NOx Generation In Dielectric Barrier Discharge(DBD)

Non – Linear Streamer Interaction Effects

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- Description of Modeling case
- Streamers Interaction
- Monte–Carlo Simulation of Multiple Streamers Pattern
- Plasma Chemical Modeling
- Conclusions
- Future Plans

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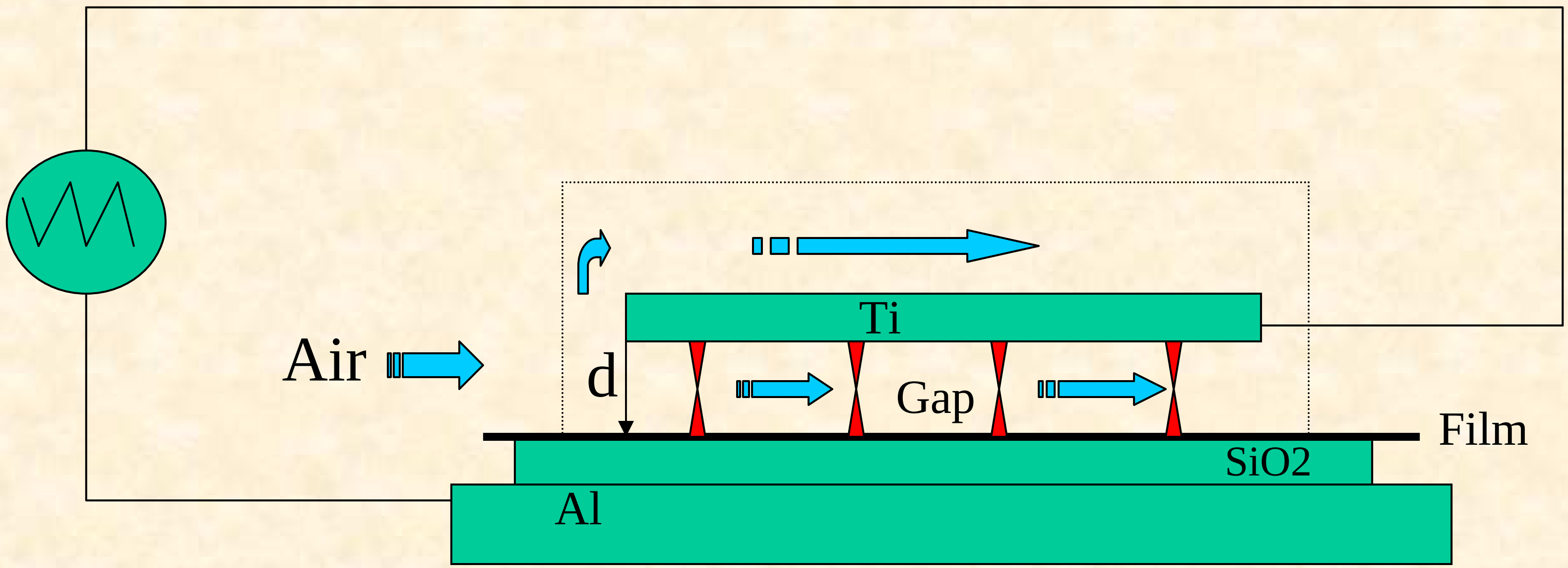
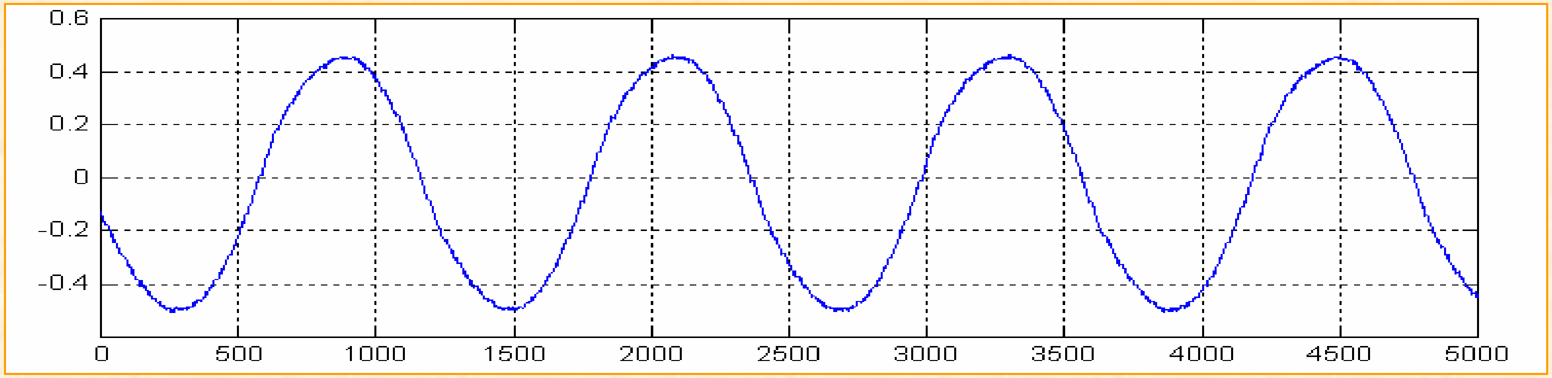


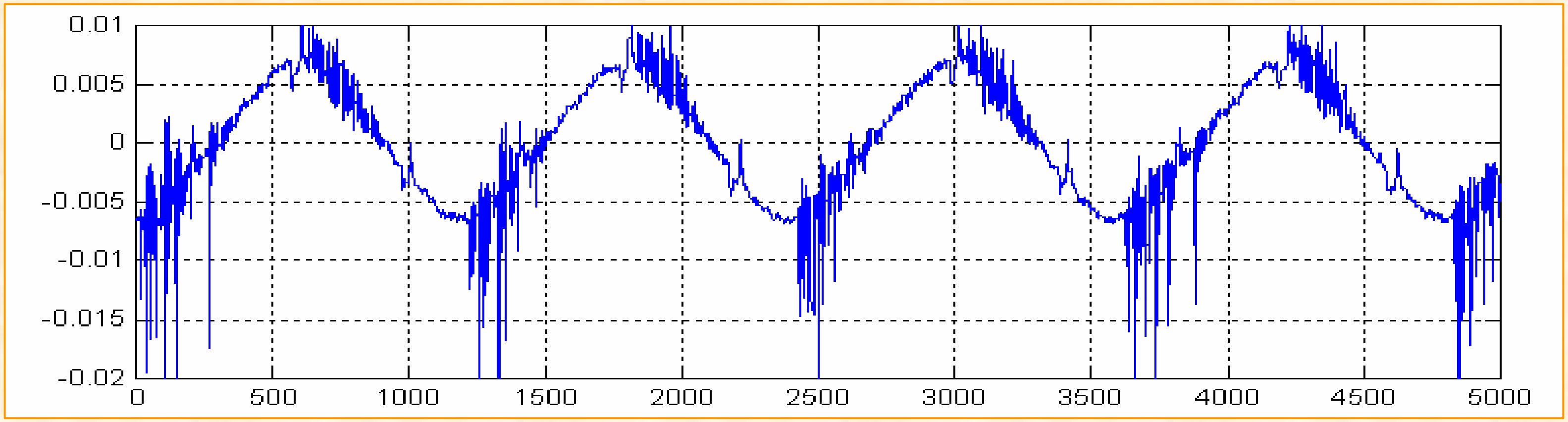
Discharge System Parameters

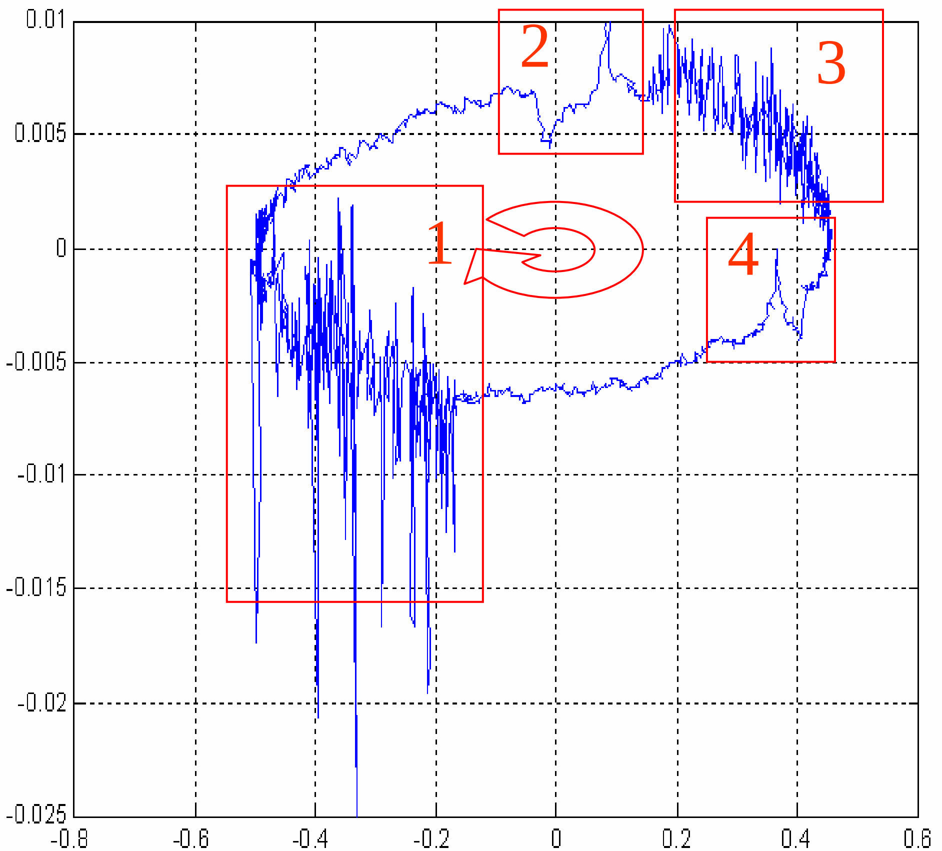
W	= 20 ÷ 150	[W]	- power
dg	= 0.89	[mm]	- gap distance
dd	= 1.00	[mm]	– dielectric thickness
V	= 1 ÷10	[sl/min]	- gas flow velocity
v	= 5	[m/sec]	– web velocity
F	= 10 ÷ 40	[kHz]	- frequency of source
P	= 1.0	[atm]	- pressure
T	= 300	[K]	- temperature

Voltage, V = 5kV, f = 20 Hz, T = 5e-5 [sec]

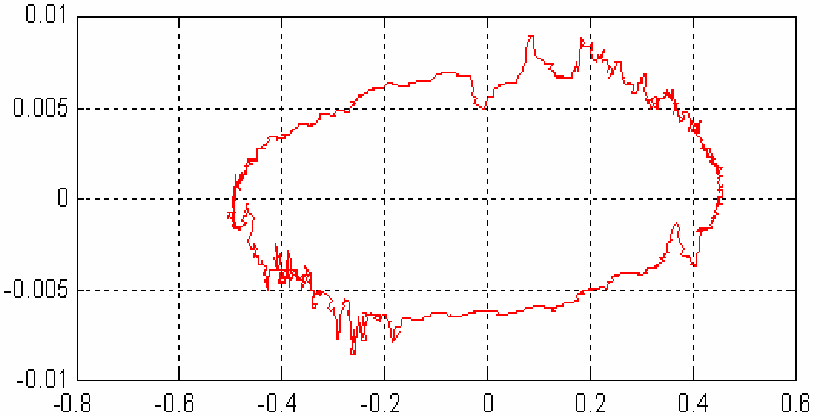


Electric Current, I = 70mA, f = 20 Hz, T = 5e-5 [sec]





Lissajous figure



1st *zone belongs to the streamers from dielectric to a metal cathode.*

2nd *zone belongs to the space charge moving during switching of voltage.*

3th *zone belongs to streamers from metal anode to the dielectric cathode. This zone more uniform because we have electron loosing on the metal anode and that is why current impulses are smaller.*

4th *zone belongs to the space charge moving during switching of voltage. This zone differs from zone 2 because there is no anode electron layer in the case of metal anode.*

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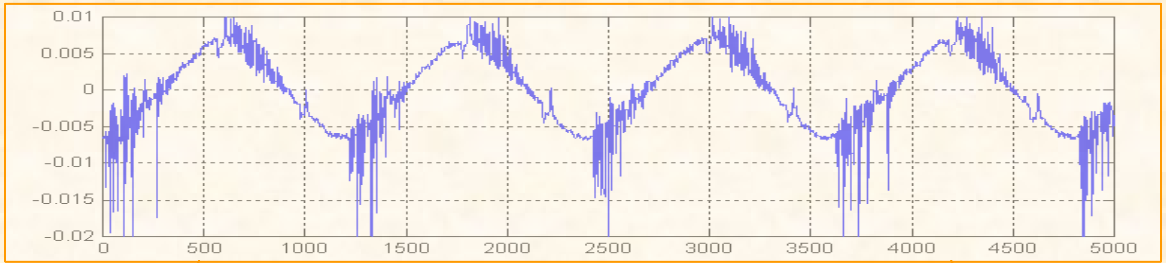
Time resolution

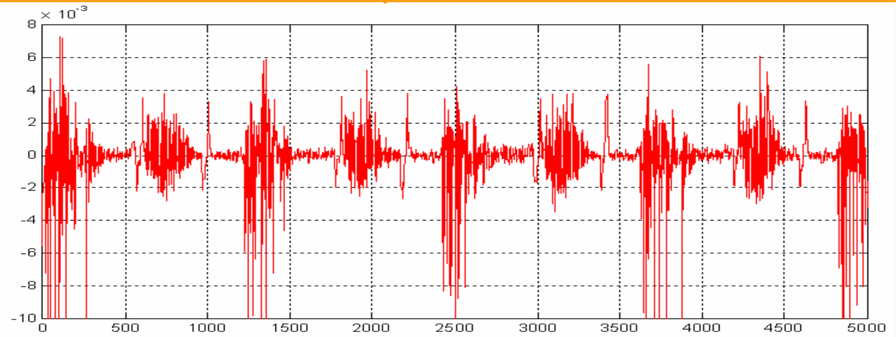
dt=4e-8 [sec]

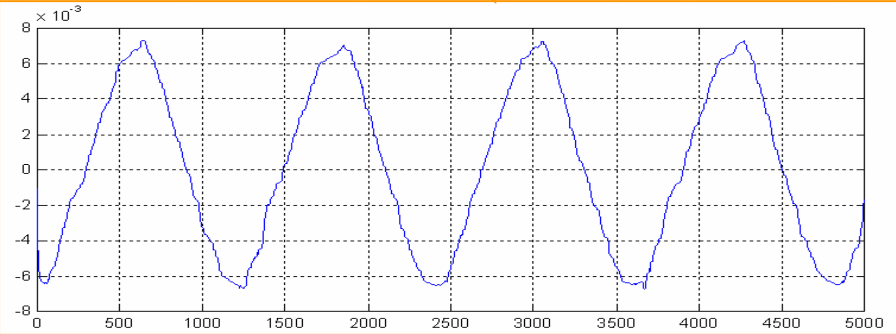


Median filtration

Window size 100 = 4e-6sec

Residuals

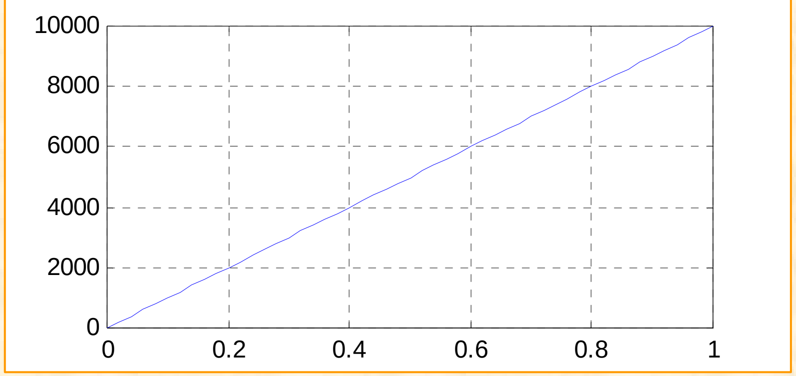




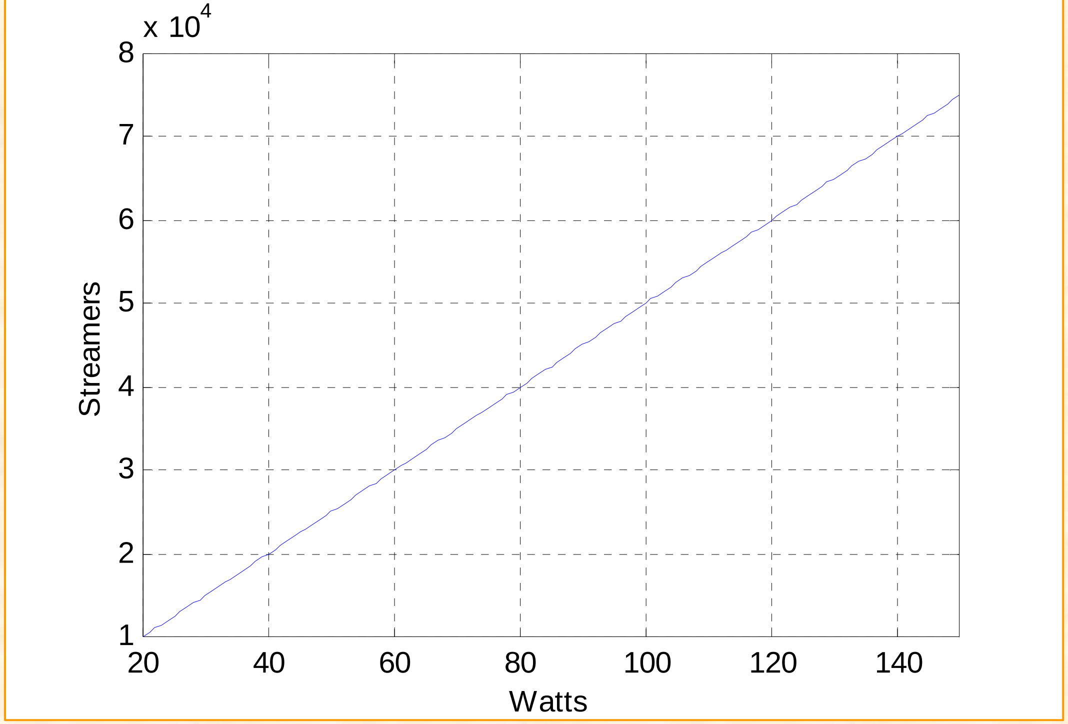
Filtered Electric current

Number of Streamers

Streamers Number Vs. time for 20Wt



Streamers Number Vs. Power for one period (20kHz)



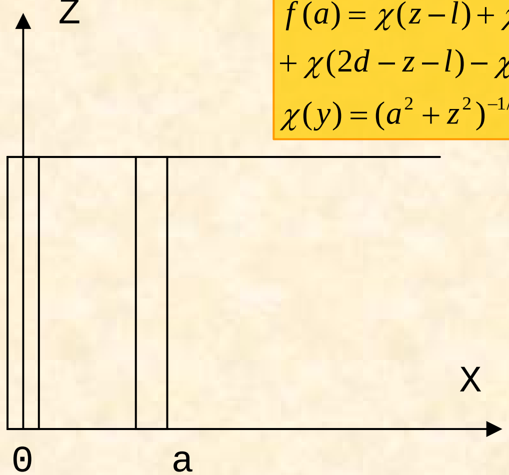
Streamer Interaction

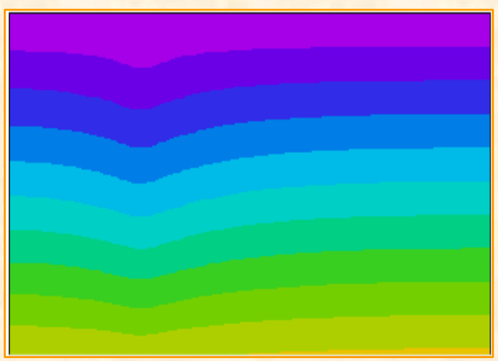
$$E^{(a)}(z,t) = \bar{\rho}(t) f(a)$$

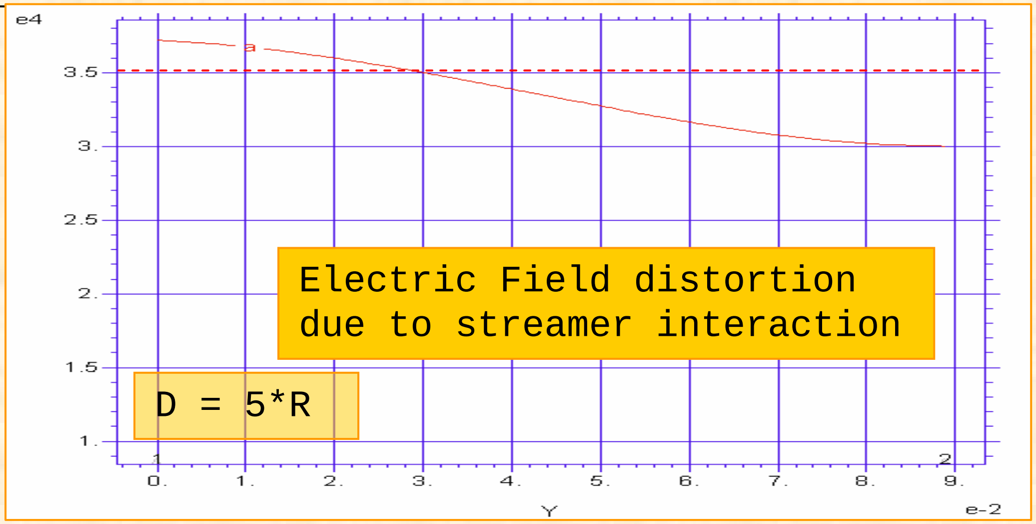
$$\bar{\rho}(t) = \int_0^{l(t)} \rho(z',t) \frac{dz'}{l(t)}$$

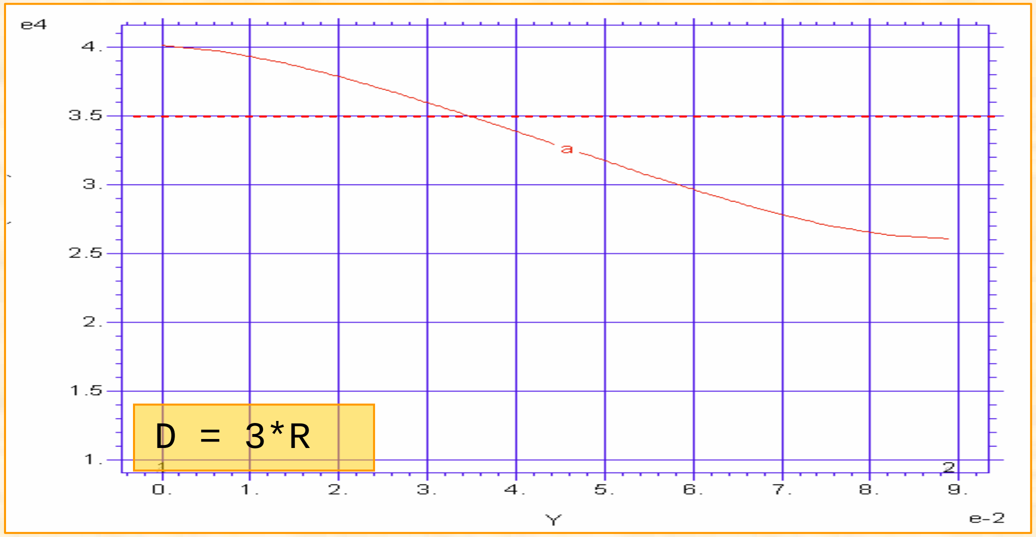
$$f(a) = \chi(z-l) + \chi(z+l) + $$
$$+ \chi(2d-z-l) - \chi(2d-z) - 2\chi(z)$$

$$\chi(y) = (a^2 + z^2)^{-1/2}$$









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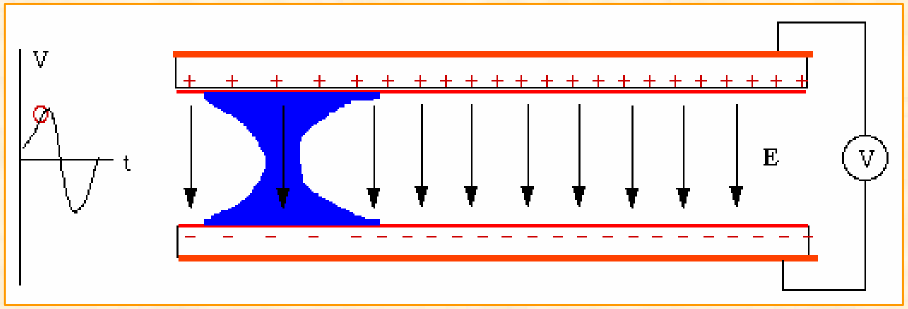
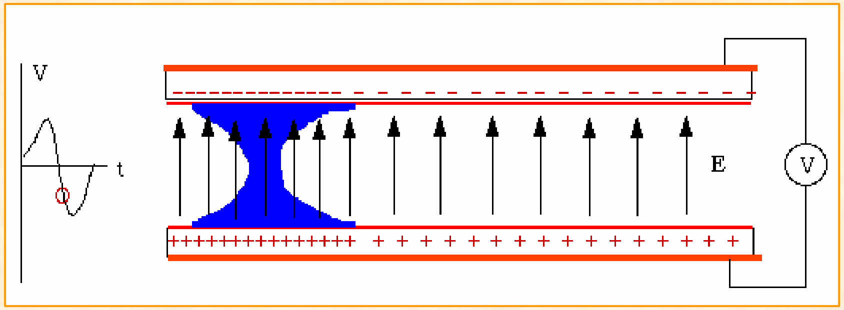
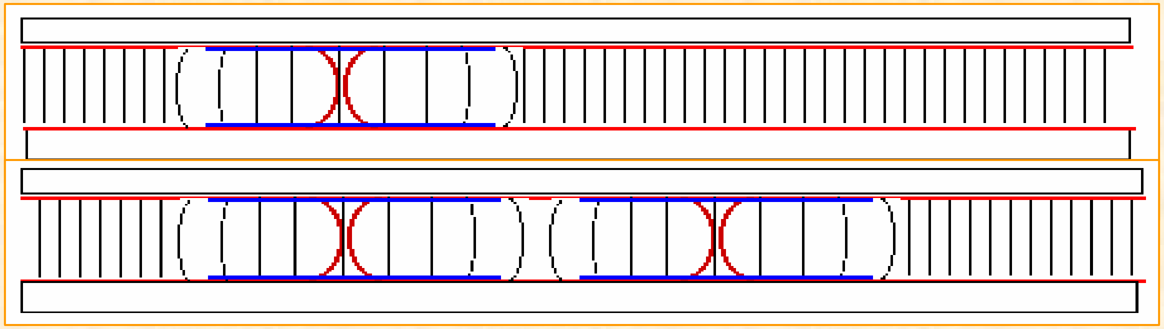


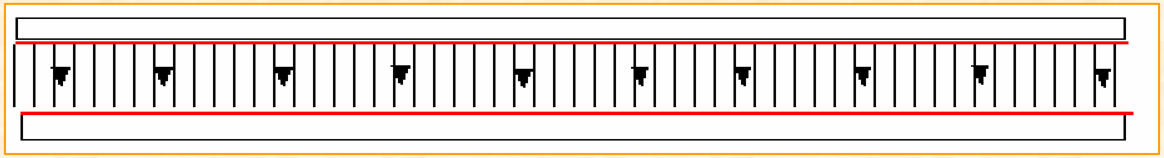


A discharge deposits charges on surface . These charges set up an electric field that opposes the applied field. Therefore, field is abruptly lowered in a localized region.

When voltage is reversed, the field is reinforced by the charge deposited during the preceding half-cycle. Therefore , it is most likely to get a discharge to occur in the position of a previous filament.

Regular Structure Formation as a Result of Streamer Interaction





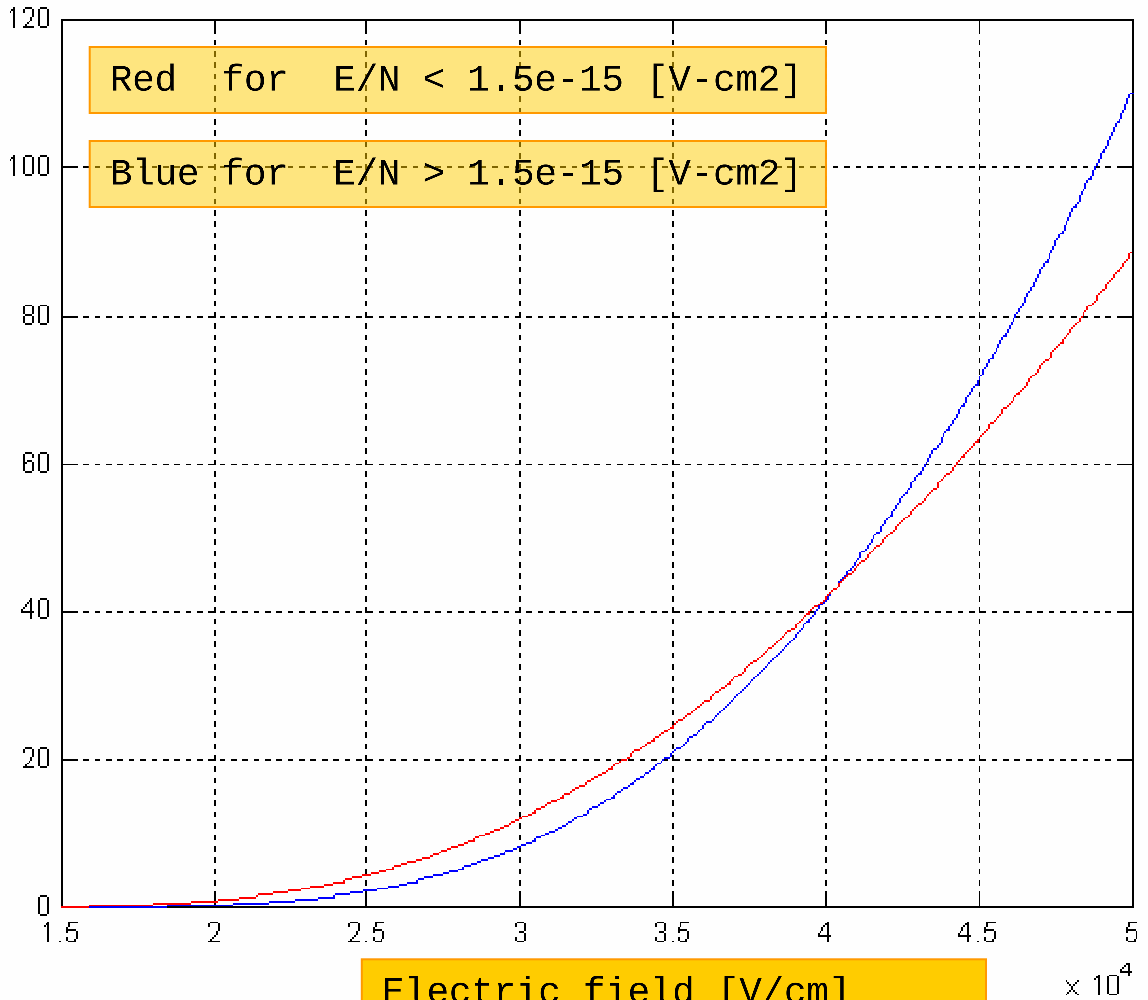
Meek streamer breakdown condition ($\alpha d \geq 20$)

$$\alpha d \cdot \left(\frac{E_0}{p}\right) = \ln\left(\frac{4\pi\varepsilon_0 E_0}{e\alpha^2}\right) \approx 20$$

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

Meek condition for streamer formation : $E' = E_0$

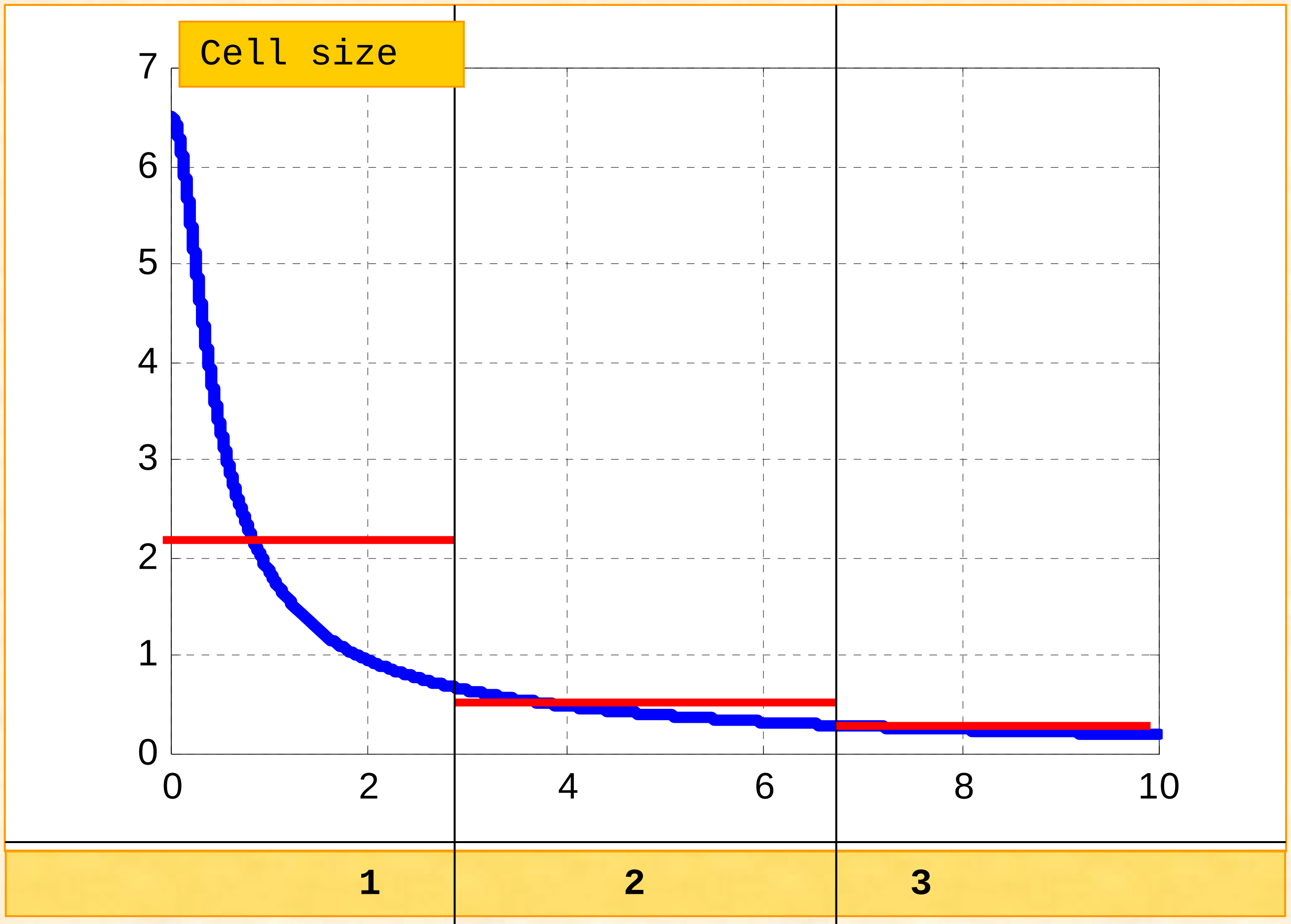
Ionization coefficient α [1/cm]



$$P = P_0 \cdot \exp\left(-\frac{(\alpha - \alpha_0)^2}{\alpha_0^{\,2}}\right)$$

Streamer formation probability

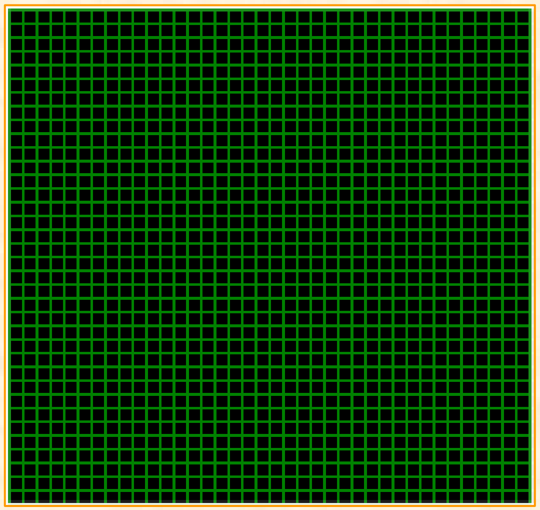
Relative decrease of Streamer Formation Probability vs. distance from streamer channel.



Electric field distortion influent by streamer channel

We divide distance from streamer into tree zones and assign probability of streamer strike in each zone using Electric field distortion from all streamers previous streamers and using Meek streamer breakdown condition.

Monte Carlo Simulation



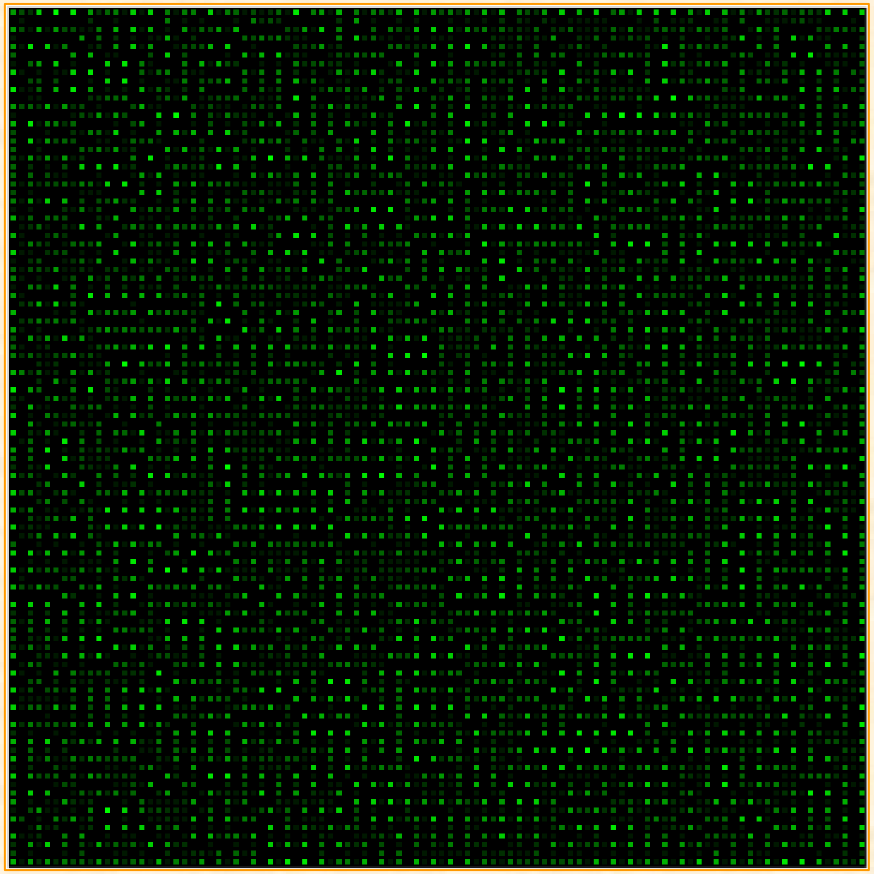
1. Divide discharge area into cells
2. Set probability of micro discharge for each cell
3. Choose location of first micro-discharge
4. Update probability for each cell
5. Choose location of next micro-discharge
6. Return to point 4

Parameters ...

Electrode	10.16*10.16 [cm2]	
Matrix	100*100	cells
Streamers	1e4-7.5e4 per period	
Streamers	4e6 - 3e7 per residence time(5 [m/sec] web moving vel.)	

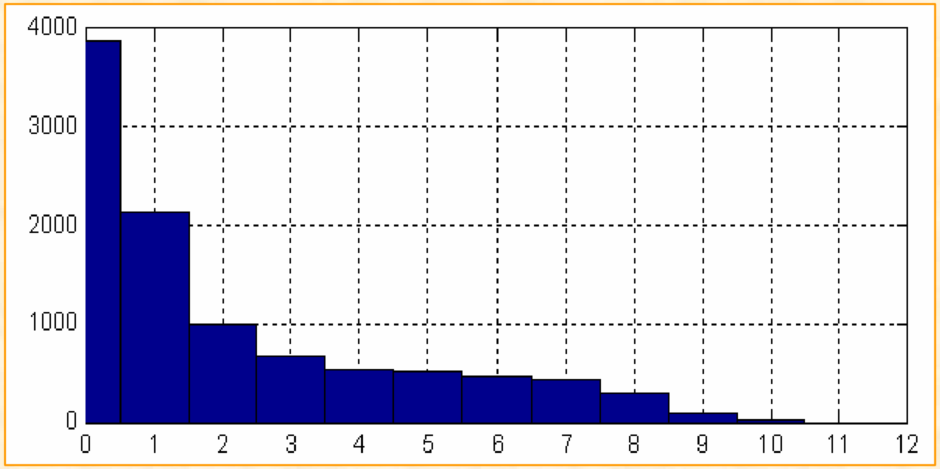
Example:
First steps of Monte Carlo Simulation on 20*20 Matrix

Monte Carlo Simulation



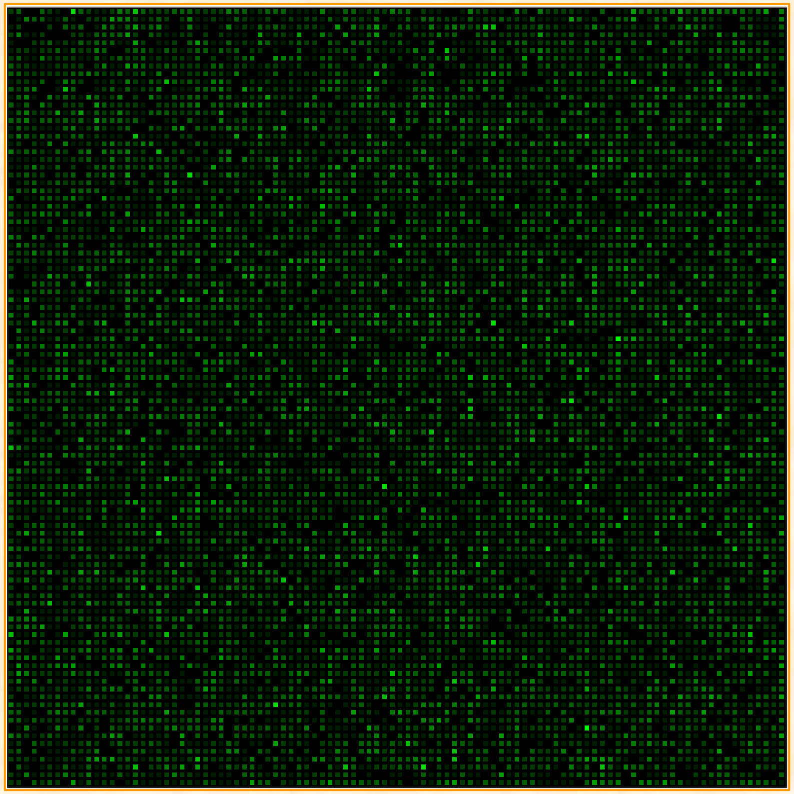
Cells	100*100
Strikes Count	2e4

Strikes Matrix histogram



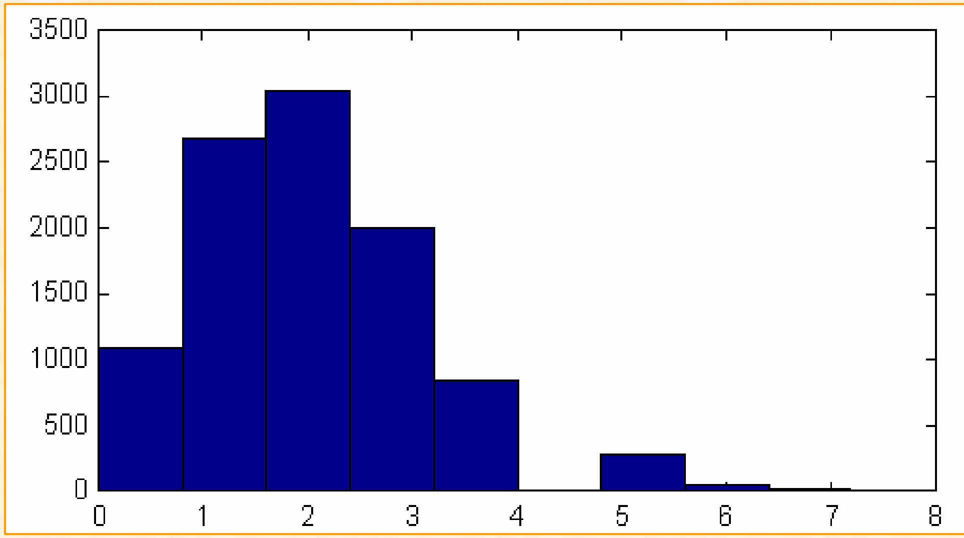
Brightness of points mean the number of streamers that strike in this area

Monte Carlo Simulation



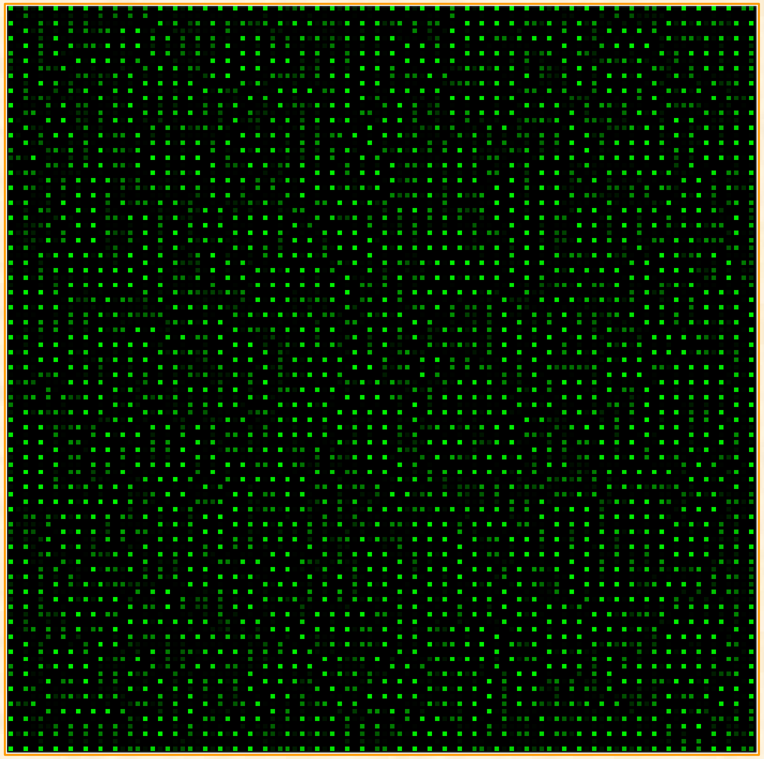
Spatial disorder effect of high applied voltage

Strikes Matrix histogram

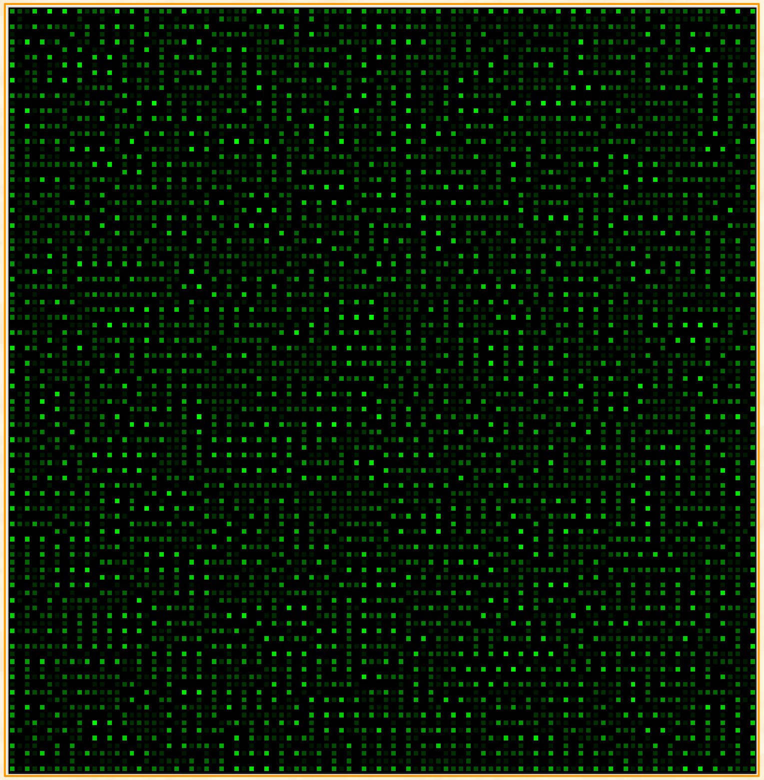


Cells	1e4
Strikes Count	2e4

Monte Carlo Simulation



Cells 100*100
Strikes Count 7.5e4



Cells 100*100
Strikes Count 2e4

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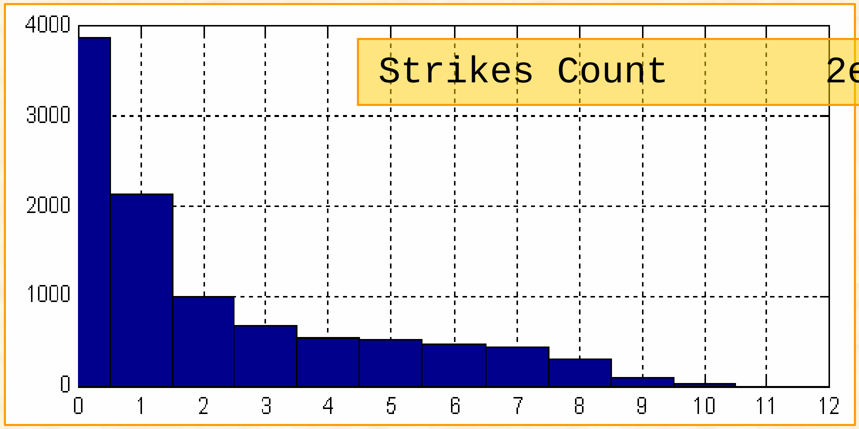
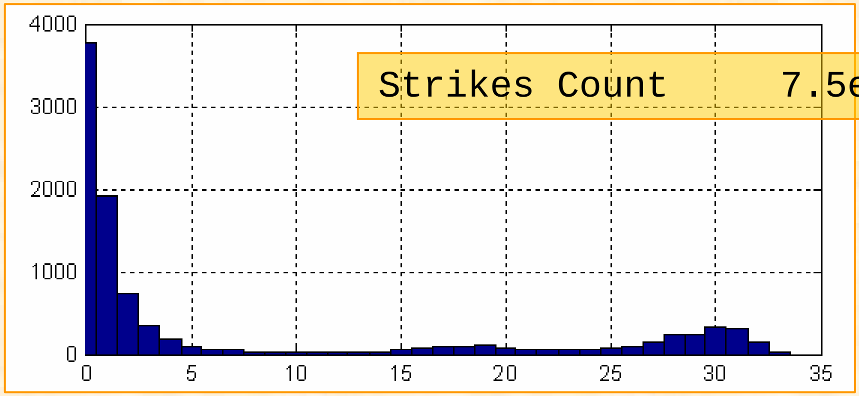
Monte Carlo Simulation

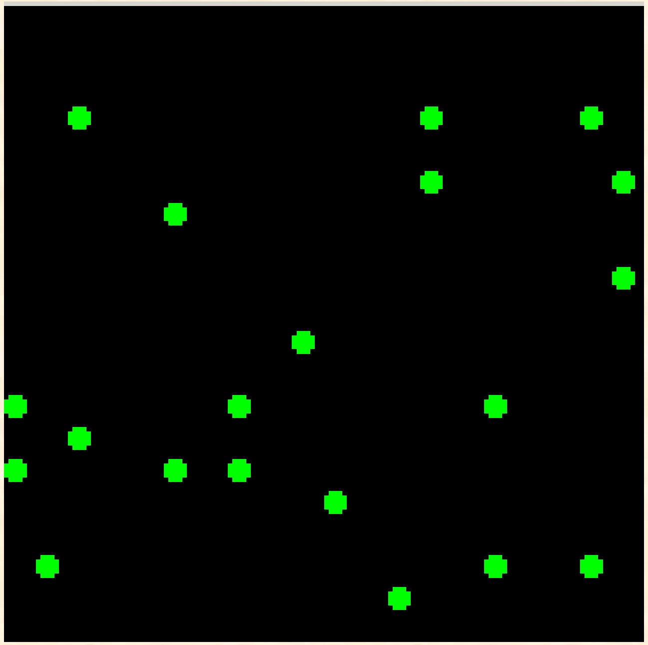
Strikes Matrix histogram



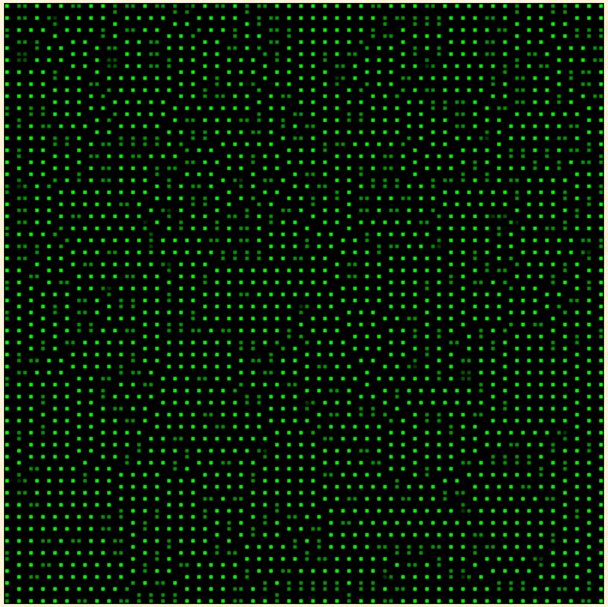


This histograms give us how many times was unit volume been treated by micro discharge.

Pattern formation example 20*20 cells 100 Monte Carlo steps every frame refresh



Monte Carlo Simulation

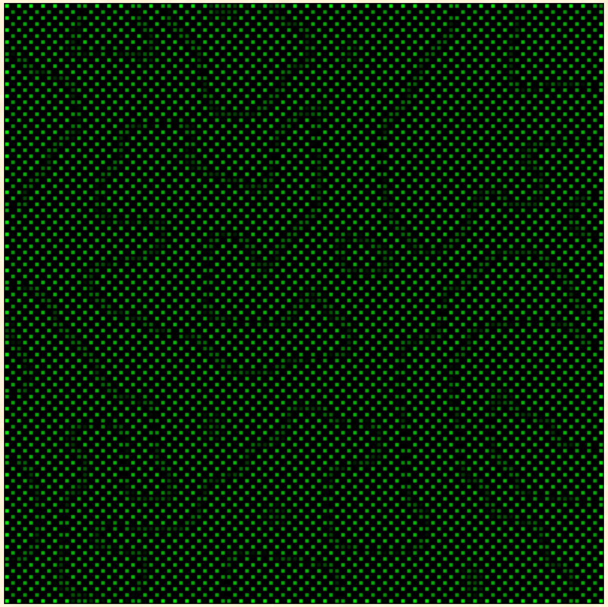


Simulation:

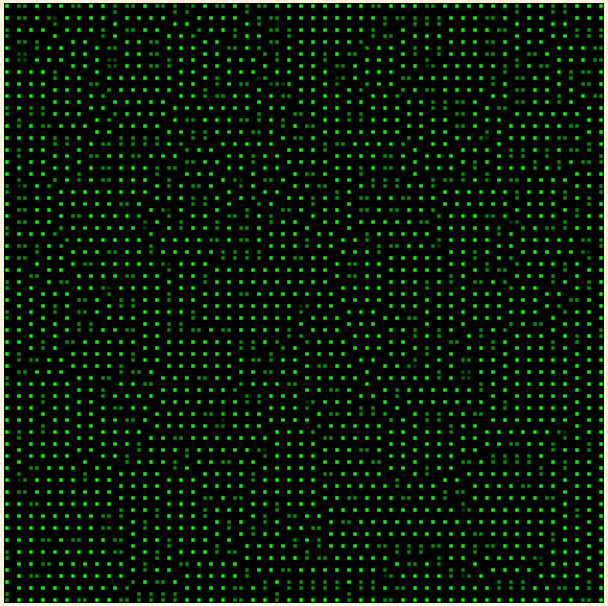
Streamers	3e7
Time residence time	20 [ms]
Power	50 [W]
Humidity [H2O]	40%

High Streamer Interaction

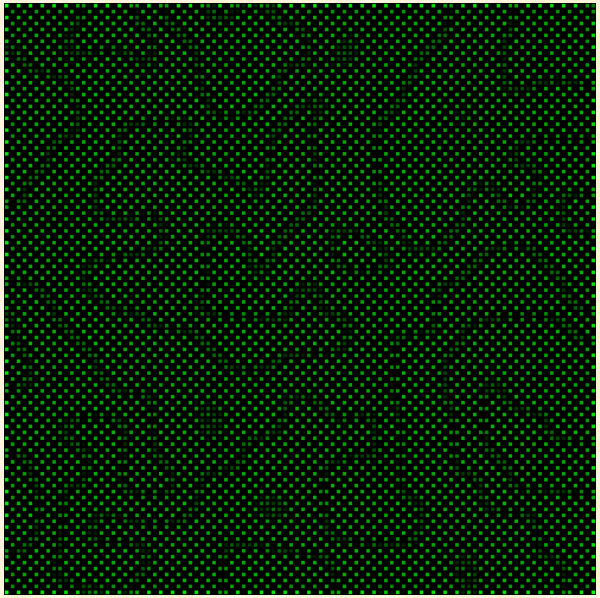
Low Streamer Interaction



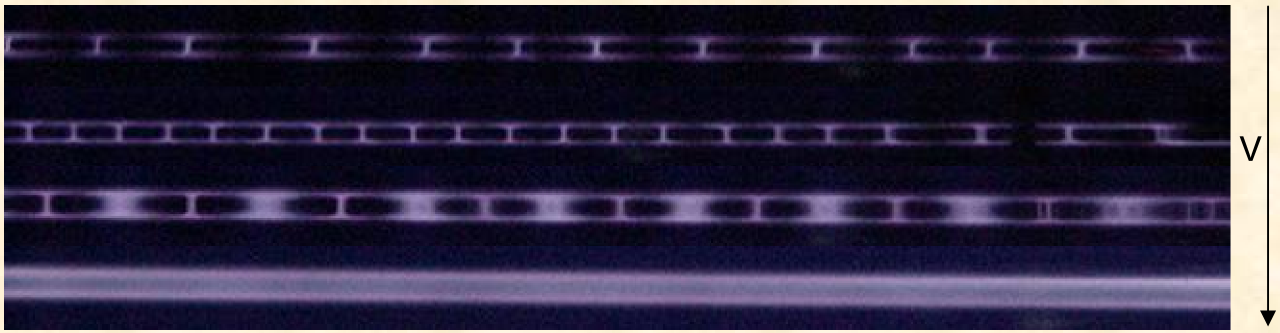
3e7 streamers



4e6 streamers

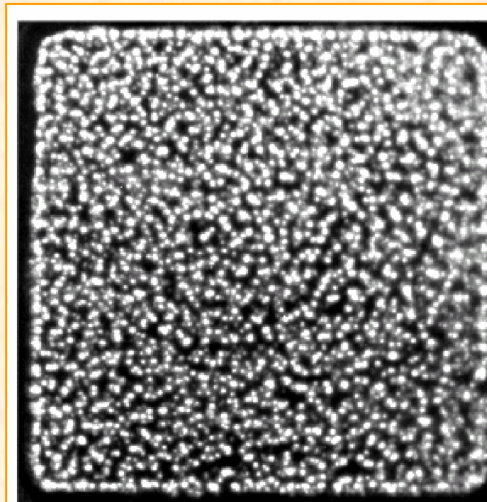


Experimental Evidence



Patterns for different applied voltage

A. narrow filaments with relatively wide separations
B. narrow filaments separated by roughly half of the typical Type A spacing
C. alternating bright, wide filaments and dim, narrow filaments.
D. Spatial disorder



B. Eliasson and U. Kogelschatz, IEEE Trans. Plasma Sci. **19**, 309 (1991).

Phys. Rev. Lett. 85, p. 3817 J. Guikema, N. Miller, J. Niehof, M. Klein, and M. Walhout.

Random Number Generator test

Standard Statistical Tests

- Birthday Spacing Test
- Chi-Squared Test
- Gap Test
- Kolomogorov-Smirnov Test
- Moments Test
- M-tuple Test
- Spectral Test
- Runs Test
- Uniformity Test

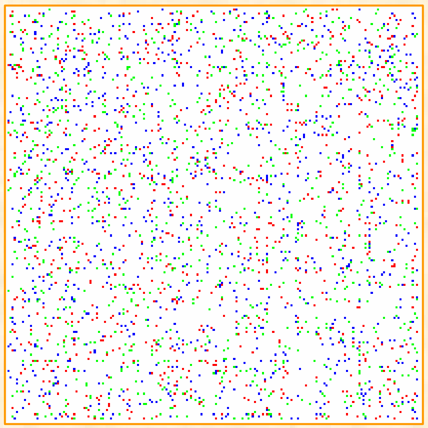
Monte Carlo Tests

- Ising Model using Metropolis Algorithm
- Ising Model using Swendsen-Wang Algorithm
- Ising Model using Wolff Algorithm
- Percolation
- Random Walk

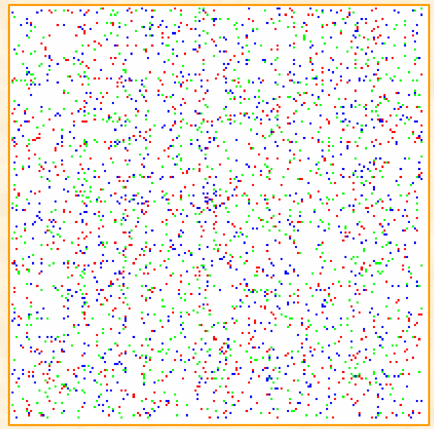
Long Period (2e18)random number generator of L'Ecuyer with Bays-Durhman shuffle was used in this Monte Carlo simulation.

Tested Generators: PIC, NR, MS

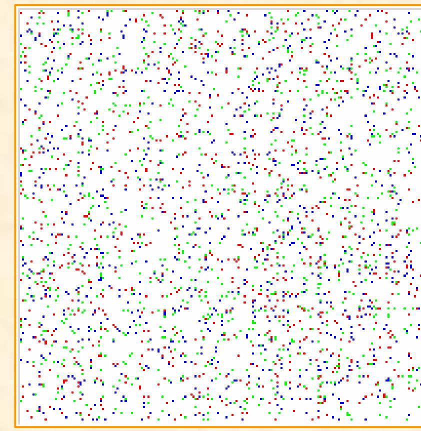
k-Space Correlation



PIC



NR



MS

NR Random number generator test for motion correlation patterns

PIC – generator used in Particle in Cell
NR - generator from Numerical Recipes
MS - system generator in Microsoft C++

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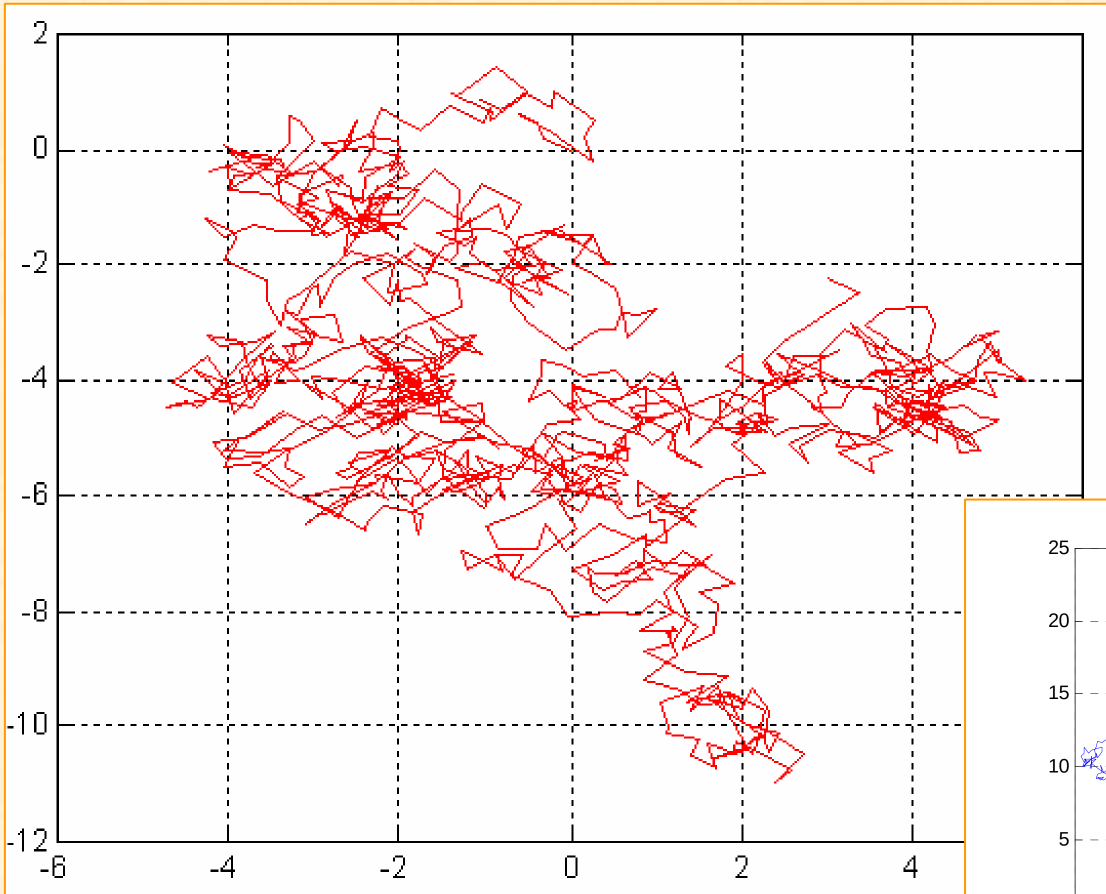
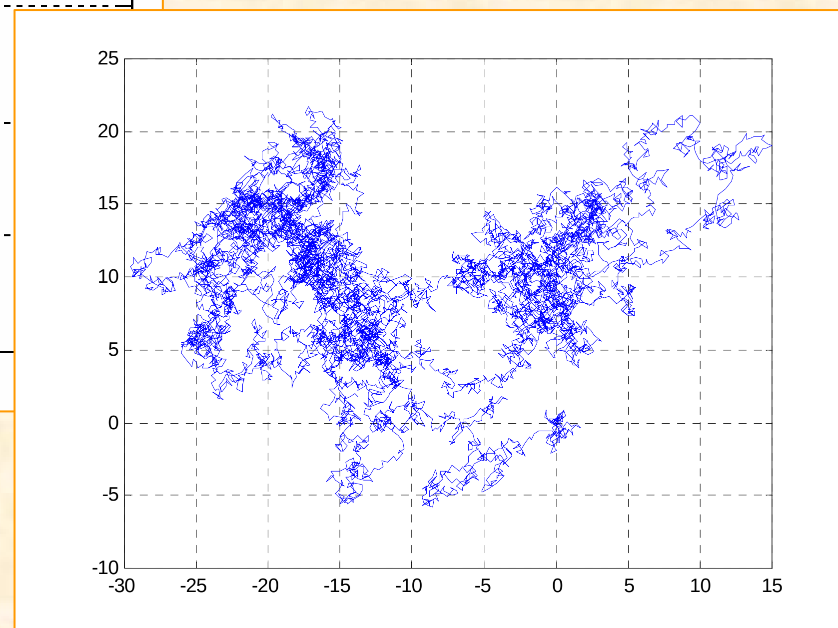
Random walk simulation

Steps: 1e3



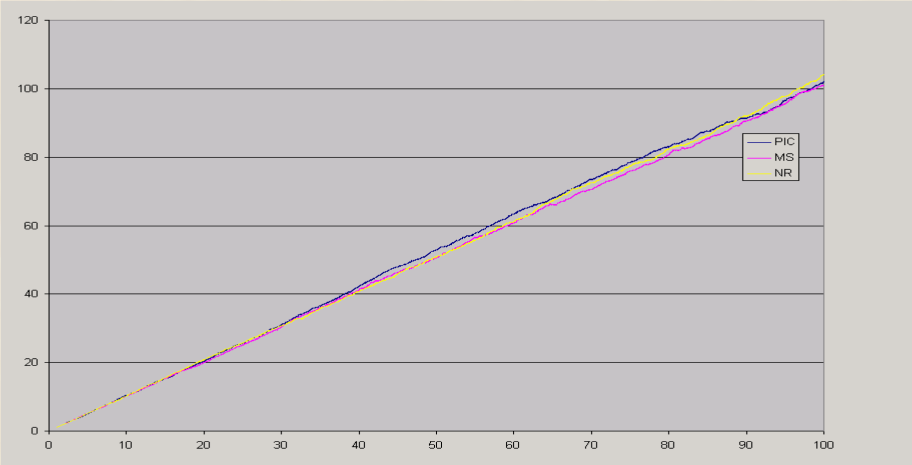
Steps: 1e4



$(\Delta x_1 \Delta y_1), (\Delta x_2 \Delta y_2), \ldots, (\Delta x_n \Delta y_n)$

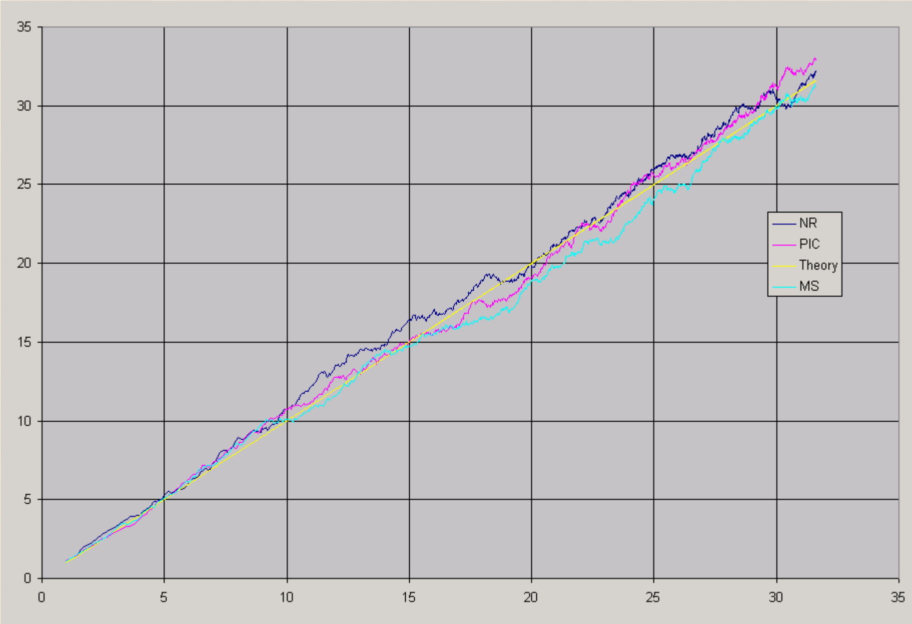
$R^2 = \Delta x_1^2 + \Delta x_2^2 + \ldots + \Delta x_n^2 + \Delta y_1^2 + \Delta y_2^2 + \ldots + \Delta y_n^2 = N < r^2 >$

$R = \sqrt{N} \cdot r_{rms}$



1e3 steps at each of
1e4 simulations

	angle	bias	R
NR	1.0312	**0.3047**	0.9996
PIC	1.0072	1.9007	0.9984
MS	**1.0011**	0.7238	**0.9997**



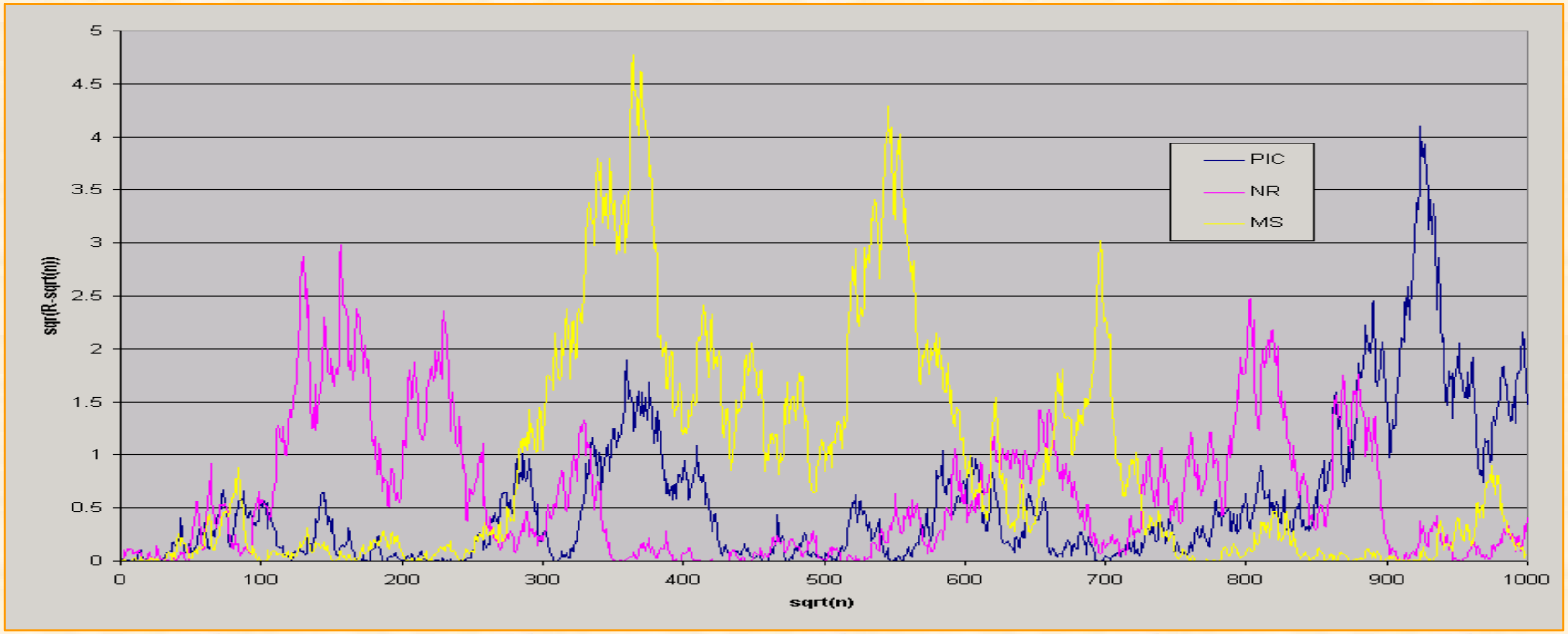
1e3 steps at each of
1e3 simulations

	angle	bias	R
NR	**0.9956**	0.6958	**0.9956**
PIC	1.0393	0.5677	0.9936
MS	0.9751	**0.1339**	0.9921

Random walk simulation

$$(\Delta x_1 \Delta y_1), (\Delta x_2 \Delta y_2), \ldots, (\Delta x_n \Delta y_n)$$
$$R^2 = \Delta x_1^2 + \Delta x_2^2 + \ldots + \Delta x_n^2 + \Delta y_1^2 + \Delta y_2^2 + \ldots + \Delta y_n^2 = N < r^2 >$$
$$R = \sqrt{N} \cdot r_{rms}$$

$(R - \sqrt{n})^2$



$\sqrt{n}$

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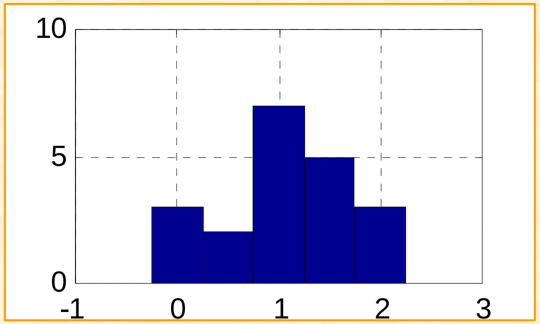
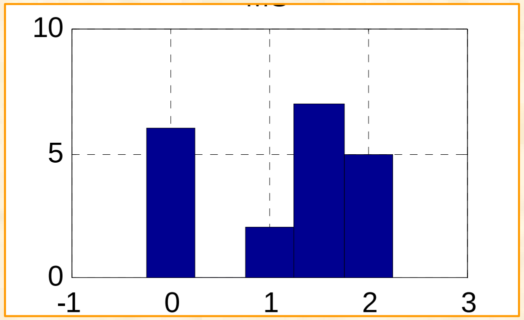
DIEHARD
a battery of tests of randomness

THE MINIMUM DISTANCE TEST

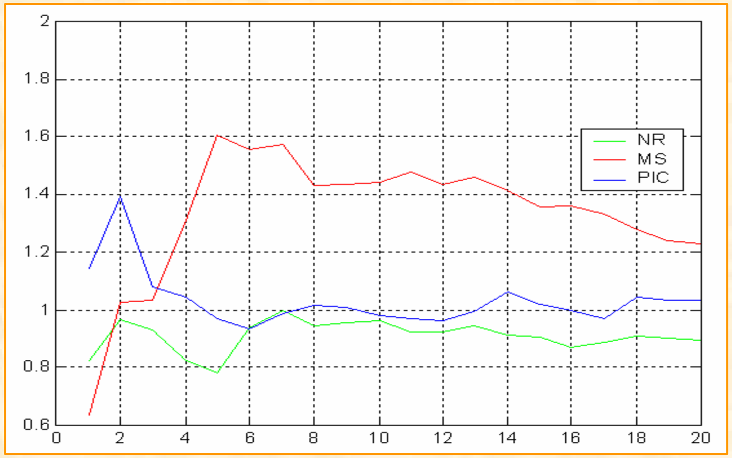
It does this 100 times choose n=8000 random points in a square of side 10000. Find d, the minimum distance between the (n^2-n)/2 pairs of points. If the points are truly independent uniform, then d^2, the square of the minimum distance should be (very close to) exponentially distributed with mean .995 Thus 1-exp(-d^2/.995) should be uniform on [0,1).

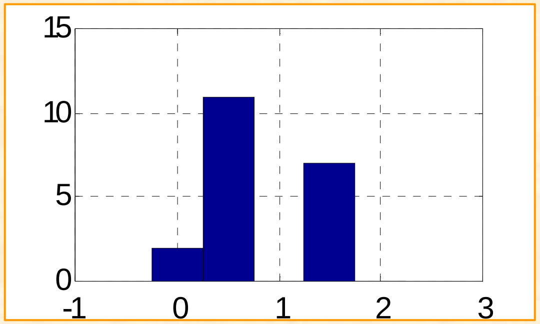


NR



MS





PIC

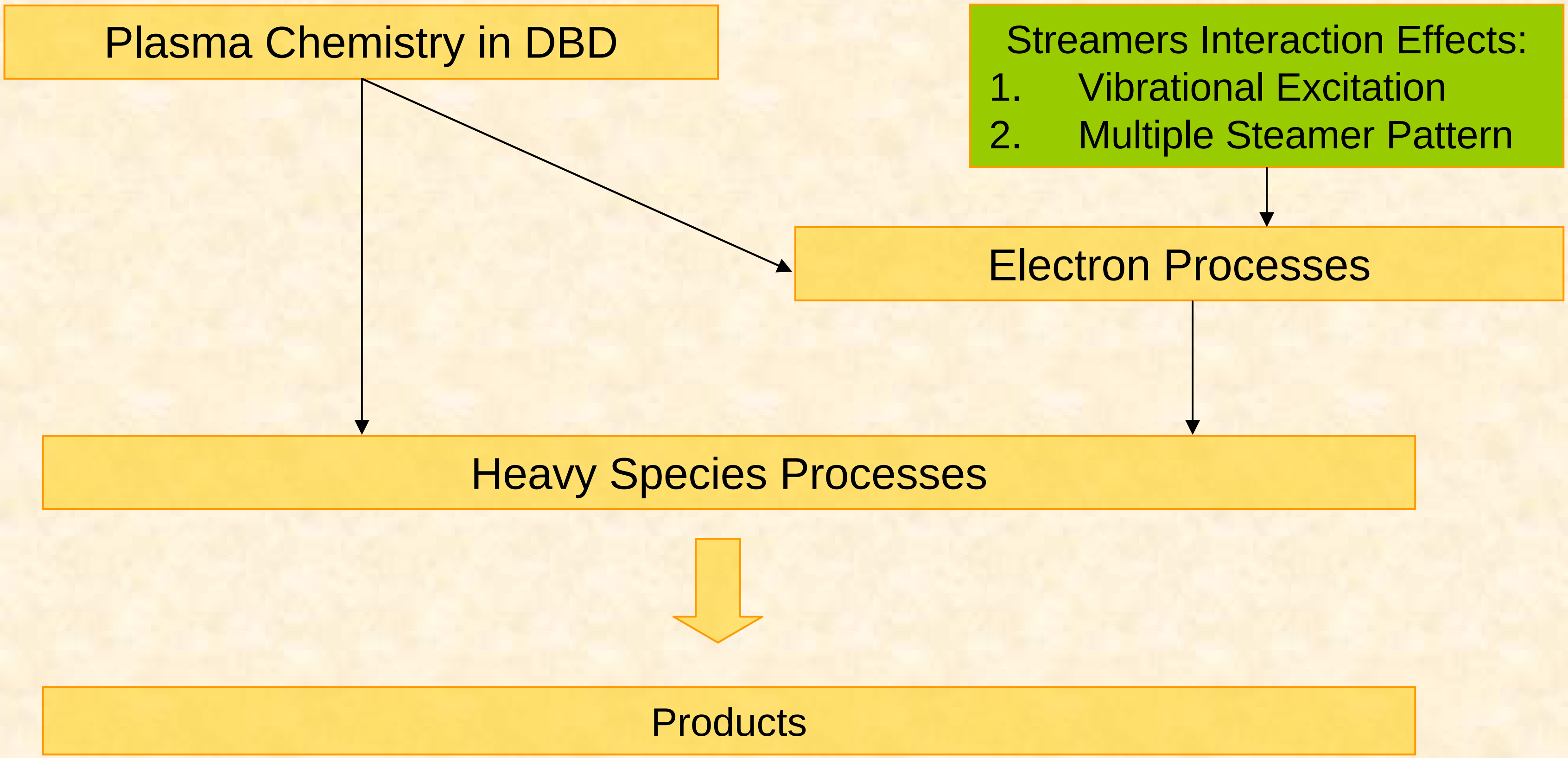
Author of DIEHARD:
George Marsaglia

Average should be 0.995

	mean	d	SDT
NR	0.9090	0.0860	**0.0535**
PIC	**1.0312**	**0.0362**	0.0971
MS	1.3310	0.3360	0.2258

Plasma Chemistry Modeling

University of Illinois at Chicago



SPECIES INVOLVED IN THE MECHANISM

57 – species ; 327 - reactions

SPECIES INVOLVED IN THE MECHANISM

57 – species ; 327 - reactions

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

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Mechanism was taken from "KINEMA" Research and Software Com. kinema.com

REACTIONS CONSIDERED

		A	b	E
1.	O2+E=>O2++2E	1.76E+14	0.0	0.0
2.	O2+E=>O2a1D+E	2.88E+15	0.0	0.0
3.	O2+E=>O2B1S+E	2.88E+15	0.0	0.0
4.	O2+E=>O2-	6.00E-08	0.0	0.0
5.	O+E=>O++2E	5.40E+15	0.0	0.0
6.	O+E=>O1D+E	2.52E+15	0.0	0.0
7.	O+E=>O1S+E	2.52E+15	0.0	0.0
8.	N2a+E=>N2++2E	1.32E+17	0.0	0.0
9.	N2A+E=>N2++2E	1.32E+17	0.0	0.0
10.	NO2++E=>NO+O	1.20E+15	0.0	0.0
11.	NO2++E=>NO+O1D	1.20E+15	0.0	0.0
12.	E+NO2=>NO2-	2.40E+16	0.0	0.0
13.	N2+E=>N2A+E	5.10E+13	0.0	0.0
14.	N2+E=>N2a+E	5.10E+13	0.0	0.0
15.	N2+E=>N2++2E	3.99E+11	0.0	0.0
16.	O2+E=>O+O+E	8.60E+14	0.0	0.0
17.	O2+E=>O-+O	3.62E+13	0.0	0.0
18.	O2a1D+E=>O+O+E	2.88E+17	0.0	0.0
19.	O2a1D+E=>O2++2E	2.88E+17	0.0	0.0
20.	O2B1S+E=>O+O+E	2.88E+17	0.0	0.0
21.	O2B1S+E=>O2++2E	2.88E+17	0.0	0.0
22.	N2O+E=>N2+O-	2.88E+17	0.0	0.0
23.	NO++E=>N+O1D	2.40E+13	0.0	0.0
24.	O3+E=>O3++2E	3.00E+14	0.0	0.0
25.	H2O+E=>H+OH+E	3.18E+13	0.0	0.0

Note: A [mole-cm-sec-K]
E [cal/mole].

(k = A T**b exp(-E/RT))

In the reactions with electrons, the temperature used is the electron temperature(Te=2eV).

26. H2O+E=>O1D+H2+E	3.54E+13	0.0	0.0
27. H2O+E=>H2O++2E	3.90E+13	0.0	0.0
28. H2O+E=>OH-+H	1.50E+14	0.0	0.0
29. H2O+E=>H-+OH	1.50E+14	0.0	0.0
30. H2O+E=>H2+O-	1.50E+14	0.0	0.0
Electron "temperature" dependent processes			
Recombination			
31. E+N2+=>N+N	3.24E+16	-0.4	0.0
32. E+N2++O2=>N2+O2	6.00E-03	0.0	0.0
33. E+O2+=>O+O	1.62E+16	-0.6	0.0
34. E+O2+=>O+O1D	1.17E+17	0.0	0.0
35. E+O2++O2=>O2+O2	4.80E-05	0.0	0.0
36. E+NO+=>N+O	3.96E+16	-0.5	0.0
37. E+NO++O2=>NO+O2	1.86E+01	-1.5	0.0
38. E+N4+=>N2+N+N	1.20E+18	0.0	0.0
39. E+O4+=>O2+O+O	1.20E+18	0.0	0.0
40. E+O4+=>O2+O2	6.60E+16	0.0	0.0
41. E+O++E=>O+E	5.25E-03	-4.5	0.0
42. E+H2O+=>H+OH	6.60E+17	-0.5	0.0
43. E+H2O+=>O+H2	2.28E+17	-0.5	0.0
44. E+H2O+=>O+H+H	2.88E+17	-0.5	0.0
45. E+H3O+=>H2O+H	1.32E+18	-0.1	0.0
Attachment:			
46. E+O2+O2=>O2-+O2	1.32E-06	0.0	0.0
47. E+O2+N2=>O2-+N2	6.00E-08	0.0	0.0
48. E+O+O2=>O-+O2	6.00E-08	0.0	0.0
49. E+O+N2=>O-+N2	6.00E-08	0.0	0.0
50. E+HO2=>H+O2-	3.00E+15	0.0	0.0
51. E+NO2=>O-+NO	2.04E+14	-2.4	3.0
52. E+O3=>O-+O2	6.00E+12	0.0	0.0
53. E+O=>O-	7.80E+08	0.0	0.0

54.	E+O3+O2=>O3-+O2	2.76E-04	0.0	0.0
55.	E+NO=>O-+N	2.04E+18	-8.2	15.2
56.	E+NO+N2=>NO-+N2	2.40E-05	0.0	0.0
57.	E+HNO2=>NO2-+H	3.00E+16	0.0	0.0
58.	E+HNO3=>NO2-+OH	3.00E+16	0.0	0.0
59.	E+N2O+N2=>N2O-+N2	1.80E-09	0.0	0.0
Dissociation				
60.	E+O3=>O2+O+E	1.34E+16	0.0	0.0
Atomic & Molecular Reactions: Neutral Chemistry				
61.	O+O+N2=>O2+N2	3.90E-11	0.0	-1039.0
62.	O+O+N=>O2+N	3.90E-11	0.0	-1039.0
63.	O+O2+O2=>O3+O2	1.45E-10	-1.0	-238.9
64.	O+O2+N2=>O3+N2	1.45E-10	-1.0	-238.9
65.	O+O2+O3=>O3+O3	8.58E-10	-2.0	0.0
66.	O+O2+O=>O3+O	1.29E-10	0.0	-345.0
67.	O+O3=>2O2	9.17E+12	0.0	2185.0
68.	O+NO+N2=>NO2+N2	6.38E-08	-1.7	46.3
69.	O+NO+O2=>NO2+O2	6.38E-08	-1.7	46.3
70.	O+NO=>NO2	1.33E+13	0.5	-92.6
71.	O+NO=>O2+N	2.53E+13	0.0	23200.0
72.	O+NO2=>O2+NO	5.45E+12	0.2	0.0
73.	O+NO2=>NO3	1.32E+13	0.0	0.0
74.	O+NO2+N2=>NO3+N2	6.39E-08	-2.2	46.6
75.	O+NO2+O2=>NO3+O2	6.39E-08	-2.2	46.6
76.	O+NO3=>O2+NO2	6.00E+12	0.0	0.0
77.	N+N+N2=>N2+N2	4.96E-10	0.0	-500.0
78.	N+N+N=>N2+N	1.40E-09	0.0	-500.0
79.	N+NO=>N2+O	2.11E+13	0.0	49.8
80.	N+O2=>NO+O	6.01E+12	0.0	3473.0
81.	N+NO2=>N2O+O	1.80E+12	0.0	0.0

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82.	N+O3=>NO+O2	6.00E+07	0.0	0.0
83.	NO+O3=>O2+NO2	2.58E+12	0.0	1560.0
84.	NO2+O3=>NO3+O2	1.14E+11	0.0	2542.0
85.	NO3+O3=>2O2+NO2	7.20E+10	0.0	2450.0
86.	NO+NO2+N2=>N2O3+N2	5.47E-09	0.0	0.0
87.	NO+NO2=>N2O3	2.04E+12	0.0	0.0
88.	NO+NO3=>2NO2	6.66E+12	0.0	-220.9
Neutral Chemistry:				
89.	H+O2=>O+OH	7.01E+13	0.3	7860.0
90.	H+O2+1H2=>1HO2+1H2	3.47E-08	-0.8	0.0
91.	H+O2+1N2=>1HO2+1N2	3.56E-08	-1.0	0.0
92.	H+O2+1O2=>1HO2+1O2	3.56E-08	-1.0	0.0
93.	H+OH+1N2=>1H2O+1N2	3.56E-08	-1.0	0.0
94.	H+OH+1O2=>1H2O+1O2	4.13E-07	-2.0	0.0
95.	H+OH+H2O=>H2O+H2O	2.62E-06	-2.0	0.0
96.	H+NO2=>NO+OH	1.32E+14	0.0	182.0
97.	H+1O3=>1O2+1OH	4.67E+13	0.3	327.8
98.	H+1O3=>1HO2+1O	4.50E+11	0.0	0.0
99.	H+1HO2=>1H2+1O2	1.54E+13	0.6	346.0
100.	H+1HO2=>1OH+1OH	1.41E+14	0.0	373.7
101.	H+1HO2=>1H2O+1O	5.51E+13	0.0	971.9
102.	H+1O2=>1HO2	4.50E+13	0.0	0.0
103.	H+1OH=>1H2O	1.62E+10	0.0	0.0
104.	H+HNO=>H2+NO	2.56E+12	0.0	-998.1
105.	H+1HNO=>1OH+1NH	1.45E+15	-0.5	9010.0
106.	H+1HNO=>1O+1NH2	6.30E+14	-0.3	14730.0
107.	H+1NO=>1NH+1O	5.57E+14	-0.1	35220.0
108.	H+1NO=>1OH+1N	1.27E+14	0.0	24330.0
109.	H+1NO+1N2=>1HNO+1N2	4.40E-08	-1.3	184.3

110.	H+1NO+1O2=>1HNO+1O2	4.40E-08	-1.3	184.3
111.	H+1NO3=>1NO2+1OH	6.60E+13	0.0	0.0
112.	H+1H2O2=>1OH+1H2O	2.40E+13	0.0	2000.0
113.	H+1H2O2=>1H2+1HO2	4.80E+13	0.0	4000.0
114.	OH+1OH=>1H2O+1O	9.29E+10	1.4	-267.3
115.	OH+1O=>1O2+1H	1.26E+13	-0.2	153.9
116.	OH+1H=>1H2+1O	6.74E+09	3.4	1233.0
117.	OH+1H2=>1H2O+1H	1.39E+12	1.5	1761.0
118.	OH+1O3=>1HO2+1O2	8.83E+11	0.0	932.7
119.	OH+1HO2=>1H2O+1O2	2.63E+13	0.0	-110.9
120.	OH+1OH+1N2=>1H2O2+1N2	3.63E-07	-3.0	0.0
121.	OH+1OH+1O2=>1H2O2+1O2	3.63E-07	-3.0	0.0
122.	OH+1OH+1H2O=>1H2O2+1H2O	9.26E-08	-2.0	-183.6
123.	OH+1H2O2=>1H2O+1HO2	2.72E+12	0.0	288.9
124.	OH+1HNO2=>1H2O+1NO2	1.08E+13	0.0	390.0
125.	OH+1N2O=>1HO2+1N2	2.22E+11	0.0	2740.0
126.	OH+1OH=>1H2O2	9.06E+12	-0.4	0.0
127.	OH+1NO+1N2=>1HNO2+1N2	2.35E-08	0.0	-794.2
128.	OH+1NO+1O2=>1HNO2+1O2	2.35E-08	0.0	-794.2
129.	OH+1NO2=>1HO2+1NO	1.98E+13	0.0	3360.0
130.	OH+1NO2+1N2=>1HNO3+1N2	5.03E-06	-3.9	409.3
131.	OH+1NO2+1O2=>1HNO3+1O2	5.03E-06	-3.9	409.3
132.	OH+1NO3=>1HO2+1NO2	1.38E+13	0.0	0.0
133.	OH+1HNO=>1H2O+1NO	7.60E+12	1.0	334.2
134.	OH+1HNO3=>1H2O+1NO3	2.40E+10	0.0	-317.6
135.	HO2+1O3=>1OH+2O2	1.05E+09	0.0	-628.3
136.	HO2+1HO2=>1H2O2+1O2	1.80E+12	0.0	0.0
137.	HO2+1O=>1OH+1O2	1.74E+13	0.0	-200.0
138.	2HO2+N2=>H2O2+O2+N2	1.14E-09	0.0	-980.0

139.	HO2+1HO2+1O2=>H2O2+2O2	1.14E-09	0.0	-980.0
140.	HO2+1NO=>1O2+1HNO	5.46E+05	0.0	-2819.0
141.	HO2+1NO=>1OH+1NO2	2.10E+12	0.0	-240.0
142.	HO2+1NO2=>1HNO2+1O2	7.20E+10	0.0	0.0
143.	HO2+1NO=>1HNO3	8.40E+10	0.0	0.0
144.	HO2+1N=>1OH+1NO	1.32E+13	0.0	0.0
145.	HO2+1NO3=>1HNO3+1O2	5.53E+11	0.0	0.0
146.	N+1OH=>1NO+1H	2.35E+13	0.0	-72.4
147.	N+1OH=>1O+1NH	1.13E+13	0.1	10700.0
148.	O+1H2=>1OH+1H	9.01E+10	2.8	2834.0
149.	O+1H2O2=>1OH+1HO2	1.08E+11	2.9	1394.0
150.	N2O3+1H2O=>2HNO2	3.78E+13	0.0	4468.0
151.	HNO2+1O=>1OH+1NO2	6.00E+08	0.0	0.0
152.	HNO3+1O=>1OH+1NO3	1.80E+07	0.0	0.0
153.	HNO2+1NO3=>1HNO3+1NO2	1.20E+09	0.0	0.0
154.	H2O2+1NO3=>1HO2+1HNO3	1.20E+09	0.0	0.0
Excited State Chemistry				
155.	N2A+H2O=>H2+N+NO	6.00E+13	0.0	0.0
156.	N2a+H2O=>H2+N+NO	6.00E+13	0.0	0.0
157.	O1D+H2O=>OH+OH	1.20E+14	0.0	0.0
158.	O1D+H2=>OH+H	1.98E+14	0.0	0.0
159.	O1D+H2O2=>H2O+O2	3.12E+14	0.0	0.0
160.	O1S+H2O=>O+H2O	1.80E+14	0.0	0.0
161.	O1S+H2O=>OH+OH	3.00E+14	0.0	0.0
162.	O1S+H2O=>H2+O2	3.00E+14	0.0	0.0
163.	O2a1D+H2O=>O2+H2O	3.00E+06	0.0	0.0
164.	O2B1S+H2O=>O2+H2O	2.40E+12	0.0	0.0
Ion - Molecule: Positive Ion				
165.	O++H2=>OH++H	6.00E+13	0.0	0.0
166.	O++H2O=>H2O++O	1.56E+15	0.0	0.0
167.	O2++2H2O=>H3O++OH+O2	1.20E-04	0.0	0.0

168. O4++2H2O=>H3O++OH+2O2	1.20E-04	0.0	0.0
169. N2++H2O=>H2O++N2	1.32E+15	0.0	0.0
170. H2O++O2=>H2O+O2+	1.98E+14	0.0	0.0
171. H2O++H2O=>H3O++OH	1.11E+15	0.0	0.0
172. OH++O2=>OH+O2+	2.28E+14	0.0	0.0
173. NO++2H2O=>H3O++HNO2	1.20E-04	0.0	0.0
Negative Ion			
174. O-+H2=>H2O+E	3.90E+14	0.0	0.0
175. O2-+1H2O=>1O2+1H2O+E	3.00E+15	0.0	5000.0
176. OH-+1O3=>1OH+1O3-	3.00E+14	0.0	0.0
177. OH-+1O3=>1O2-+1HO2	6.00E+12	0.0	0.0
178. H-+1H2O=>1OH-+1H2	6.00E+14	0.0	0.0
Ionic Recombination			
179. H3O++NO2-=>H2O+OH+NO	1.13E+18	0.0	0.0
180. H3O++O3-=>H2O+OH+O2	6.00E+17	0.0	0.0
Electron temperature			
181. H2O+O2+E=>O2-+H2O	8.40E-06	0.0	0.0
Atomic & Molecular Reactions: Excited State Chemistry			
182. N2a+N2a=>N2+N2++E	6.00E+13	0.0	0.0
183. N2a+O2=>N2+2O	1.68E+13	0.0	0.0
184. N2a+N2=>N2+N2	1.20E+11	0.0	0.0
185. N2a+NO=>N2+N+O	2.16E+14	0.0	0.0
186. N2A+N2=>N2+N2	1.80E+06	0.0	0.0
187. N2A+O2=>N2+2O	7.74E+11	0.0	0.0
188. N2A+O2=>N2O+O	4.68E+10	0.0	0.0
189. N2A+NO=>N2+NO	4.20E+13	0.0	0.0
190. N2A+O=>NO+N	4.20E+12	0.0	0.0
191. N2A+O=>N2+O1S	1.26E+13	0.0	0.0
192. N2A+N=>N2+N	3.00E+13	0.0	0.0
193. N2A+N2O=>N2+N+NO	6.00E+12	0.0	0.0
194. O1D+N2=>O+N2	1.08E+13	0.0	-107.0
195. O1D+O2=>O+O2B1S	1.54E+13	0.0	-67.0
196. O1D+O2=>O+O2a1D	6.00E+11	0.0	0.0

197.	O1D+NO=>O2+N	1.02E+14	0.0	0.0
198.	O1D+NO2=>O2+NO	1.80E+14	0.0	0.0
199.	O1D+N2O=>NO+NO	4.32E+13	0.0	0.0
200.	O1D+N2O=>N+NO2	1.47E+11	0.0	0.0
201.	O1D+N2O=>N2+O2	2.94E+13	0.0	0.0
202.	O1D+O3=>2O+O2	7.20E+22	0.0	0.0
203.	O1D+O3=>2O2	1.44E+14	0.0	0.0
204.	O1D+O3=>O+O3	1.44E+14	0.0	0.0
205.	O1D+O3=>O2B1S+O2	2.16E+13	0.0	0.0
206.	O1S+NO=>O2+N	3.00E+14	0.0	0.0
207.	O1S+O2=>O2+O	1.80E+11	0.0	850.0
208.	O1S+O3=>O2+O+O1D	1.74E+14	0.0	0.0
209.	O1S+O3=>2O2	5.40E+13	0.0	0.0
210.	O1S+O2a1D=>O2+O1D	3.60E+12	0.0	0.0
211.	O1S+O2a1D=>3O	2.40E+12	0.0	0.0
212.	O1S+O2a1D=>O+O2B1S	7.80E+13	0.0	0.0
213.	O1S+O=>O+O1D	3.00E+12	0.0	301.0
214.	O2a1D+N=>O+NO	1.20E+10	0.0	600.0
215.	O2a1D+O=>O+O2	4.20E+10	0.0	0.0
216.	O2a1D+NO=>NO+O2	1.50E+13	0.0	0.0
217.	O2a1D+O3=>2O2+O	1.43E+12	0.0	2876.0
218.	O2a1D+O2=>O2+O2	1.32E+23	0.8	0.0
219.	O2a1D+N2=>O2+N2	8.40E+04	0.0	0.0
220.	O2a1D+NO=>O+NO2	2.93E+06	0.0	0.0
221.	O2B1S+N2=>O2a1D+N2	2.94E+09	0.0	253.0
222.	O2B1S+O2=>O2a1D+O2	2.24E+08	2.4	241.0
223.	O2B1S+O3=>2O2a1D+O	1.08E+13	0.0	0.0
224.	O2B1S+O=>O2+O	4.80E+10	0.0	0.0
225.	O2B1S+NO=>O2a1D+NO	2.40E+10	0.0	0.0

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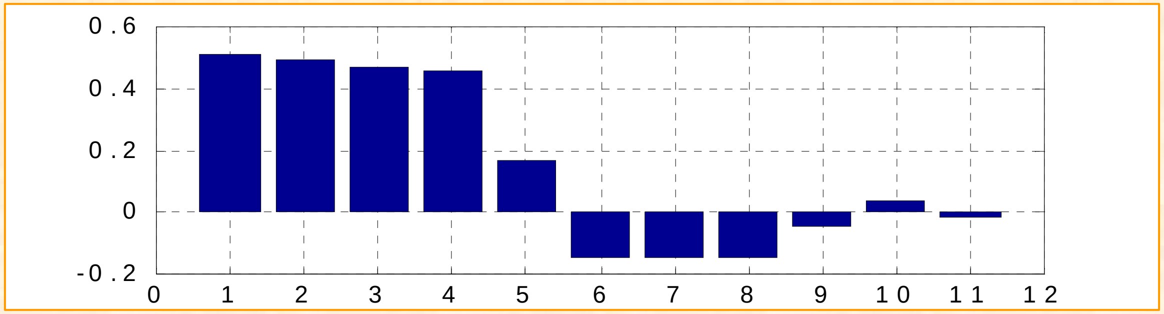
Ion - Molecule Reactions: Positive Ions				
226.	O++N2=>NO++N	1.80E+23	0.0	0.0
227.	O2++NO=>O2+NO+	2.64E+14	0.0	0.0
228.	O2++O2+N2=>O4++N2	1.44E+21	-3.2	0.0
229.	O2++O2+N=>O4++N	1.44E-06	-3.2	0.0
230.	O2++N=>NO++O	7.20E+13	0.0	0.0
231.	O2++N2=>NO++NO	6.00E+06	0.0	0.0
232.	O3++O2=>O2++O3	6.00E+12	0.0	0.0
233.	O4++O2a1D=>O2++O2+O2	6.00E+13	0.0	0.0
234.	O4++O2B1S=>O2++O2+O2	6.00E+13	0.0	0.0
235.	O4++NO=>NO++O2+O2	6.00E+13	0.0	0.0
236.	O4++O=>O3++1O2	1.80E+14	0.0	0.0
237.	O4++O=>O2++1O3	1.80E+14	0.0	0.0
238.	O4++O2=>O2++O2+O2	1.20E+11	0.0	0.0
239.	N2++O=>N2+O+	6.00E+12	-0.2	0.0
240.	N2++O=>NO++N	7.80E+13	-0.5	0.0
241.	N2++O2=>N2+O2+	3.60E+13	-0.5	0.0
242.	N2++NO=>N2+NO+	1.98E+14	0.0	0.0
243.	N2++N2+N2=>N4++N2	3.00E-05	-1.0	0.0
244.	N2++N2+N=>N4++N	3.00E-05	-1.0	0.0
245.	N4++O2=>O2++N2+N2	1.50E+14	0.0	0.0
246.	N4++O=>O++N2+N2	1.50E+14	0.0	0.0
Negative Ions				
247.	1O-+1N2=>1N2O+1E	6.00E+11	0.0	0.0
248.	O-+1O2=>1O3+1E	3.00E+09	0.0	0.0
249.	O-+1O=>1O2+1E	3.00E+14	0.0	0.0
250.	O-+1N=>1NO+1E	1.56E+14	0.0	0.0
251.	O-+1N2A=>1O+1N2+1E	1.32E+15	0.0	0.0
252.	O-+1O2a1D=>1O3+1E	1.80E+14	0.0	0.0
253.	O-+1O3=>2O2+1E	3.18E+14	0.0	0.0

254.	O-+1NO=>1NO2+1E	1.56E+14	0.0	0.0
255.	O-+1N2O=>1NO-+1NO	1.26E+14	0.0	0.0
256.	O-+1NO2=>1O+1NO2-	7.20E+14	0.0	0.0
257.	O-+1NO2=>1O2-+1NO	1.20E+13	0.0	0.0
258.	O-+1O2+1O2=>1O3-+1O2	6.60E-07	0.0	0.0
259.	O-+1O3=>1O3-+1O	3.30E+14	0.0	0.0
260.	O-+1O3=>1O2-+1O2	6.00E+12	0.0	0.0
261.	O2-+1O=>1O-+1O2	1.99E+14	0.0	0.0
262.	O2-+1O=>1O3+1E	9.00E+13	0.0	0.0
263.	O2-+1O2=>1O2+1O2+E	1.62E+06	0.5	5590.0
264.	O2-+1O2a1D=>1O2+O2+E	1.20E+14	0.0	0.0
265.	O2-+1O2B1S=>1O2+O2+E	2.16E+14	0.0	0.0
266.	O2-+1N2=>1O2+N2+E	6.60E+04	0.0	0.0
267.	O2-+1NO2=>1NO2-+1O2	4.80E+14	0.0	0.0
268.	O2-+1N=>1NO2+1E	3.00E+14	0.0	0.0
269.	O2-+1O3=>1O2+1O3-	2.40E+14	0.0	0.0
270.	O3-+1O=>1O2-+1O2	6.60E+12	0.0	0.0
271.	O3-+1O=>2O2+1E	8.40E+13	0.0	0.0
272.	O3-+1N2=>1NO2-+1NO	6.00E+03	0.0	0.0
273.	O3-+1NO=>1NO3-+1O	6.00E+12	0.0	0.0
274.	O3-+1NO2=>1O3+1NO2-	4.20E+14	0.0	0.0
275.	O3-+1NO2=>1NO3-+1O2	1.20E+13	0.0	0.0
276.	NO-+1O2=>1O2-+1NO	3.00E+14	0.0	0.0
277.	NO-+1NO2=>1NO2-+1NO	4.44E+08	0.0	0.0
278.	NO-+1N2O=>1NO2-+1N2	1.68E+10	0.0	0.0
279.	NO2-+1O3=>1O2+1NO3-	5.40E+13	0.0	0.0
Negative Ion Clusters:				
280.	O-+1H2O+1N2=>H2O2-+N2	7.80E-05	0.0	0.0
281.	O-+1H2O+1O2=>H2O2-+O2	7.80E-05	0.0	0.0

282.	O2-+1H2O+1N2=>H2O3-+N2	1.32E-04	0.0	0.0
283.	O2-+1H2O+1O2=>H2O3-+O2	1.32E-04	0.0	0.0
284.	O3-+1H2O+1N2=>H2O4-+N2	1.62E-04	0.0	0.0
285.	O3-+1H2O+1O2=>H2O4-+O2	1.62E-04	0.0	0.0
286.	OH-+1H2O+1N2=>H3O2-+N2	1.50E-04	0.0	0.0
287.	OH-+1H2O+1O2=>H3O2-+O2	1.50E-04	0.0	0.0
288.	NO-+H2O+N2=>NO2H2-+N2	6.00E-05	0.0	0.0
289.	NO-+H2O+O2=>NO2H2-+O2	6.00E-05	0.0	0.0
290.	NO2-+H2O+N2=>NO2H2O-+N2	9.60E-05	0.0	0.0
291.	NO2-+H2O+O2=>NO2H2O-+O2	9.60E-05	0.0	0.0
Ionic Recombination of + & - Clusters:				
292.	H3O++1H2O2-=>2H2O+1OH	6.00E+17	0.0	0.0
293.	H3O++1H2O3-=>2H2O+1HO2	6.00E+17	0.0	0.0
294.	H3O++1H2O4-=>2H2O+OH+O2	6.00E+17	0.0	0.0
295.	H3O++1H3O2-=>3H2O	6.00E+17	0.0	0.0
296.	H3O++1NO2H2-=>2H2O+HNO	6.00E+17	0.0	0.0
297.	H3O++1NO2H2O-=>2H2O+HNO2	6.00E+17	0.0	0.0
298.	OH++1H2O2-=>1H2O+1HO2	6.00E+17	0.0	0.0
299.	OH++1H2O3-=>H2O+OH+O2	6.00E+17	0.0	0.0
300.	OH++1H2O4-=>H2O+HO2+O2	6.00E+17	0.0	0.0
301.	OH++1H3O2-=>2H2O+O	6.00E+17	0.0	0.0
302.	OH++1NO2H2-=>HNO2+H2O	6.00E+17	0.0	0.0
303.	OH++1NO2H2O-=>HNO3+H2O	6.00E+17	0.0	0.0
304.	O2++1H2O2-=>1H2O+1O3	6.00E+17	0.0	0.0
305.	O2++1H2O3-=>1H2O+2O2	6.00E+17	0.0	0.0
306.	O2++1H2O4-=>H2O+O3+O2	6.00E+17	0.0	0.0
307.	O2++1H3O2-=>H2O2+HO2	6.00E+17	0.0	0.0
308.	O2++NO2H2-=>H2O+NO3	6.00E+17	0.0	0.0

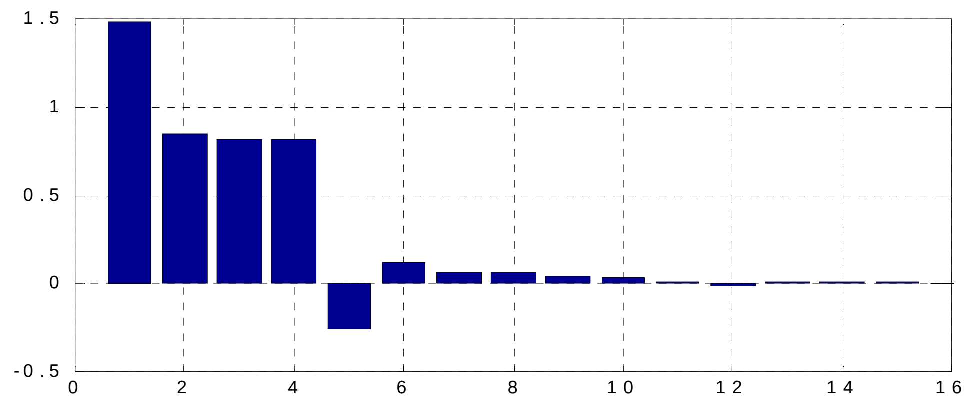
309.	O2++NO2H2O-=>H2O+NO2+O2	6.00E+17	0.0	0.0
310.	NO++1H2O2-=>1H2O+1NO2	6.00E+17	0.0	0.0
311.	NO++1H2O3-=>1H2O+1NO3	6.00E+17	0.0	0.0
312.	NO++1H2O4-=>H2O+NO2+O2	6.00E+17	0.0	0.0
313.	NO++1H3O2-=>H2O+HNO2	6.00E+17	0.0	0.0
314.	NO++1NO2H2-=>2NO+H2O	6.00E+17	0.0	0.0
315.	NO++NO2H2O-=>NO2+NO+H2O	6.00E+17	0.0	0.0
316.	O2-+NO+=>O2+N+O	6.00E+16	0.0	0.0
317.	O3-+O+=>O3+O	1.20E+17	0.0	0.0
318.	O3-+O2+=>O3+O2	1.20E+17	0.0	0.0
319.	O3-+O2+=>2O+1O3	6.00E+16	0.0	0.0
320.	O3-+NO+=>O3+1NO	1.20E+17	0.0	0.0
321.	NO3-+NO+=>NO3+1N+1O	6.00E+16	0.0	0.0
322.	NO3-+O2+=>NO3+O+O	6.00E+16	0.0	0.0
323.	O-+O2+=>O+O2	1.20E+17	0.0	0.0
324.	O-+O2++1O2=>O3+O2	1.20E+22	0.0	0.0
325.	O-+NO++1O2=>NO2+O2	1.20E+22	0.0	0.0
326.	O2-+O2+=>O2+O2	2.52E+17	0.0	0.0
327.	O2-+NO++O2=>2O2+NO	1.20E+22	0.0	0.0



Sensitivity of the concentration of NO in humid air

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
12	-5.51172E-03	N2A+E=>N2++2E
13	-5.23243E-03	N2a+E=>N2++2E
14	4.89278E-03	O2+E=>2O+E
15	-1.98218E-03	E+O2+=>O+O1D
16	1.38832E-03	O+E=>O++2E

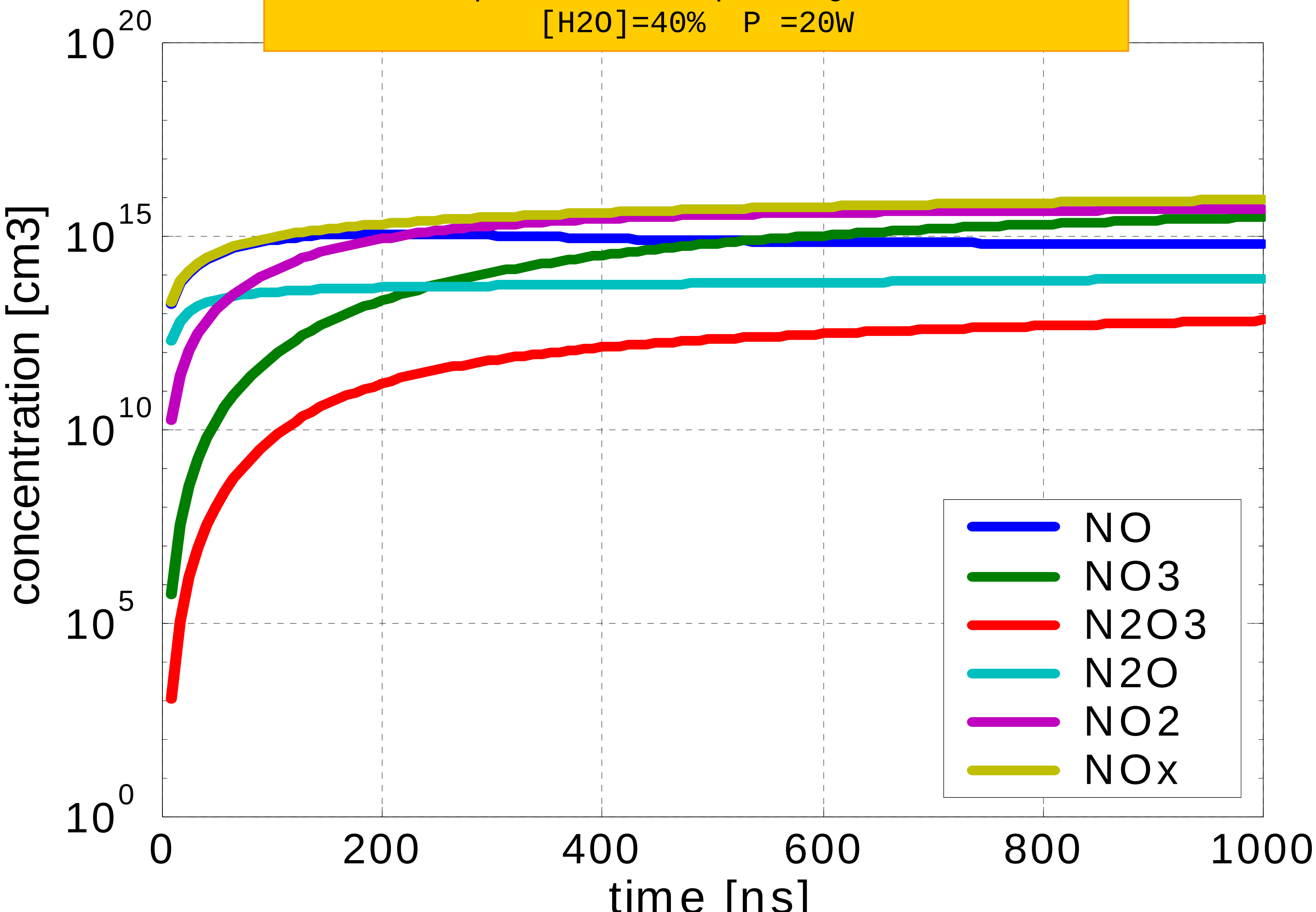
NOTE : normalized sensitivity matrix are printed out in descending order.Listing is ceased after 3 orders of magnitude.

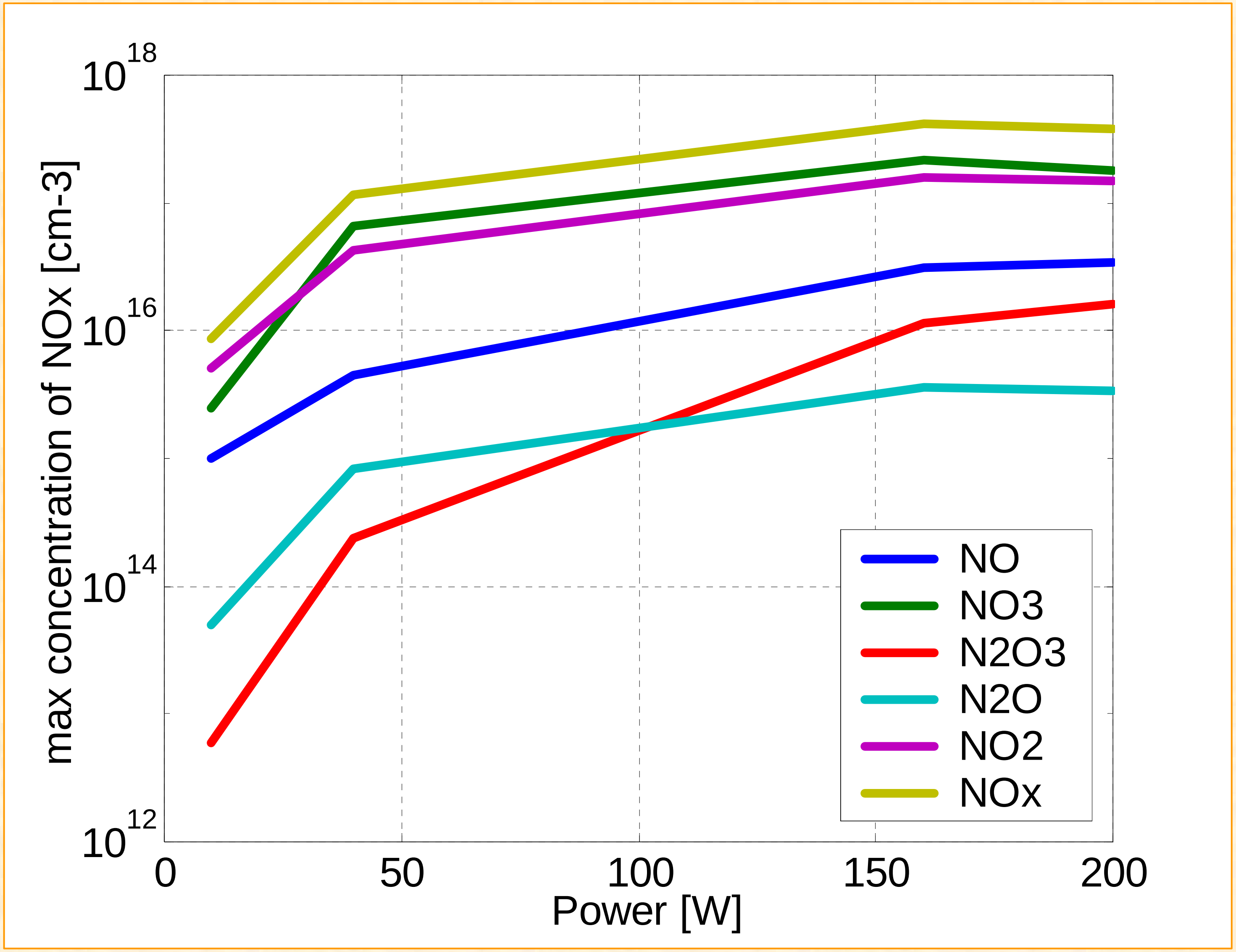


Sensitivity of the concentration of NO in dry air

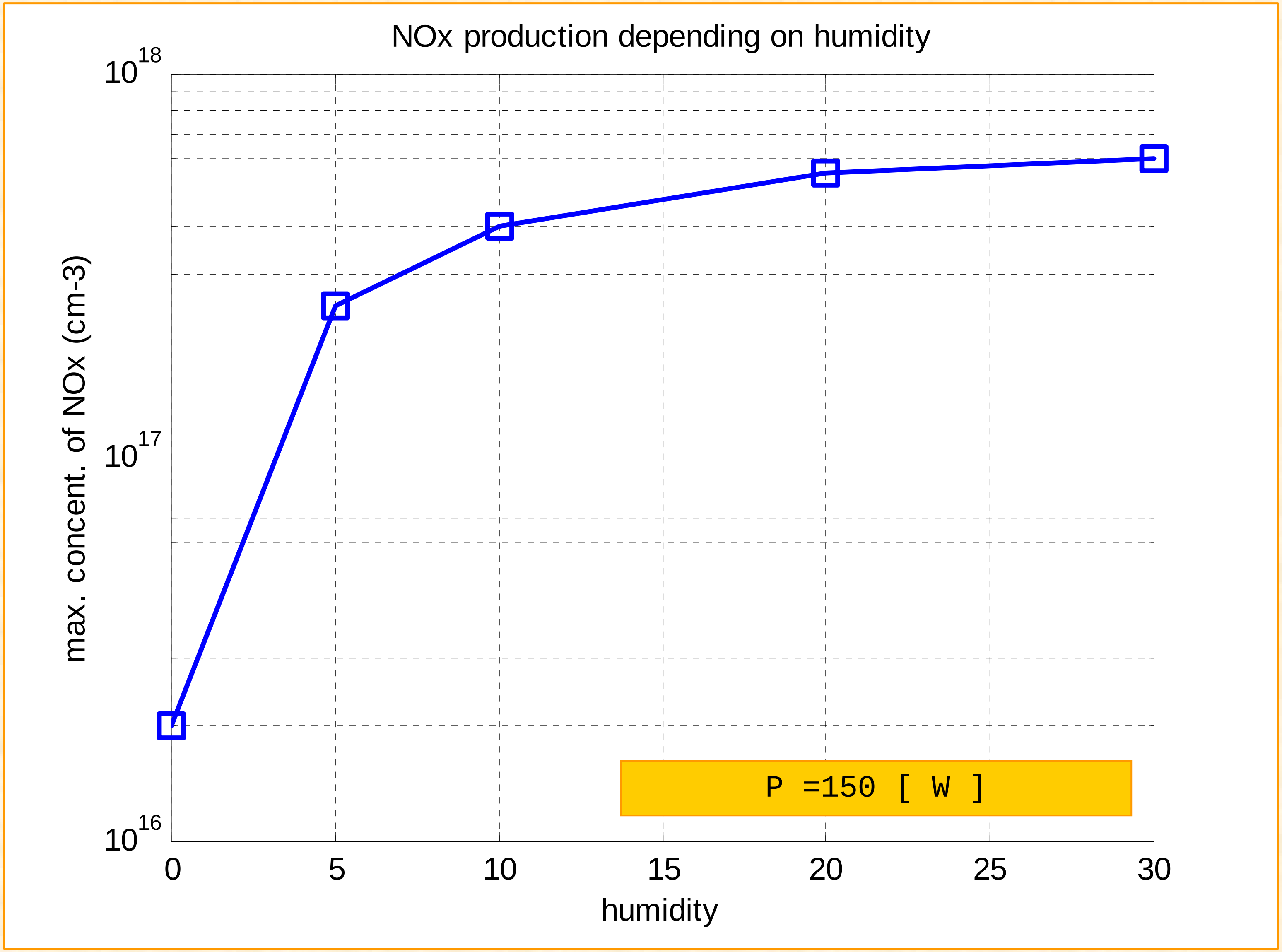
1	1.48537E+00	O2+E=>O2++2E
2	8.45766E-01	O2+E=>2O+E
3	8.17030E-01	N2+E=>N2A+E
4	8.15169E-01	N2A+O=>NO+N
5	-2.60547E-01	O2+E=>O-+O
6	1.20548E-01	O2++N2=>NO++NO
7	6.36030E-02	O+E=>O++2E
8	6.28990E-02	N+O2=>NO+O
9	4.34527E-02	O2+E=>O2B1S+E
10	3.67916E-02	O2B1S+E=>O2++2E
11	1.09363E-02	N2+E=>N2++2E
12	-1.03377E-02	O2B1S+O2=>O2a1D+O2
13	9.19929E-03	N2+E=>N2a+E
14	7.71050E-03	N2a+O2=>N2+2O
15	6.57281E-03	O2B1S+E=>2O+E
16	2.10552E-03	O-+N2=>N2O+E

NOx production depending on time
[H2O]=40% P =20W





max concentration of NOx [cm-3]
10^{18}
10^{16}
10^{14}
10^{12}
0
50
100
150
200
Power [W]
NO
NO3
N2O3
N2O
NO2
NOx


NOx production depending on humidity
10^{18}
10^{17}
10^{16}
max. concent. of NOx (cm-3)
0
5
10
15
20
25
30
humidity
P =150 [W]

NOx production depending on microdischarge pattern

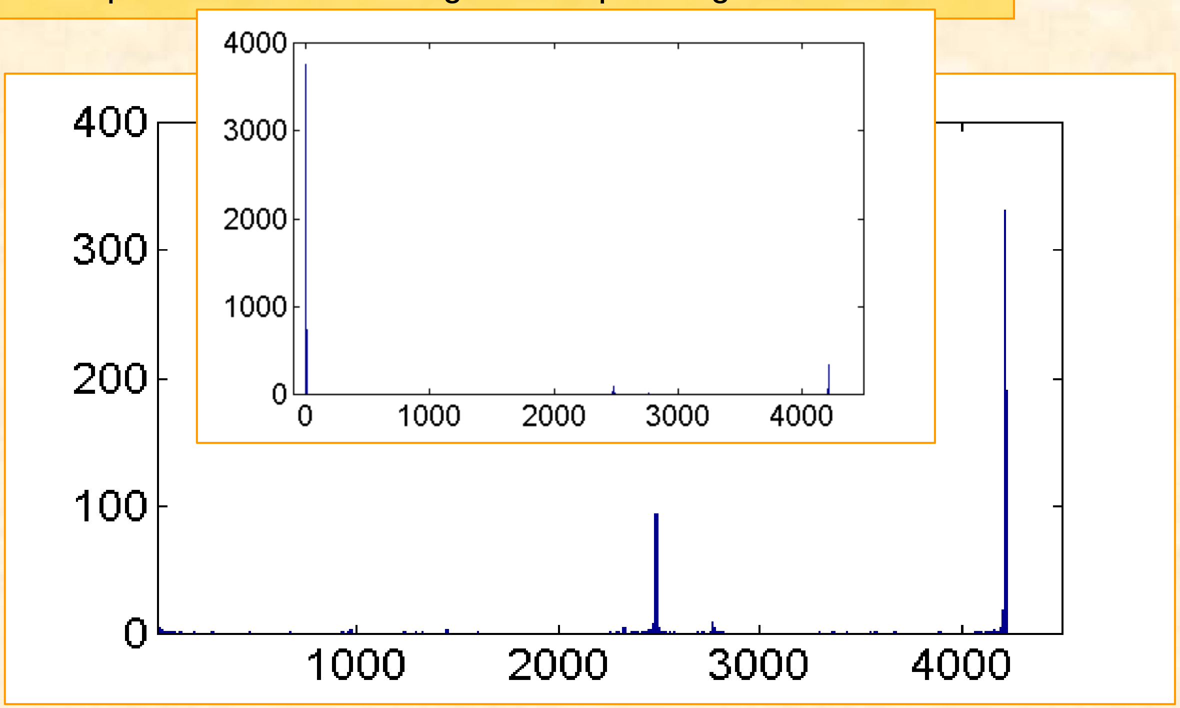
We will answer the question where NOx production will be higher in uniformly distributed microdischarge pattern or in some pattern with regular spacing.

$$P_{cell} = N_{cell} \cdot \frac{E_{str}}{t \cdot V_{cell}}$$

Ncell – number of streamer strikes in cell
Estr – energy of single streamer
Vcell - volume of simulation cell

Simulation:

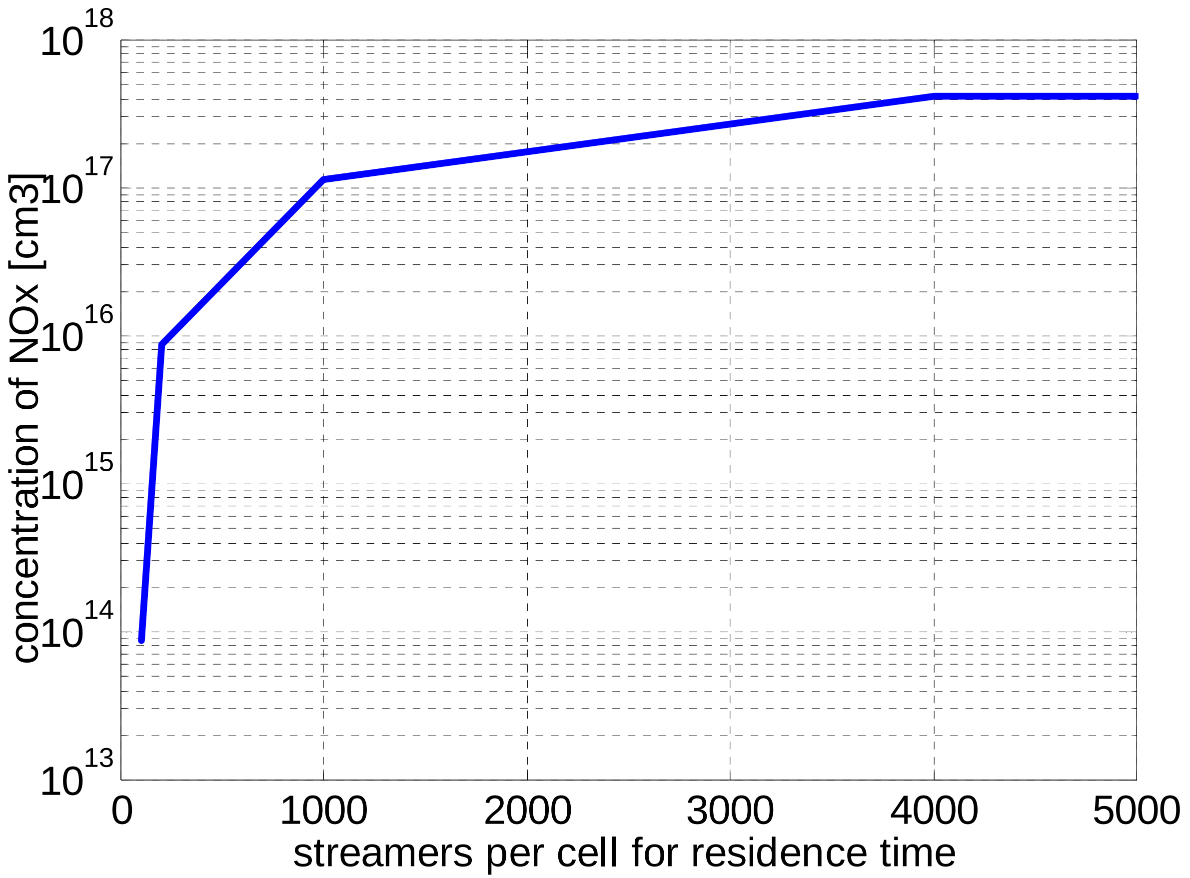
Streamers	1e7
Time	20 [ms]
residence time	
Power	100 [W]
Humidity [H2O]	40%

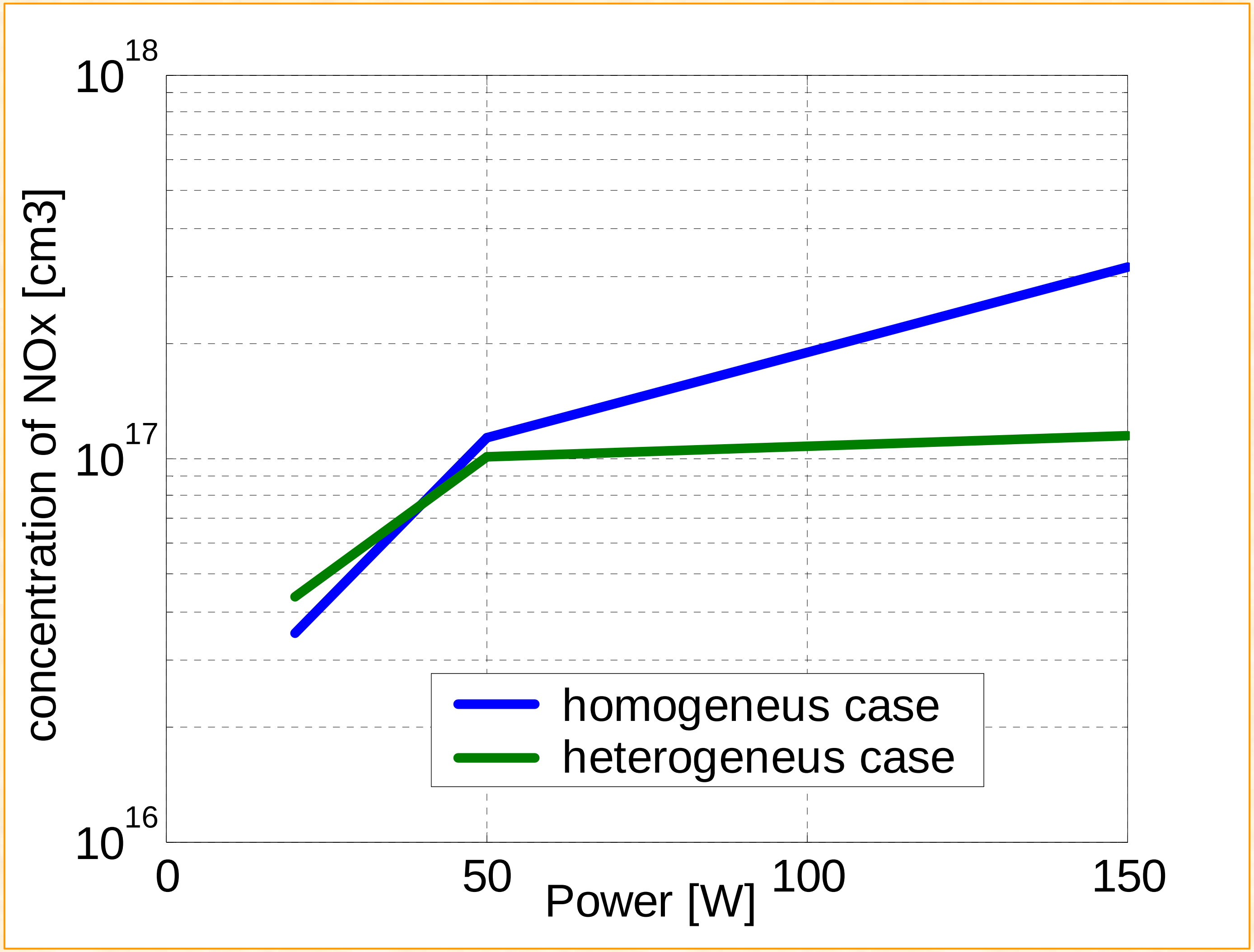


Number of streamers vs. number of cells

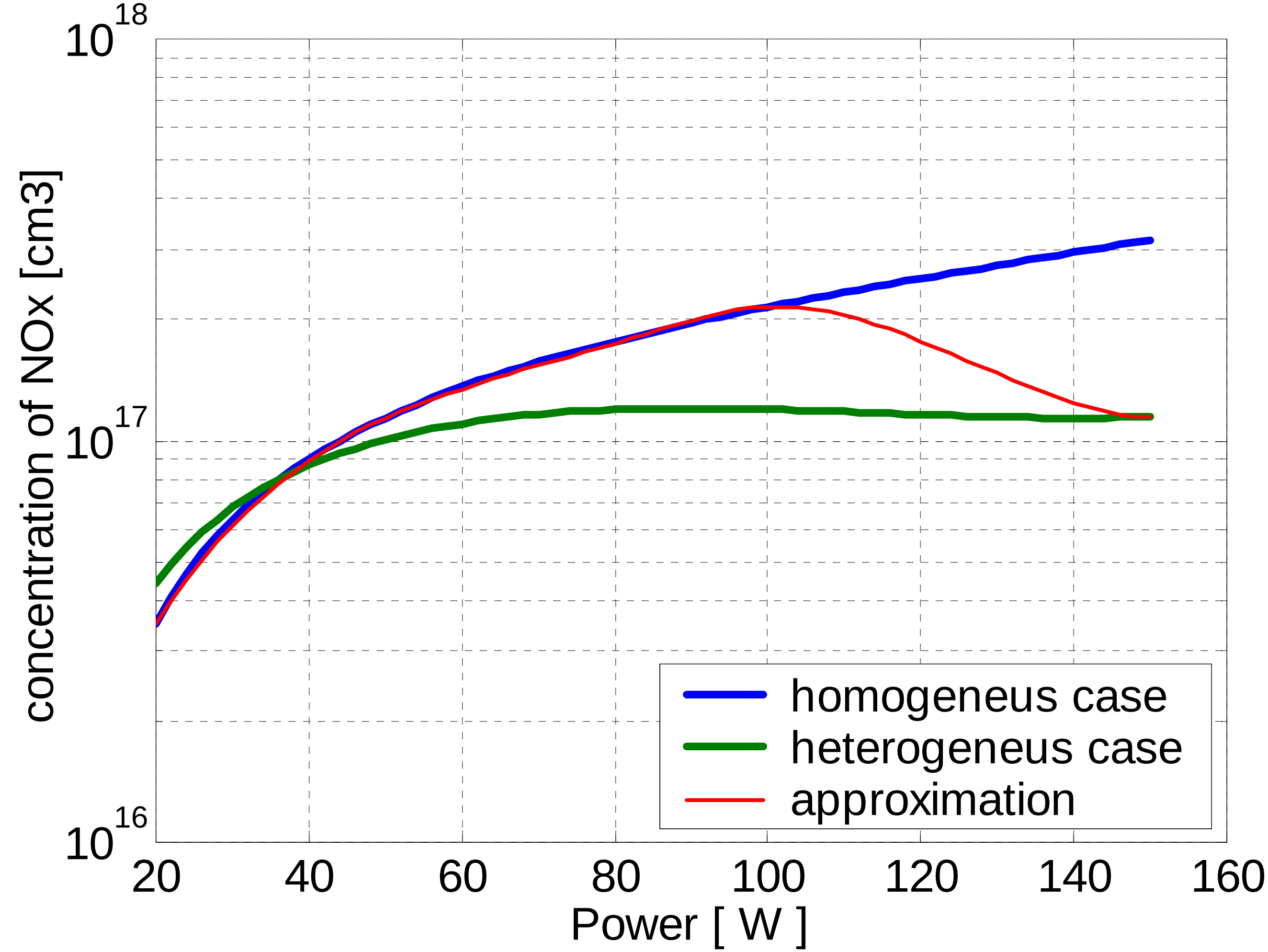
Streamers Pattern occurs at power about 100 [W]

NOx production depending on microdischarge pattern





10^{18}
10^{17}
10^{16}
concentration of NOx [cm3]
0
50
100
150
Power [W]
homogeneus case
heterogeneus case


10^{18}
10^{17}
10^{16}
concentration of NOx [cm3]
20
40
60
80
100
120
140
160
Power [W]
homogeneus case
heterogeneus case
approximation

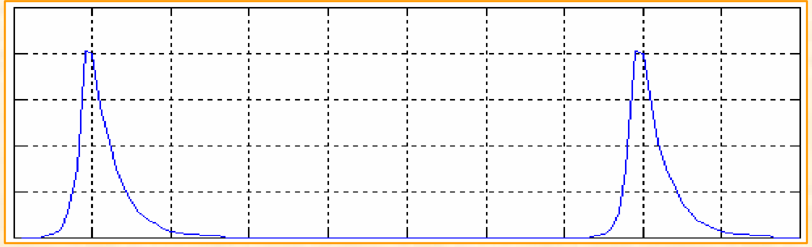
Conclusions

Effect of Power supply operation regime on NOx production is opposite for high and low power

For High Power Density (more than about 10 W/cm3)

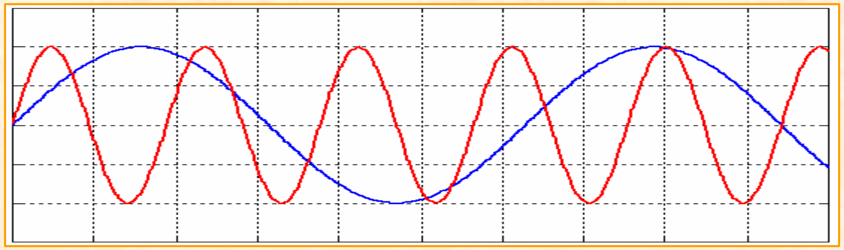
Effect of Waveform Type

NOx production is higher when Pulse type waveform is used



Effect of Frequency

NOx production increases with increasing frequency



When we increase frequency or change waveform type from sine to pulse we actually **decrease rise time of applied voltage** and we decrease effect of streamer interaction. This leads to more **uniform streamers pattern**. And according to our calculations we **increase NOx production**.

Summary

- Analytical consideration of DBD and streamer phenomena taking into account non-equilibrium between translational and vibrational temperatures of molecules.
- Numerical modeling of Avalanche&Streamer formation/propagation and Avalanche to Streamer Transition.
- Numerical simulation of chemical kinetics in streamer channel (CHEMKIN software) together with the developed program for taking into account vibrational excitation
- Sensitivity analysis of chemical mechanism (SENKIN software and KINALC postprocessor).
- Specially created Monte-Carlo modeling of Streamers interaction in discharge gap(Random generator was carefully and thoroughly tested).
- Results include the dependence of NO_x concentration in streamer channel on experimental parameters. Average NO_x concentration in the gap is calculated using data on streamer activity in gap obtained from Monte Carlo streamer modeling.
- NO_x concentration in streamer channel depends on power, humidity
- NO_x relative concentration may be as high as 1.5 % and as low as 0.03%.
- NO_x concentration increases with increase of humidity in all cases.
- NO_x concentration increases with increase of driving frequency.
- NO_x production is higher in case of pulse waveform and lower in case of sine waveform.
- The highest NO_x concentration may be reached in humid air in the case of high power, low frequency, sine waveform, and high power (vibrational temperature is high, but translational one is low).
- The lowest NO_x concentration may be reached in dry air in the case of high frequency, pulse waveform, and low power.

Future Plans

TwoPnt
Boundary Value Problems Solver

TwoPnt was successfully used in Premix, Opdiff.

$$\dot{M}\frac{dY_k}{dx}+\frac{d}{dx}(\rho A Y_k V_k)-A\dot{\omega}W_k=0$$

$$\rho=\frac{p\overline{W}}{RT}$$

Heterogeneous chemical reactions in clusters

Surface Reactions on Web

1D Chemistry Modeling

Species concentration depending on length of the DBD reactor