Fluid Modeling of Low Temperature Atmospheric Pressure Plasmas: What can and cannot be done with Commercial Software

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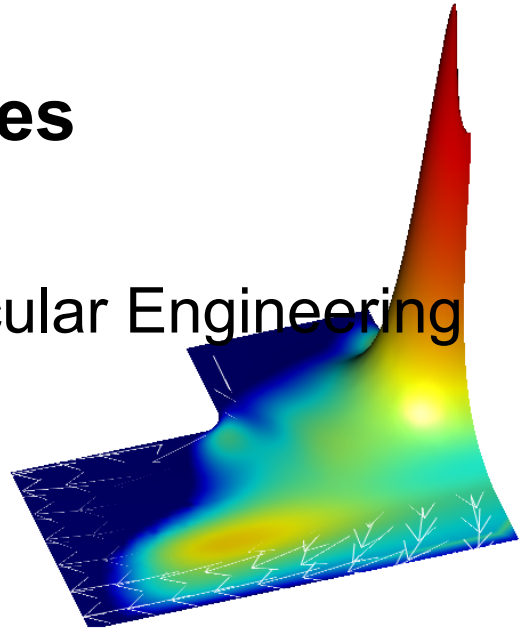


Outline

1. Introduction
    - Motivation: plasma medicine
    - Problem setting: RF plasma needle

2. Modeling and the results
    - Model description
    - Solver and computational environment
    - Coupling with neutral gas flows
    - Coupling with air chemistry

3. Use of commercial software
    - Commercial software available for fluid modeling
    - Advantage and disadvantage

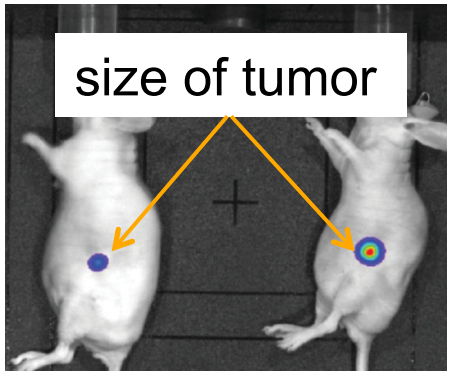
4. Concluding Remarks

Motivation: plasma '*medicine*'

Tumor treatment

M. Vandamme, *Plasma Process. Polym.* **7** (2010) 264

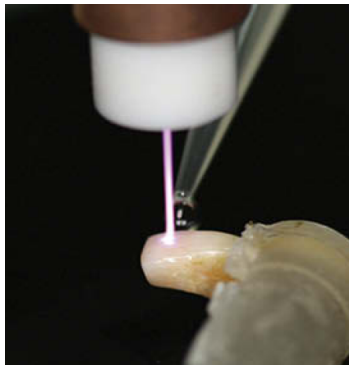
6 min
x
5 days



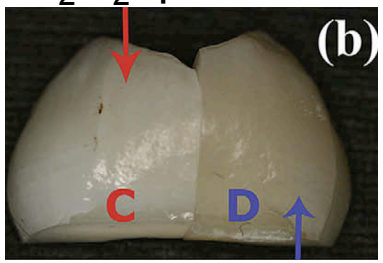
control

Dental application

H. W. Lee, et al., *J. Endod* **35** (2009) 587



H_2O_2+plasma

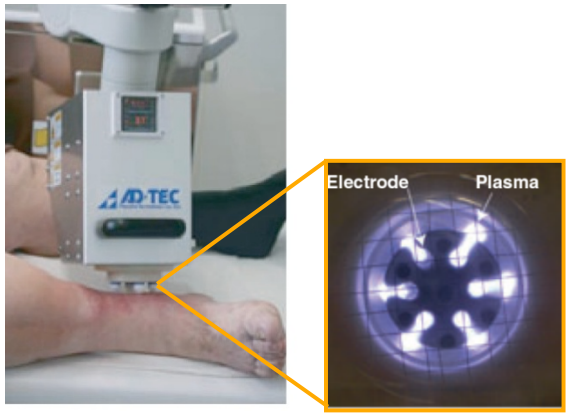


H_2O_2

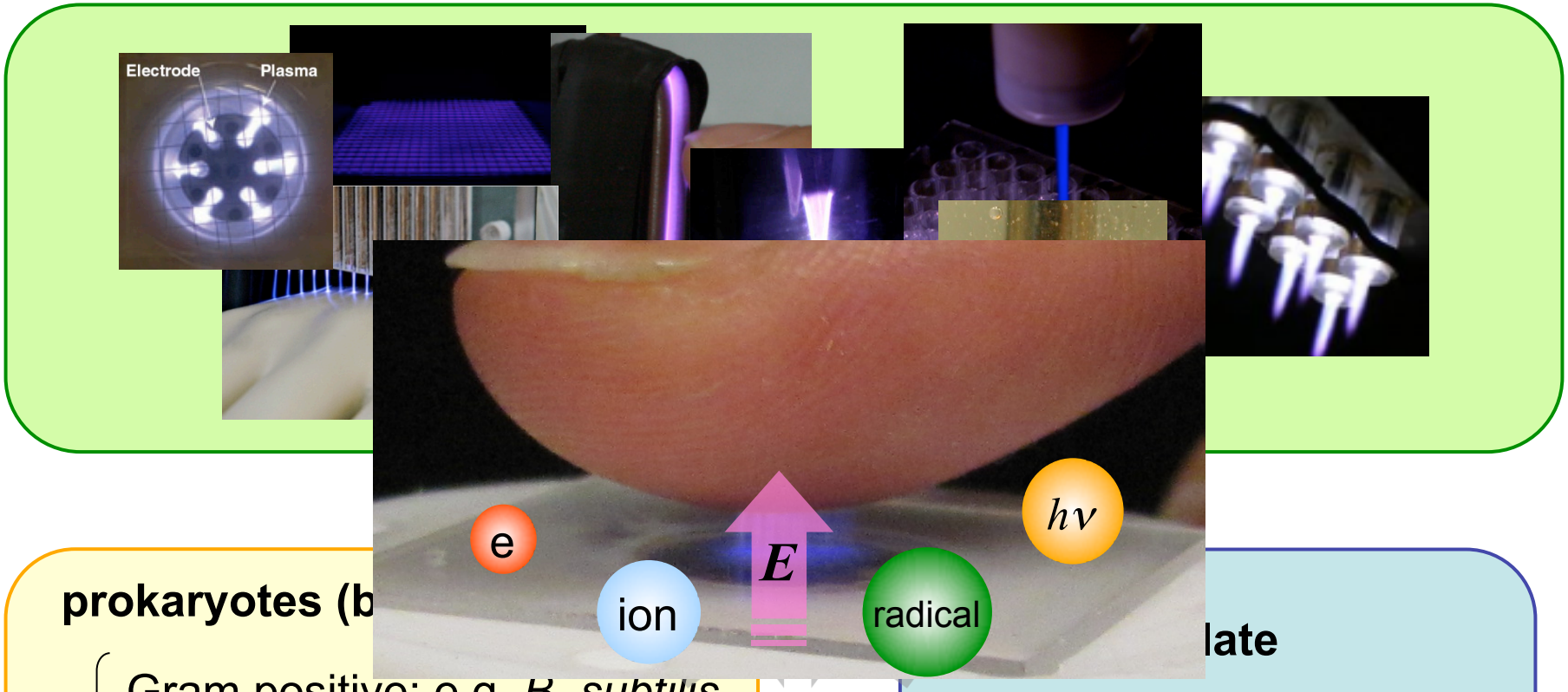
Wound healing

J. Heinlin, *JDDG* **8** (2010) 968, G. Isbary, Br. J. Dermatol. 163 (2010) 78

Microwave Ar plasma torch



Plasma-biomaterial interaction: complex nature



prokaryotes (b

- Gram positive: e.g. *B. subtilis* (vegetative cell or spore)
- Gram negative: e.g. *E. coli*

eukaryotes (animal or plant)

late

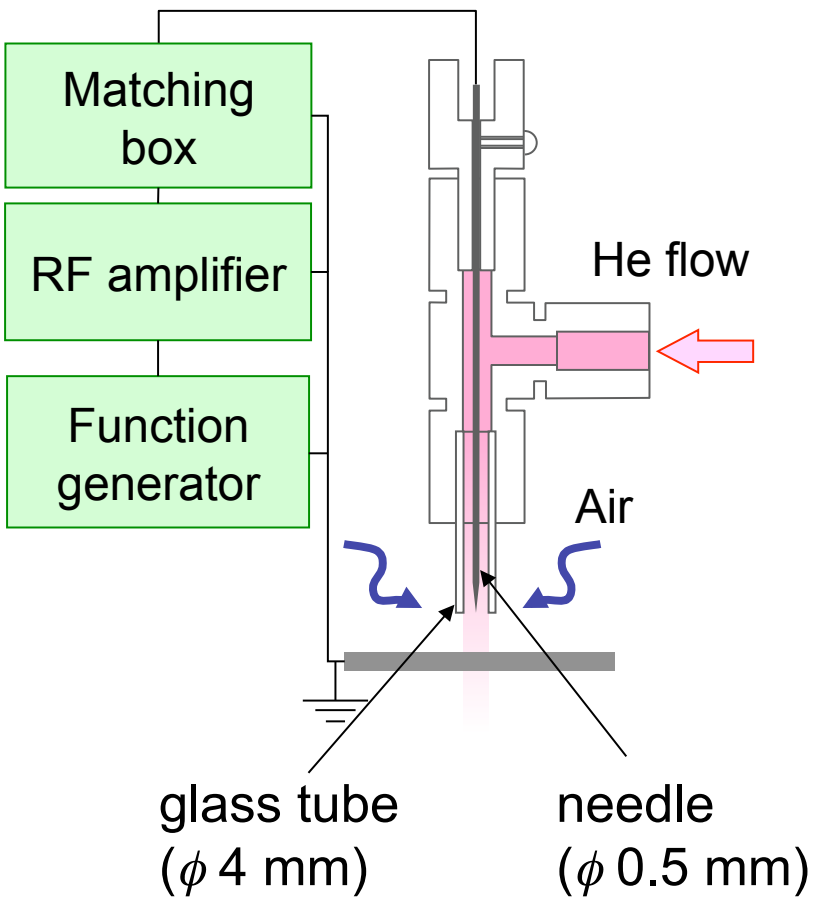
in liquid

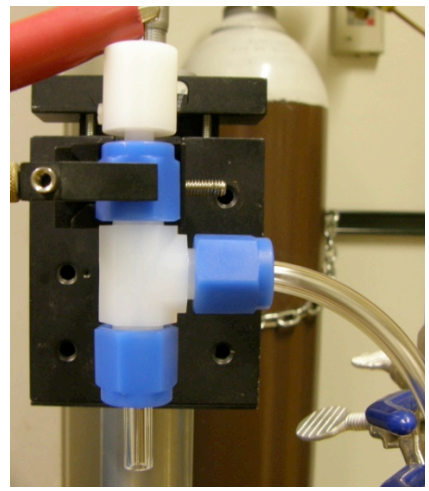
biofilm

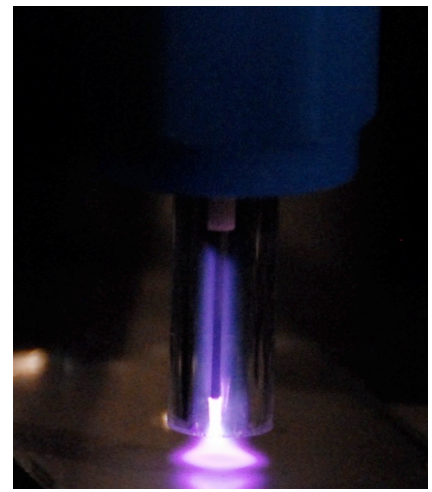
in vivo

Problem setting: RF plasma needle - 1

E. Stoffels, et al., *Plasma Sources Sci. Tehcnol*. 11 (2002) 383.



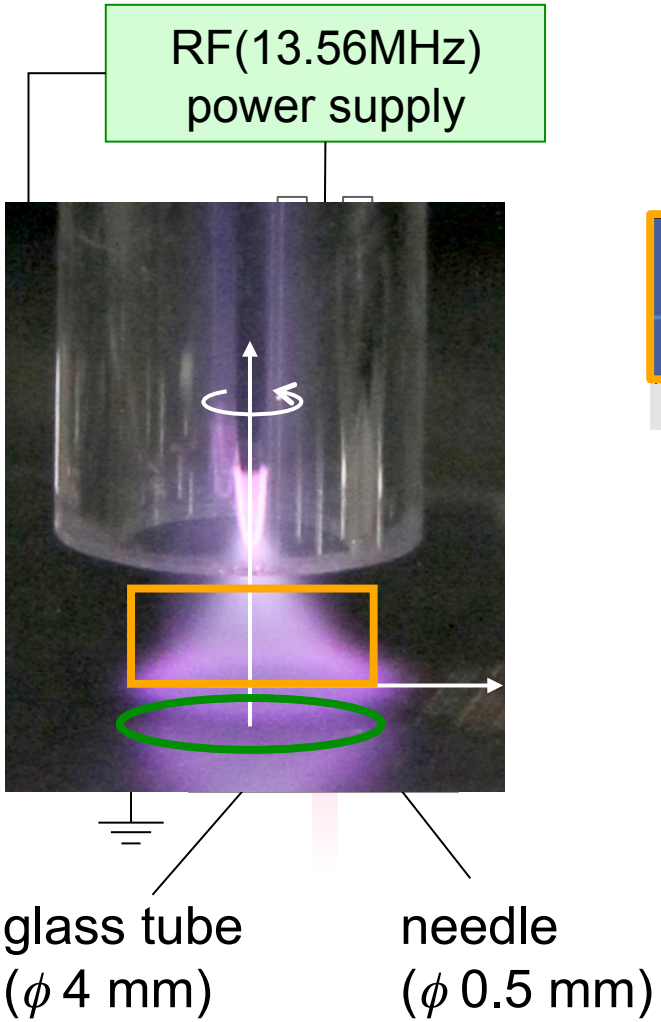


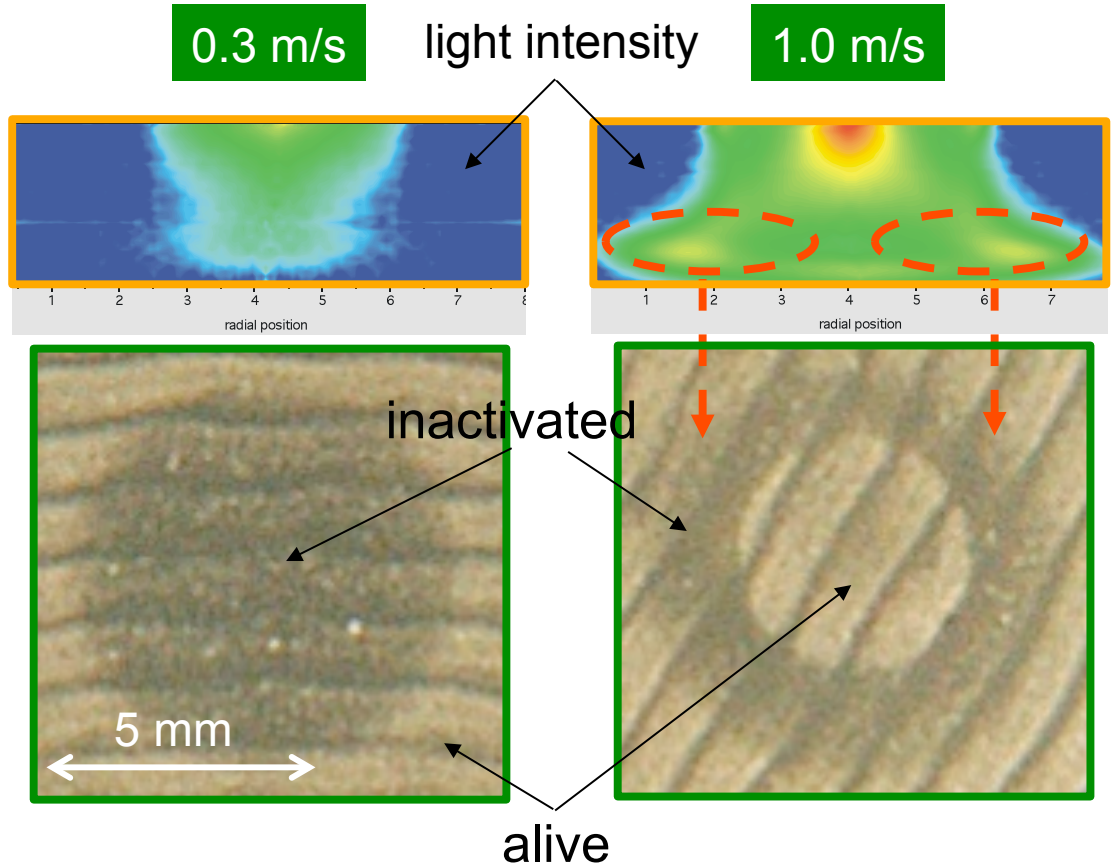


- Frequency: RF (13.56MHz)
- Voltage: 200-400 V_{pkpk}
- He flow rate: ~1 slpm (Re_d < 100)
- Power consumption: ~1 W
- Distance to sample: 1-5 mm

Problem setting: RF plasma needle - 2

J.Goree, et al, *J.Phys.D.* **39** 3479 (2006) and *IEEE Trans.Plasma Sci.* **34,** 1317 (2006)





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Solver and computational environment

Solver

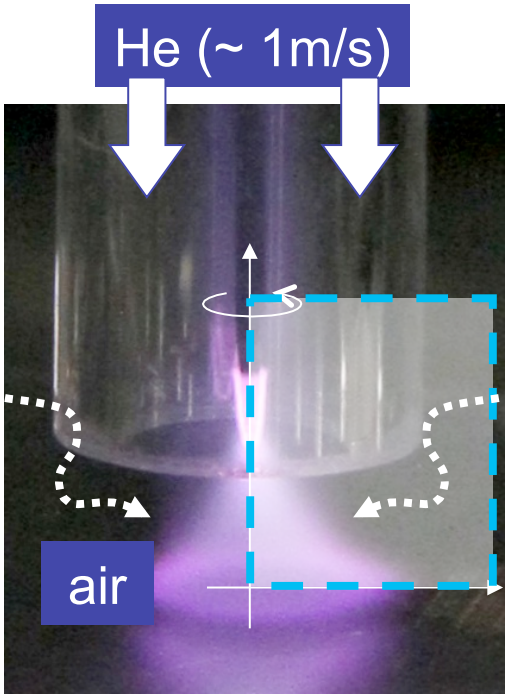
COMSOL Multiphysics
- FEM (finite element method) solver
- By Comsol: www.comsol.com

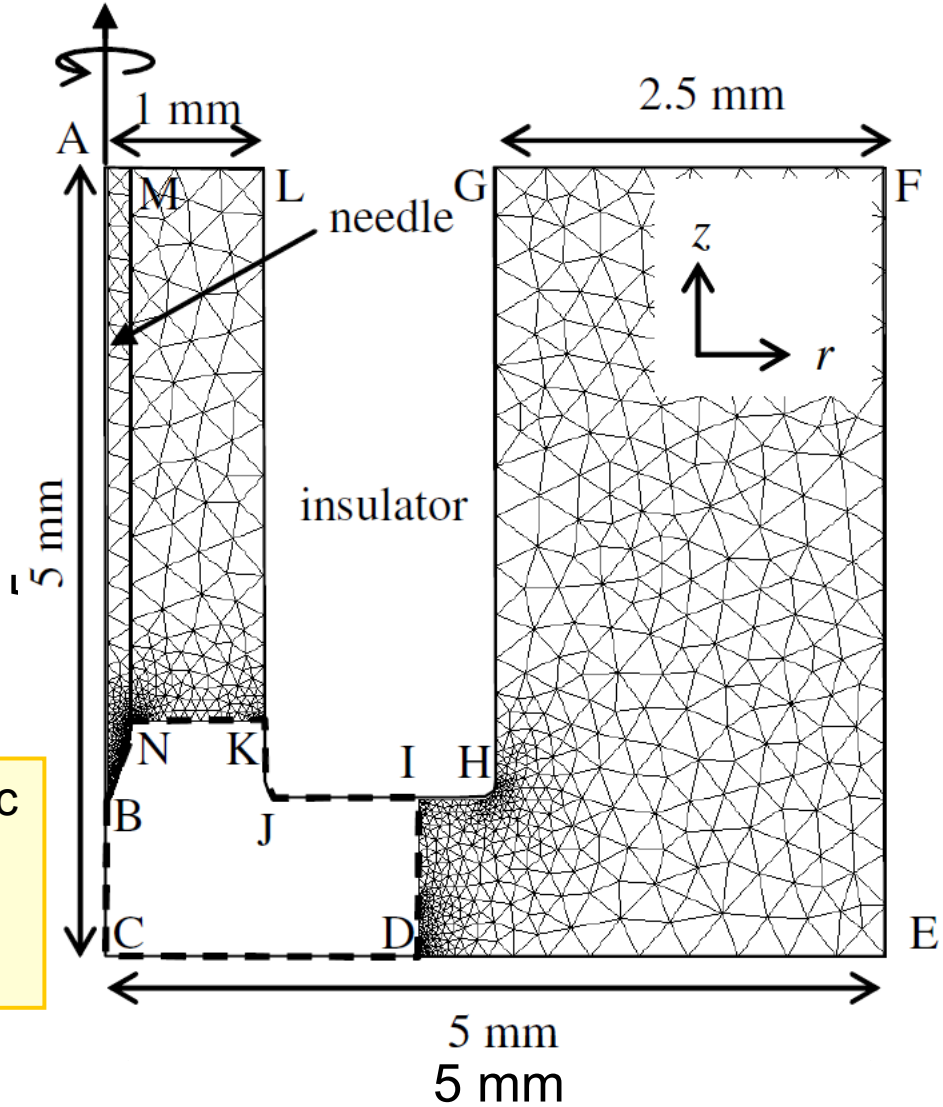
MATLAB
- Custom control of COMSOL
- By MathWroks: www.mathworks.com

Computational environment

- Desktop workstations
- CPU: AMD Opteron (4 quad cores)
- Memory: 8-16 GB
- OS: Open Suse
- CPU time: from ~10 min/RF cycle (1D model) to ~10 hr/RF cycle (2D model)

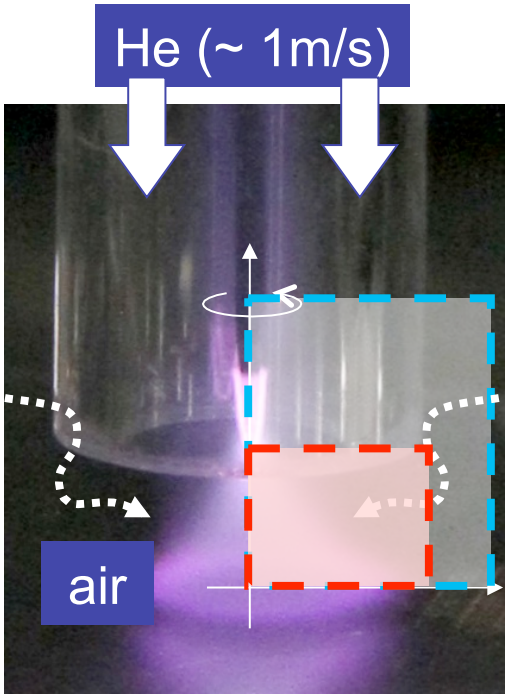
Model description: neutral flow domain

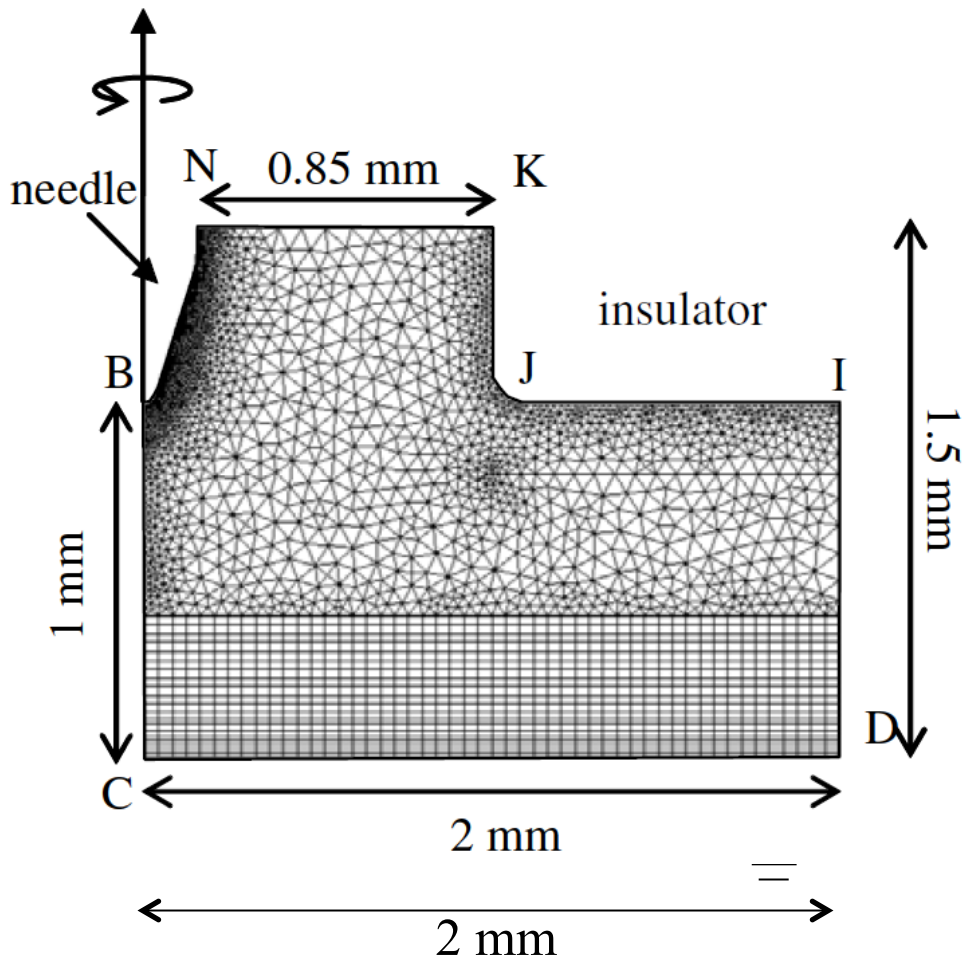




Basis function: Lagrange-quadratic
Number of meshes: ~10,000
Number of DOF: ~250,000
Mesh size: 3-500 μm

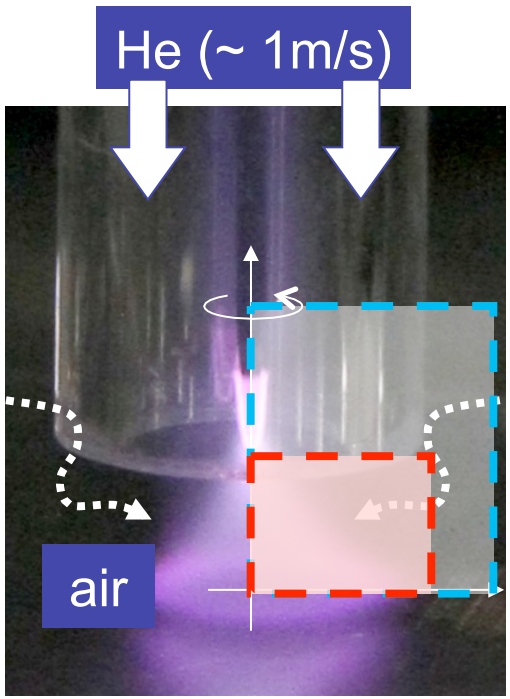
Model description: plasma domain





Basis function: Lagrange-quadratic
Number of meshes: ~10,000
Number of DOF: ~250,000
Mesh size: 3-500 μm

Model description: governing equations



Neutral Gas flow (He, Air)

$$\nabla\cdot(\rho\mathbf{u})=0,\ \nabla\cdot(\rho\omega_{\mathrm{air}}\mathbf{u}-\rho D\nabla\omega_{\mathrm{air}})=0 \qquad \text{(mass conservation)}$$

$$\nabla\cdot(\rho\mathbf{u}\mathbf{u}_i)=-\nabla p\mathbf{E}-\nabla\cdot\overline{\overline{\ }}+\sum q_i n_i \qquad \text{(momentum conservation)}$$

$$\nabla\cdot(-\lambda\nabla T+\mathbf{u}\Gamma_{\mathrm{p}}\mathbf{E})=\Phi+\sum q_i\ {}_i+Q_{el} \qquad \text{(energy conservation)}$$

ion momentum
collisional heating

temperature
velocity
species density

Plasma dynamics

$$\frac{\partial n_i}{\partial t}+\nabla\cdot\mathbf{\Gamma}_i=S_i \qquad \text{(mass conservation)}$$

$$\mathbf{\Gamma}_i=\mathrm{sgn}(q_i)n_i\mu_i\mathbf{E}-D_i\nabla n_i+n_i\mathbf{u} \qquad \text{(drift-diffusion)}$$

$$\frac{\partial(n_e\varepsilon)}{\partial t}+\nabla\cdot\left(\frac{5}{3}\varepsilon\mathbf{\Gamma}_e-\frac{5}{3}n_eD_e\nabla\varepsilon\right)=-\mathbf{\Gamma}_e\cdot\mathbf{E}-Q \qquad \text{(electron energy)}$$

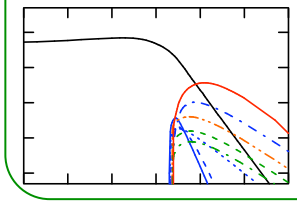
$$\varepsilon_0\nabla\cdot\mathbf{E}=\sum q_i n_i \qquad \text{(Poisson's equation)}$$

Y. Sakyiama et al, Plasma Sources Sci. Tchnol. 18 (2009) 025022

Simulation procedure: pre-processing

Look-up tables

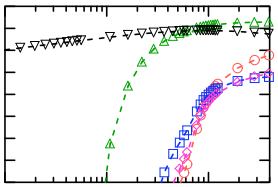
cross section data



$He + e \rightarrow He + e$
$\rightarrow He^{*} + e$
$\rightarrow He^{+} + 2e$

electron Boltzmann eq.
(BOLSIG+)

reaction/transport rate const.



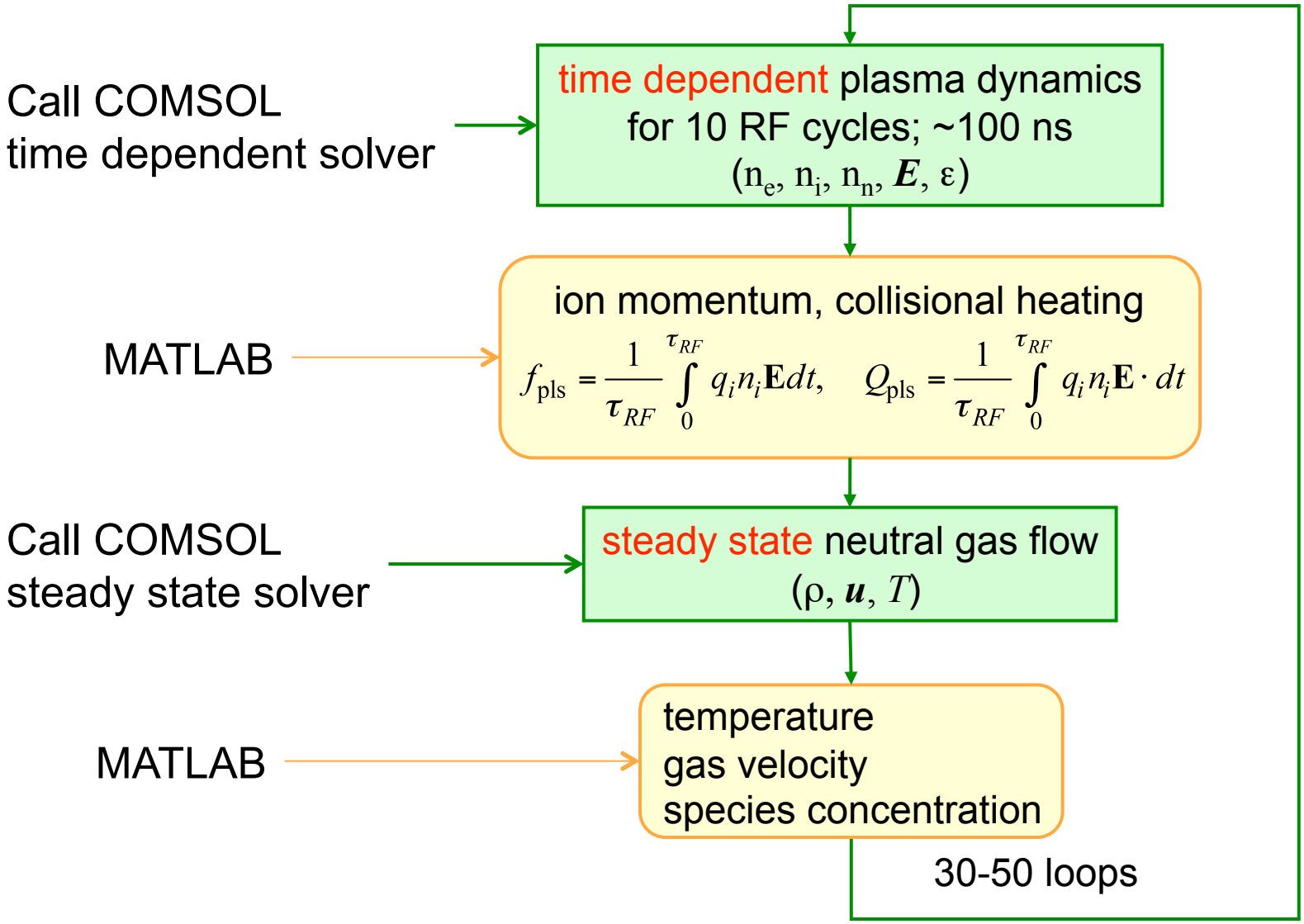
$k = f(\varepsilon)$

electron energy

Initialization (COMSOL)

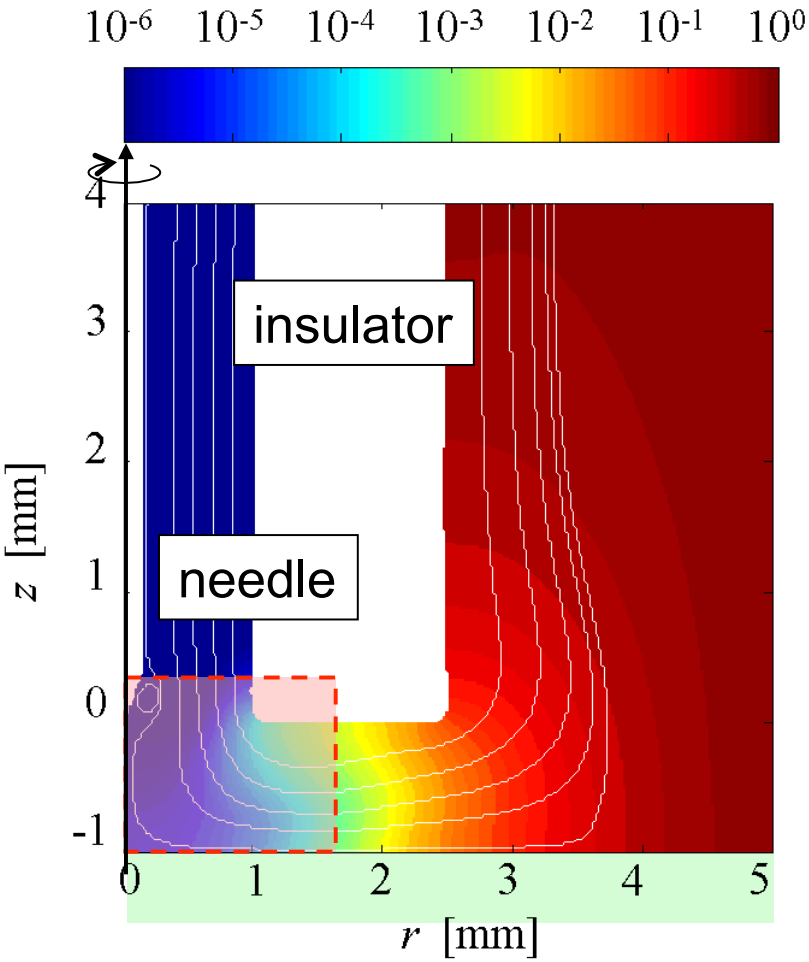
- Constants/variables
- Geometry
- Mesh generation
- Governing equations
- Boundary conditions
- Initial conditions

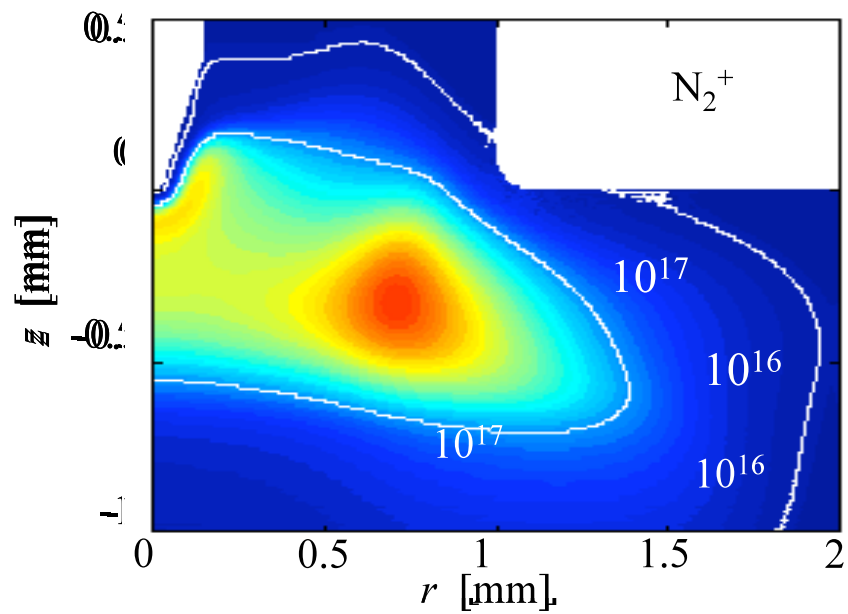
Simulation procedure: MATLAB script



Coupling with gas flow: simulation results

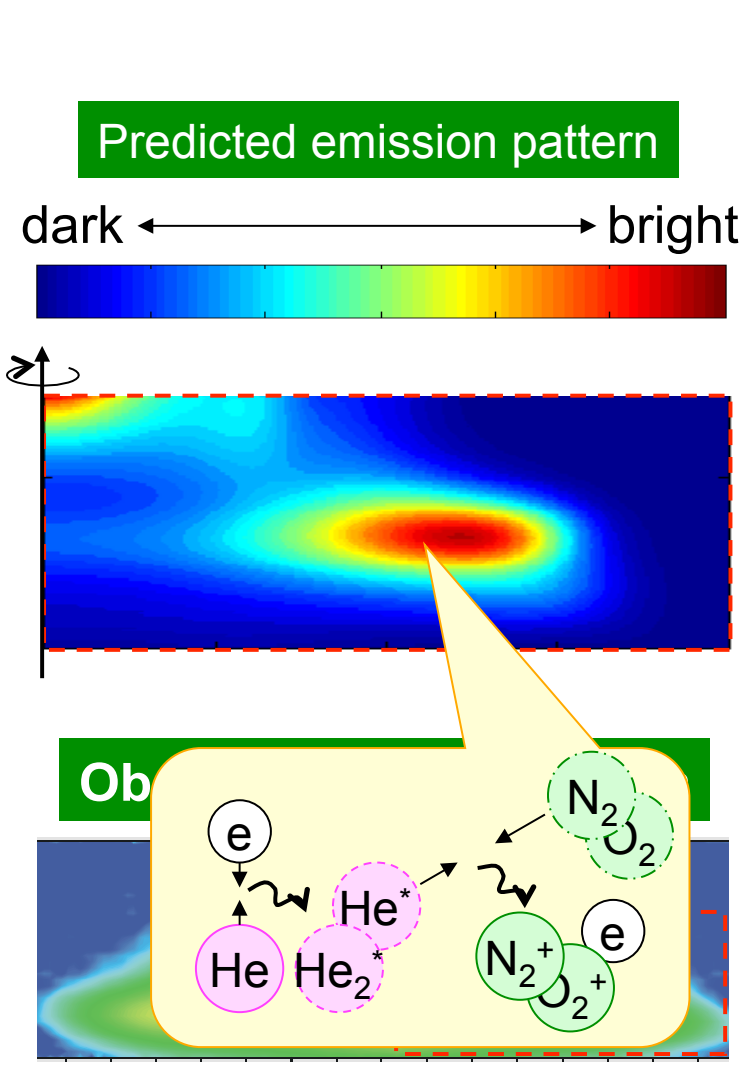
Mole fraction of air (log scale)



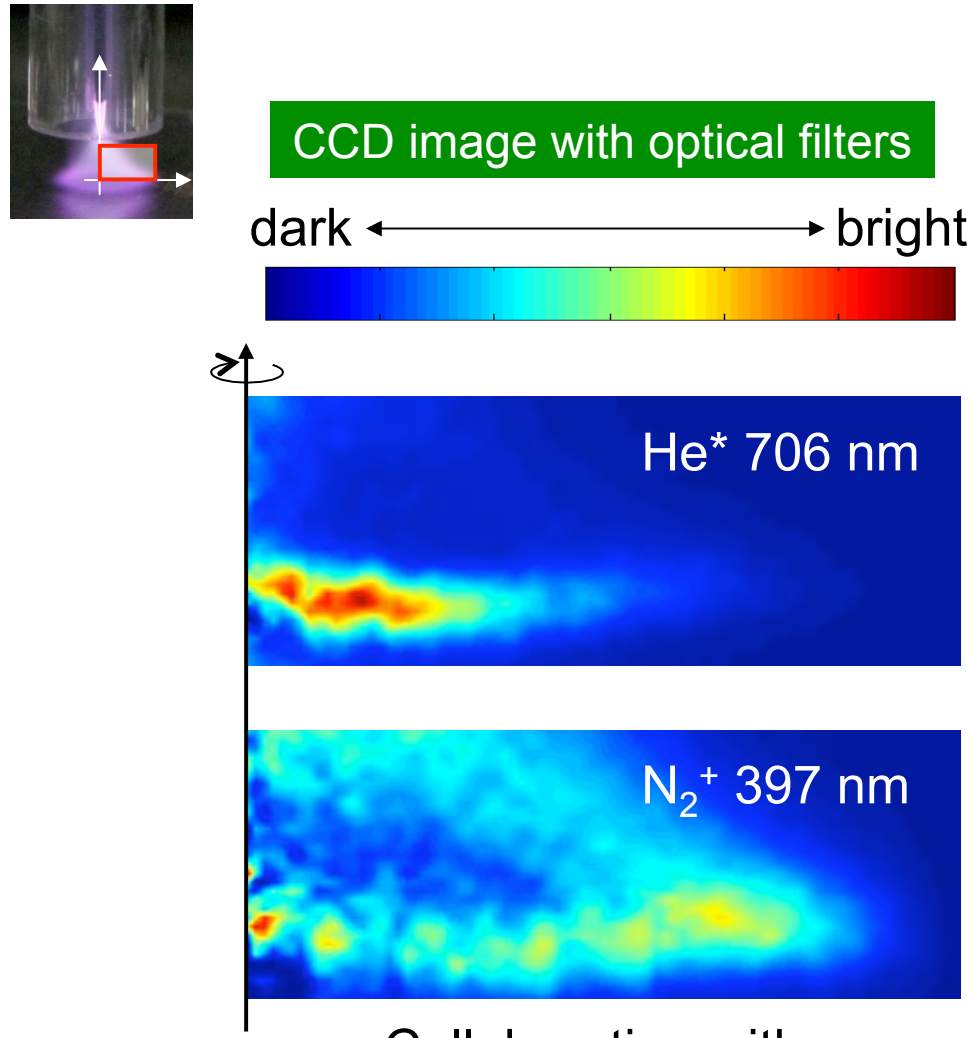


Y. Sakyiama et al, Plasma Sources Sci. Tchnol. 18 (2009) 025022

Coupling with gas flow: comparison with experiment



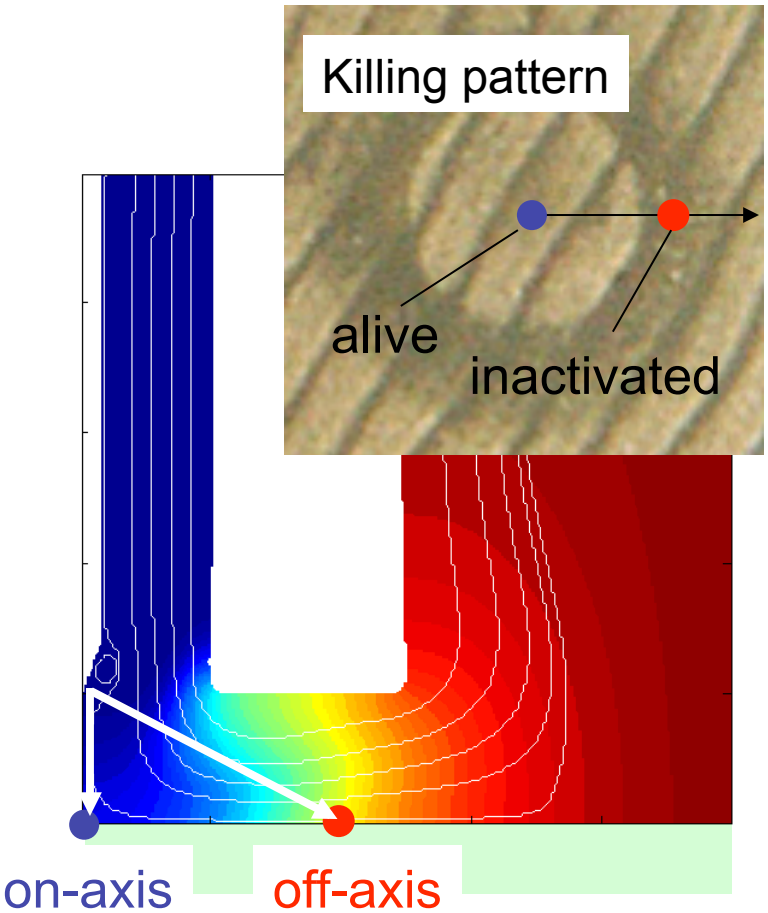
Courtesy of J. Goree



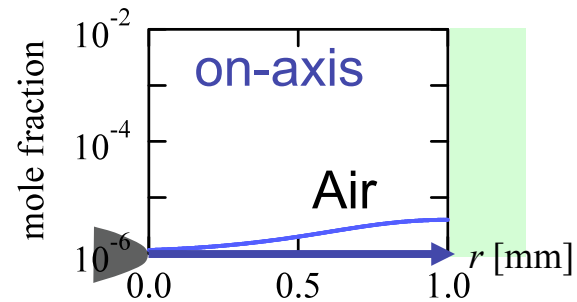
Collaboration with
Schulz-von der Gathen

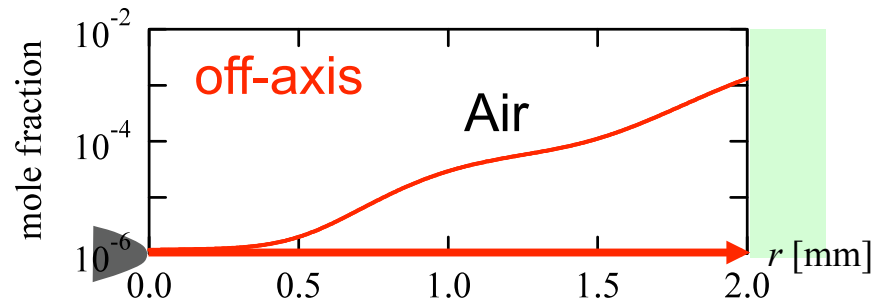
Plasma chemistry: model description

Mole fraction of air (log scale)



1D plasma model





Plasma chemistry: He/humid air chemistry

46 species

negative particles: e, O^-, O_2^-, O_3^-, O_4^-, H^-, OH^-

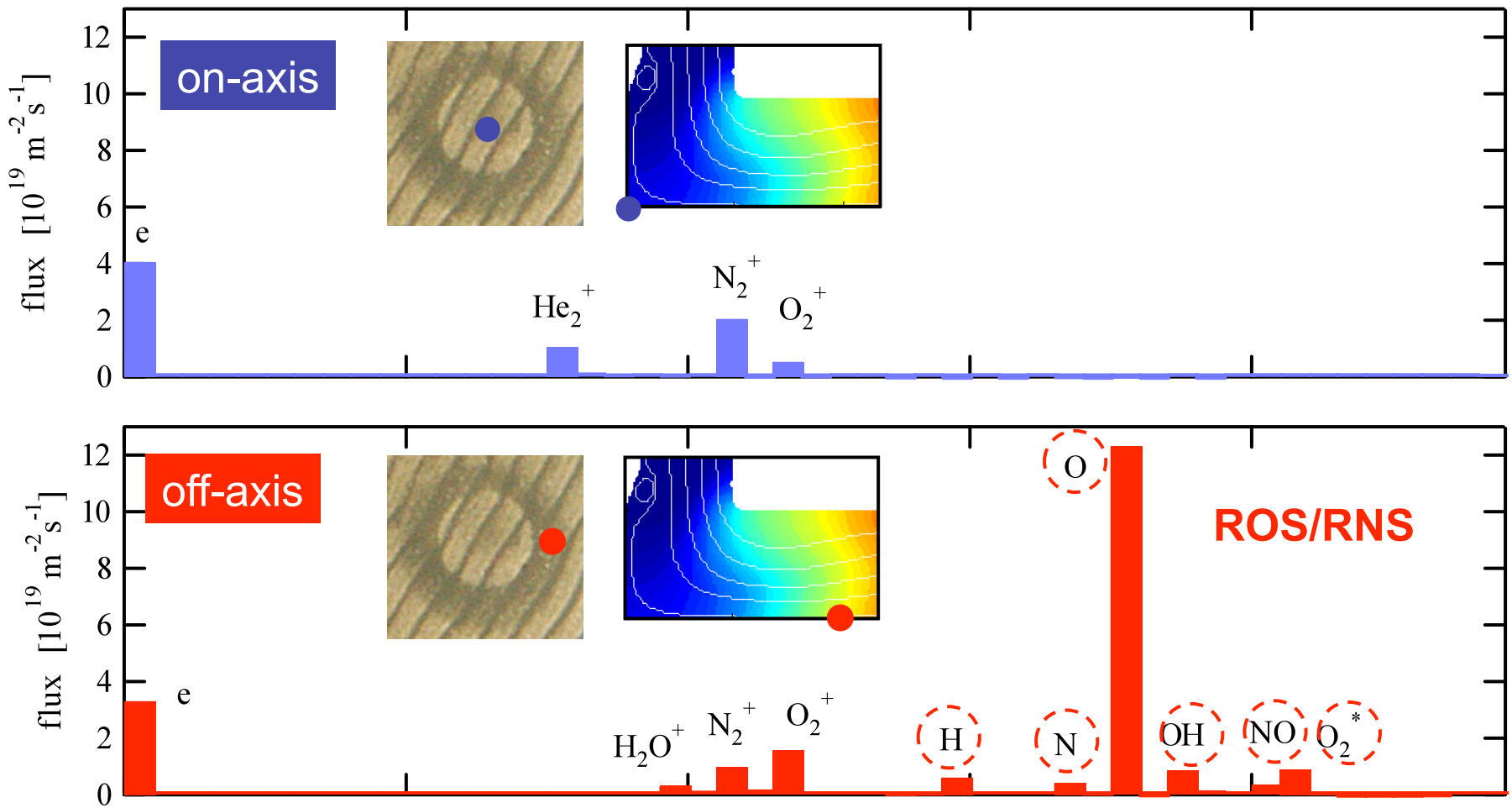
positive particles: He^+, He_2^+, N^+, N_2^+, N_3^+, N_4^+, O^+, O_2^+, O_4^+, NO^+, N_2O^+, NO_2^+, H^+, OH^+, H_2O^+, H_3O^+

neutrals: He, He^*, He_2^*, N, N^*, N_2, N_2^*, N_2^{**}, O, O^*, O_2, O_2^*, O_3, NO, N_2O, NO_2, NO_3, H, H_2, OH, H_2O, HO_2, H_2O_2

214 elementary reactions

- 21 electron impact excitation/ionization/dissociation reactions
- 20 Penning and associative ionization reactions
- 26 electron recombination/attachment reactions
- 65 charge transfer reactions
- 51 ion recombination reactions
- 31 neutral-neutral reactions

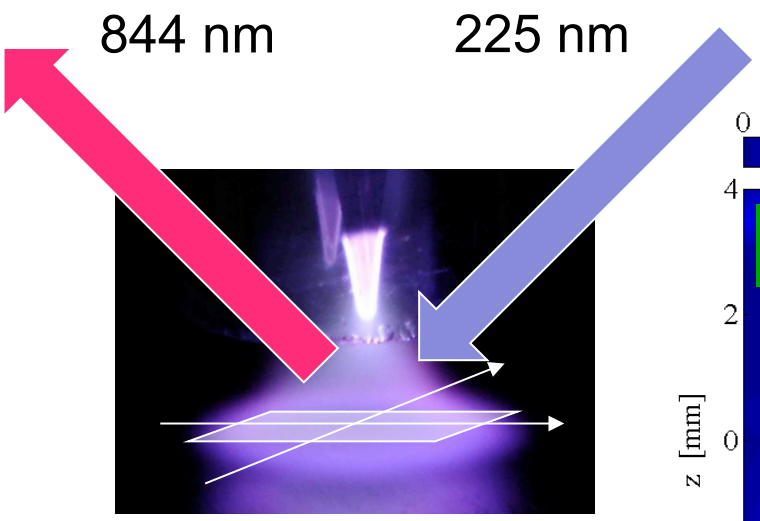
Plasma chemistry: simulation results

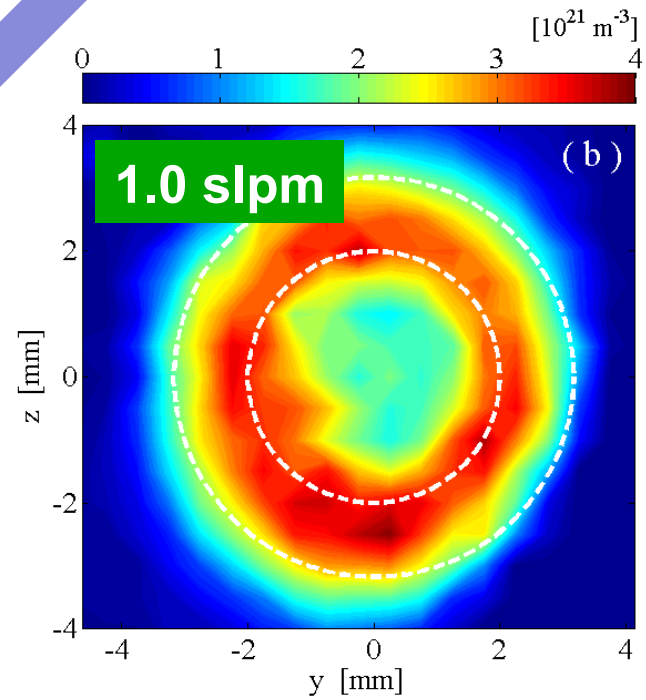


Plasma chemistry: comparison with experiment

TALIF (two photon absorbed laser induced fluorescence)

- Collaboration with Ruhr-Universitat Bochum (Germany)
- Absolute density of O atom





Y. Sakiyama, et al., *Appl. Phys. Lett.* **97** (2010) 151501.

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Commercial software available for fluid modeling

CFD-ACE+: ESI Group (http://www.esi-group.com/)

- general PDE solver
- plasma physics module available

ANSYS Fluent: ANSYS Inc. (http://www.ansys.com/)

- general fluid dynamics solver
- applicable to low pressure CVD simulation

COMSOL Multiphysics: Comsol, Inc. (http://www.comsol.com/)

- FE (finite element) solver
- ~20 pre-defined application modules from fluid dynamics to mechanics
- plasma module included in the latest version (after 4.1)

SIGLO and SIPDP: Kinema Research (http://www.kinema.com/)

- plasma fluid solver in 1-D and 2-D from AC to RF

Advantages of commercial software

- Mesh generation for complicated geometries through GUI
- Easy to add multi-physics problems
- Hybrid simulation possible with MATLAB script
- Beneficial especially for non-professionals in numerical modeling (e.g. experimentalists)
- Saving time to write/debug simulation codes
- Sharing/exchanging models and results with others

Disadvantages of commercial software

- No direct access to algorithm (“black box”)
- Non-full control of solvers (e.g. error control, tolerance)
- Limited options to advanced techniques (e.g. numerical diffusion)
- (Slightly) slower computational speed
- Need to learn how to use GUI/CUI
  (frequent version up is problematic…?)
- Commercial (license fee required)

Publications for plasma needle modeling

- Y. Sakiyama and D. B. Graves, *J. Phys. D* **39** (2006) 3451.
- Y. Sakiyama and D. B. Graves, *J. Phys. D* **39** (2006) 3644.
- Y. Sakiyama and D. B. Graves, *J. Appl. Phys.* **101** (2007) 073306.
- Y. Sakiyama and D. B. Graves, *IEEE Trans. Plasma Sci*. **35** (2007) 1279.
- Y. Sakiyama, et al., *J. Phys. D* **41** (2008) 95204.
- Y. Sakiyama and D. B. Graves, *Plasma Sources Sci. Technol*. **18** (2009) 25022.
- Y. Sakiyama, et al., *Appl. Phys. Lett*. **96** (2010) 041501
- Y. Sakiyama, et al., *Appl. Phys. Lett*. **97** (2010) 151501.

Related publications using COMSOL/MATLAB

- E. Kawamura et al., *Plasma Sources Sci. Technol.* **20** (2011) 035009. (2D hybrid fluid-analytical simulation)
- I. Lee et al., *Plasma Sources Sci. Technol.* **17** (2008) 015018. (2D EM-plasma coupling)
- C. Corr et al., *J. Phys. D: Appl. Phys.* **41** (2008) 185202. (2D inductively coupled Ar/Cl_2 plasmas)
- Y. Kabouzi, et al., *Phys. Rev. E* **75** (2007) 016402. (surface wave-sustained plasmas)
- C.-C. Hsu et al., *J. Phys. D* 39 (2006) 3272. (Ar/O2/Cl2 inductively coupled plasmas)

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Concluding Remarks

- Commercial software (COMSOL/MATLAB) is a powerful tool for modeling of low-temperature atmospheric pressure plasmas.

- Neutral gas flows and ROS/RNS play crucial roles in plasma-biomaterial interaction.

Q. If you do not have a simulation code and need to run numerical simulations, are you going to write your own home-made code from scratch…?

Acknowledgements

Gregor E. Morfill and *The team plasma health care* (Max-Planck Institute, DE)

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John Goree (University of Iowa)

Eva Stoffels.