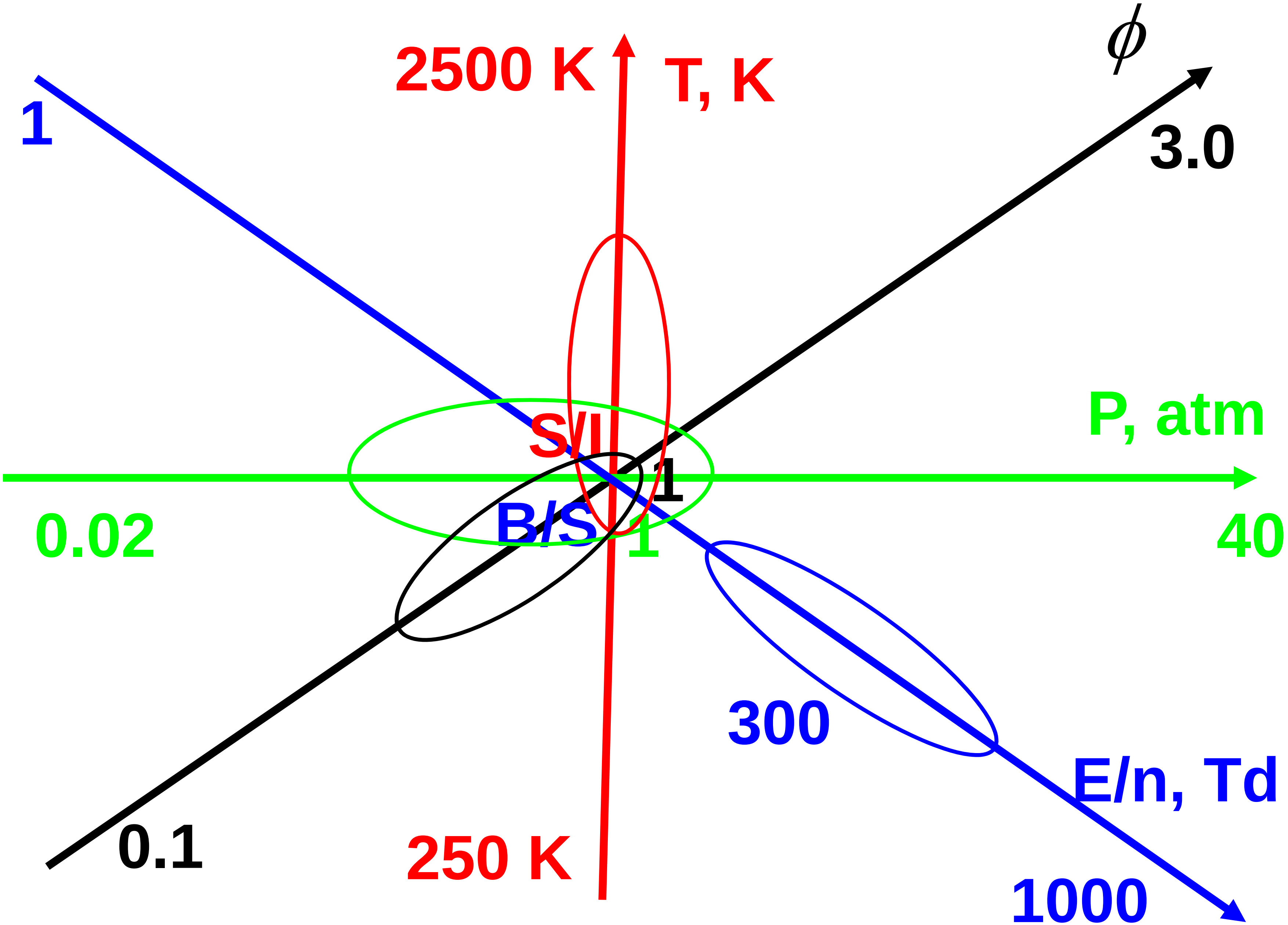
$N_2O^* + H \rightarrow N_2^* + OH$

$CO + OH \rightarrow CO_2^* + H$

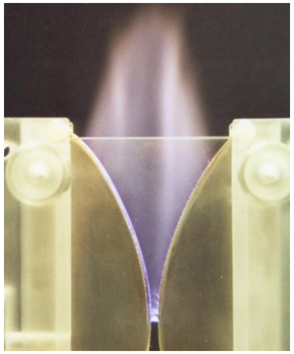
$CO_2^* + N_2O \rightarrow N_2O^* + CO_2$

$N_2^* + N_2O \rightarrow N_2O^* + N_2$

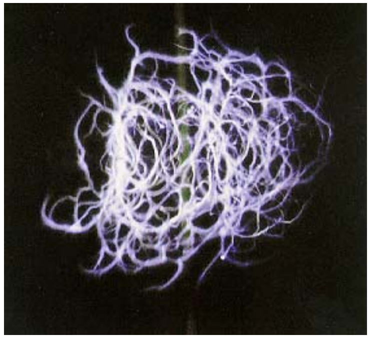
PAC: Where we are



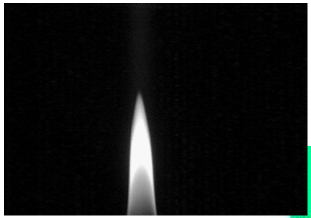
Mechanisms of Plasma Influence



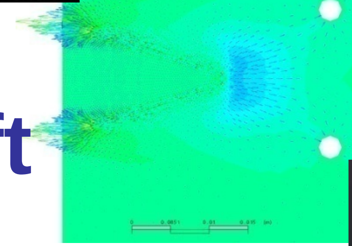
1. **Heating**



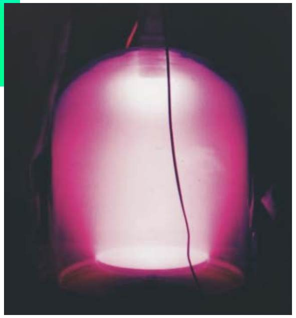
2. **Turbulization**



3. **Momentum Transfer**

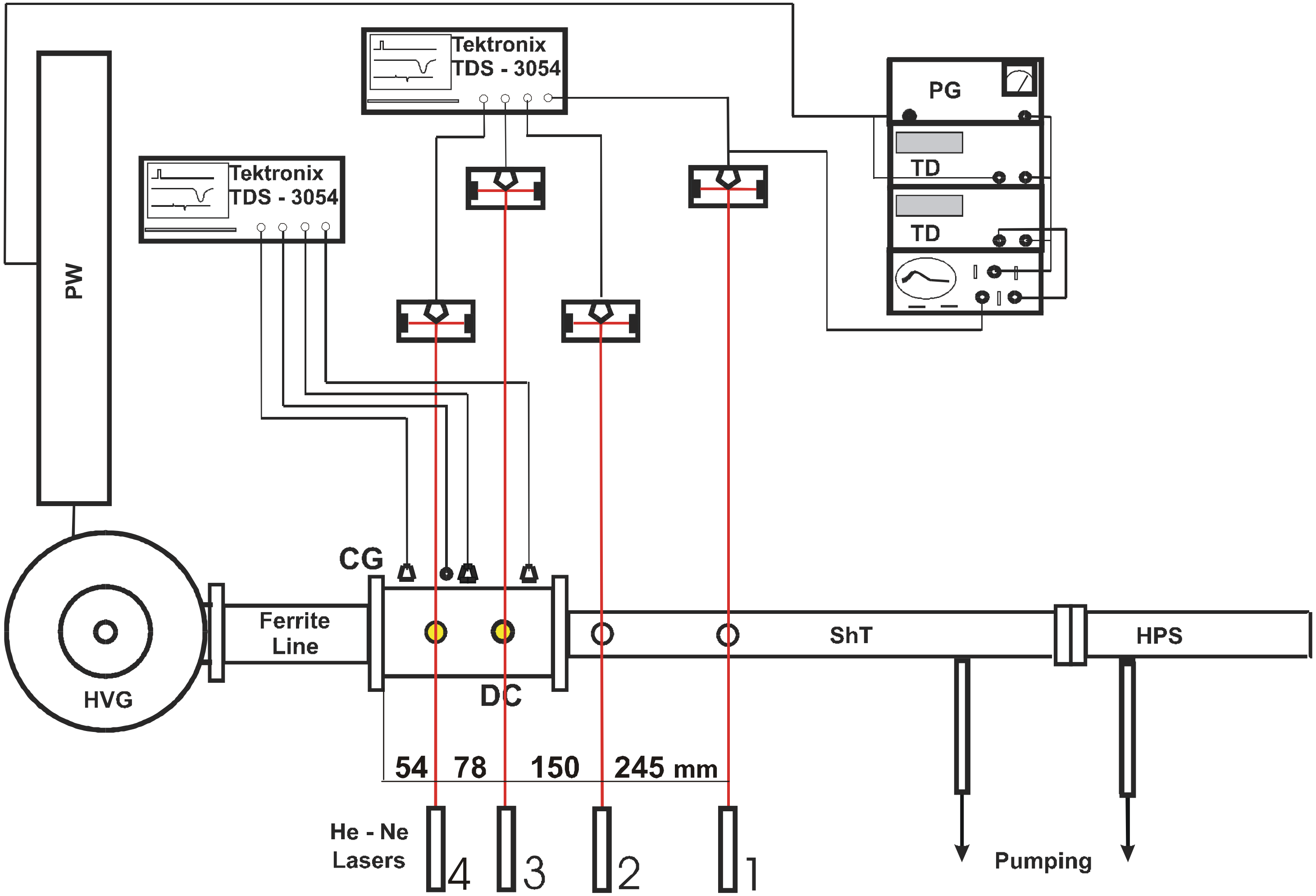


4. **Electrons/Ions Diffusion/Drift**



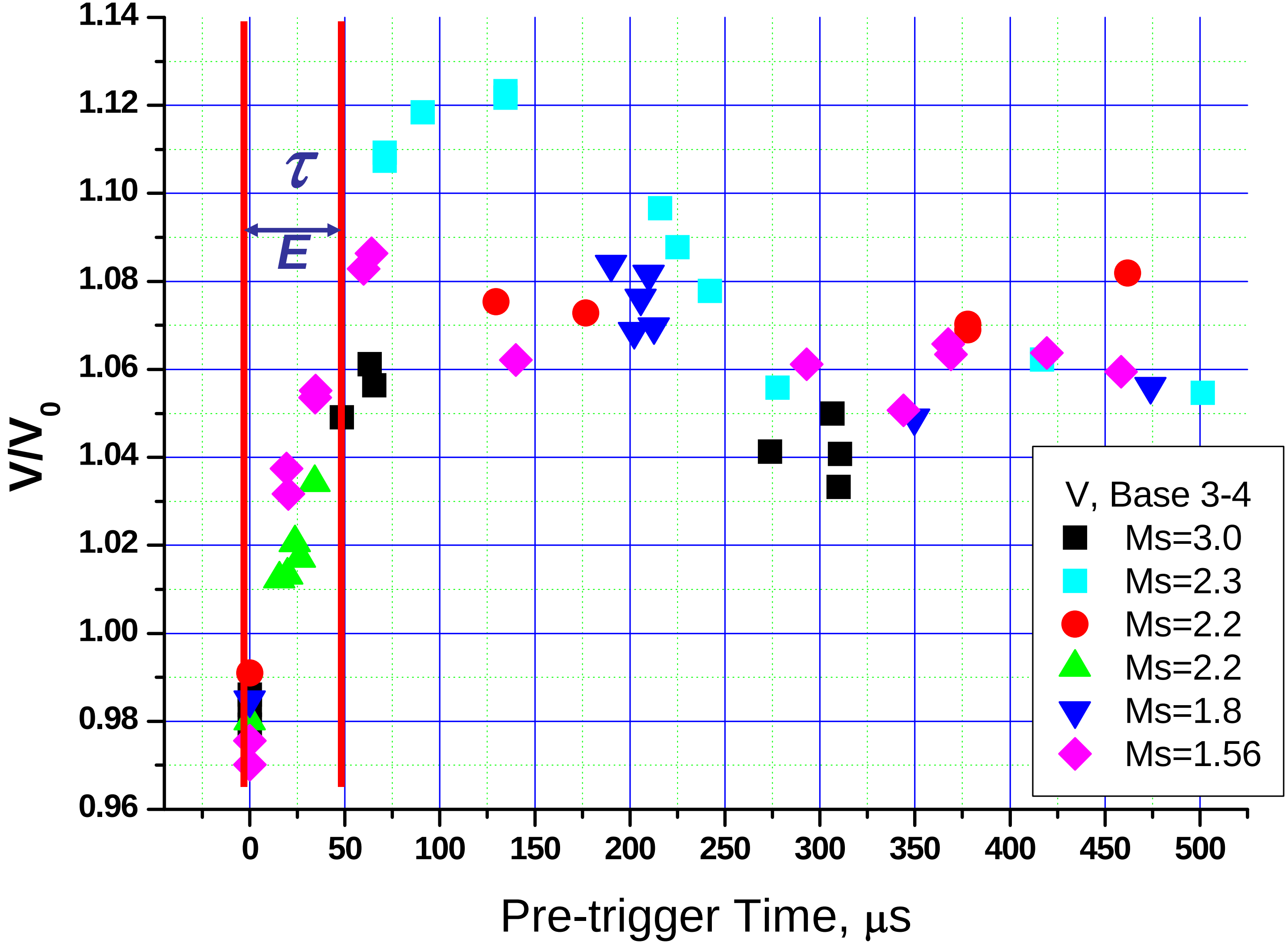
5. **Dissociation, Ionization**

Shock Wave - Nonequilibrium Plasma Interaction



Relaxation of Nonequilibrium Plasma.

Air. P_1 ~ 20 Torr



Relaxation of Nonequilibrium Plasma.
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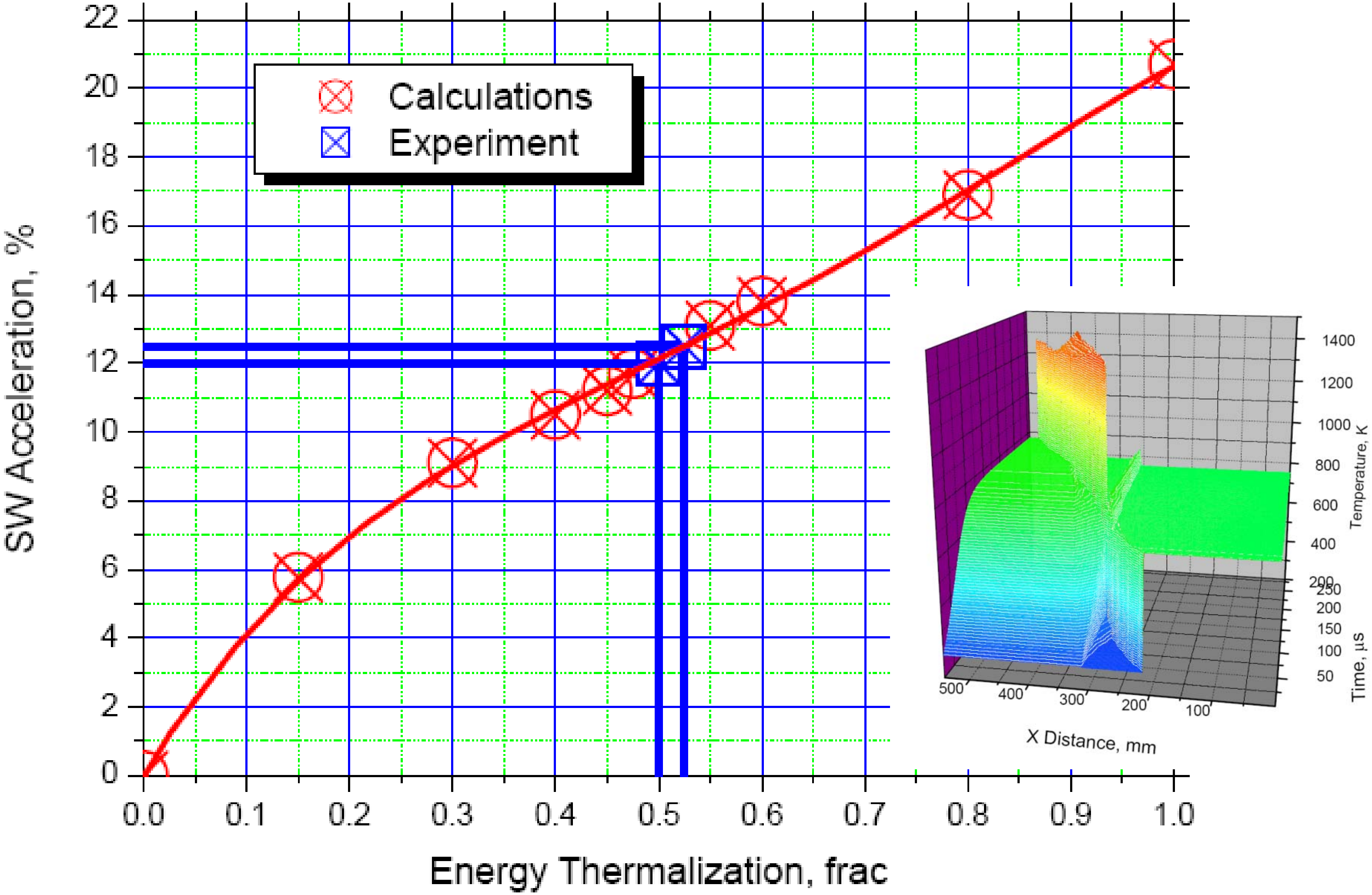
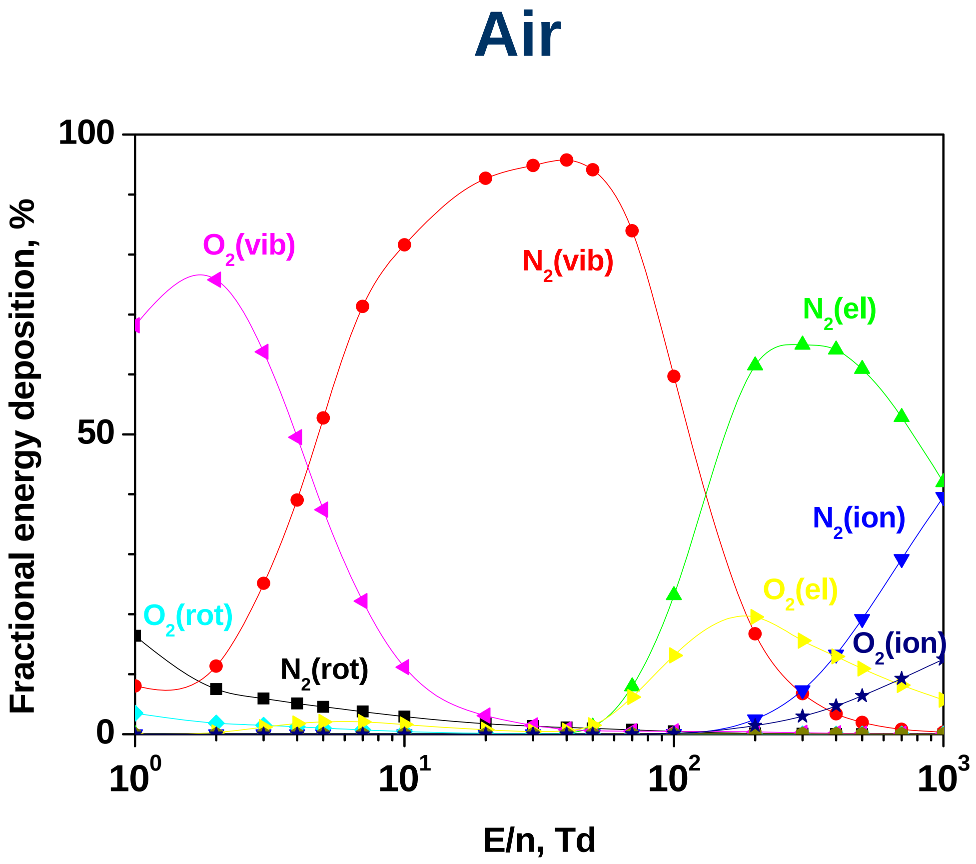


Mechanism of fast heating in discharge plasmas (low E/N)



Low (< 20 Td) E/N:

e + N_2 , O_2

- **elastic scattering**

- **rotational excitation**

Mechanism of fast heating in discharges (moderate E/N)

Moderate (20 - 200 Td) E/N:

Popov (2001) heating → 28 % of power spent on $N_2^* + O_2^*$

$e + O_2 \rightarrow e + 2O + \Delta E$

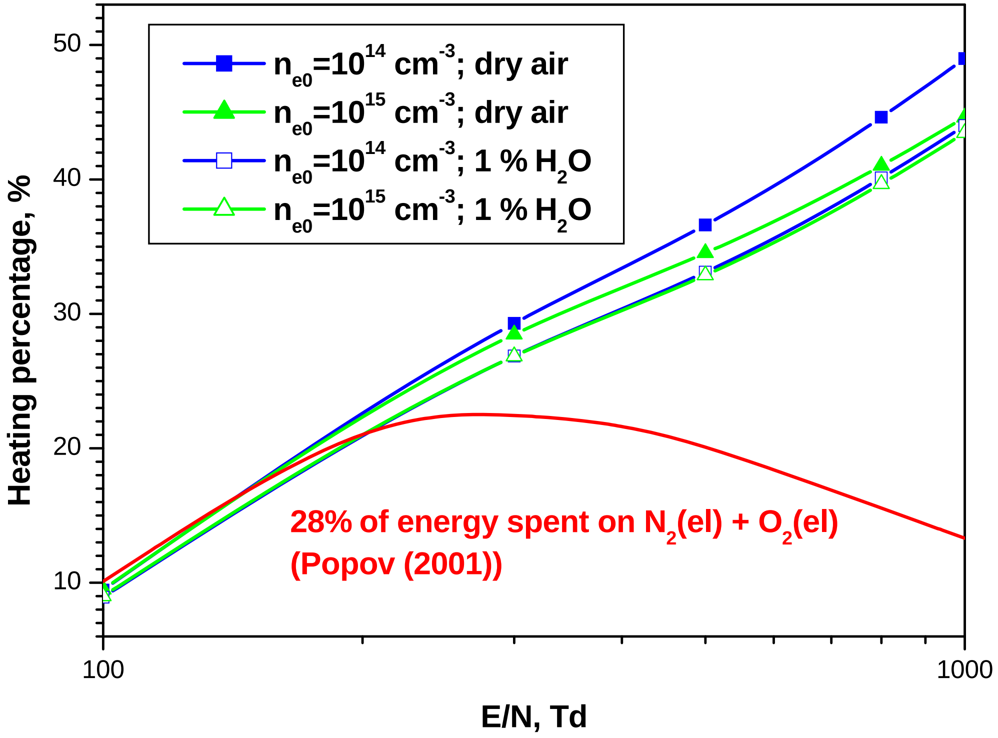
$e + N_2 \rightarrow e + N_2^*(A, B, C, a', \ldots)$

$N_2^*(A, B, C, a', \ldots) + O_2 \rightarrow N_2 + 2O + \Delta E$

$O(^1D) + N_2 \rightarrow O + N_2 + \Delta E$ $k \sim 10^{-10}\ cm^3/s$

Mechanism of fast heating in discharge plasmas (high E/N)

Aleksandrov et al. (2009)



28% of energy spent on N_2(el) + O_2(el) (Popov (2001))

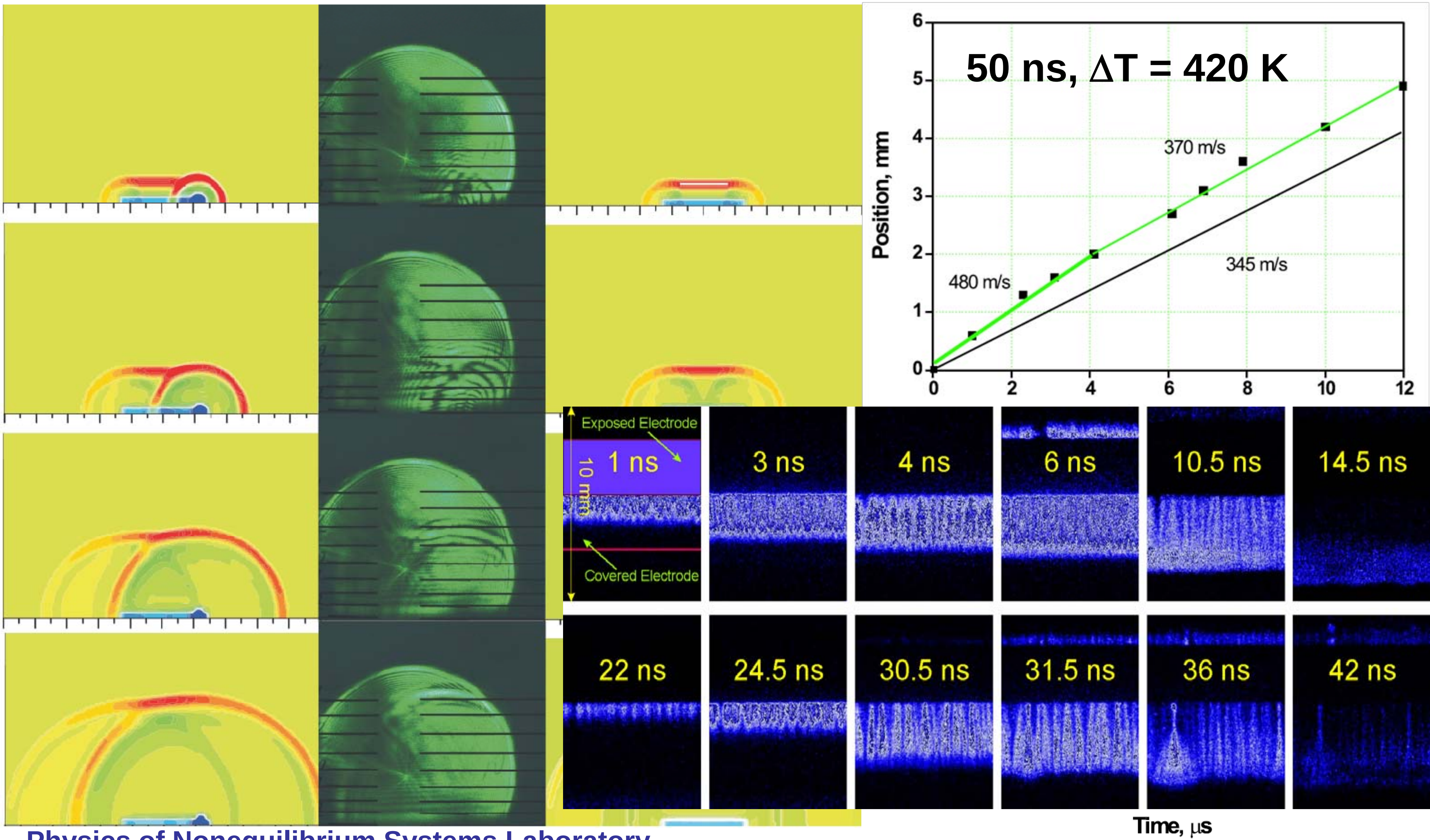
High (> 200 Td) E/N:

electron-ion and ion-ion recombination kinetics

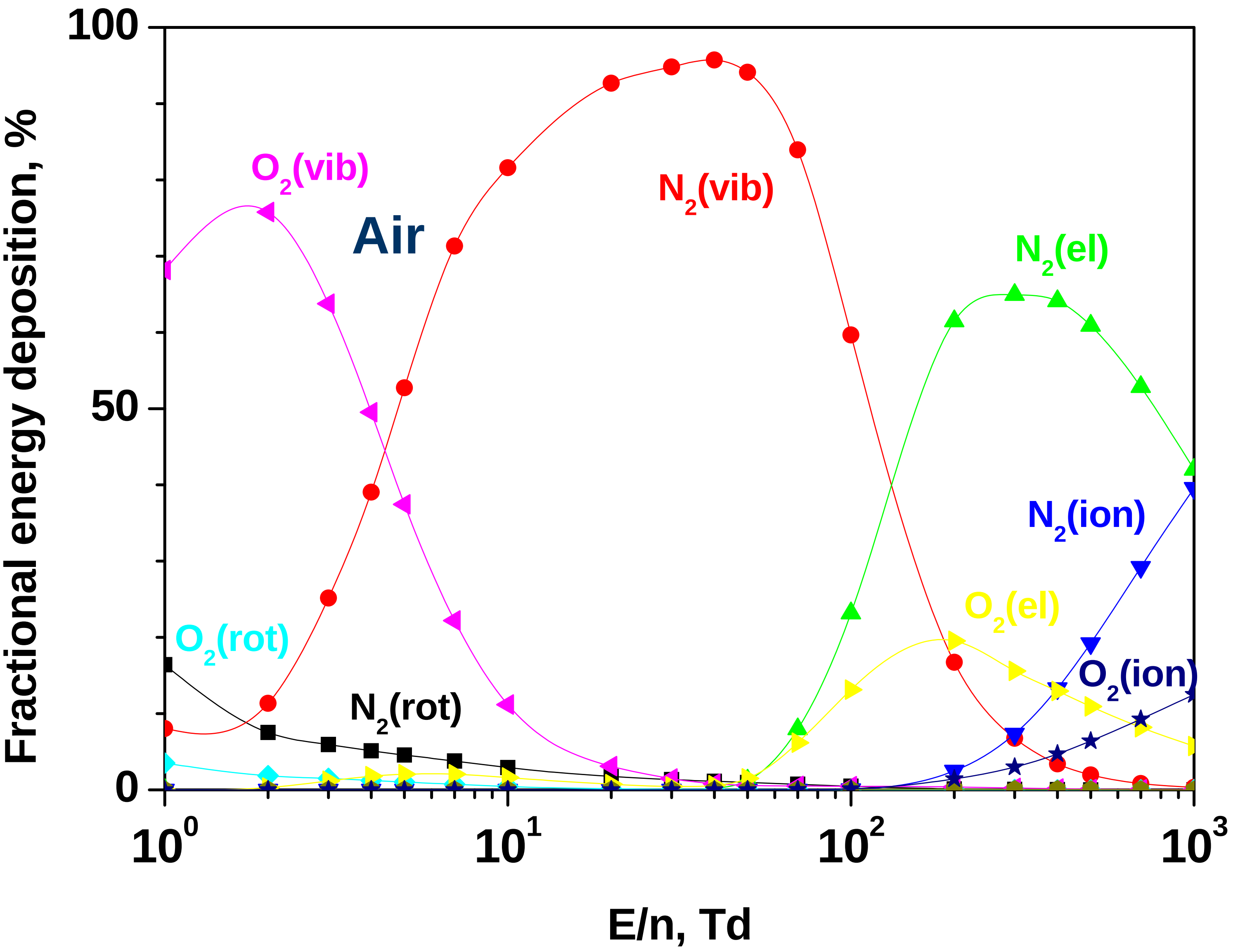
$$e + O_2^+ \rightarrow O + O^* + \Delta E$$

$$O_2^- + O_2^+ + M \rightarrow 2O_2 + M + \Delta E$$

Heat Release and Shock Waves Formation by "Nonequilibrium" Plasma

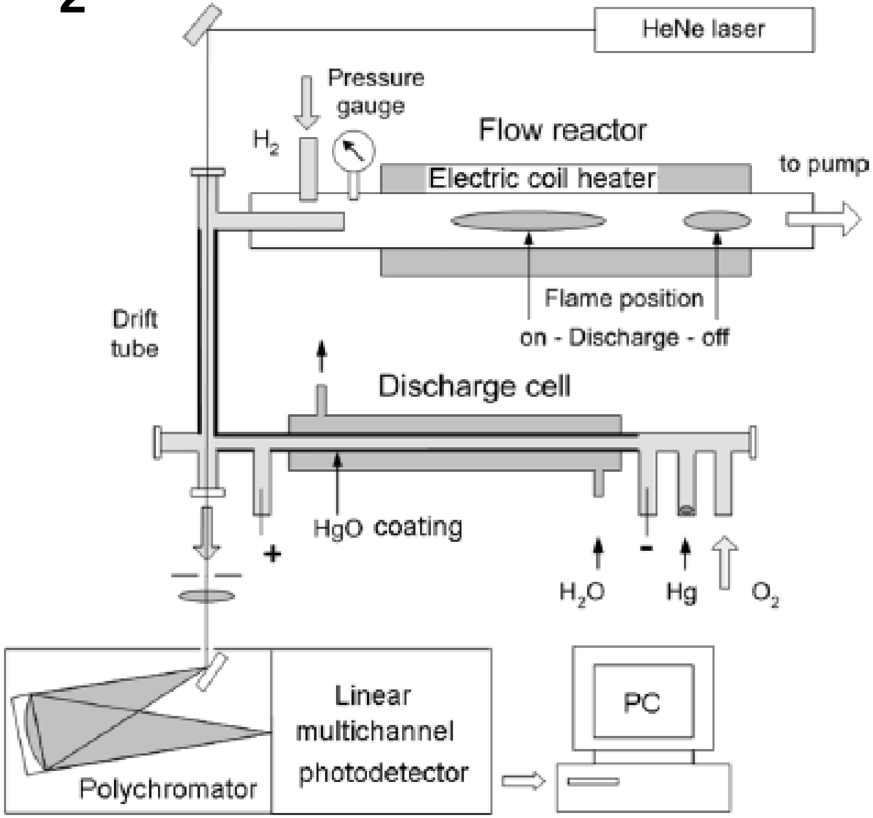


Energy Distribution in Gas Discharge



Molecular Oxygen Excitation

To directly observe the influence of SDO on the combustion of H_2-O_2 mixture



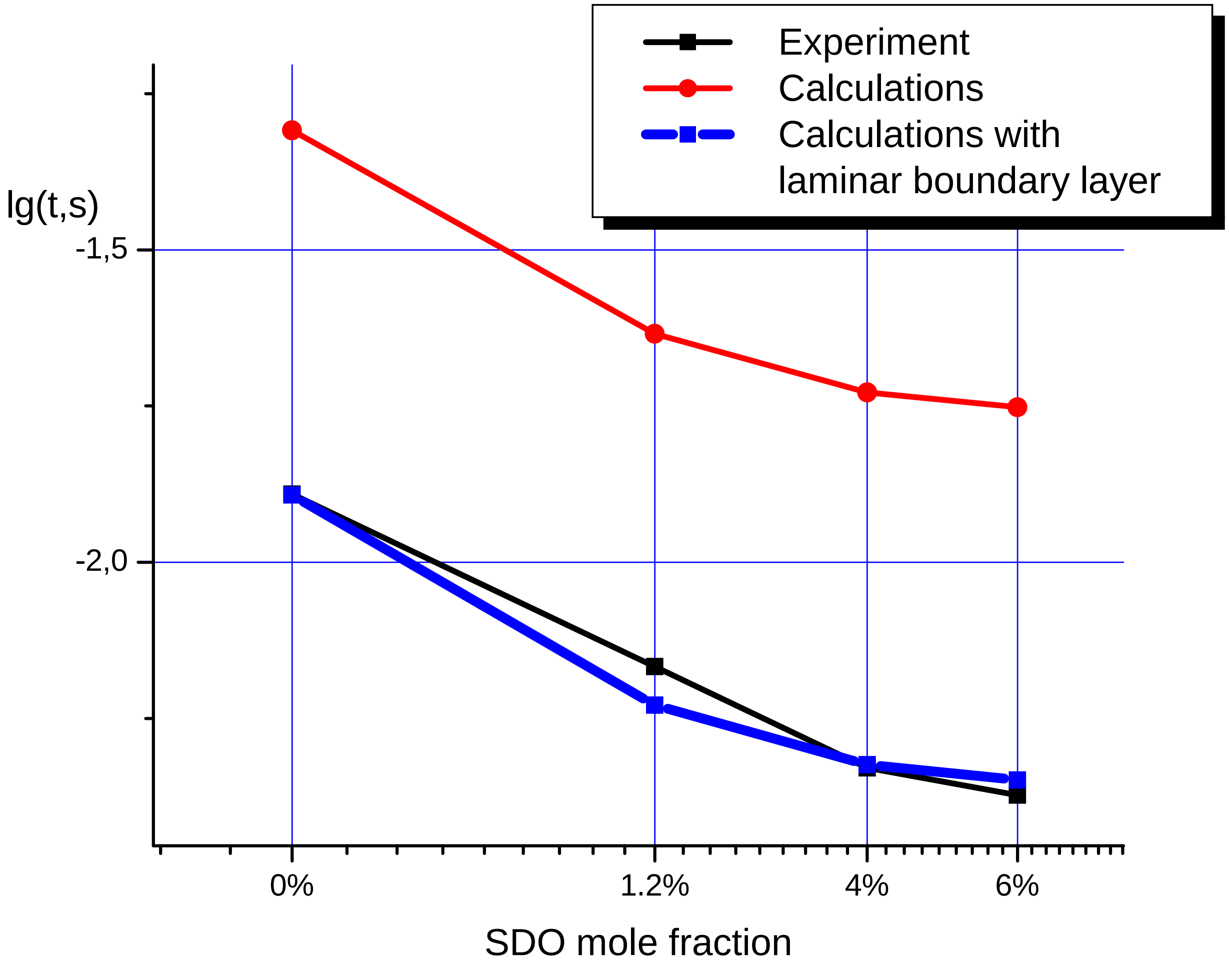
Delivering sufficient amount of SDO

Minimizing the effect of O atom

Lower the inlet temperature

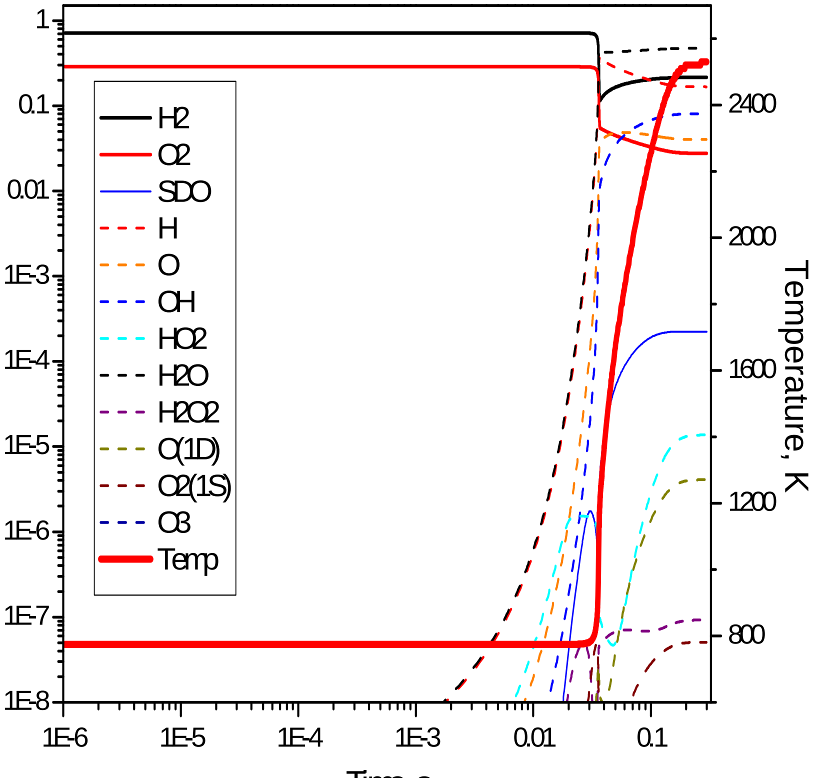
V V Smirnov, O M Stelmakh, V I Fabelinsky, D N Kozlov, A M Starik and N S Titova,
***J. Phys. D: Appl. Phys*. 41 (2008)**

SDO kinetic analysis



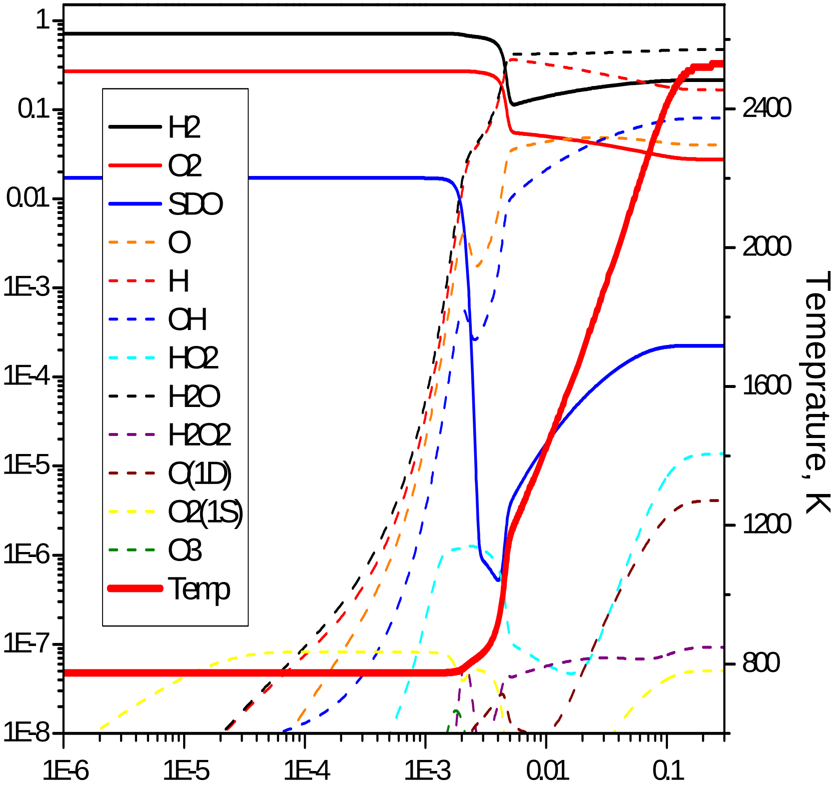
The ignition time as a function of SDO mole fraction in oxygen. T=775 K and P=10 Torr in the H_2:O_2=5:2 mixture

SDO kinetic analysis



Auto-ignition

6% SDO



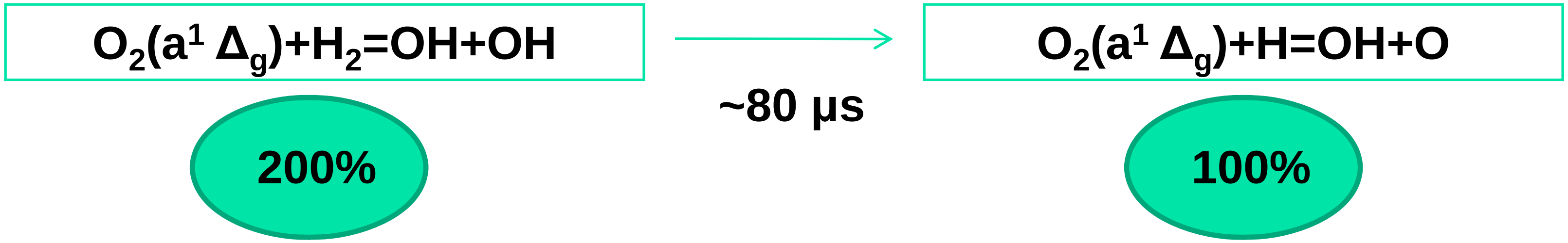
The evolution in time of the mole fractions of the main component for autoignition (a) and ignition with 6% singlet delta oxygen. The gas temperature evolution is represented by the thick red line.

SDO kinetic analysis

Possible reasons

Auto	SDO
$O_2+M=O+O+M$ (slow) $H_2+O=OH+H$ $O_2+H=OH+O$ $OH+OH=H_2O+O$ … …	$O_2(a^1\Delta_g)+H_2=OH+OH$ (fast) $OH+H_2=H_2O+H$ $O_2(a^1\Delta_g)+H=OH+O$ $O_2+H=OH+O$ $OH+OH=H_2O+O$ …

Radical generation efficiency



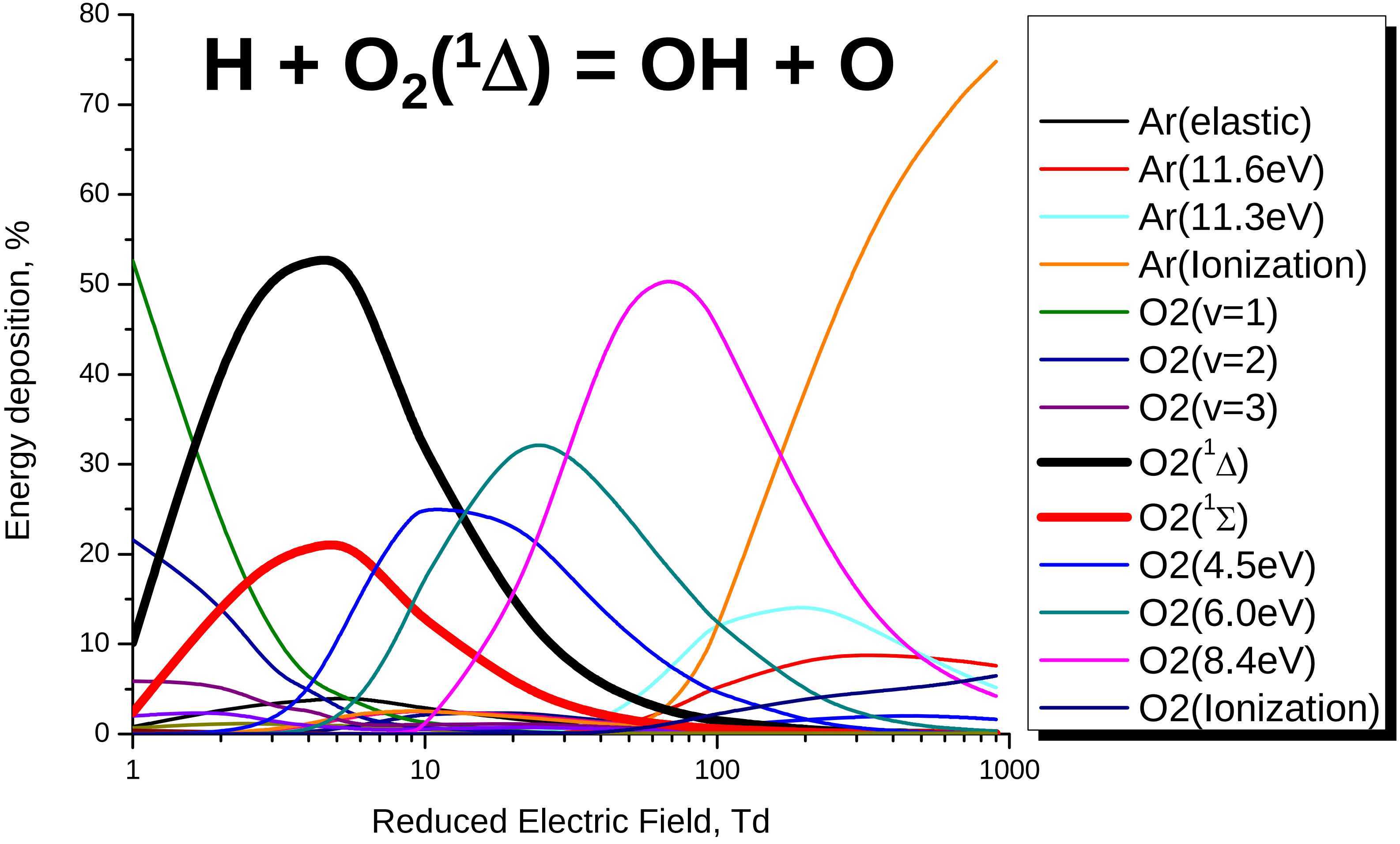
$O_2(a^1\Delta_g)+H_2=OH+OH$ $\longrightarrow$ **$O_2(a^1\Delta_g)+H=OH+O$**

~80 μs

200%

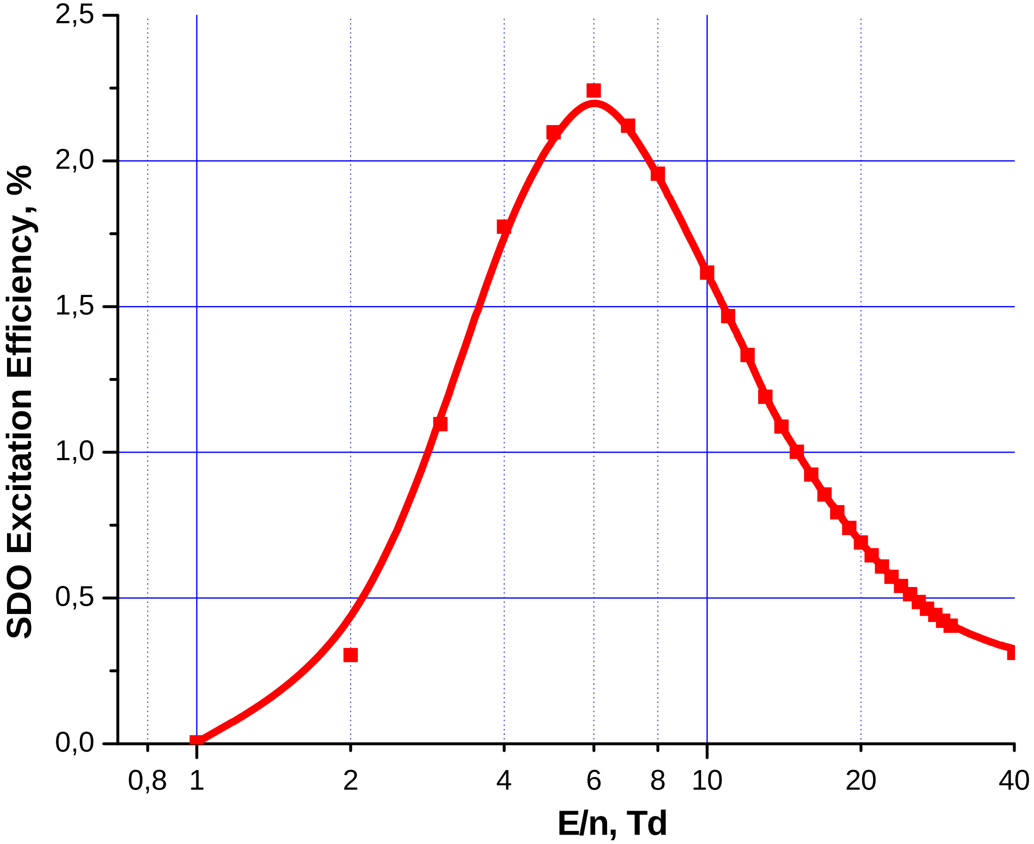
100%

Energy Distribution in O_2-Ar (15%:85%) Mixture



- **74% energy in excitation of singlet oxygen at E/n= 5 Td**
  - **Approximately 53% in singlet delta state**
  - **About 21% in singlet sigma state**

SDO Excitation efficiency in air plasma



Air Plasma

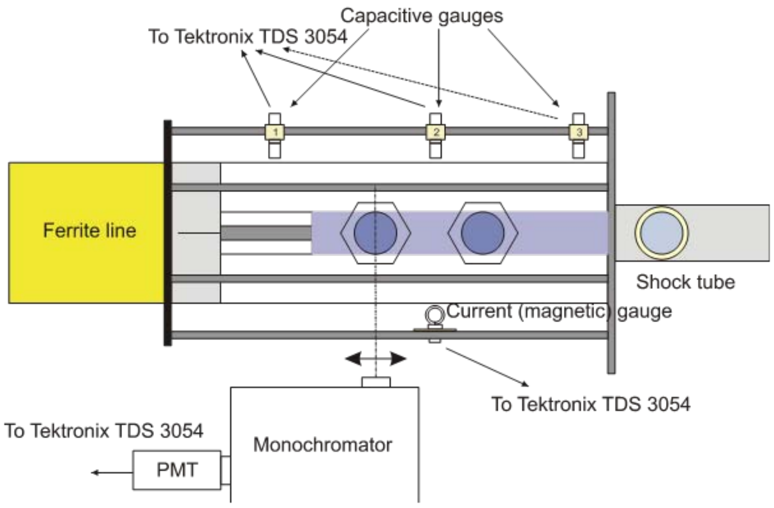
E/n = 6 Td (=10^{-17} Vcm^2)

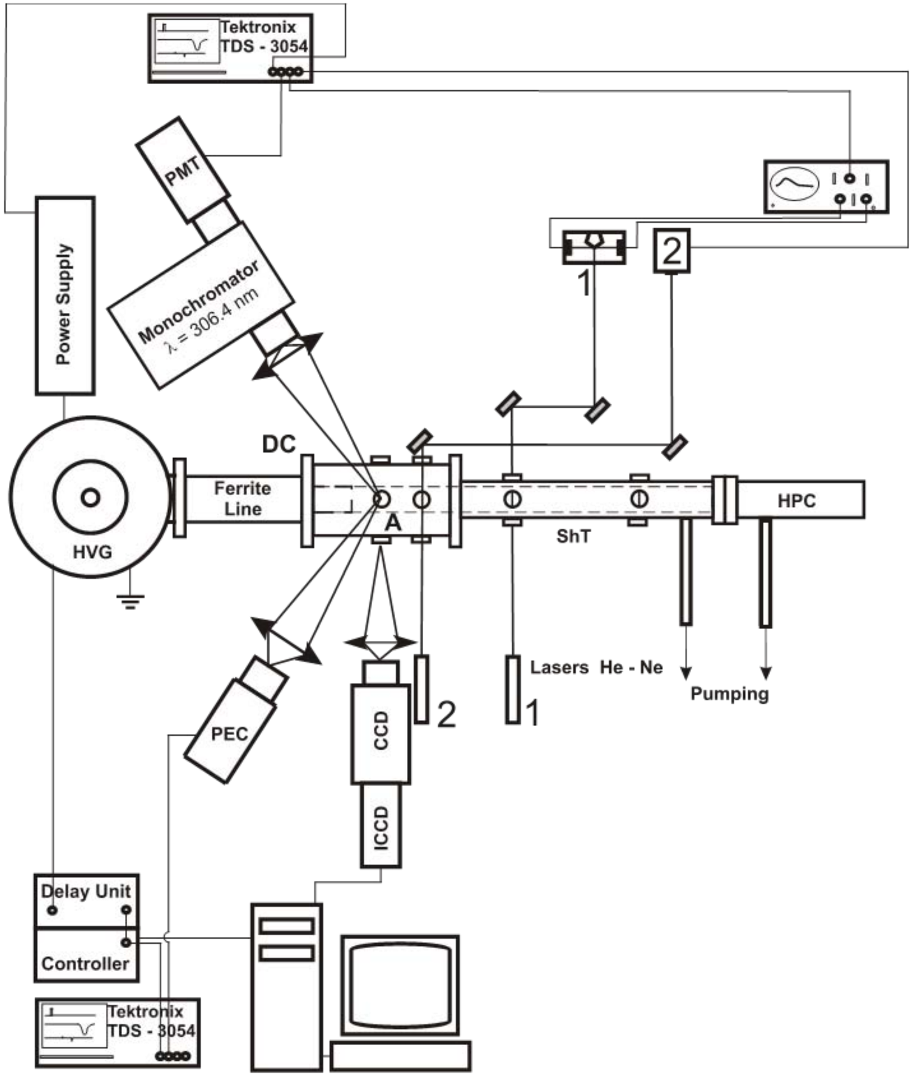
N2 Elastique	1.8 %
N2(ROT)	4 %
N2 (V=1)	49 %
N2 (V=2)	7.3 %
N2 (V=3)	1.4 %
N2 (V=4)	0.2 %
O2 Elastique	0.3 %
O2 (ROT)	0.2 %
O2 (V=1)	17 %
O2 (V=2)	11 %
O2 (V=3)	4.1 %
O2 (V=4)	1.4 %
O2 (a$^1\Delta_g$)	2.2 %
O2 (b$^1\Sigma$)	0.1%

Shock Tube with Discharge Section.
$U \leq 0.3$ MV, $M \leq 3$

Starikovskaya et al

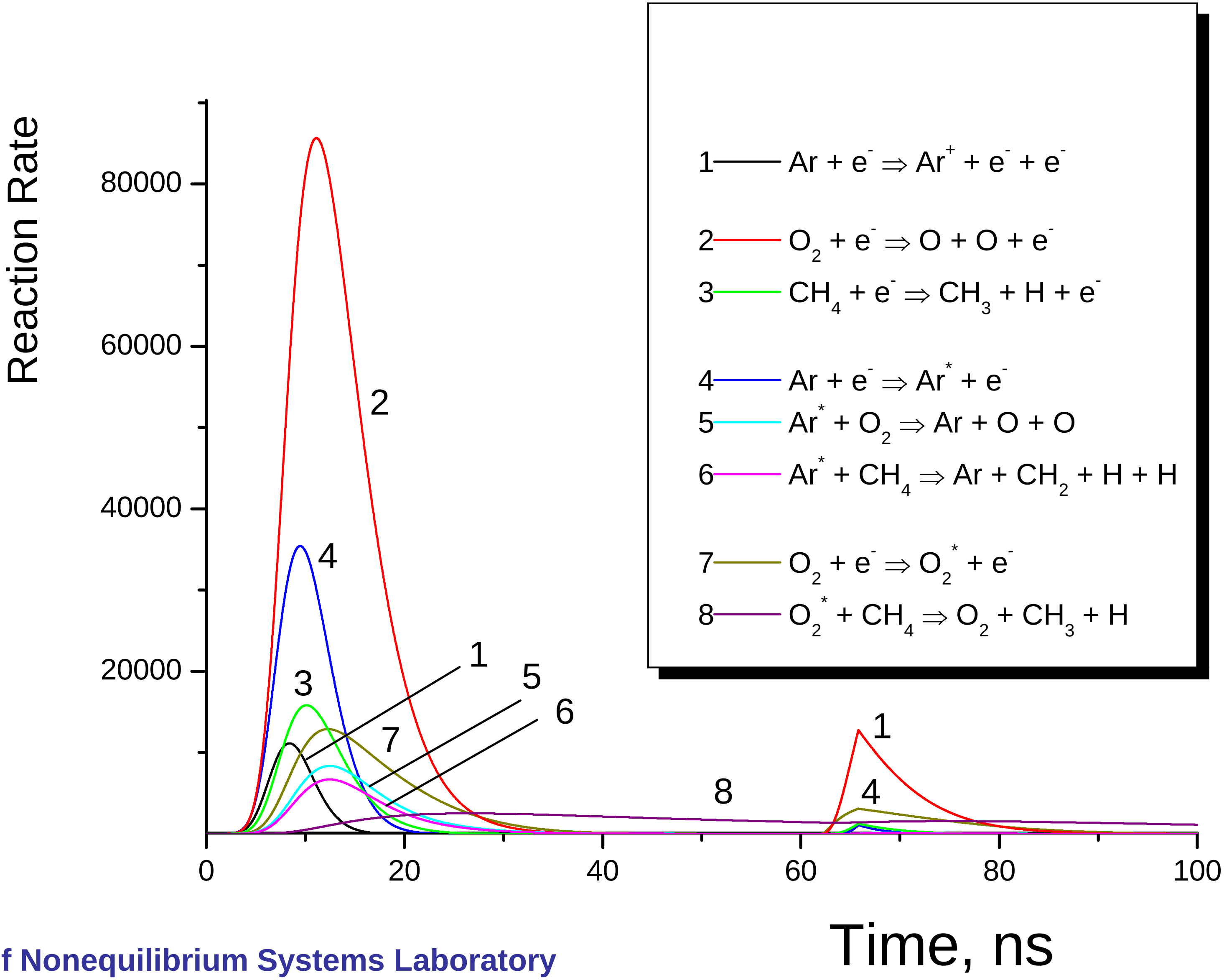
Test Section of the Shock Tube



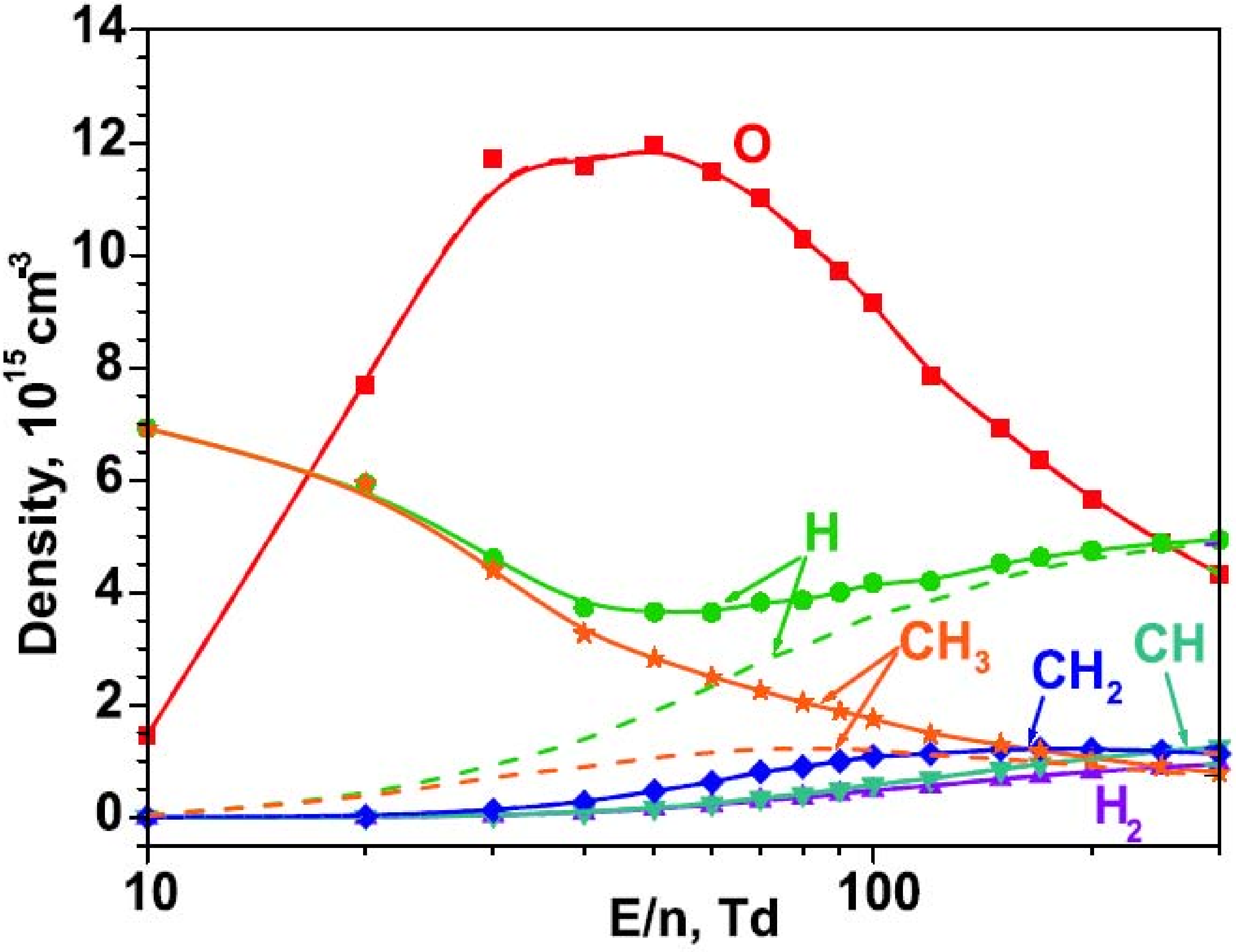


Physics of Nonequilibrium Systems Laboratory

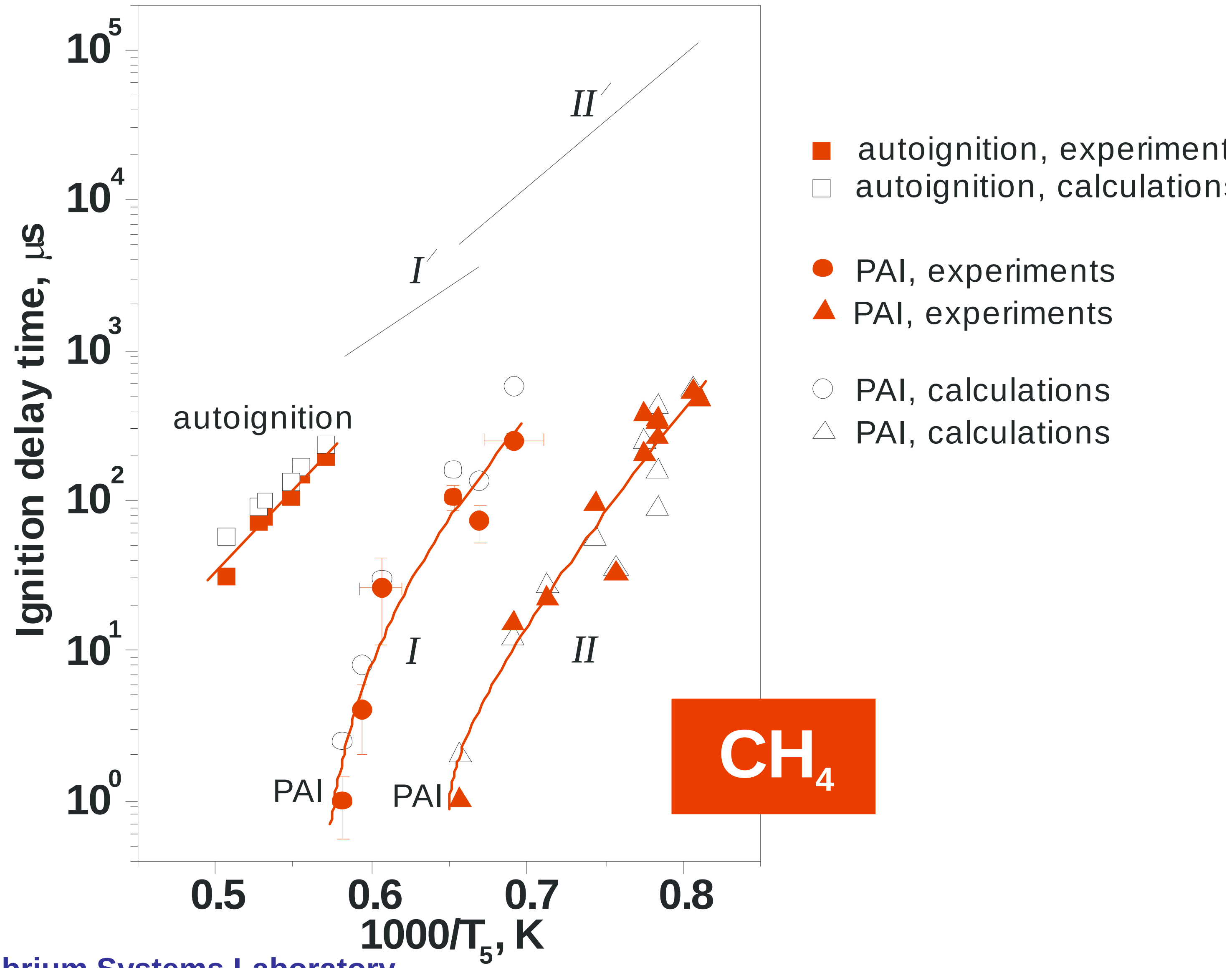
Main Processes During Discharge Phase



Radicals Production in Discharge CH_4-containing mixture

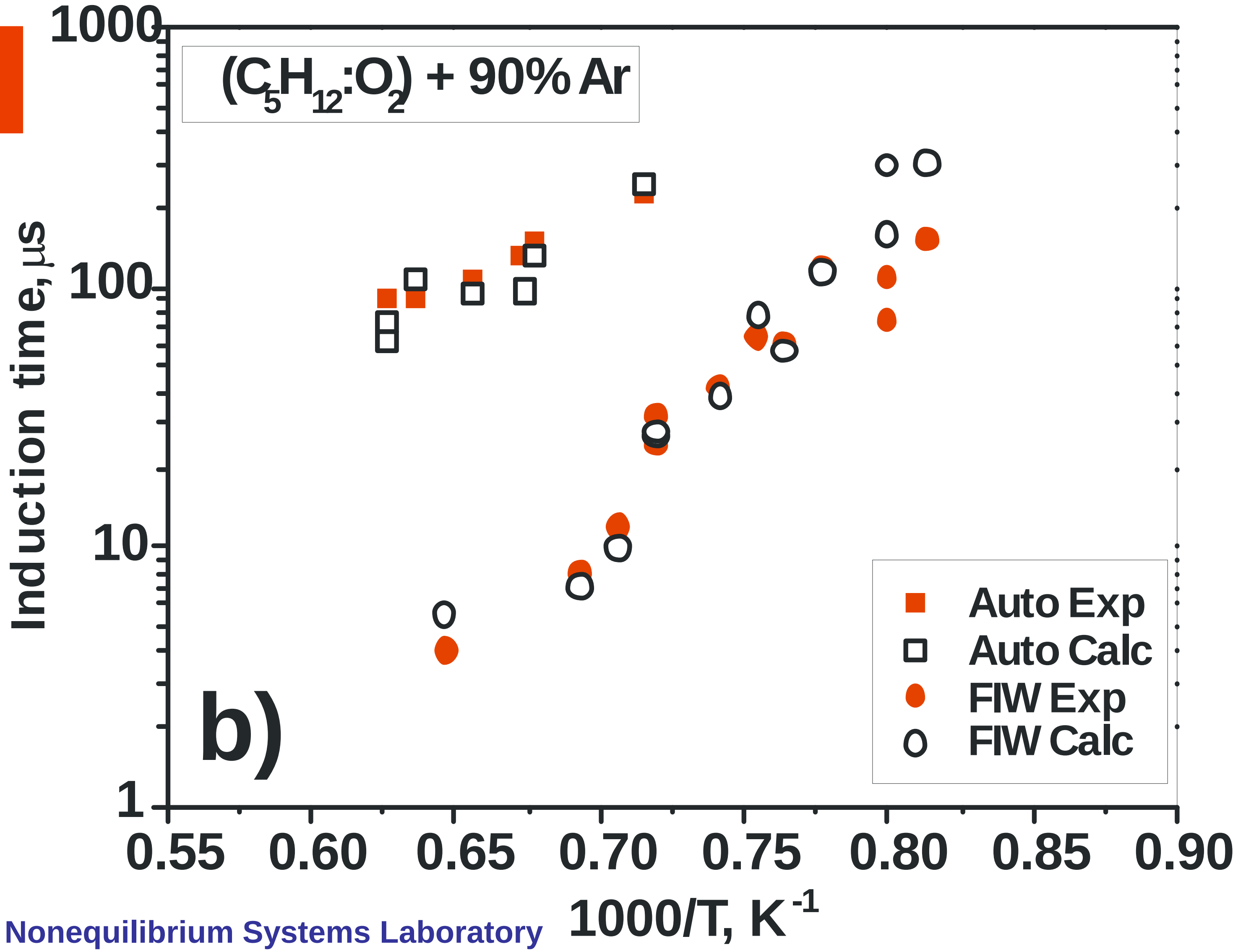


Ignition Delay Time: Methane-Containing Mixture

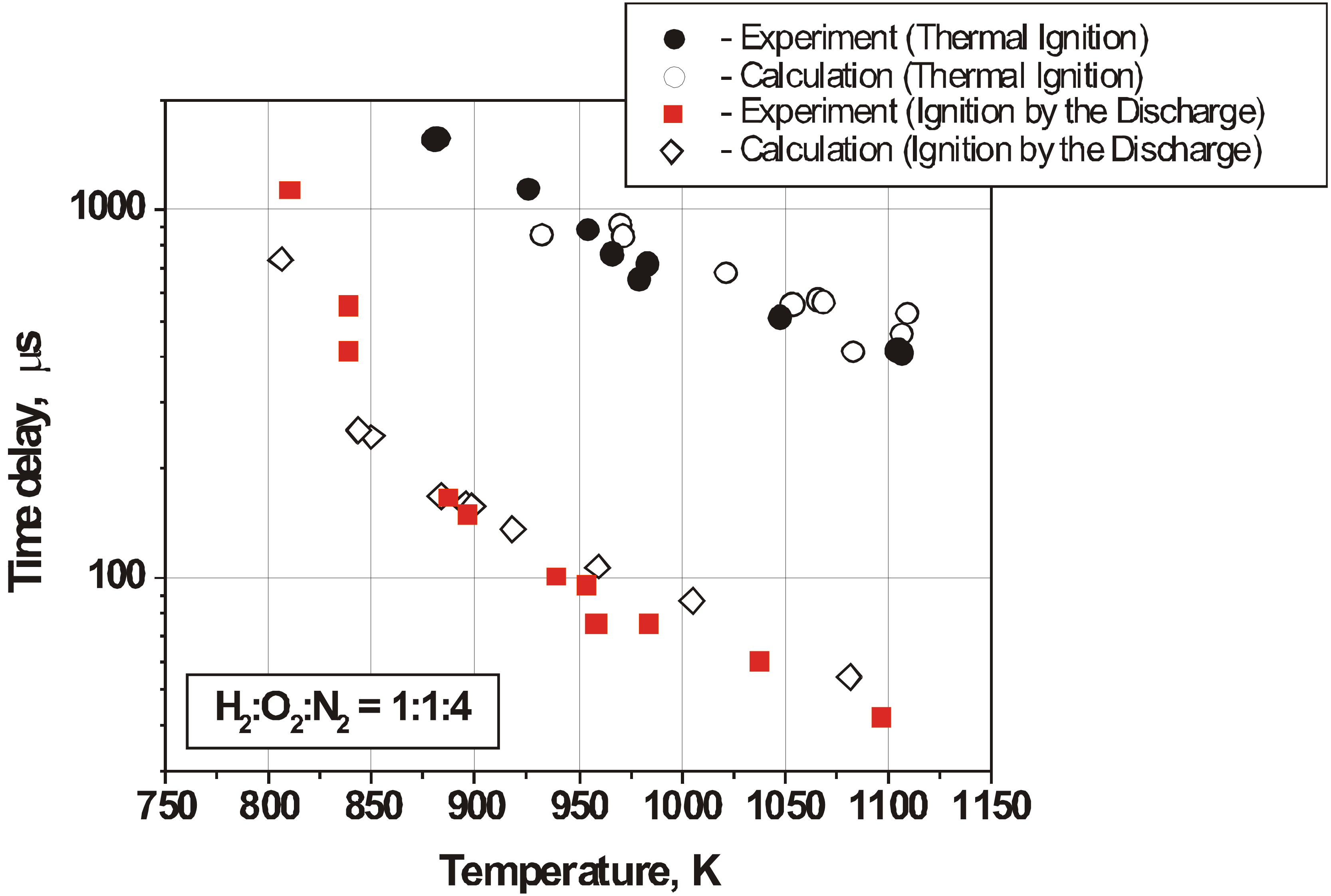


RAMEC (for C1) + Westbrook (C2-C7) + High Pressure Adjustment

C_5H_{12}

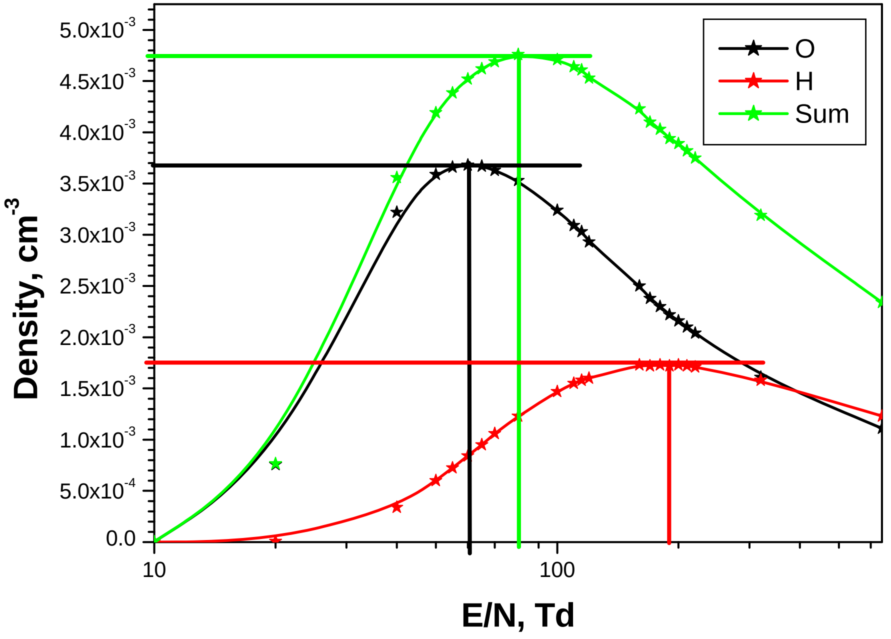


Experiment and Calculations in H_2-Air Mixture

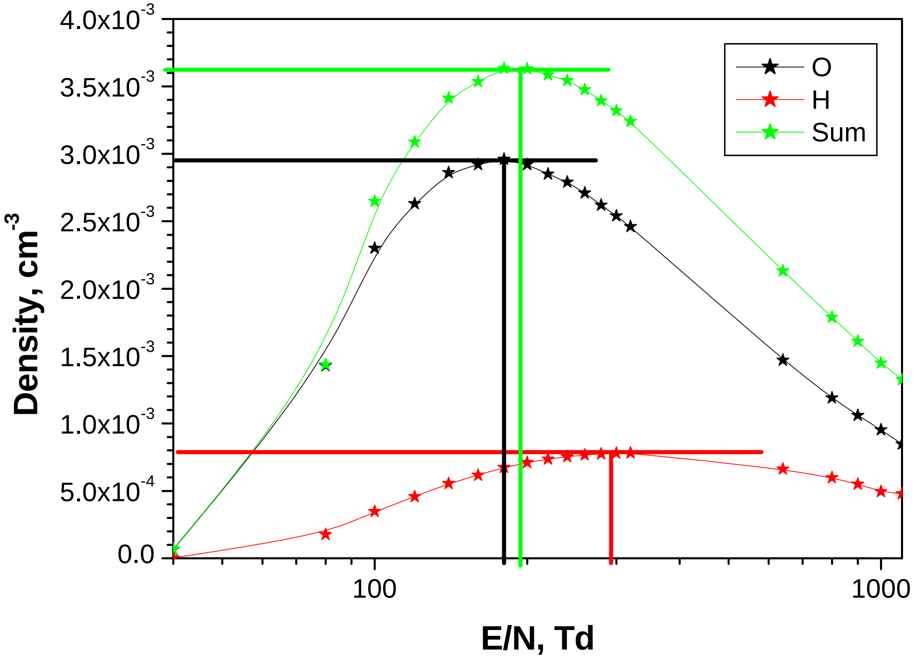


Modeling of Radicals Formation vs E/n (W=14 mJ/cm^3)

H2:O2:Ar=29.5:14.75:55.75

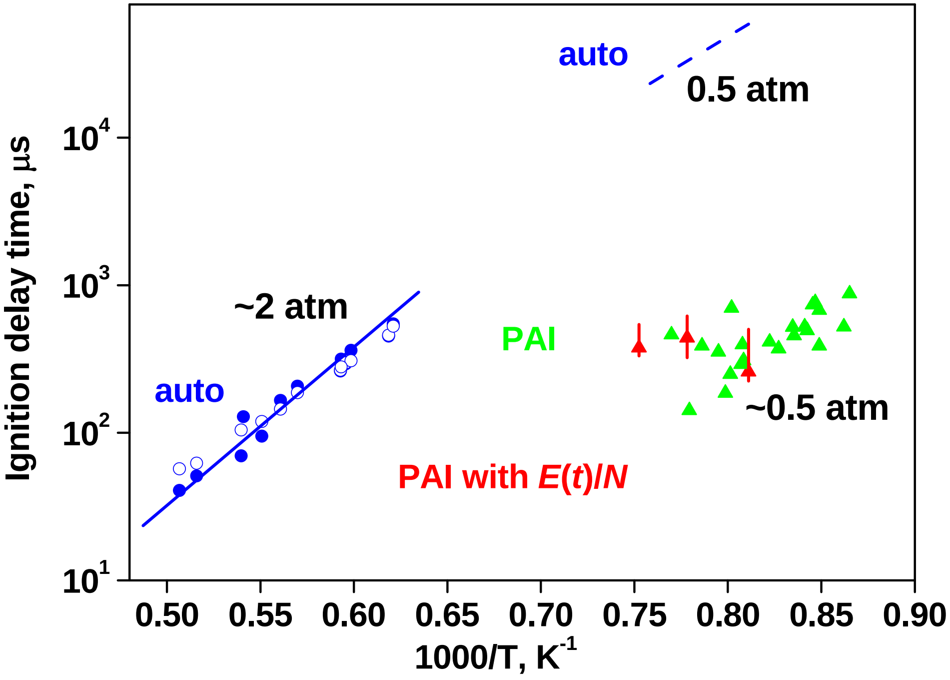


H2:O2:N2=29.5:14.75:55.75

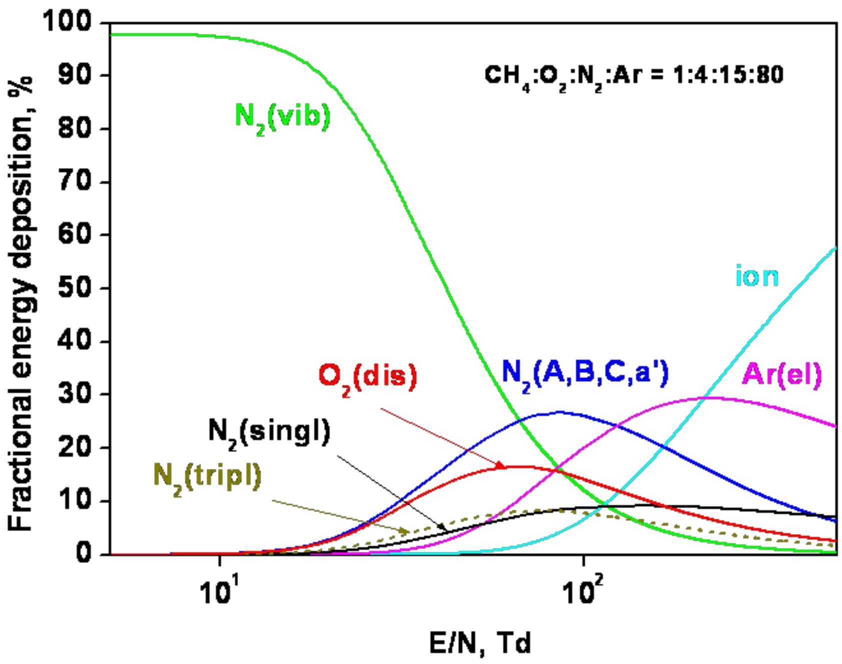


Delay time for autoignition and plasma assisted ignition in CH_4-containing mixture

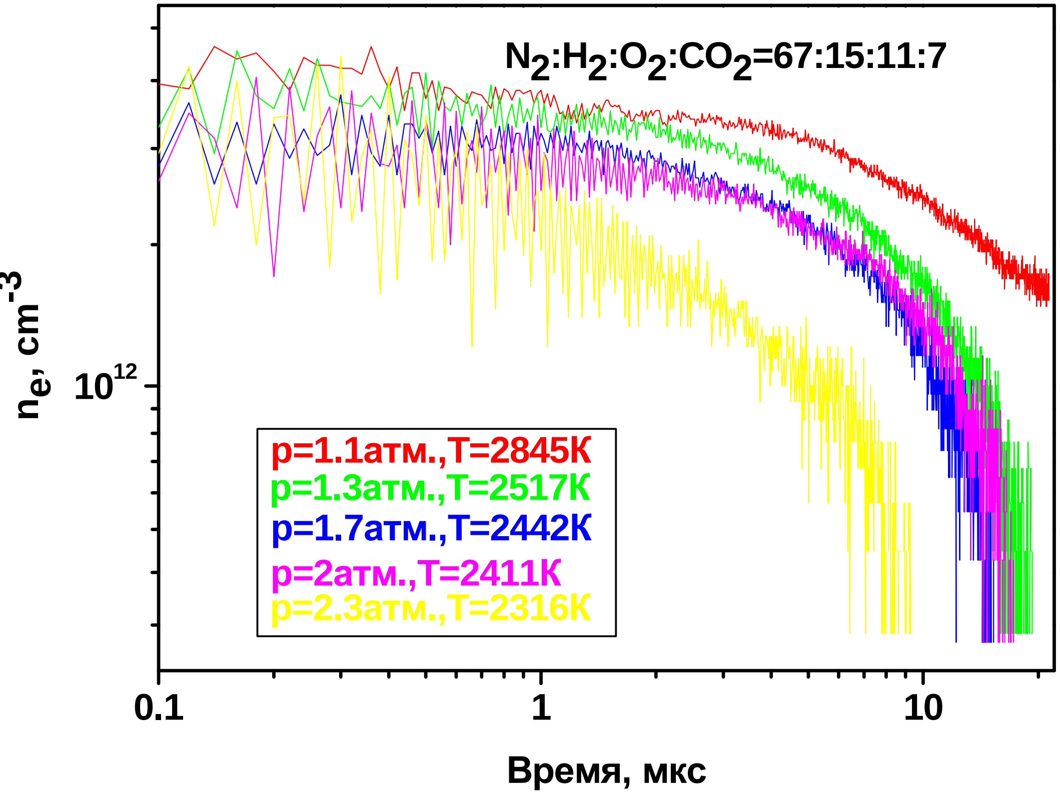
Aleksandrov et al. (2009)

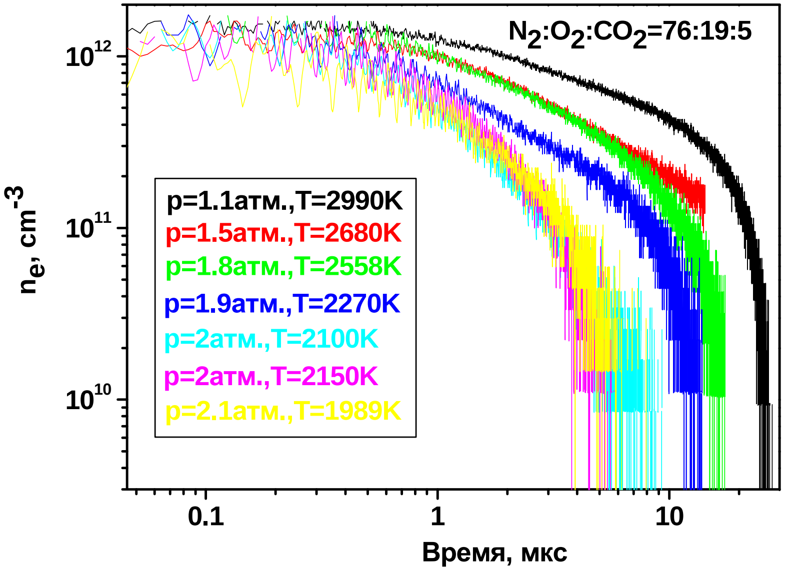


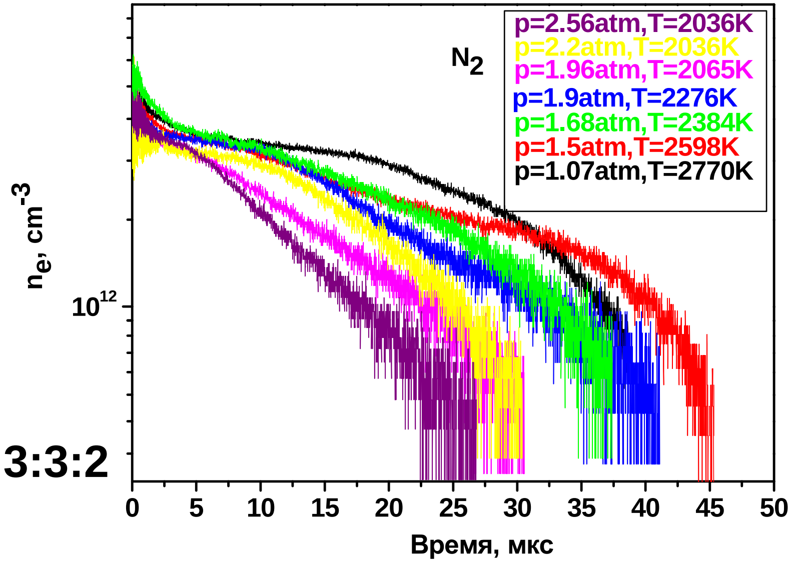
$CH_4:O_2:N_2:Ar$ = 1:4:15:80



Plasma Recombination at High Pressures and Temperatures







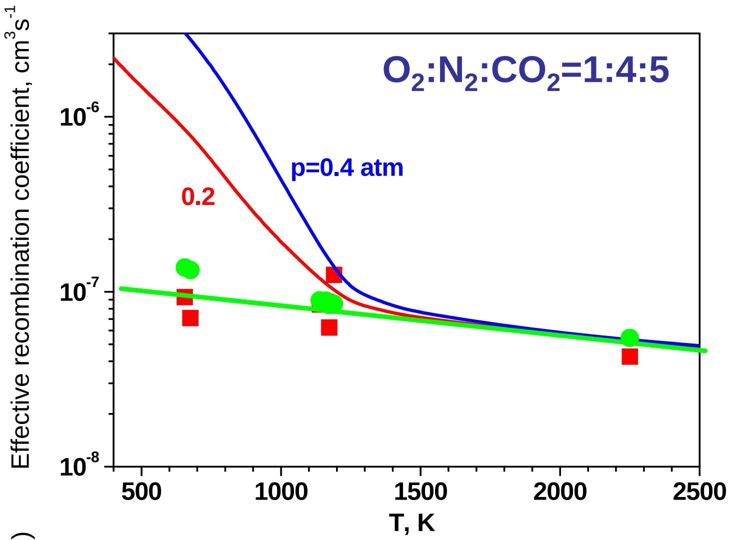
N2:H2:O2:CO2=67:15:11:7

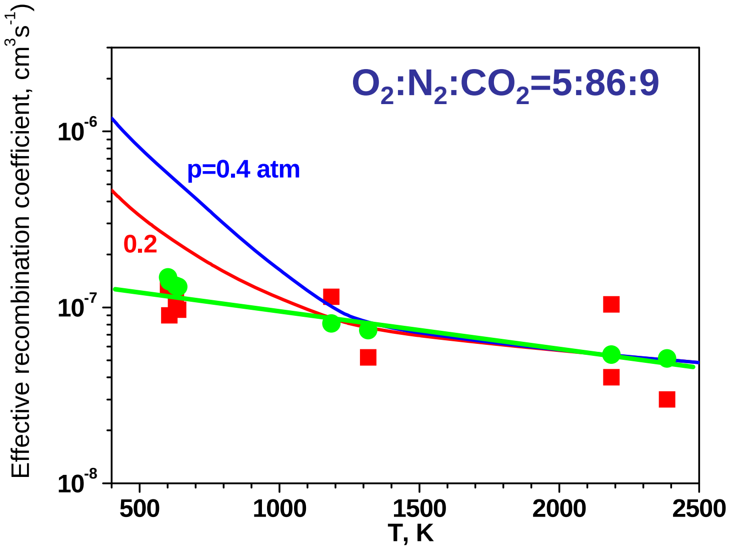
↓

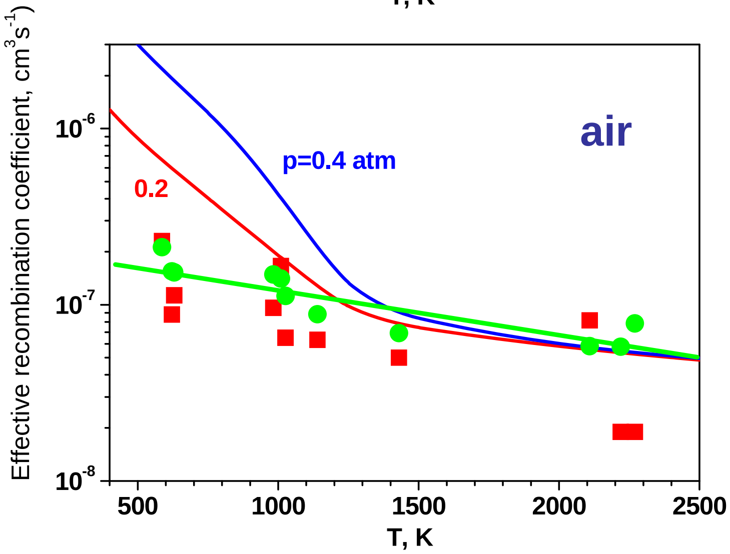
After 10 μs, at 1atm., 2800К

$N_2:H_2O:O_2:OH:CO:CO_2:H:O:H_2=67:10:5:4:3.5:3:3:3:2$

Evolution in Time of Electron Density During Plasma Decay







Dissociative electron-ion recombination

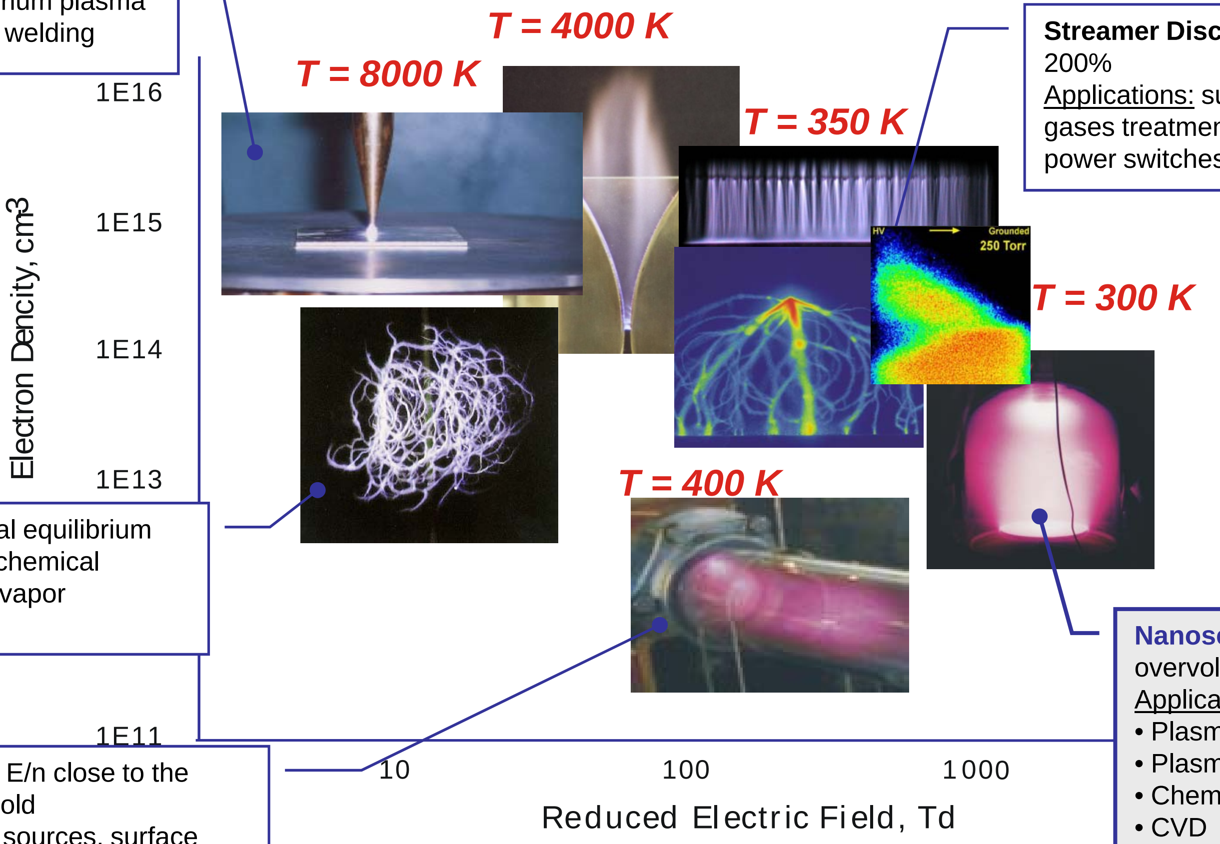
$$e + O_2^+ \rightarrow O + O$$

Electron attachment and detachment

$$e + O_2 + M \rightarrow O_2^- + M$$

$$O_2^- + O \rightarrow e + O_3$$

Types of Gas Discharges and Their Applications



Arc Discharge: equilibrium plasma
Applications: melting & welding

Streamer Discharge: overvoltage up to 200%
Applications: surface treatment, flue gases treatment, electrical breakdown, power switches

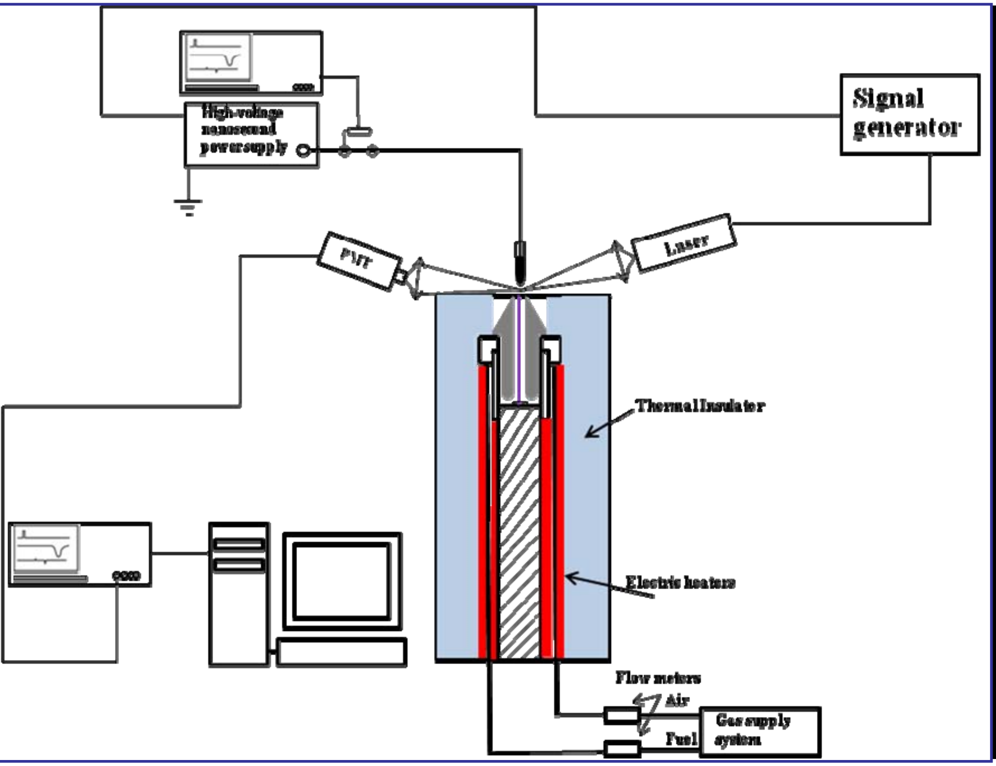
MW Discharge: partial equilibrium
Applications: plasma chemical conversion, chemical vapor deposition (CVD)

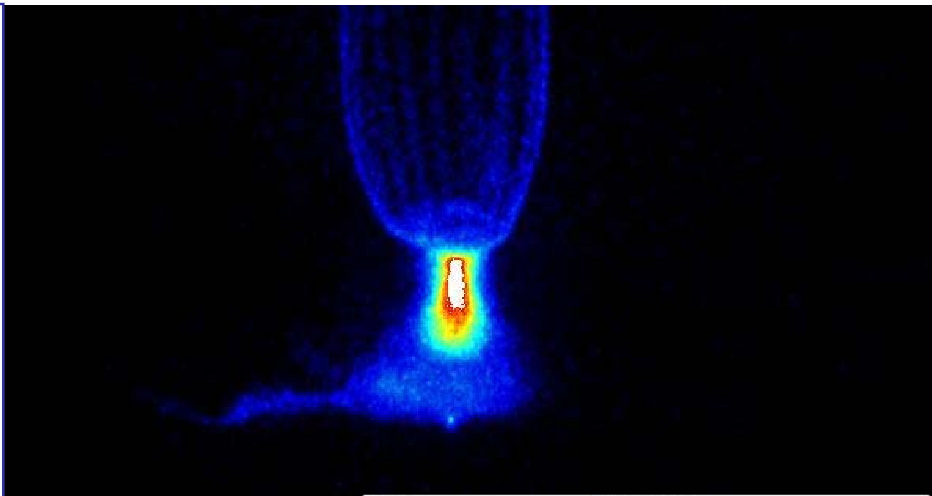
Nanosecond Pulsed Discharge: overvoltage up to 10 times
Applications:
- Plasma supported combustion
- Plasma supported aerodynamics
- Chemical conversion
- CVD

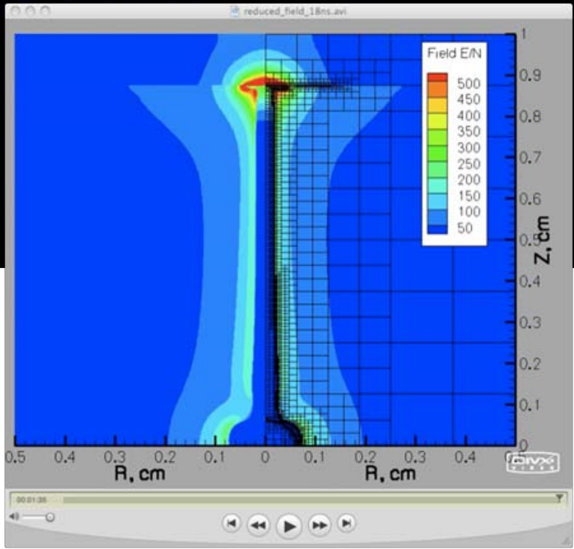
Glow Discharge: E/n close to the breakdown threshold
Applications: light sources, surface treatment, CVD

Discharge Development at Different Overvoltage and Plasma Generation

Setup for OH Dynamic Measurements in Streamer Channel Afterglow



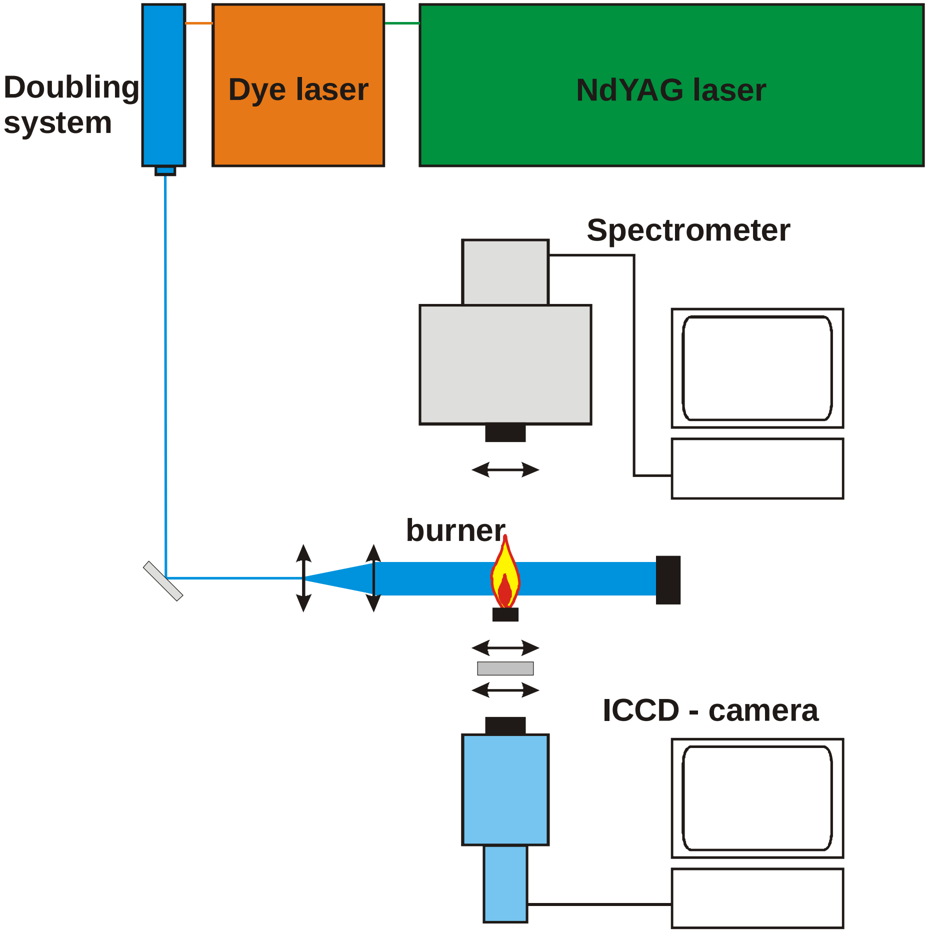




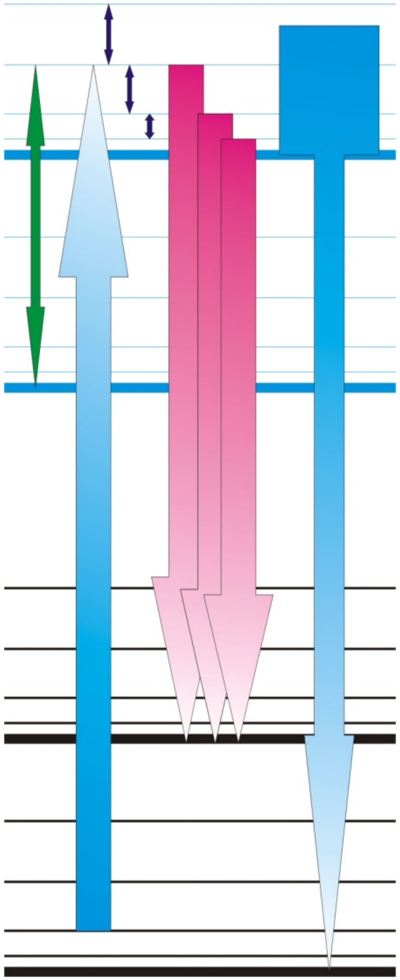
Pancheshnyi et al

LIF Diagnostics Setup: OH Profile Control

LIF OH



LIF OH



OH (X-A):

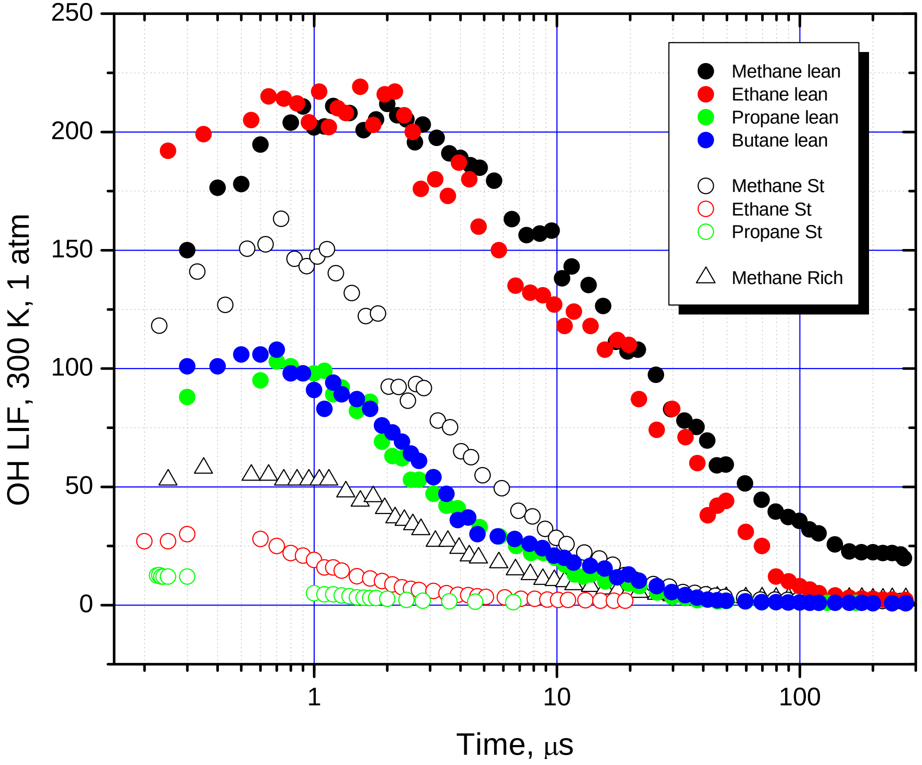
Excitation: $Q_1(6)$ 282.92 nm;

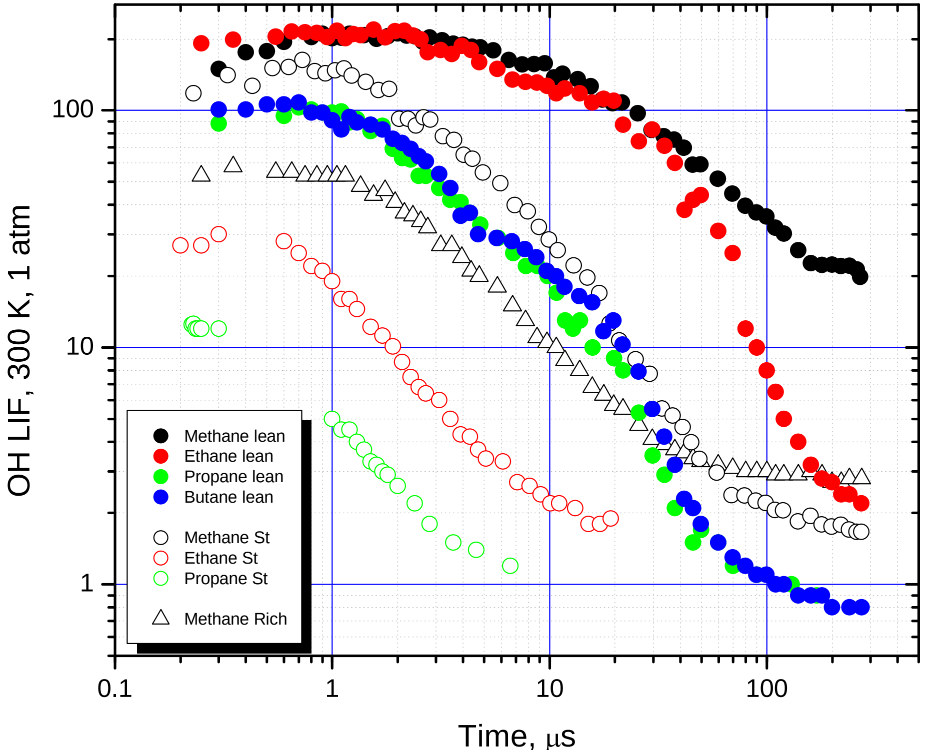
Emission:

315nm, $\delta\lambda$=1.8 нм;

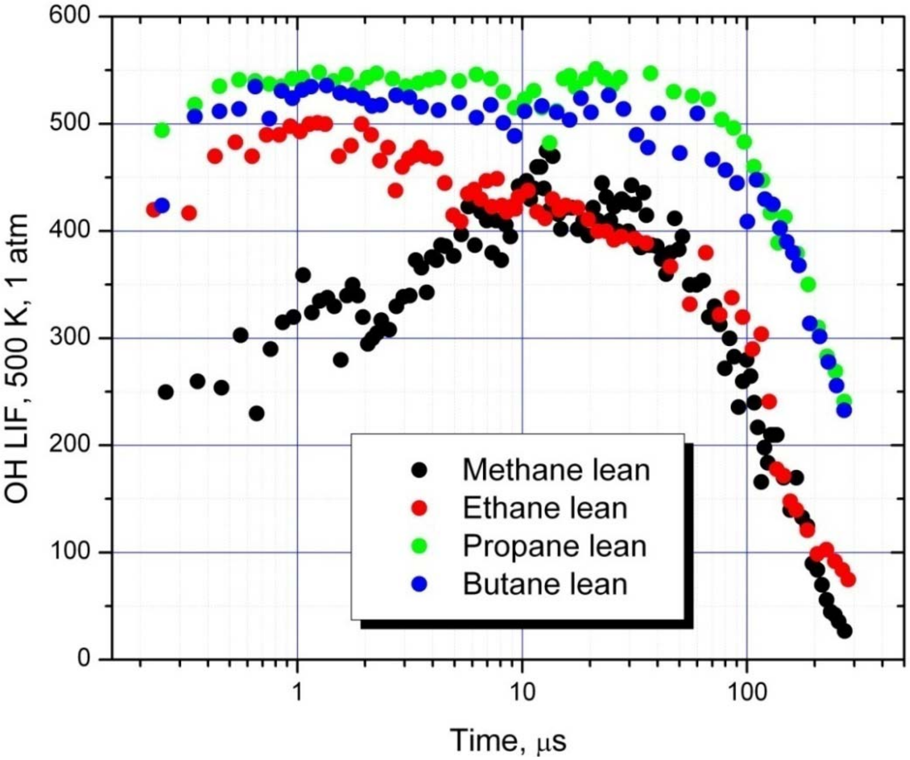
Registration – PicoStar LaVision ICCD камера

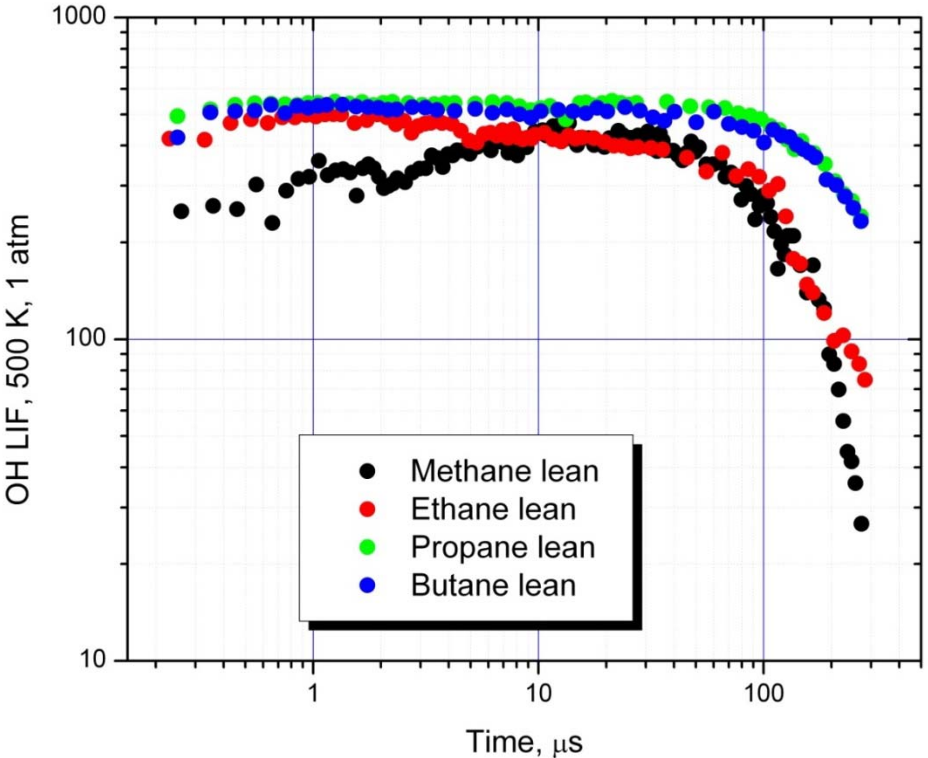
LIF Emission of OH at 300 K





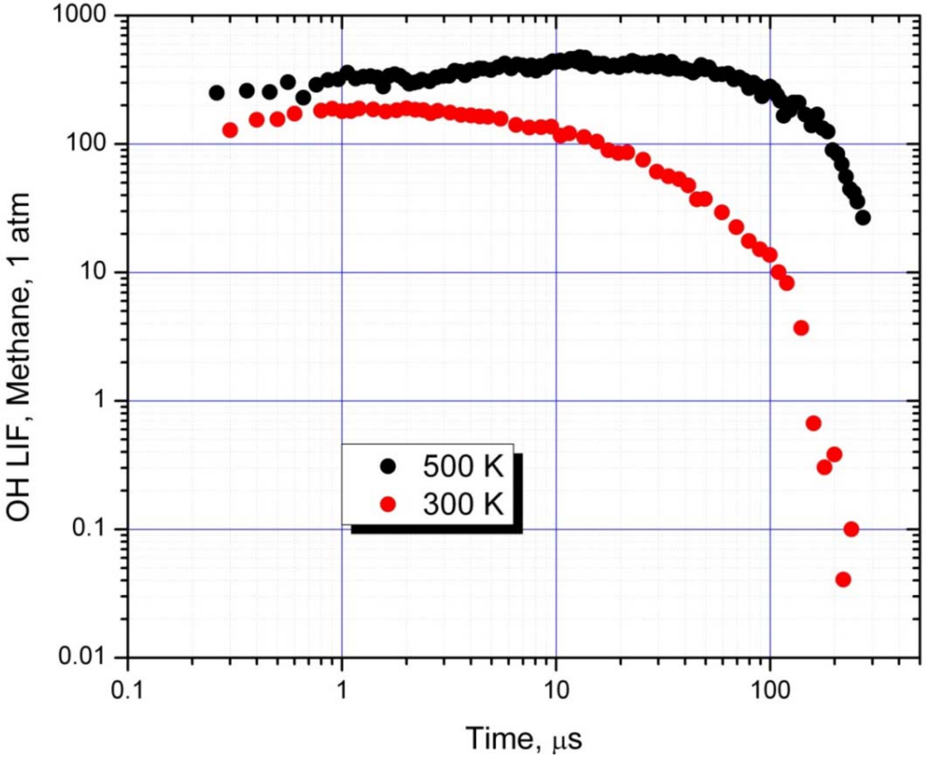
LIF Emission of OH at 500 K

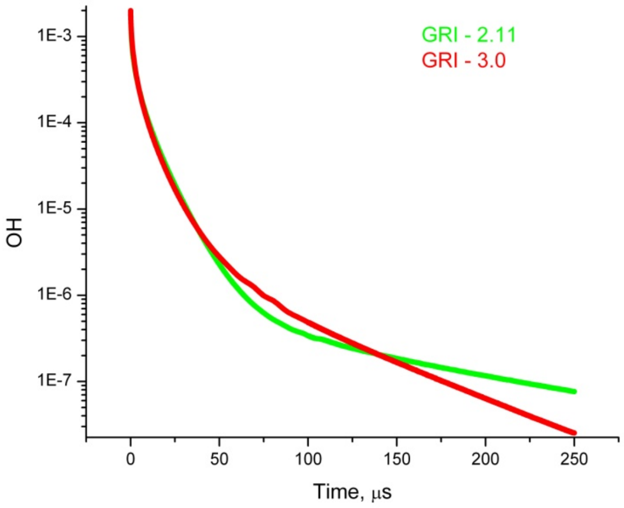




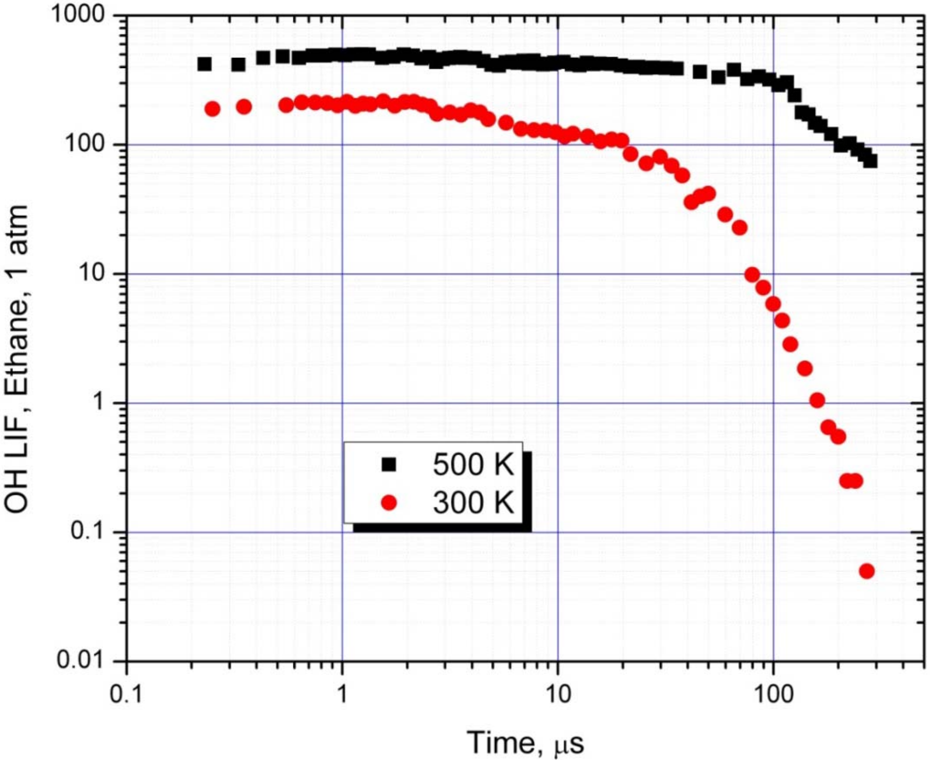
300 K Versus 500 K LIF of OH

Methane

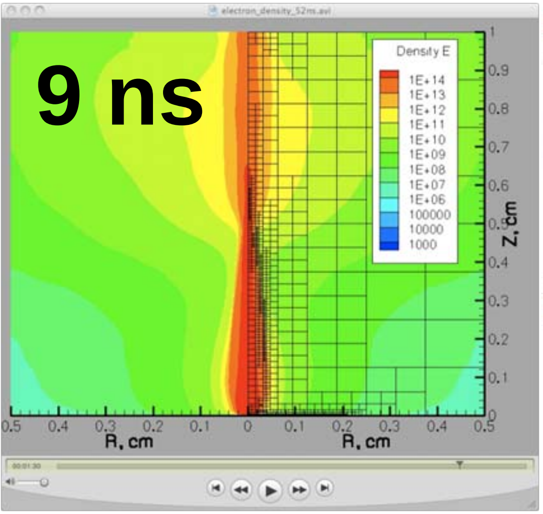


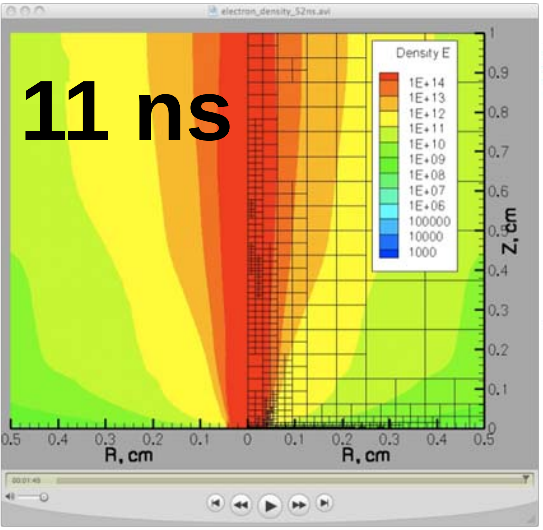


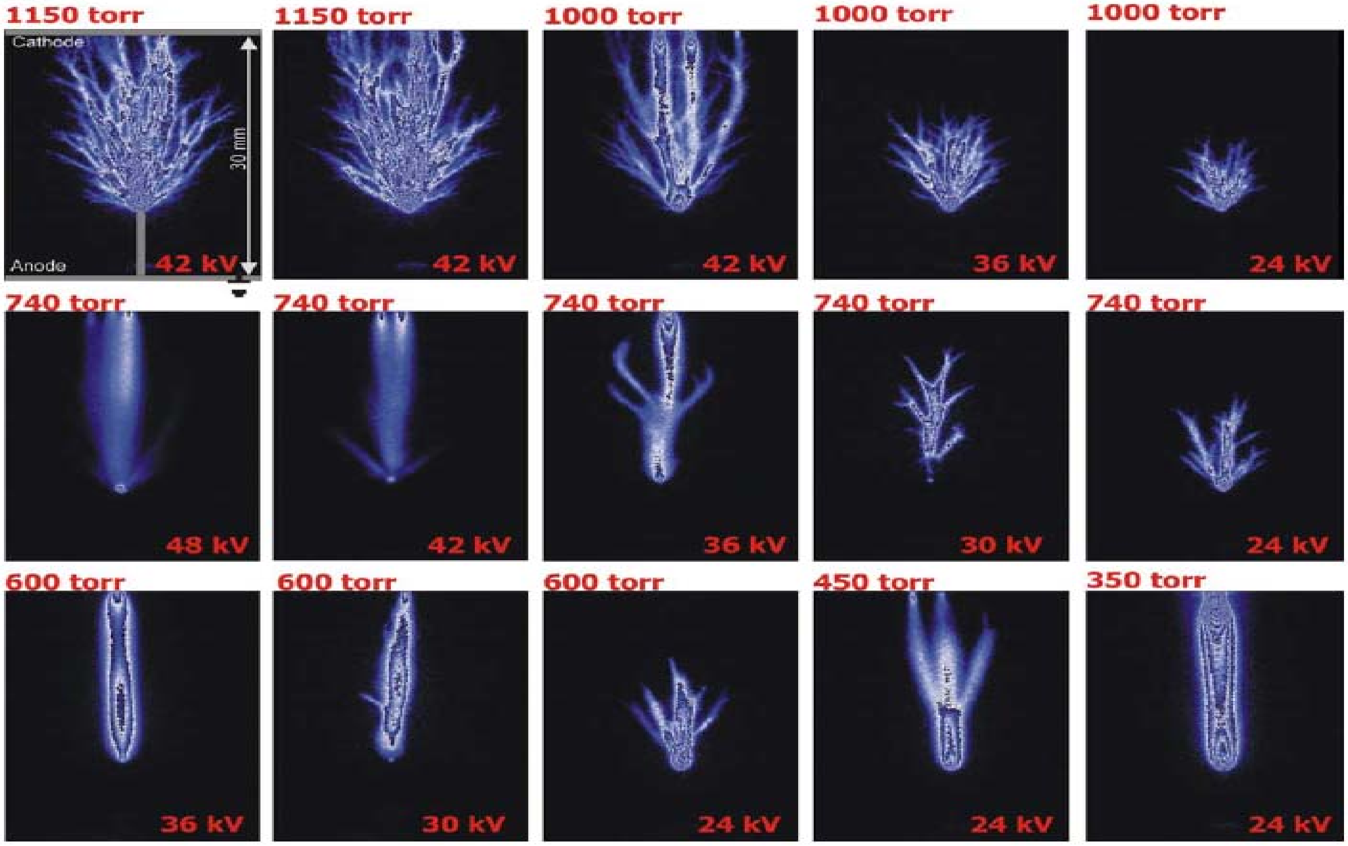
Ethane



High-pressure Conditions: Always Non-Uniform

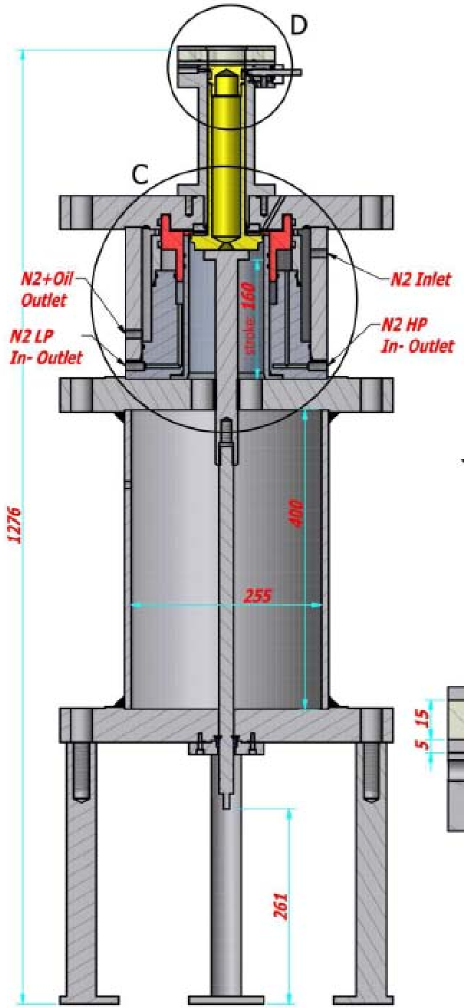


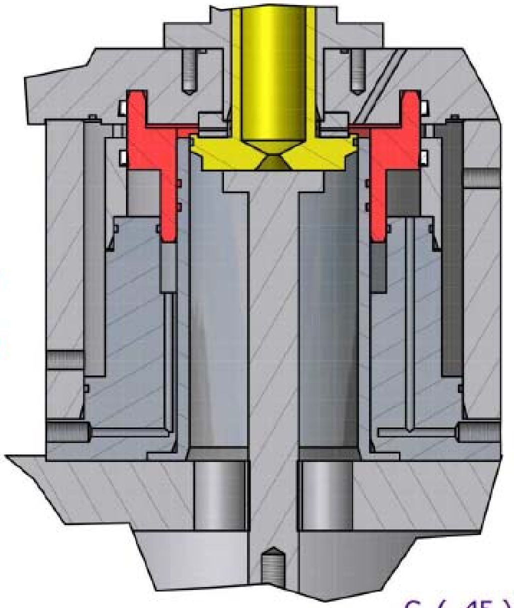




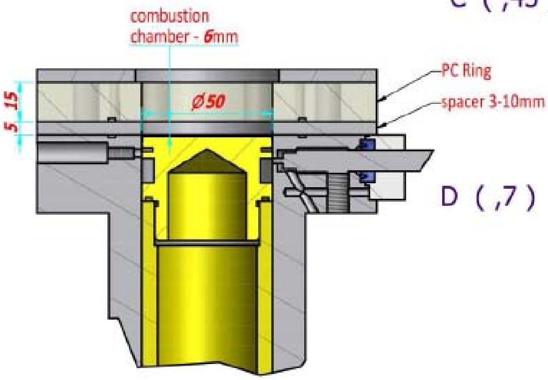
Pancheshnyi et al

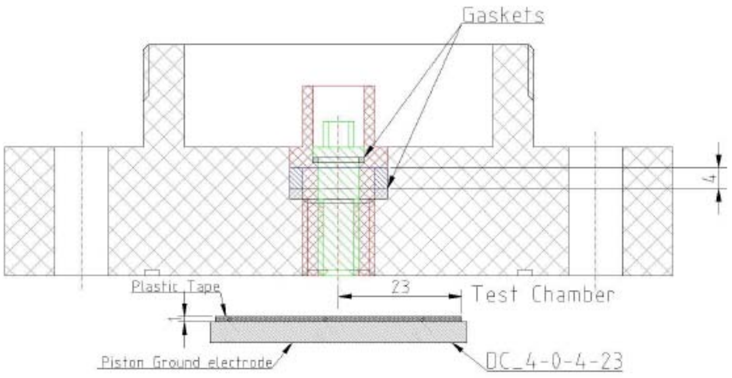
Rapid Compression Machine: High-Pressure, Low-Temperature

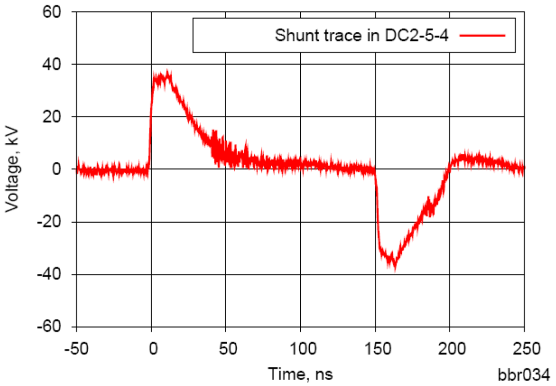


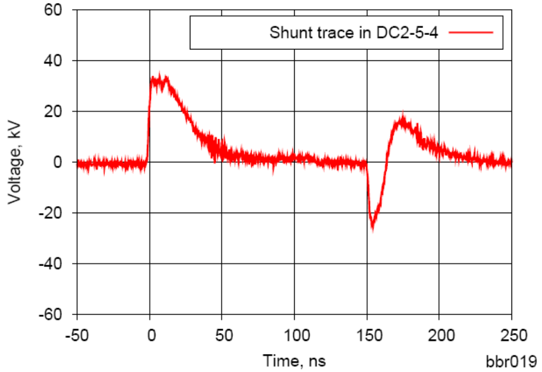


C (,45)

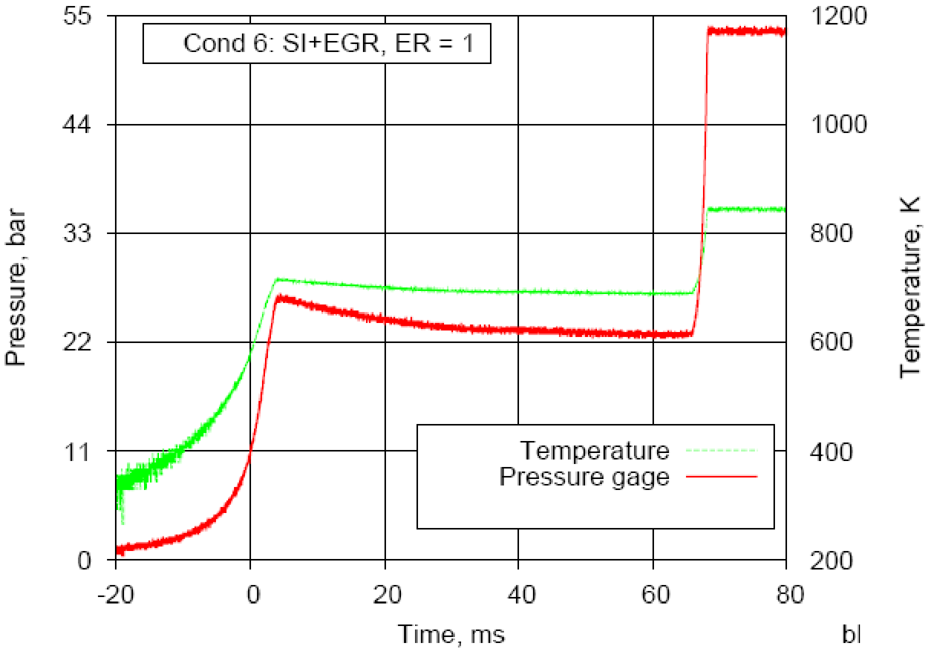






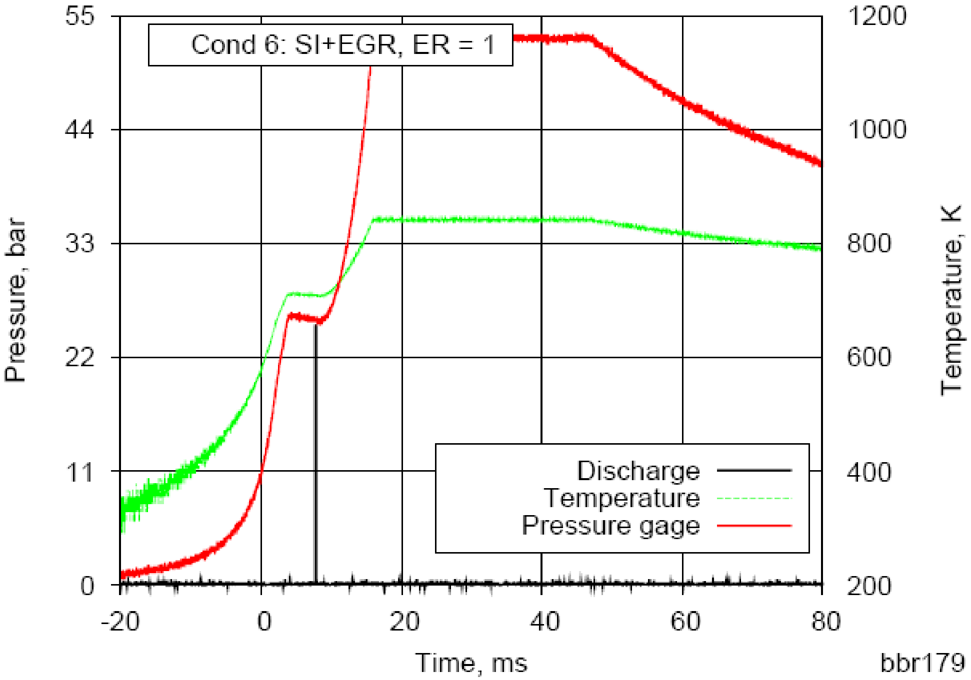


PAC at High Pressure: ER = 1 (Rakitin et al)



T2 = 713 K

P2 = 26.5 bar

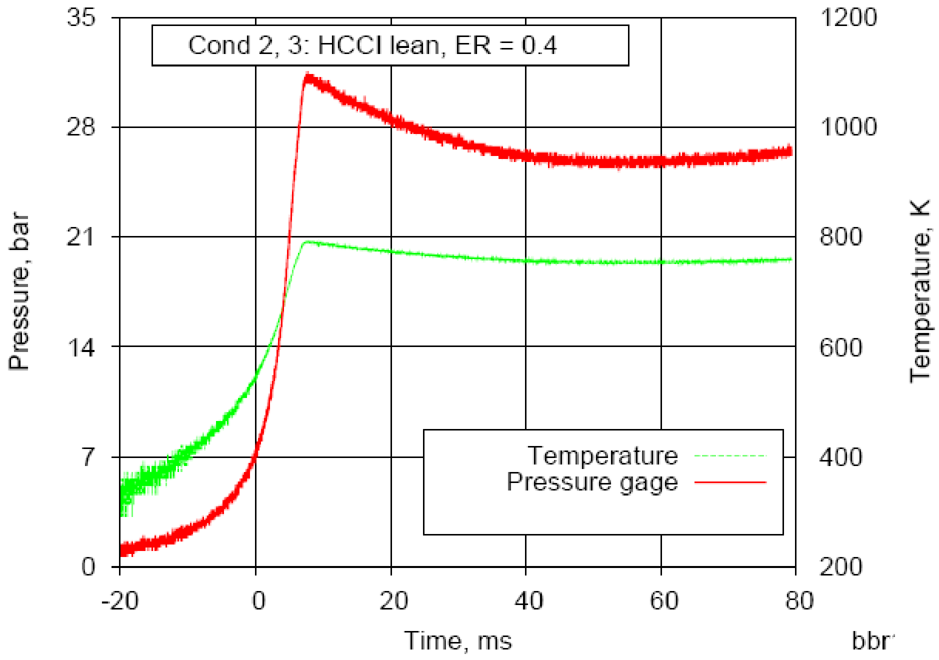


Propane,

Surface DBD,

< 50mJ

PAC at High Pressure: ER = 0.4 (Rakitin et al)



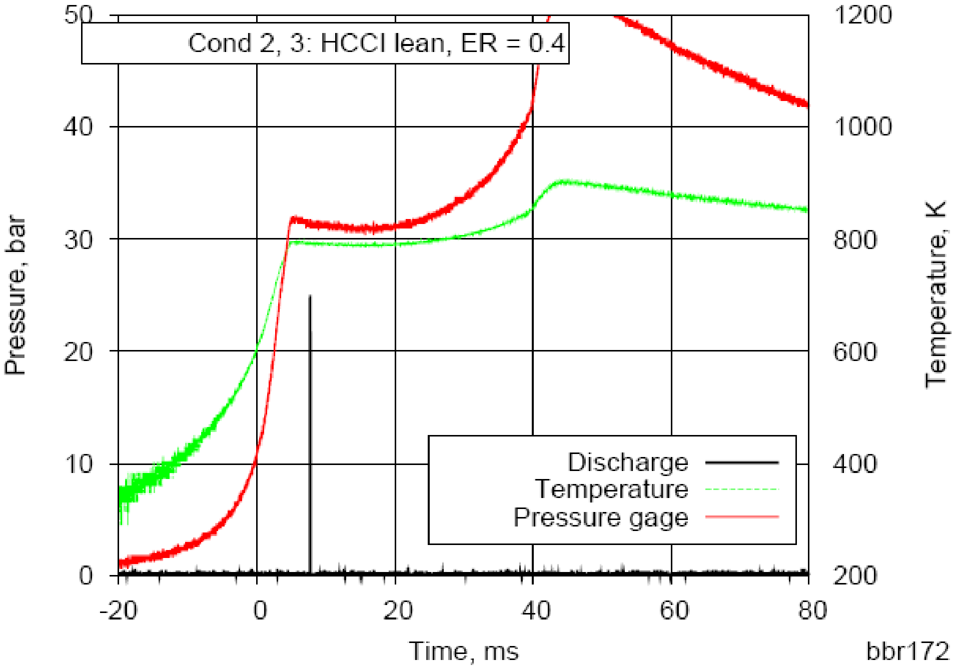
T2 = 794 K

P2 = 32 bar

Propane,

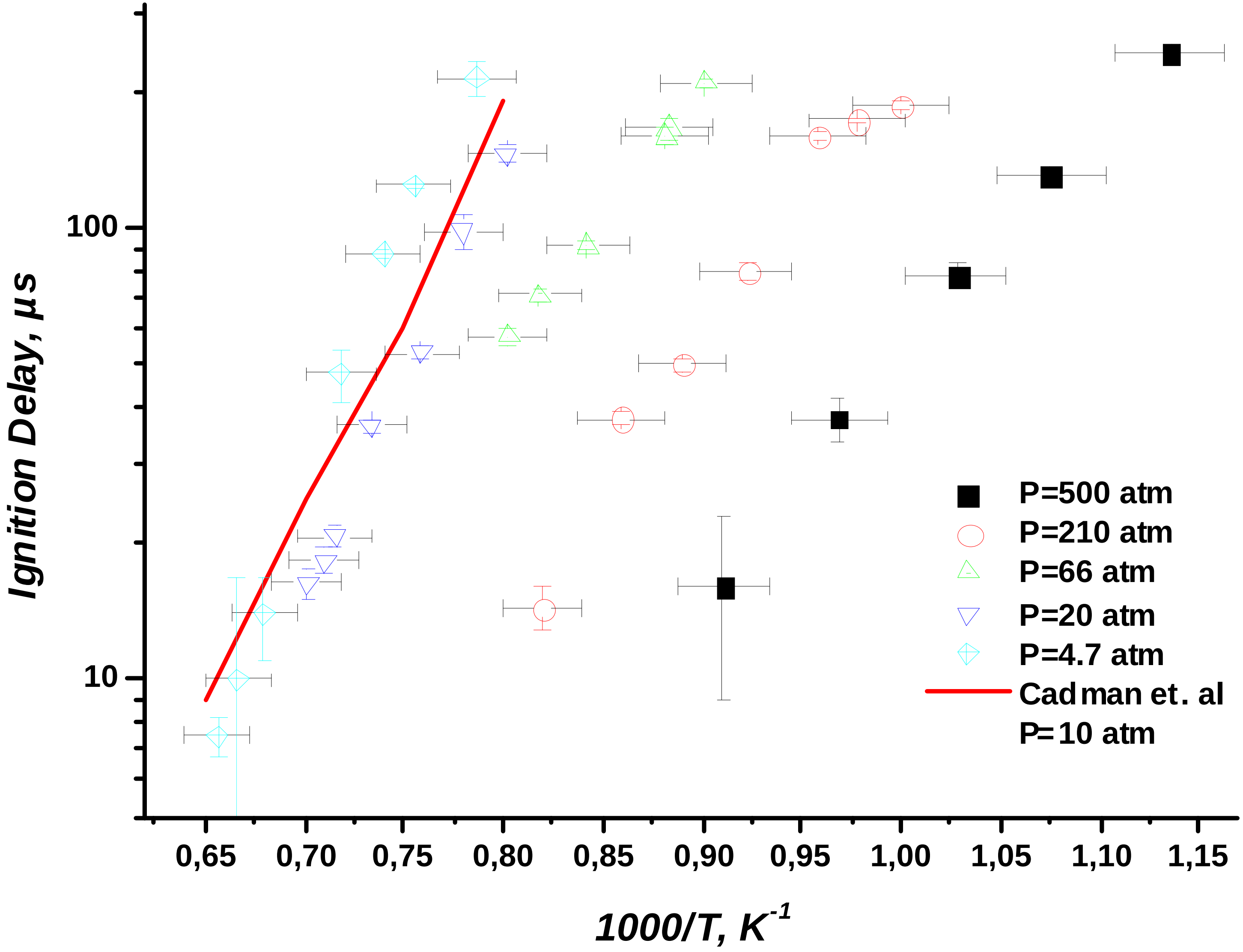
Surface DBD,

< 50mJ

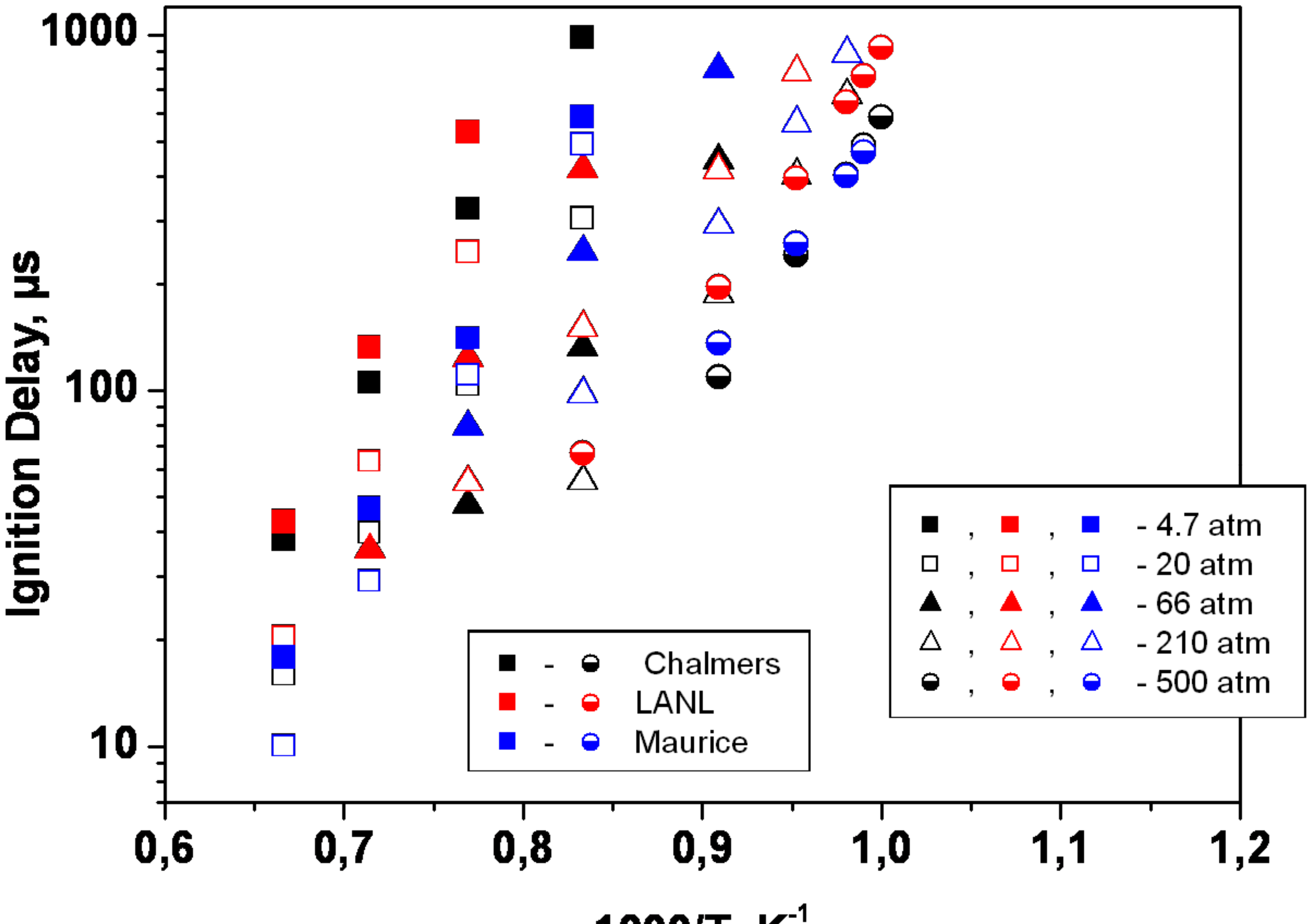


Propane-Butane-Air Lean Mixtures.

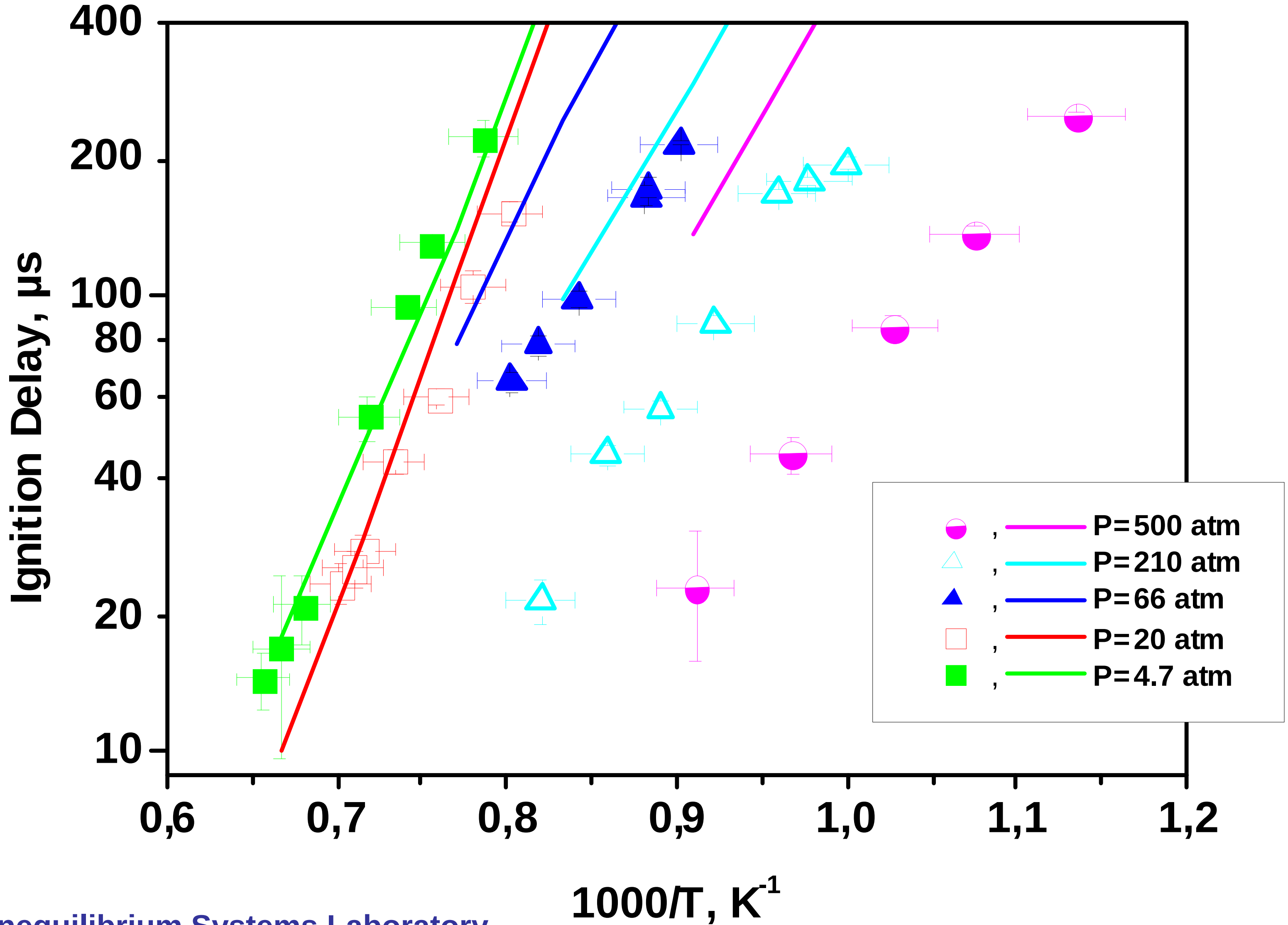
φ = 0.5 (C_3:C_4=85:15)



Propane-Butane-Air Mixture Ignition. φ = 0.5 (C_3:C_4=85:15). Calculations



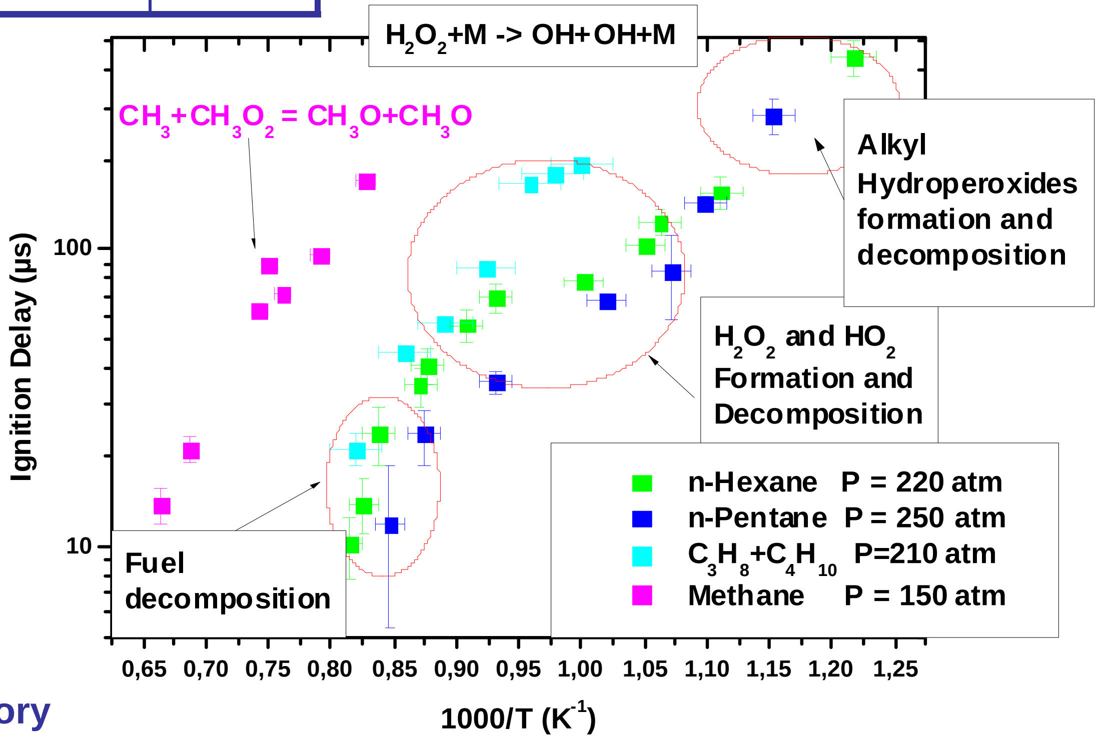
Propane-Butane-Air Mixture Ignition. Experiment vs Calculations.



Channels of Kinetic Scheme Optimization

Reaction	T	k
$C_3H_8 + HO_2 = C\grave{}H_2C_2H_5 + H_2O_2$	1200	2.5
$C_3H_8 + HO_2 = CH_3C\grave{}HCH_3 + H_2O_2$	1200	2.5
$O_2C_3H_7 = HOOCH_2C\grave{}HCH_3$	800-1000	0.2
$CH_3CHO_2CH_3 = CH_3CH(OOH)C\grave{}H_2$	800-1000	0.2
$OCHCH(OOH)CH_3 = CH_3CHO + HCO + OH$	800	0.2
$OCHCH_2CH(OOH)_2 = CH_2O + CH_2CHO + OH$	800	0.2
$CH_3COCH_2(OOH) = CH_2O + CH_3CO + OH$	800	0.2

Konnov, Potapkin



$H_2O_2+M \rightarrow OH+OH+M$

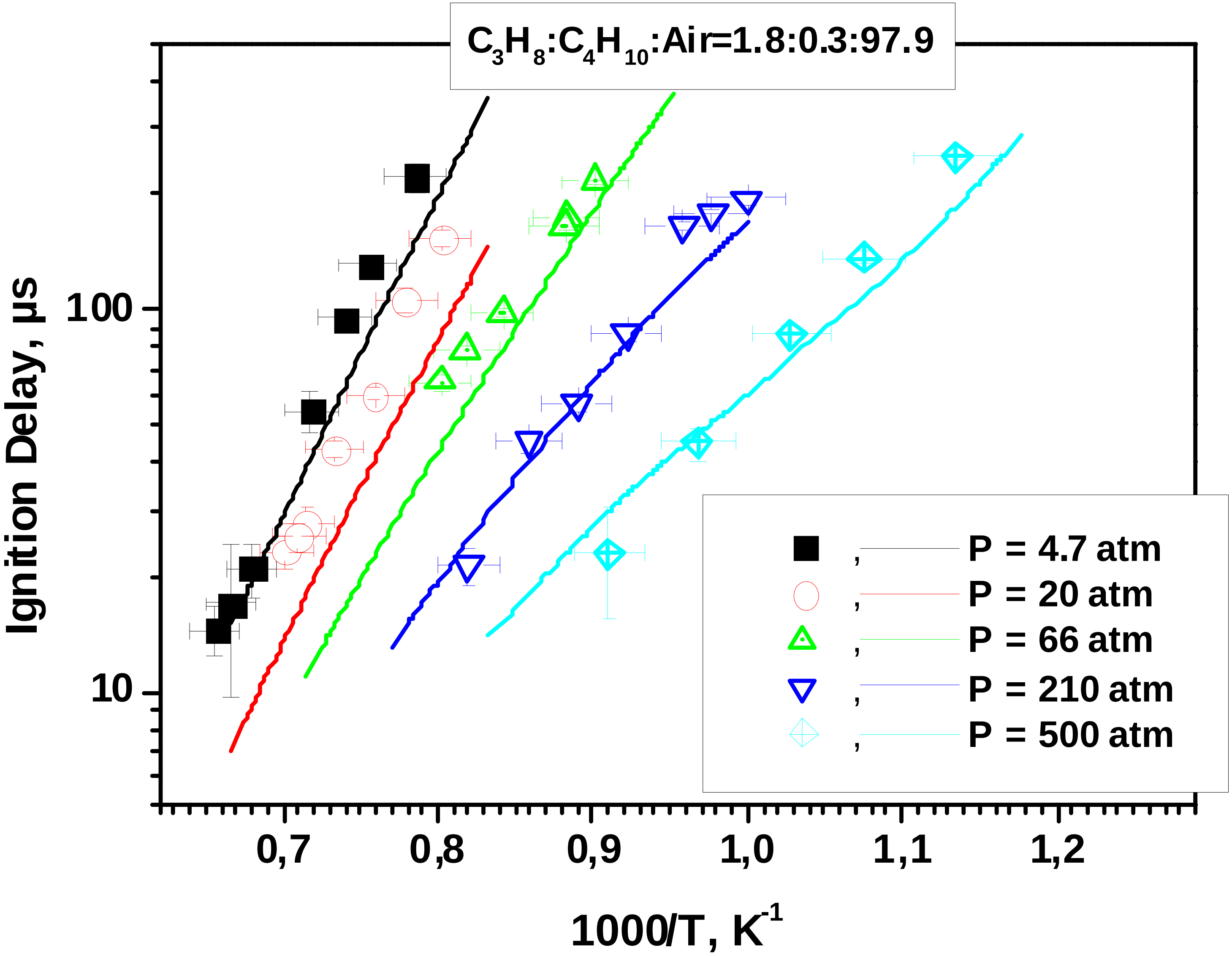
$CH_3+CH_3O_2 = CH_3O+CH_3O$

Alkyl Hydroperoxides formation and decomposition

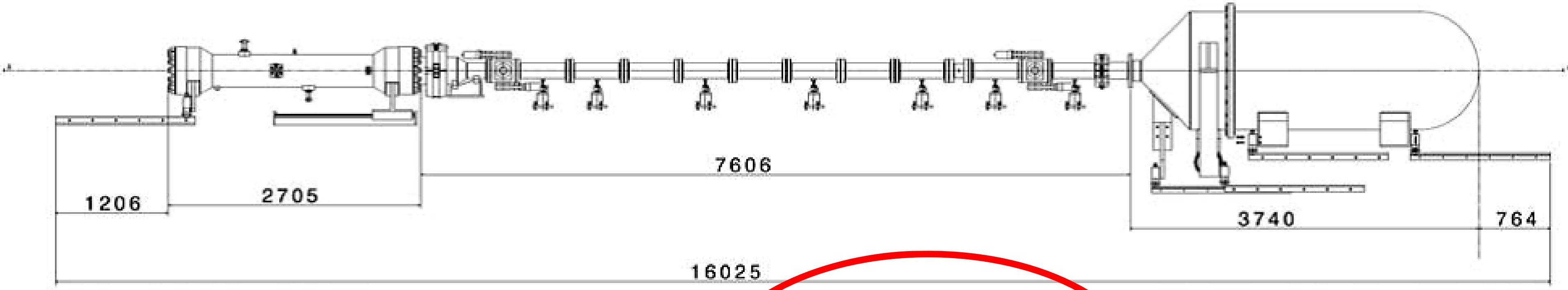
H_2O_2 and HO_2 Formation and Decomposition

Fuel decomposition

Mixture $C_3H_8:C_4H_{10}:Air = 1.8:0.3:97.9$

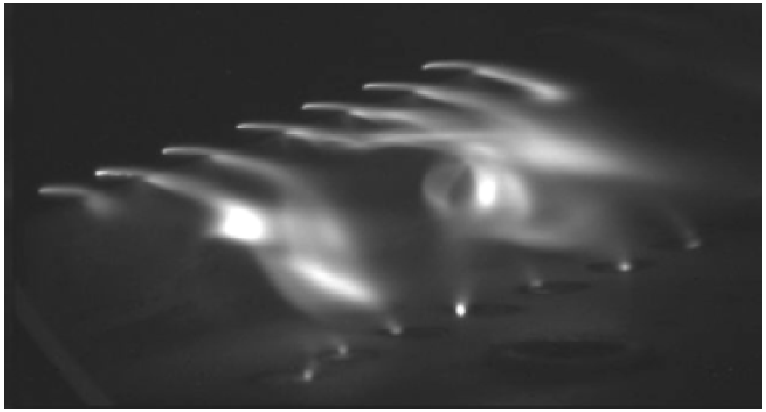


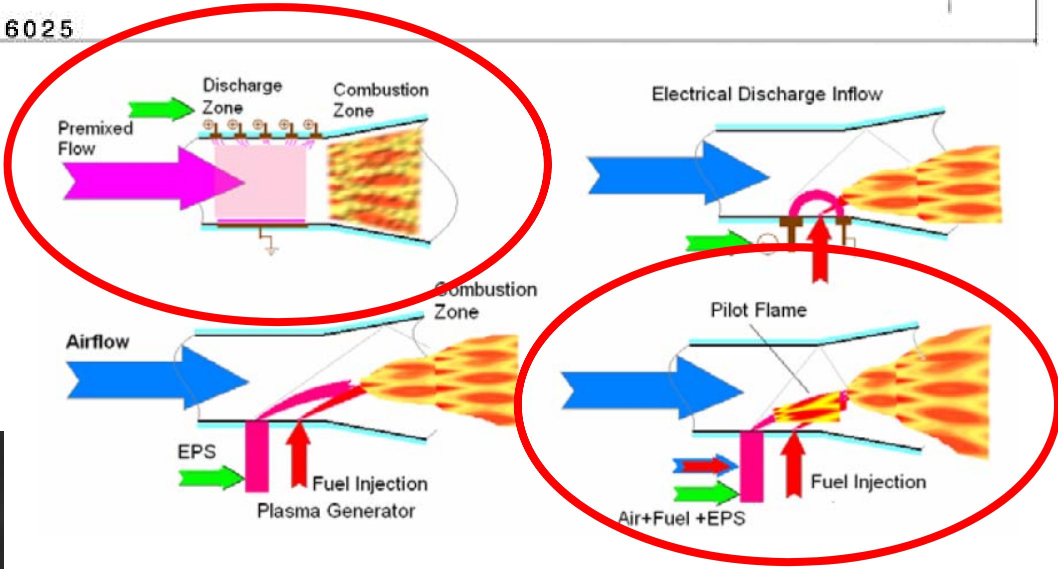
Discharge Formation and Flame Stabilization in High Speed Flow



IVTAN (Sergey Leonov):

M = 2
Maximal stagnation pressure 1.8 Bar
Stagnation temperature 670 K
Discharge Power ~ 1 kW





DPI Shock Tunnel:

M = 2-5
Static pressure 0.1 - 1 Bar
Static temperature 700-1000 K
Discharge Power ~ 1 kW

Summary

Range of Parameters

P = 0.1 – 70 atm
T = 300 – 2000 K
M = 0 - 5
ϕ = 0.01 – 1
E/n = 200-500 Td (Air)
Fuels: H_2, C_1 – C_4
Acetones, Alcohols, CO

Experiment:

Shock Tube
Shock Tunnel
Rapid Compression Machine
Premixed Flow Nozzle

Theory:

Discharge Models
Plasma Models
Chemical Kinetic Models