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Simulation of NOx Formation in Dielectric Barrier Discharge

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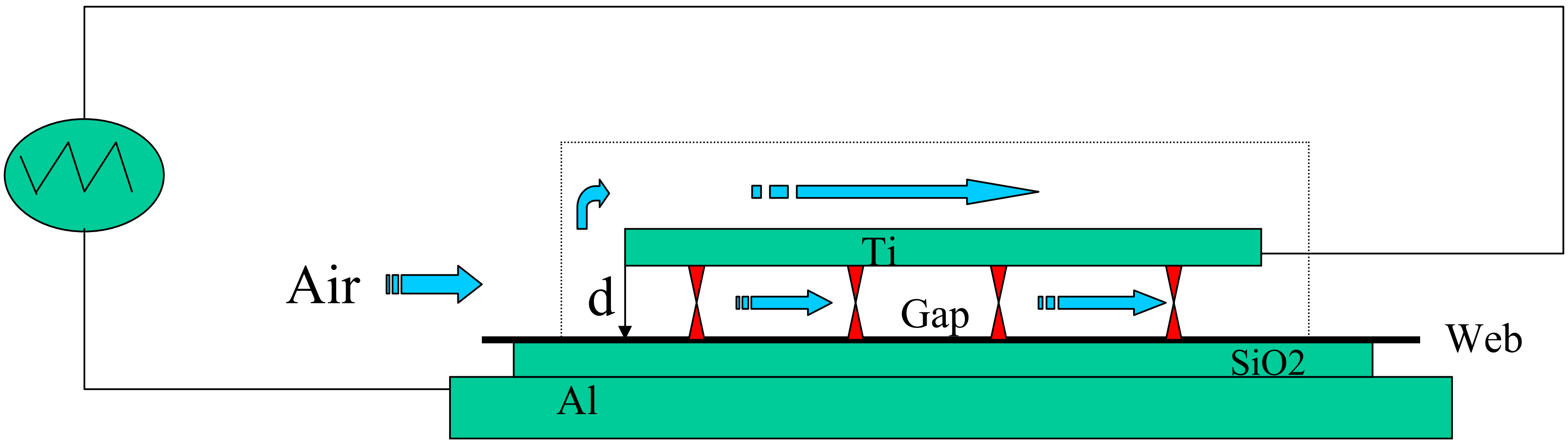
- DBD plasma treatment of organic web (photographic paper)
- Negative NO – influence on chemical quality of the web
- Factors controlling NO generation in streamers
- Fluid mechanics model and plasma chemical reaction mechanism
- Effect of specific power and humidity on NO generation.

Dielectric Barrier Discharge for Web Treatment



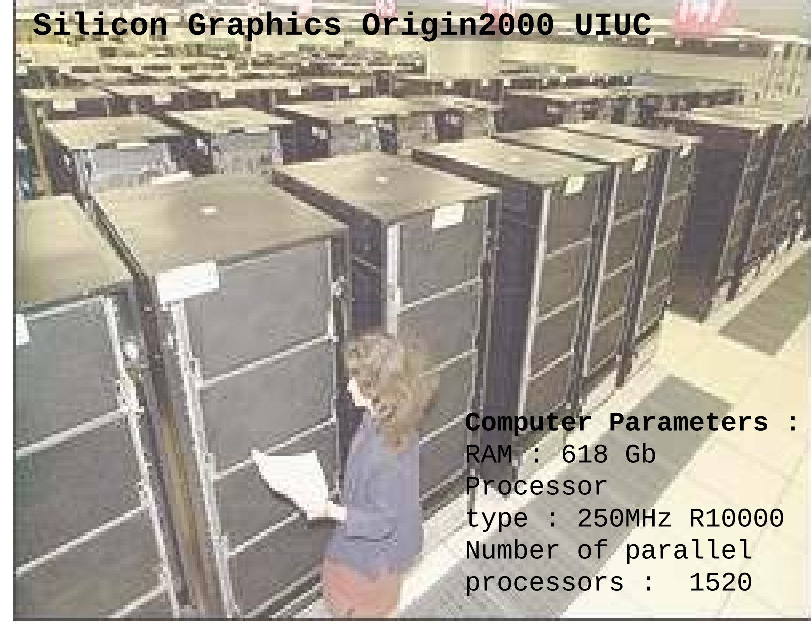
W = 20 ÷150	[W]	- power
d = 0.89	[mm]	- gap distance
V = 1 ÷ 10	[sl/min]	- gas flow rate
u = 0 ÷ 5	[m/sec]	– web velocity
F = 10 ÷ 40	[kHz]	- frequency
P = 1	[atm]	- pressure
T = 300	[K]	- temperature

NO yield depends on :

1. *Specific power (power/flow rate)—>vibrational temperature —> electron energy —> dissociation rate.*
2. *Humidity (N2A+H2O=>H2+N+NO).*
3. *Discharge parameters (electron temperature and concentration).*

INPUT :
- temperature
- pressure
- power
- flow rate
- discharge geometry

K
A
M
A
L



INPUT:
- distance between electrodes
- gas composition
- pressure
- power and current

FLUENT
for fluid dynamics and energy balance

STREAMER KINETICS
for discharge parameters

PLASMA CHEMISTRY *ChemKin*
for plasma chemistry simulation

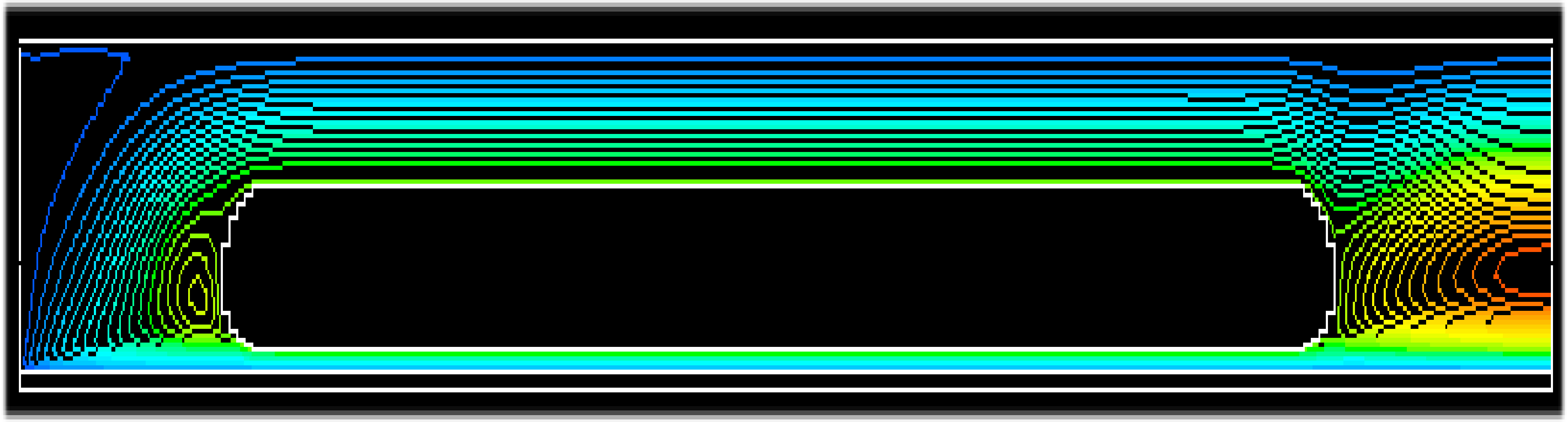
NO
(P/Q, [H2O], p, d)

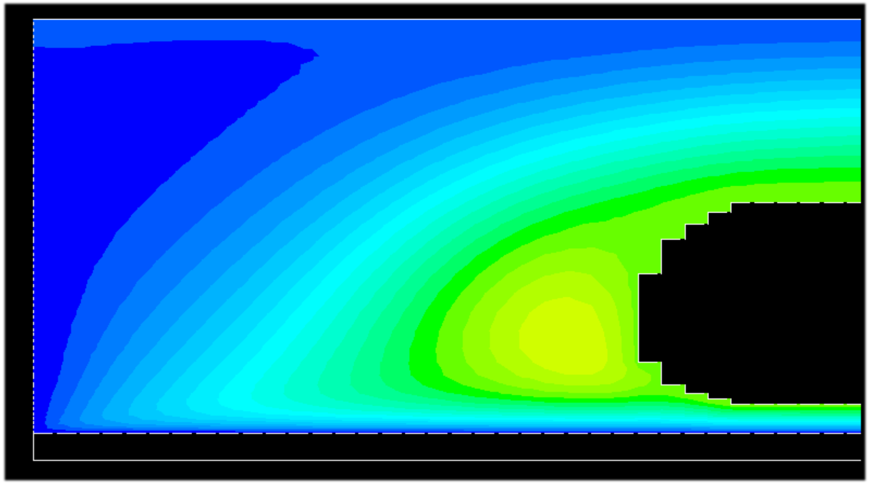
OUTPUT:
- temperature distribution
- stream lines

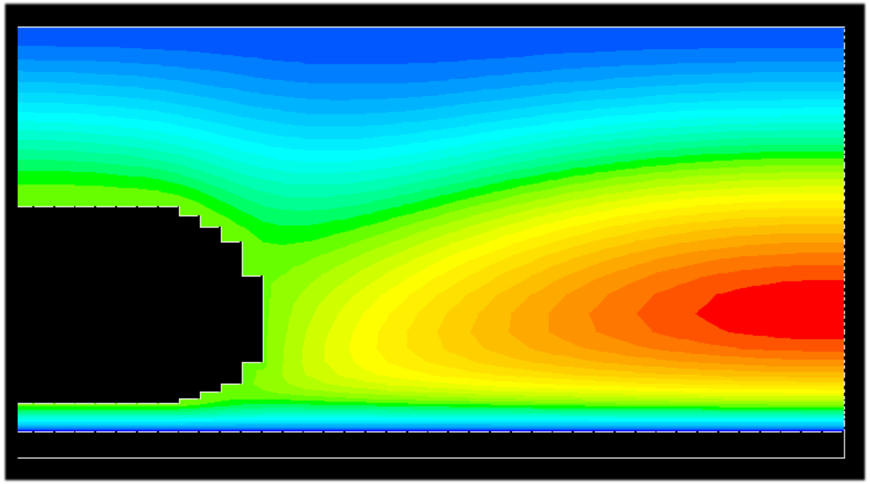
OUTPUT:
- electron temperature
- electron concentration
- number of streamers

Stream Function

FLUENT 4.5





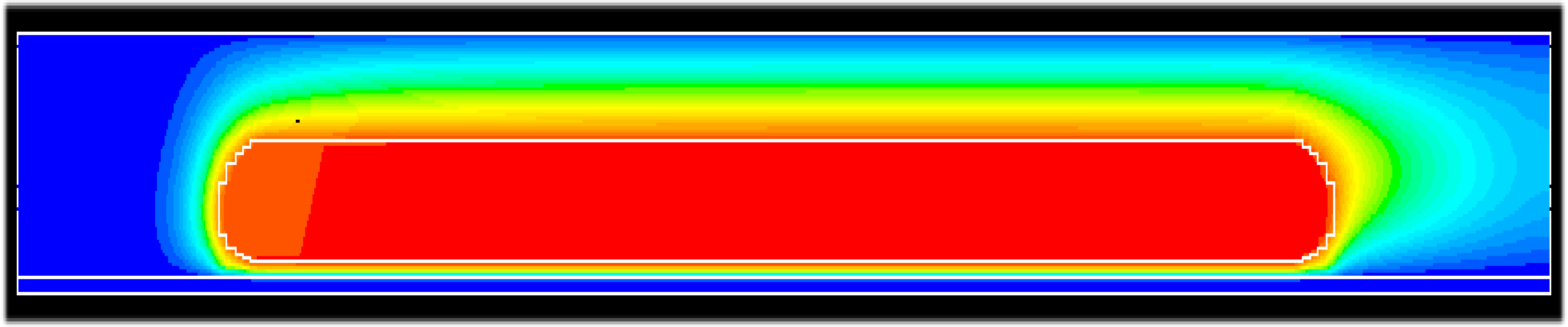


min. and max. values of stream function : **[0.0 4.57E-4] [m2/sec]**

Flow rate through the discharge gap is determined mostly by web velocity when it is moving.

Translational Temperature Distribution

Stationary Film



P = 150.0 Watt
U = 0.0117 m/sec

temperature range:

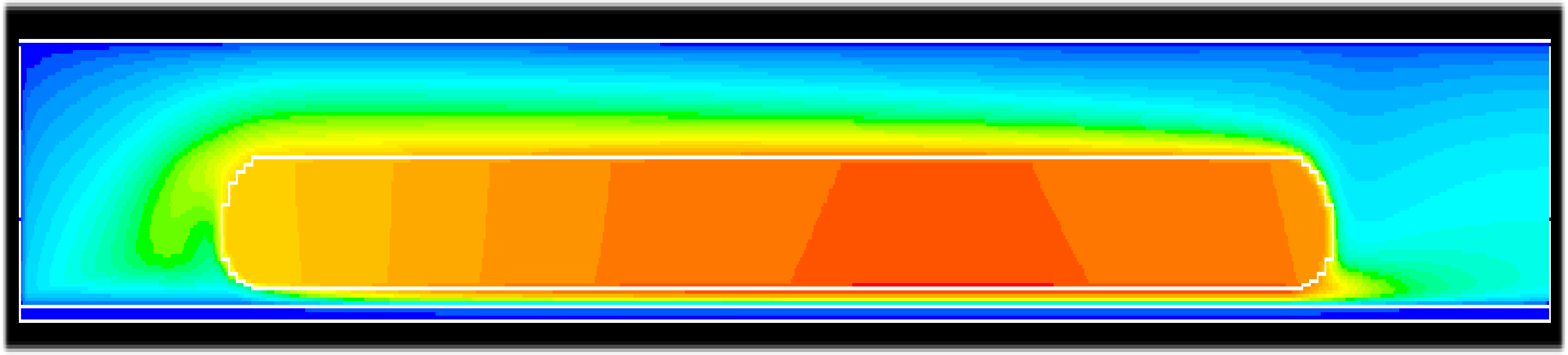
[300-511] K

Moving Film

P = 150.0 Watt
U = 0.0117 m/sec

temperature range:

[300-397] K



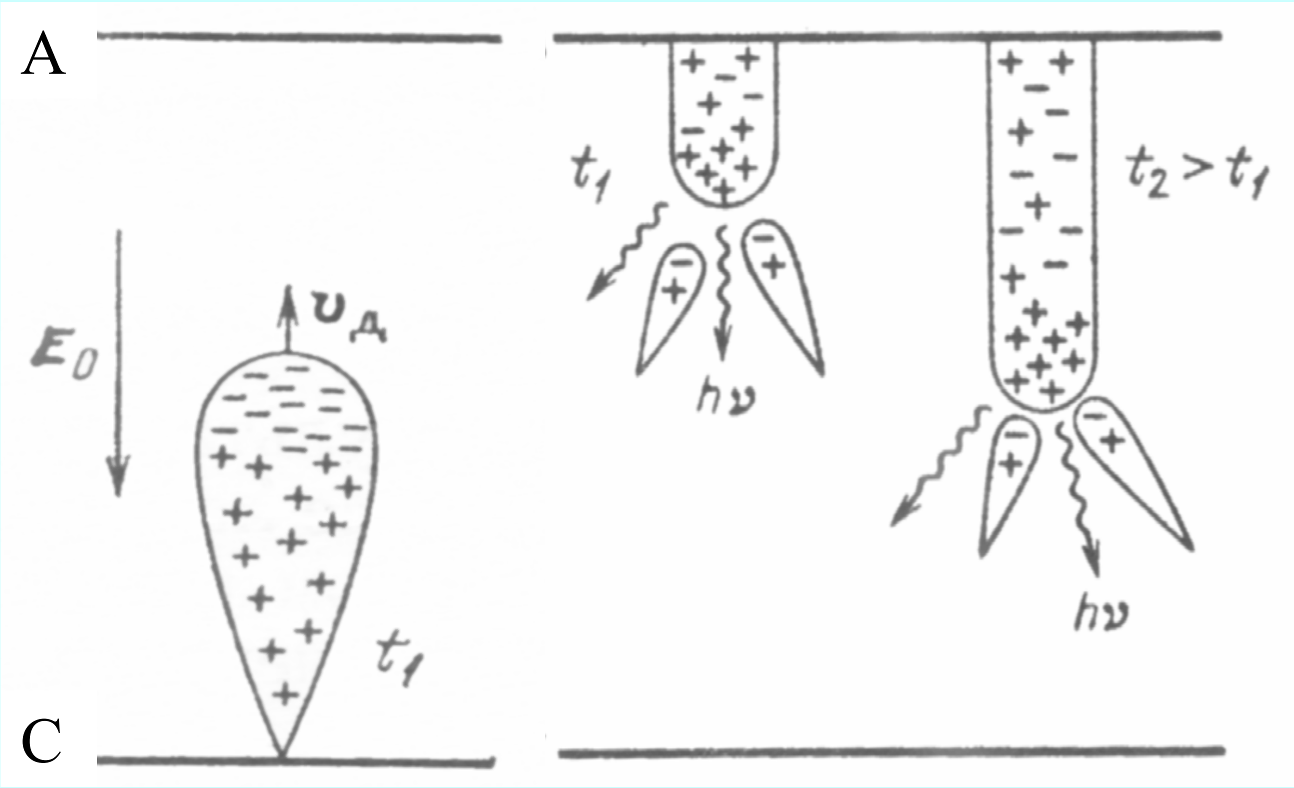
Avalanche to Streamer Transition

$$\alpha\cdot\left(\frac{E_0}{p}\right)\cdot d = \ln\frac{4\pi\varepsilon_o E_0}{e\cdot\alpha^2} \approx 20$$

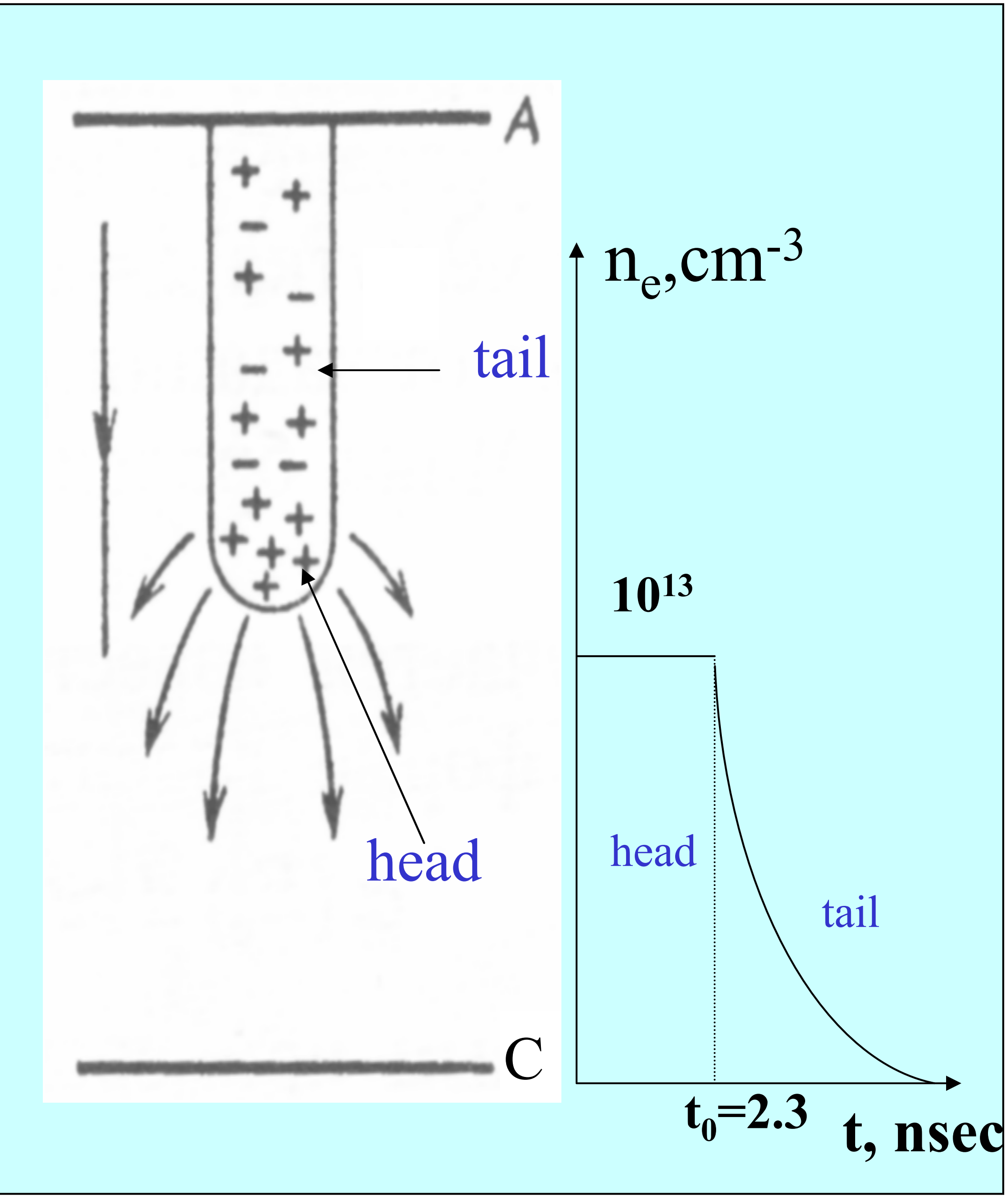
$$n_e = \exp(\alpha\cdot d) \approx 3\cdot 10^8$$

Meek streamer breakdown condition ($E > E'$, $\alpha d \geq 20$)

Breakdown Field :
≈ 4 (kV/mm)
Drift Velocity :
$V_d = \mu\cdot E_0 = 10^7$ (cm/sec)
Radius :
$5\cdot10^{-3}\div10^{-2}$ (cm)
Electron Energy :
$2\div5$ (eV)
Electron Density :
$10^{13}\div10^{15}$ (cm^{-3})



Model of an Individual Streamer



Input Parameters:

- d –distance between the electrodes
- pressure
- gas composition
- power and current

Output Parameters:

- electron temperature
- electron concentration
- α –1st Townsend coefficient
- number of streamers

Electron Concentration in Tail :

$n_e = n_{e0} \cdot \exp[-(t \cdot \mu \cdot E_0)/d]$

$t_0 = (\alpha \cdot \mu \cdot E_0)^{-1}$

streamer lifetime: 10^{-8} sec

ion drift : 10^{-4} sec

Where :

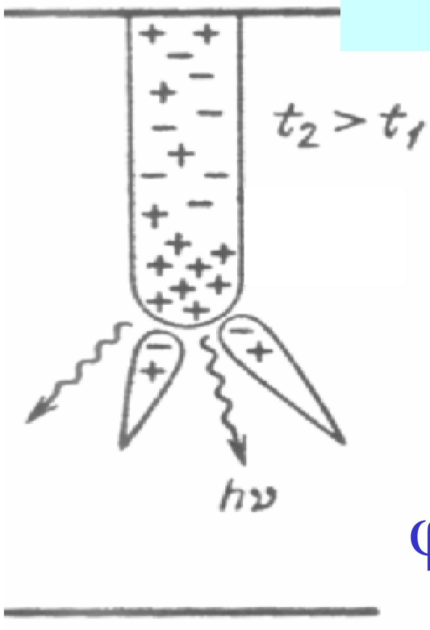
$\mu \cdot E_0 = 10^7$ cm/sec

$d = 0.1$ cm

$n_{e0} = 10^{13}$ cm^{-3}

$\alpha = 44.35$ cm^{-1}

Model of Streamer Interactions
(streamer's synergy)



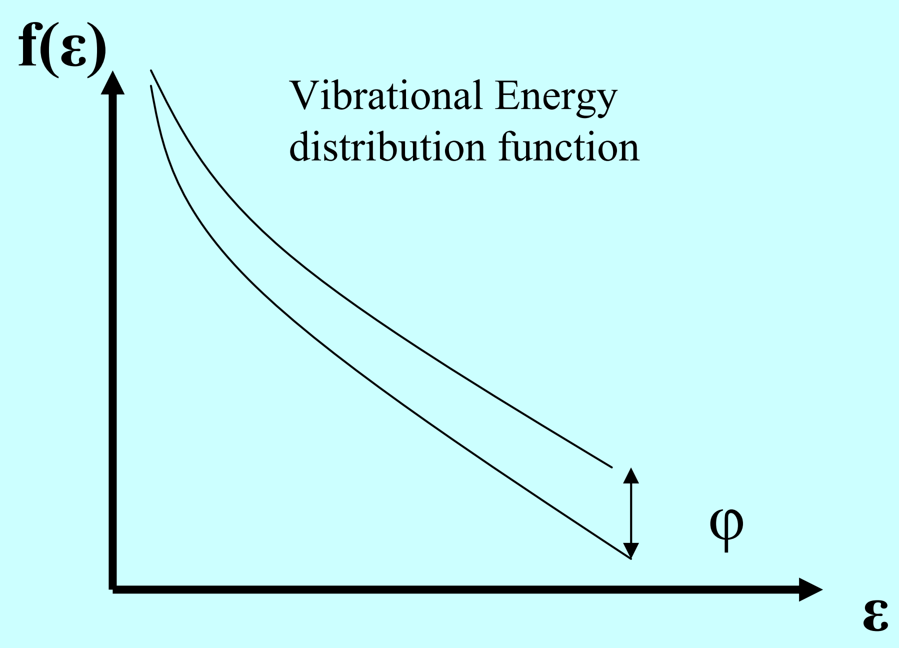
the higher specific power P/Q →

the higher vibrational temperature T_v →

the longer EEDF (electron energy distribution function) $f(\varepsilon)$ →

the higher dissociation rate coefficient k_d

$$\varphi(T_v) \approx \exp\left\{-\frac{2M}{m} P^{o}_{ev}\, \hbar\omega \,\frac{\varepsilon_2 - \varepsilon_1}{\langle\varepsilon\rangle}\left(1 - \exp\left(-\frac{\hbar\omega}{T_v}\right)\right)\right\}$$



$$\varphi(T_v) = \exp\left\{b\cdot\exp\left(-\frac{\hbar\omega}{T_v}\right)\right\}$$

$$K_e(T_e, T_v) = K(T_e)\cdot\varphi(T_v)$$

$$E_v = \frac{\hbar\omega}{\exp\left(-\frac{\hbar\omega}{T_v}\right) - 1}$$

Plasma Chemical Reaction Mechanism in Humid Air

57 – species ; 327 - reactions

SPECIES INVOLVED IN THE MECHANISM

NEUTRAL SPECIES

O <u>NO</u> H_2O HO_2 N_2 O_2 <u>NO_3</u> OH H_2O_2 N NH HNO_3 <u>N_2O_3</u> H_2 NH_2

HNO_2 <u>N_2O</u> HNO H O_3 <u>NO_2</u>

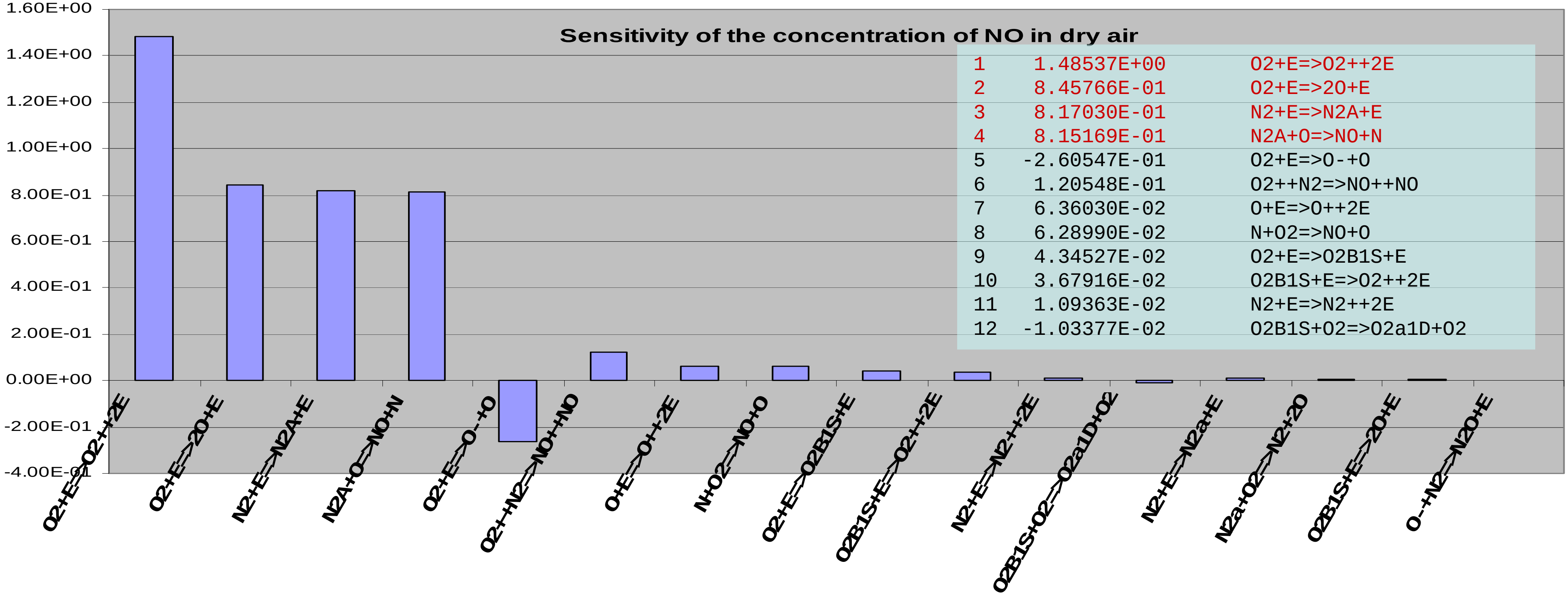
CHARGED SPECIES

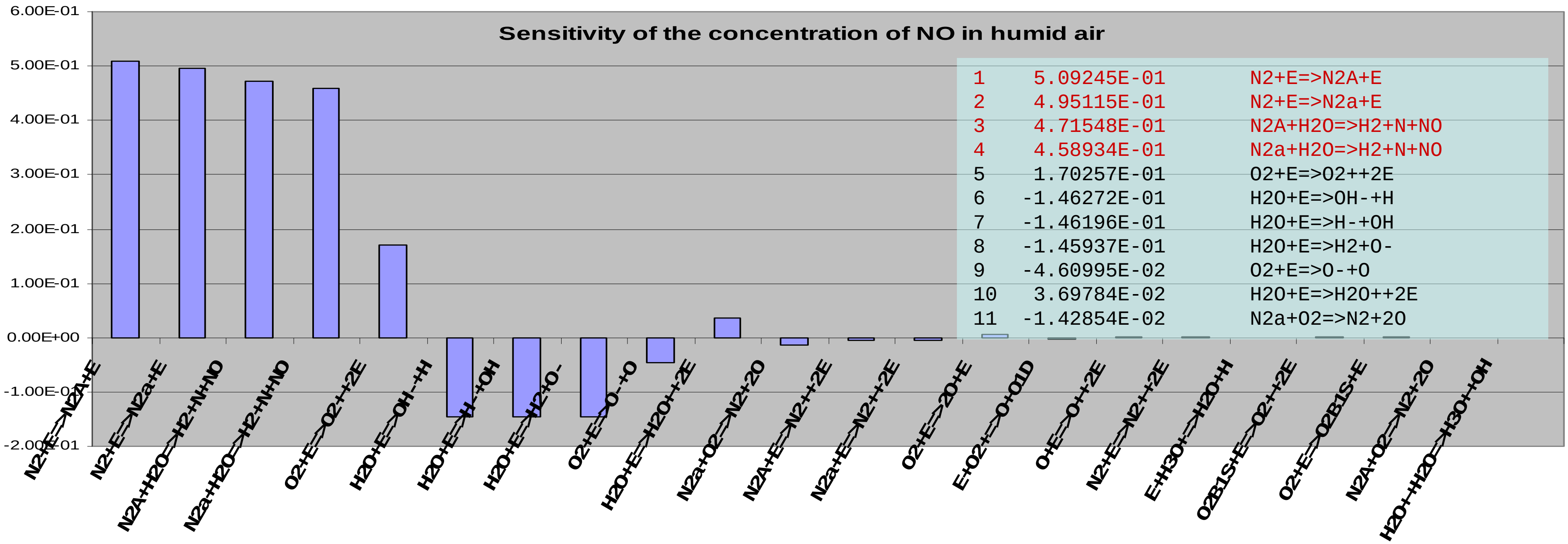
O_3^+ O_3^- NO_2^+ O_4^- O_2^- $NO_2H_2O^-$ NO_3^- OH^- $H_2O_4^-$ $H_3O_2^-$ $NO_2H_2^-$ $H_2O_2^-$

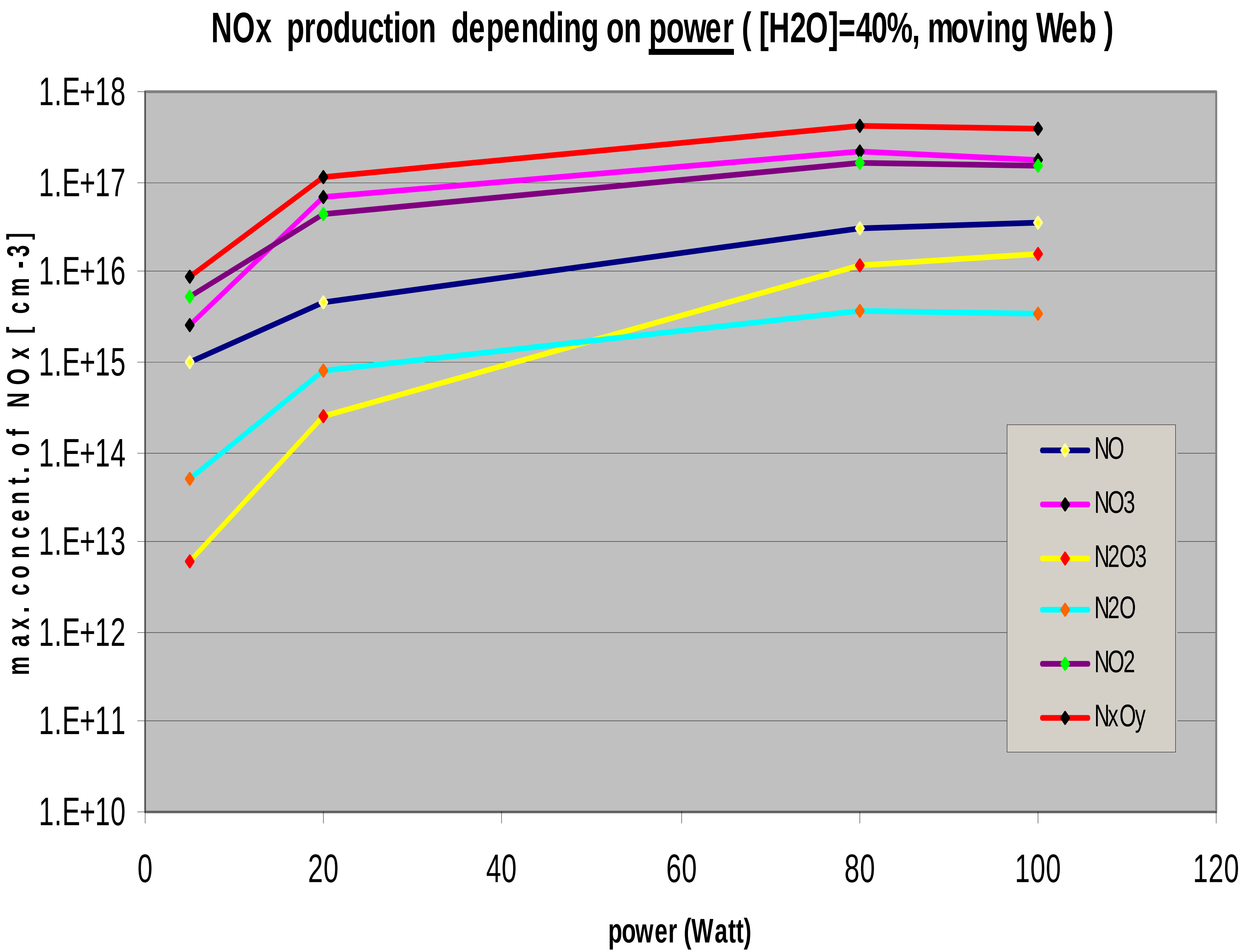
N_2O^- O^+ NO^+ H_2O^+ $H_2O_3^-$ N_2^+ O_2^+ O^- NO^- H_3O^+ N_4^+ O_4^+ OH^+

EXCITED SPECIES

O2v O2a1D O2B1S O1D N2a O1S N2v N2A

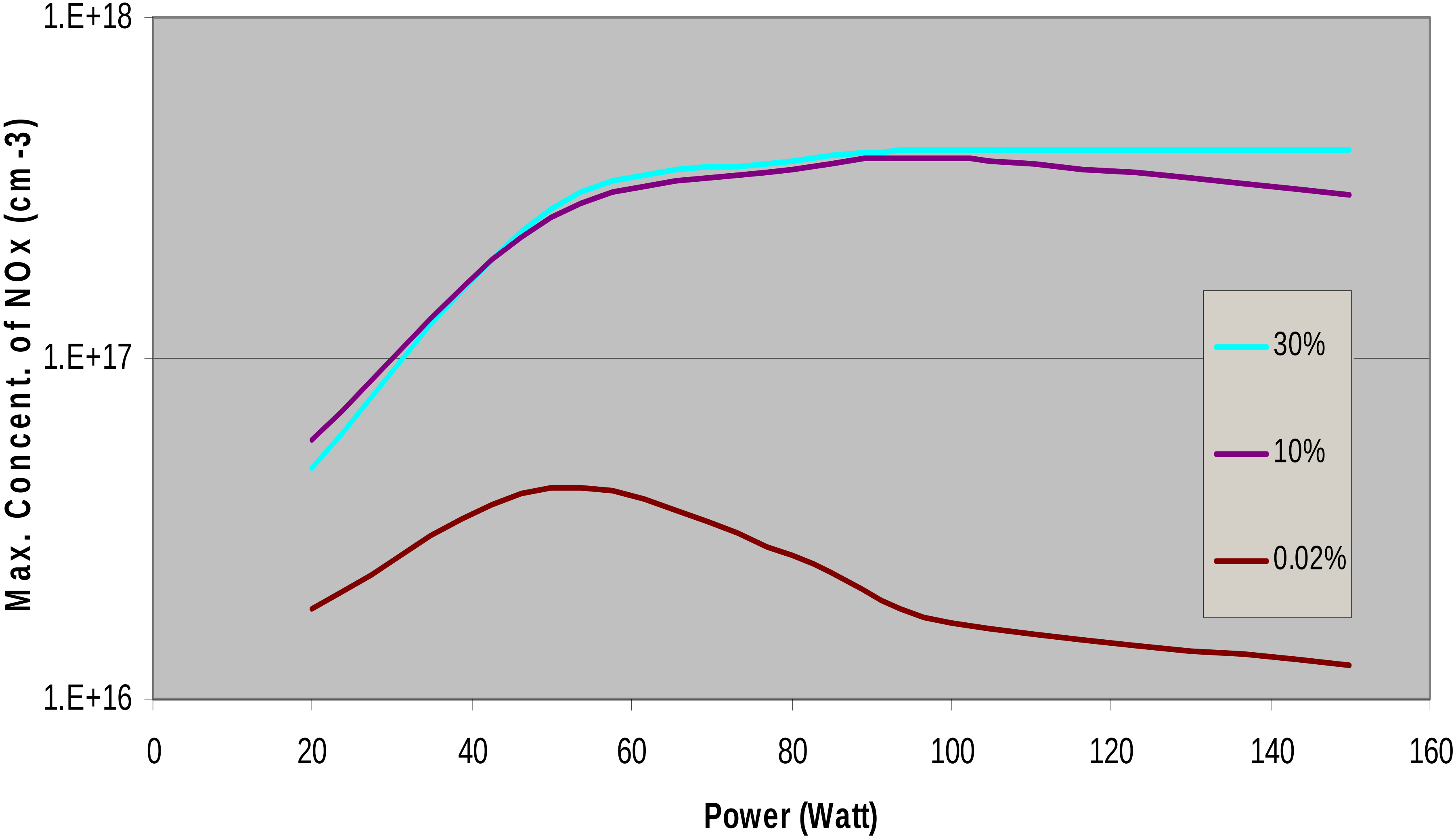

Sensitivity of the concentration of NO in dry air
1.60E+00
1.40E+00
1.20E+00
1.00E+00
8.00E-01
6.00E-01
4.00E-01
2.00E-01
0.00E+00
-2.00E-01
-4.00E-01
1 1.48537E+00 O2+E=>O2++2E
2 8.45766E-01 O2+E=>2O+E
3 8.17030E-01 N2+E=>N2A+E
4 8.15169E-01 N2A+O=>NO+N
5 -2.60547E-01 O2+E=>O-+O
6 1.20548E-01 O2++N2=>NO++NO
7 6.36030E-02 O+E=>O++2E
8 6.28990E-02 N+O2=>NO+O
9 4.34527E-02 O2+E=>O2B1S+E
10 3.67916E-02 O2B1S+E=>O2++2E
11 1.09363E-02 N2+E=>N2++2E
12 -1.03377E-02 O2B1S+O2=>O2a1D+O2
O2+E=>O2++2E
O2+E=>2O+E
N2+E=>N2A+E
N2A+O=>NO+N
O2+E=>O-+O
O2++N2=>NO++NO
O+E=>O++2E
N+O2=>NO+O
O2+E=>O2B1S+E
O2B1S+E=>O2++2E
N2+E=>N2++2E
O2B1S+O2=>O2a1D+O2
N2+E=>N2a+E
N2a+O2=>N2+2O
O2B1S+E=>2O+E
O-+N2=>N2O+E


Sensitivity of the concentration of NO in humid air
6.00E-01
5.00E-01
4.00E-01
3.00E-01
2.00E-01
1.00E-01
0.00E+00
-1.00E-01
-2.00E-01
1 5.09245E-01 N2+E=>N2A+E
2 4.95115E-01 N2+E=>N2a+E
3 4.71548E-01 N2A+H2O=>H2+N+NO
4 4.58934E-01 N2a+H2O=>H2+N+NO
5 1.70257E-01 O2+E=>O2++2E
6 -1.46272E-01 H2O+E=>OH-+H
7 -1.46196E-01 H2O+E=>H-+OH
8 -1.45937E-01 H2O+E=>H2+O-
9 -4.60995E-02 O2+E=>O-+O
10 3.69784E-02 H2O+E=>H2O++2E
11 -1.42854E-02 N2a+O2=>N2+2O
N2+E=>N2A+E
N2+E=>N2a+E
N2A+H2O=>H2+N+NO
N2a+H2O=>H2+N+NO
O2+E=>O2++2E
H2O+E=>OH-+H
H2O+E=>H-+OH
H2O+E=>H2+O-
O2+E=>O-+O
H2O+E=>H2O++2E
N2a+O2=>N2+2O
N2A+E=>N2++2E
N2a+E=>N2++2E
O2+E=>2O+E
E+O2+=>O+O1D
O+E=>O++2E
N2+E=>N2++2E
E+H3O+=>H2O+H
O2B1S+E=>O2++2E
O2+E=>O2B1S+E
N2A+O2=>N2+2O
H2O++H2O=>H3O++OH



NOx production depending on power ([H2O]=40%, moving Web)
1.E+18
1.E+17
1.E+16
1.E+15
1.E+14
1.E+13
1.E+12
1.E+11
1.E+10
max. concent. of NOx [cm-3]
0
20
40
60
80
100
120
power (Watt)
NO
NO3
N2O3
N2O
NO2
NxOy

NOx production depending on power and humidity



NOx production depending on power and humidity