「プラズマ科学における分光計測の高度化と原子分子過程研究の新展開」
「原子分子データ応用フォーラムセミナー」合同研究会

日時：平成28年1月27日 13:40 から 1月29日 16:30 まで
場所：核融合科学研究所 管理棟4階 第一会議室

プラズマ医療の物理機構：プラズマ照射により溶液中に生成される反応活性種

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Acknowledgements

Numerical Simulation:

T. Kanazawa,   M. Isobe (Eng. Sch, Osaka U.)

outline

1. Introduction: cold atmospheric-pressure plasma (CAP) and plasma medicine
2. One dimensional numerical simulation for generation of reactive species in pure water: effects of transport due to drift, diffusion, and advection
   a) reactive neutral species
   b) currents (electrons and ions)
3. Summary

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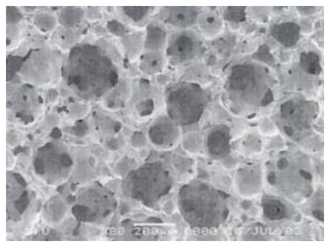
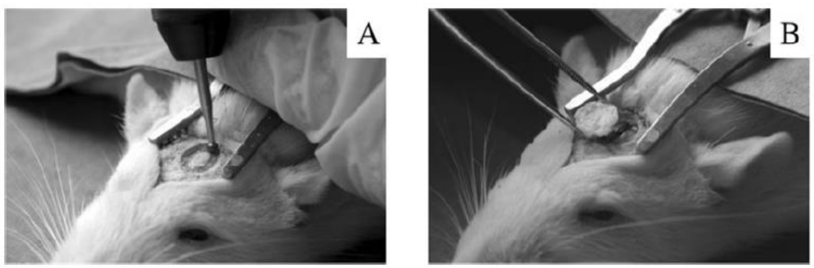
Medical applications of plasma technologies

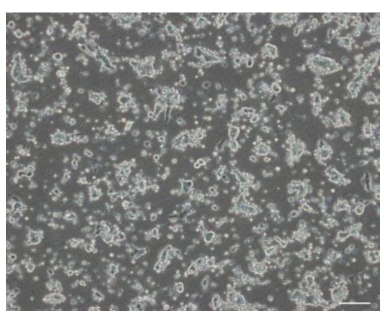
processing of biologically functional surfaces

surface processing of artificial bones

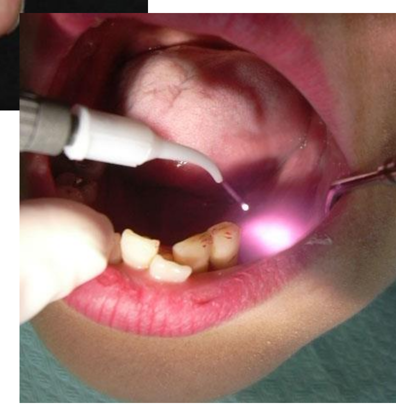




surface functionalization of cell culture dishes

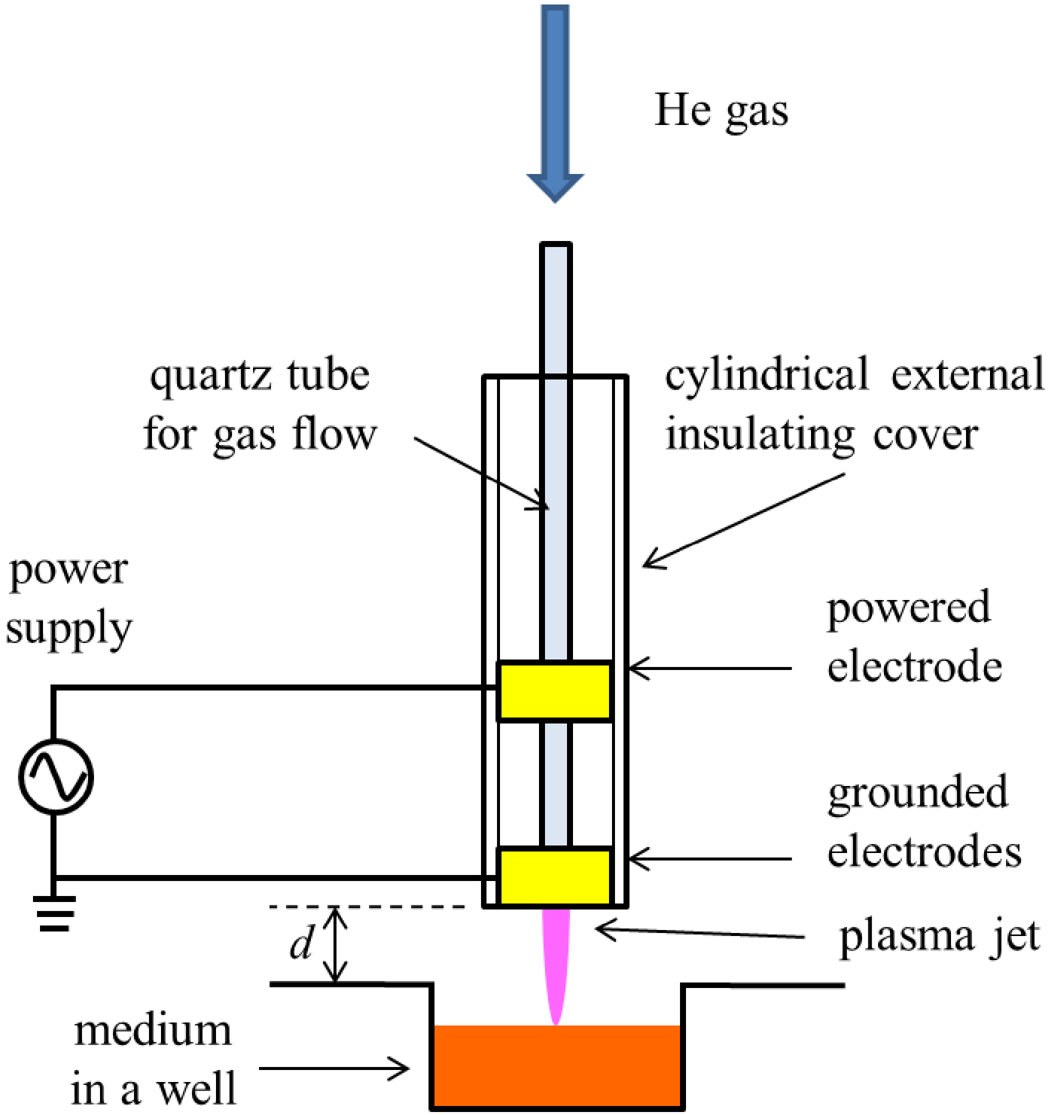


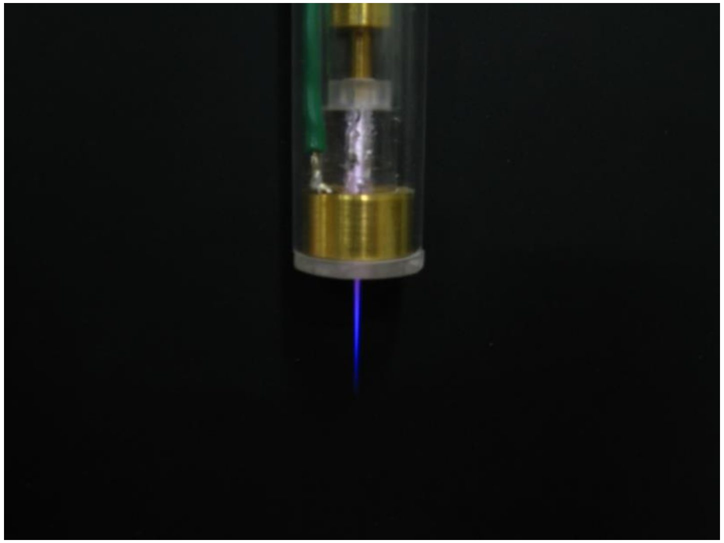
plasma based therapies



wound healing, cancer therapy, blood coagulation, sterilization, ...

Plasma System





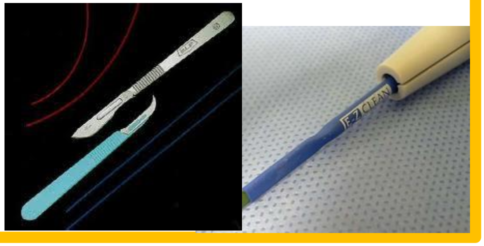
Typical Parameters:
Vpp = 10kV
frequency : 27kHz (sinusoidal)
He gas floe : 3L/min

Plasma medicine

traditional surgical devices

scalpels・electrical scalpels

mechanical force/ heat



radiations

X-ray, heavy ions

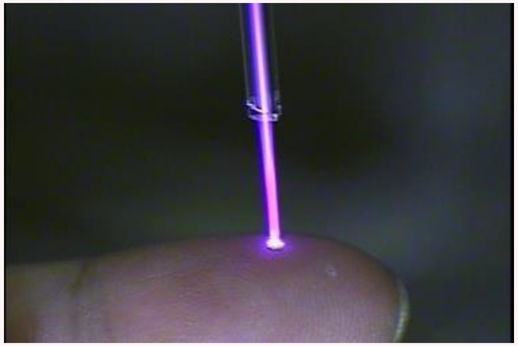
ionization

low-temperature plasma

new generation of plasma device

free radicals, ROS, RNS

blood coagulation, would healing, local sterilization, cell proliferation etc.



laser

laser scalpels

heat

thermal plasma

argon plasma coagulator

heat

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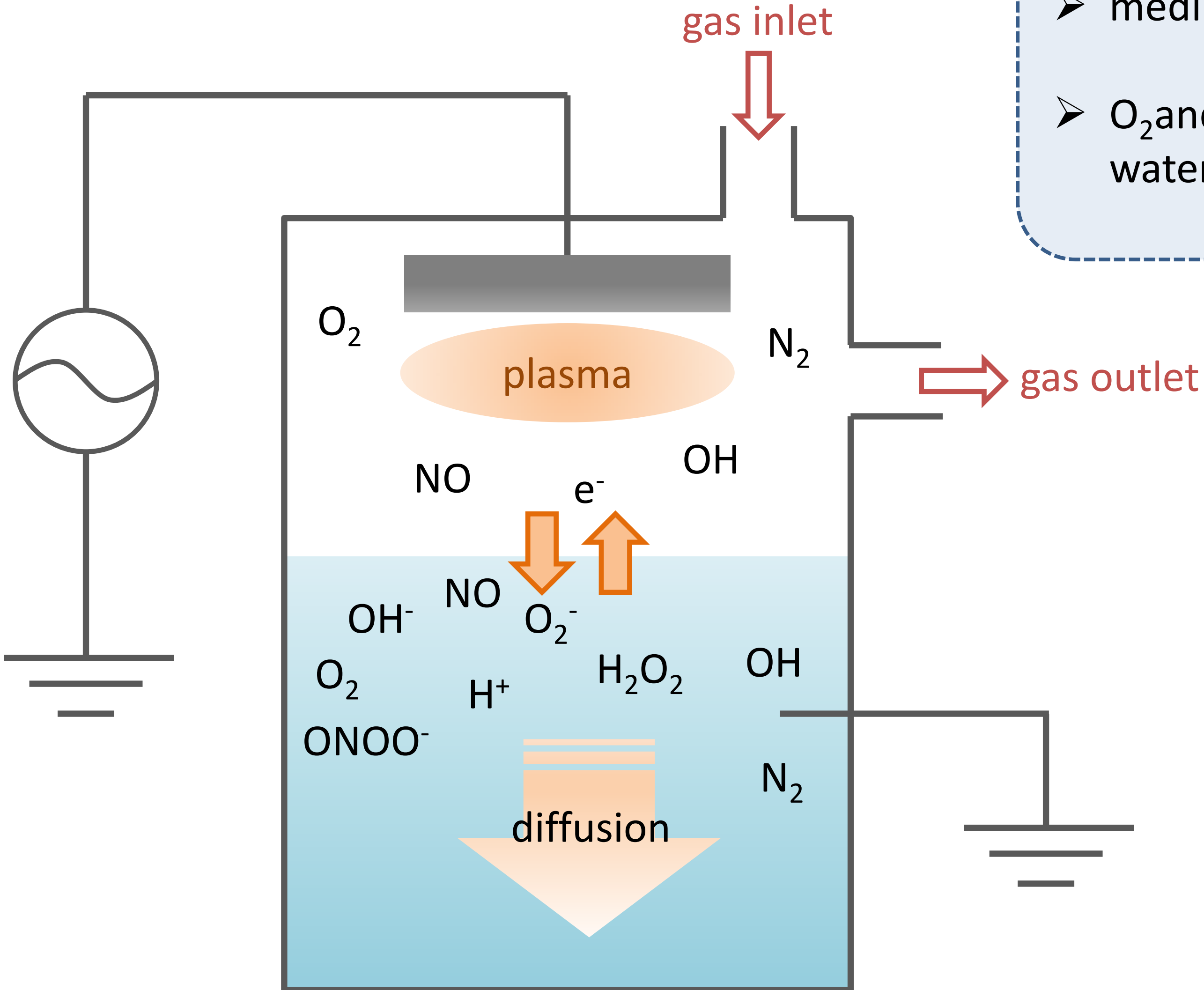
– Simulation Model –

1D Reaction-Diffusion equations

- 37species with
- 111 reaction equations
- chemical reactions and diffusion in water



Initial Conditions

- medium: pure water
- O_2 and N_2 dissolved in water at 1atm

Transport terms connecting the gas and liquid phases

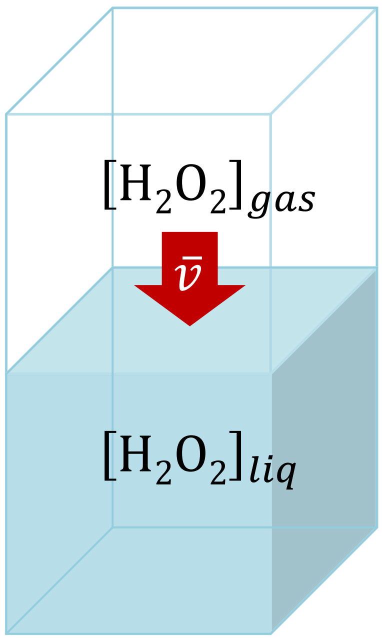
one dimensional reaction diffusion equations in the liquid phase

$$\frac{d[\mathrm{OH}]}{dt} = \underbrace{k_{ij}[\mathrm{H}][\mathrm{H_2O_2}] + \ \cdots}_{\text{reaction terms}} \ \underbrace{+ \frac{d}{dx}\Gamma_{\mathrm{OH}}}_{\text{transport term}}$$

reaction terms *transport term*

k_{ij} : rate constant Γ_{OH} : flux

for example $\mathrm{H + H_2O_2 \rightarrow OH + H_2O}$



Assumptions

- ✓ All gaseous species enter the liquid surface at thermal speed.
- ✓ Fluxes of charged particles are specified by their electric currents.
- ✓ Neutral particles desorb by Henry's law
- ✓ No charged particle leaves the liquid

Model equations

Mass conservation

diffusion — advection

$$\frac{\partial n_i}{\partial t} = \tilde{R}_i - \nabla \cdot \left(- D_i \nabla n_i + \mu_i n_i \mathbf{E} \right) - \mathbf{v}_c \nabla n_i$$

chemical reactions — drift by electrical field

Chemical reaction term (source term)

$$\tilde{R}_i = -\xi_{ij} n_i n_j + \xi_{kl} n_k n_l + \cdots$$

annihilation — production

Poisson's equation

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_w}$$

n_i : concentration of species i in liquid

t : time

D_i : diffusion coefficient of species i

μ_i : mobility of species i

$\mathbf{E}$: electric field

$\mathbf{v}_c$: flow velocity

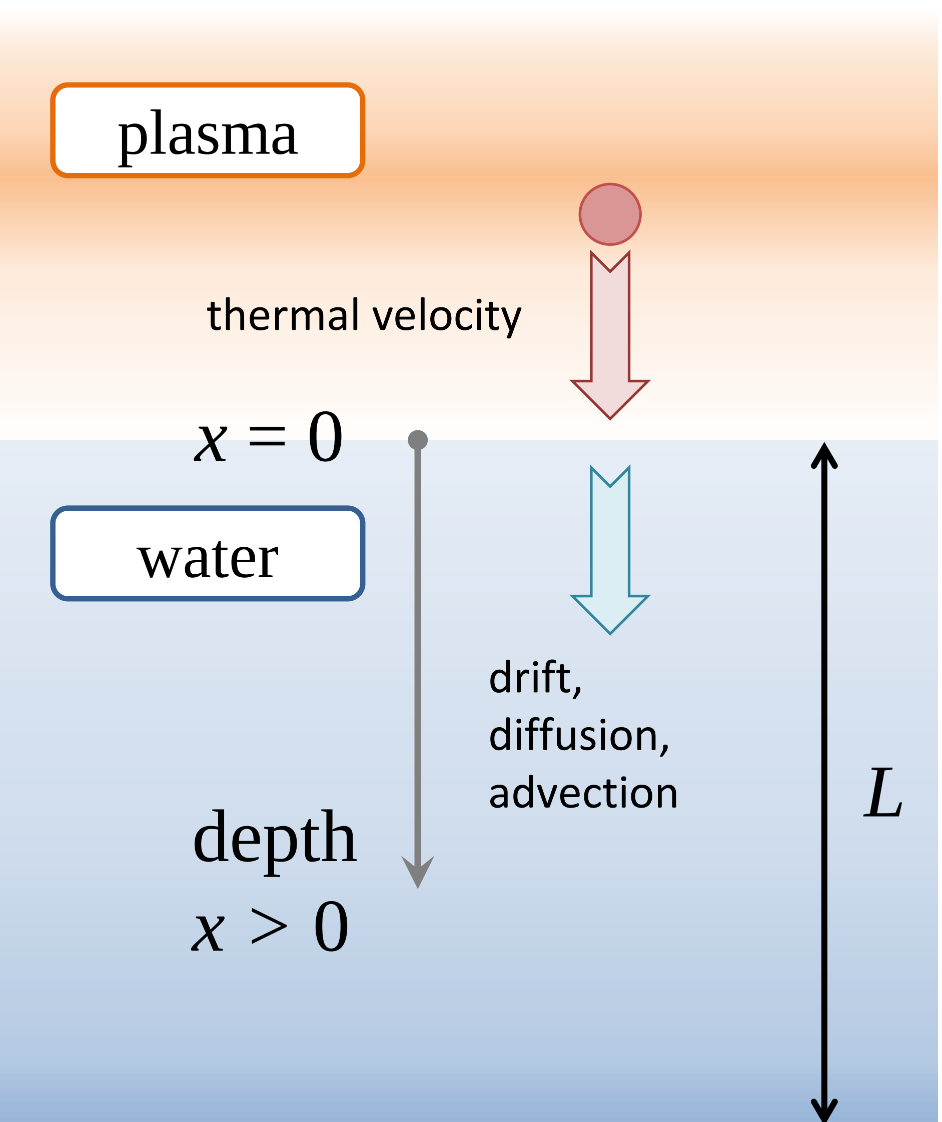
$(\nabla \cdot \mathbf{v}_c = 0.)$

ξ : reaction rate

ρ : charge density

ε_w : dielectric constant of water

Boundary Conditions



Surface

$$v_i^{th}\left(n_i^{gas} - \frac{n_i}{k_i^H R T_g}\right) = \left(-D_i \frac{\partial n_i}{\partial x} + \mu_i n_i E\right)\bigg|_{x=0}$$

v_i^{th} : thermal velocity (gas)

n_i^{gas} : concentration (gas)

k_i^H : Henry's constant

R : gas constance

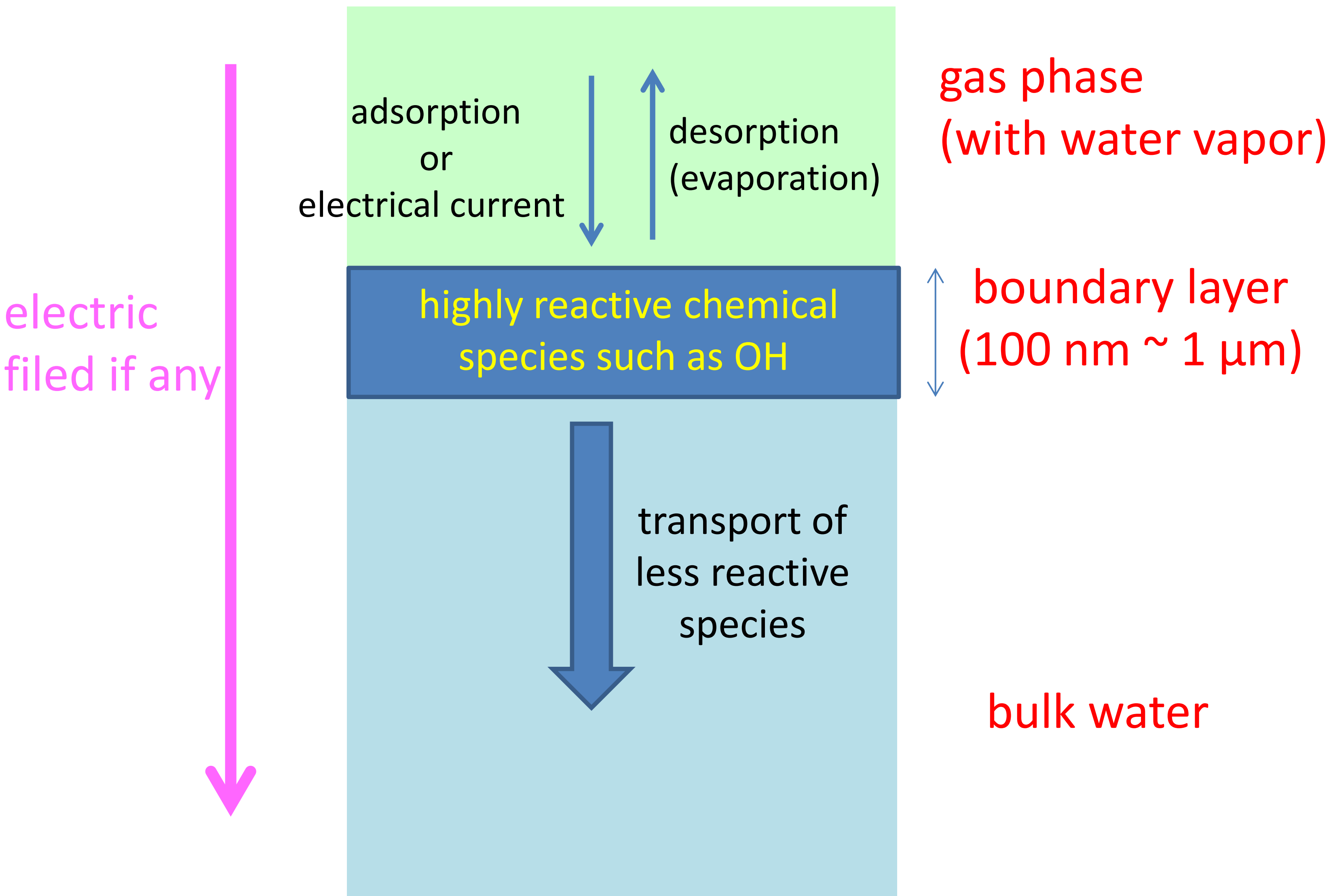
T_g : gas temperature

Bottom   if L is sufficiently large

$$0 = \left(-D_i \frac{\partial n_i}{\partial x} + \mu_i n_i E\right)\bigg|_{x=L}$$

L : bottom depth

gas-liquid interface



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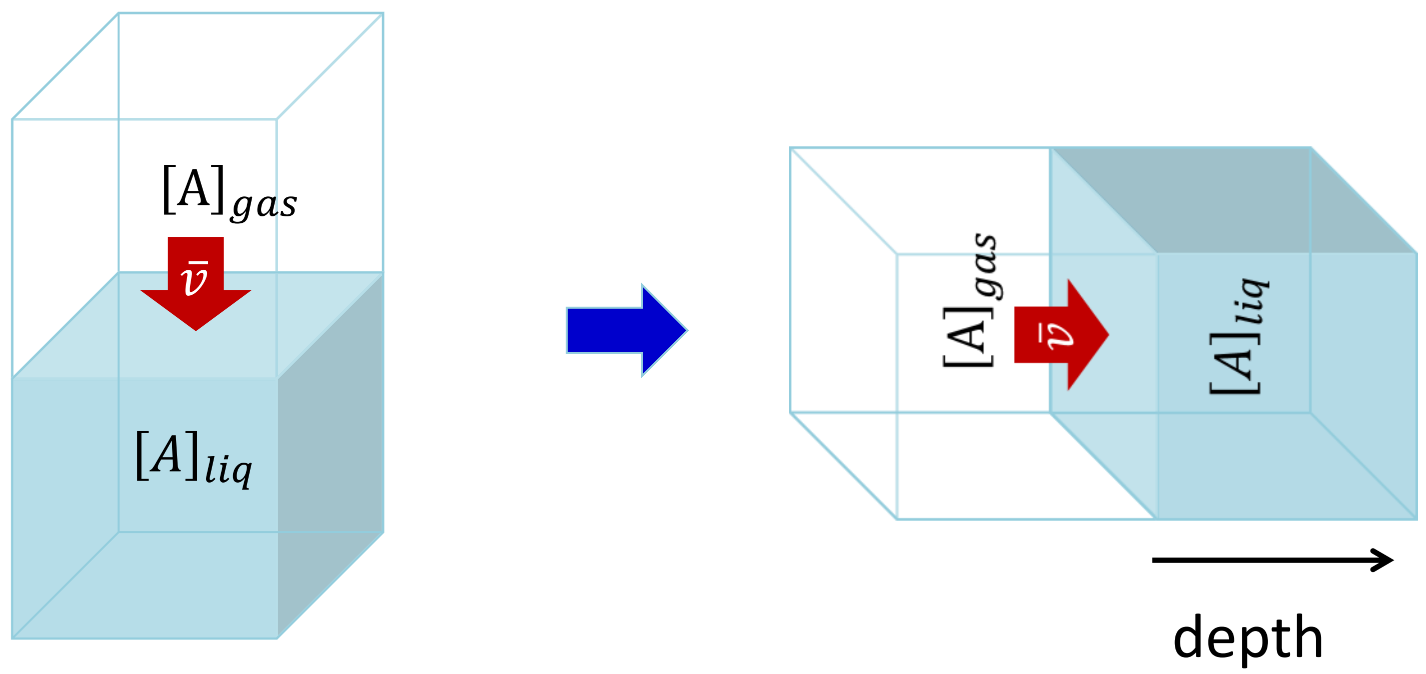
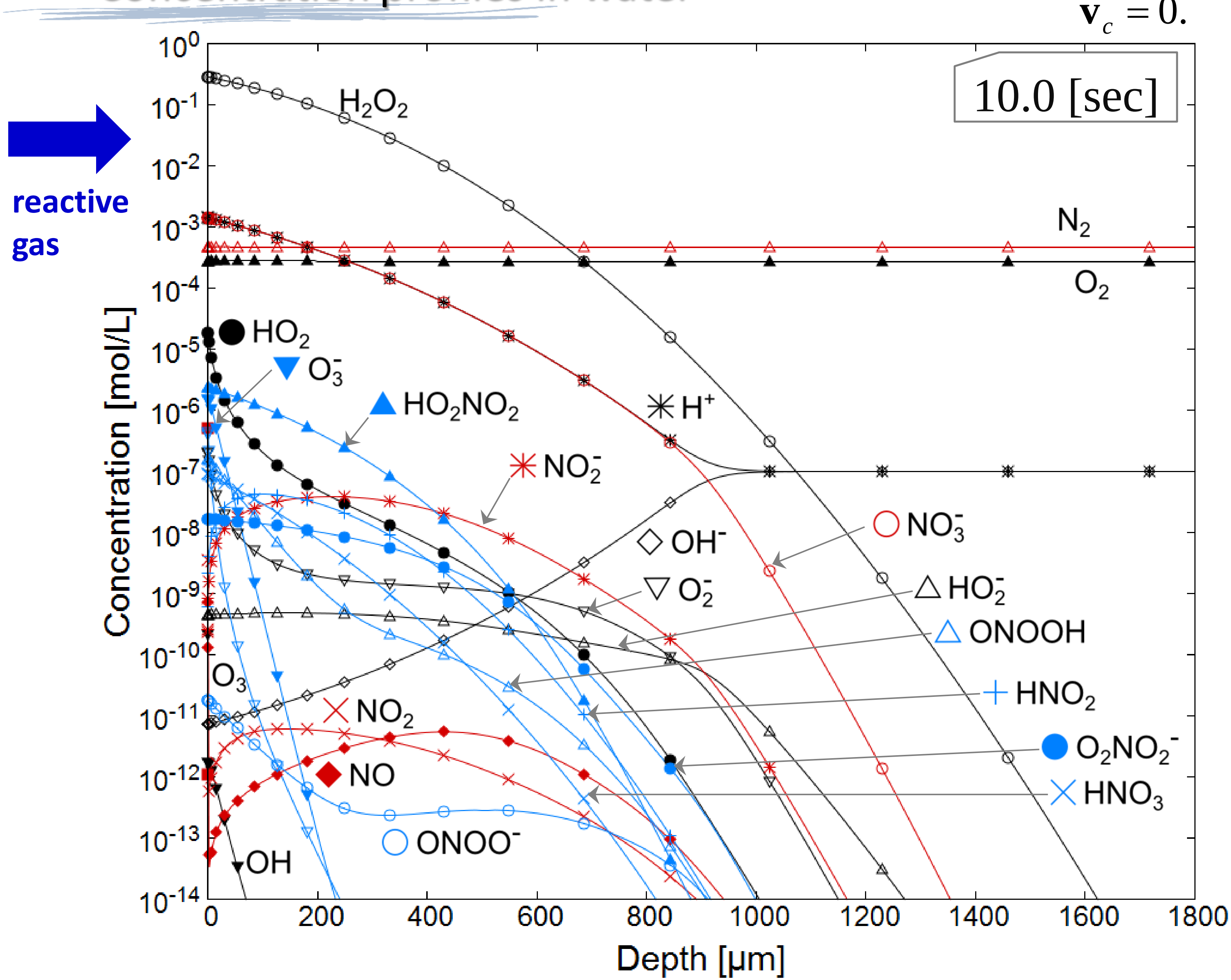
6 species supplied to pure water

species	Gas density (cm^{-3})	Incident flux ($mol \cdot cm^2 \cdot s^{-1}$)
H_2O_2	1×10^{14}	1.8×10^{-6}
HO_2	3×10^{9}	5.5×10^{-11}
NO	1×10^{13}	1.9×10^{-7}
NO_2	8×10^{12}	1.2×10^{-7}
NO_3	1×10^{13}	1.3×10^{-7}
O_3	1×10^{15}	1.5×10^{-5}



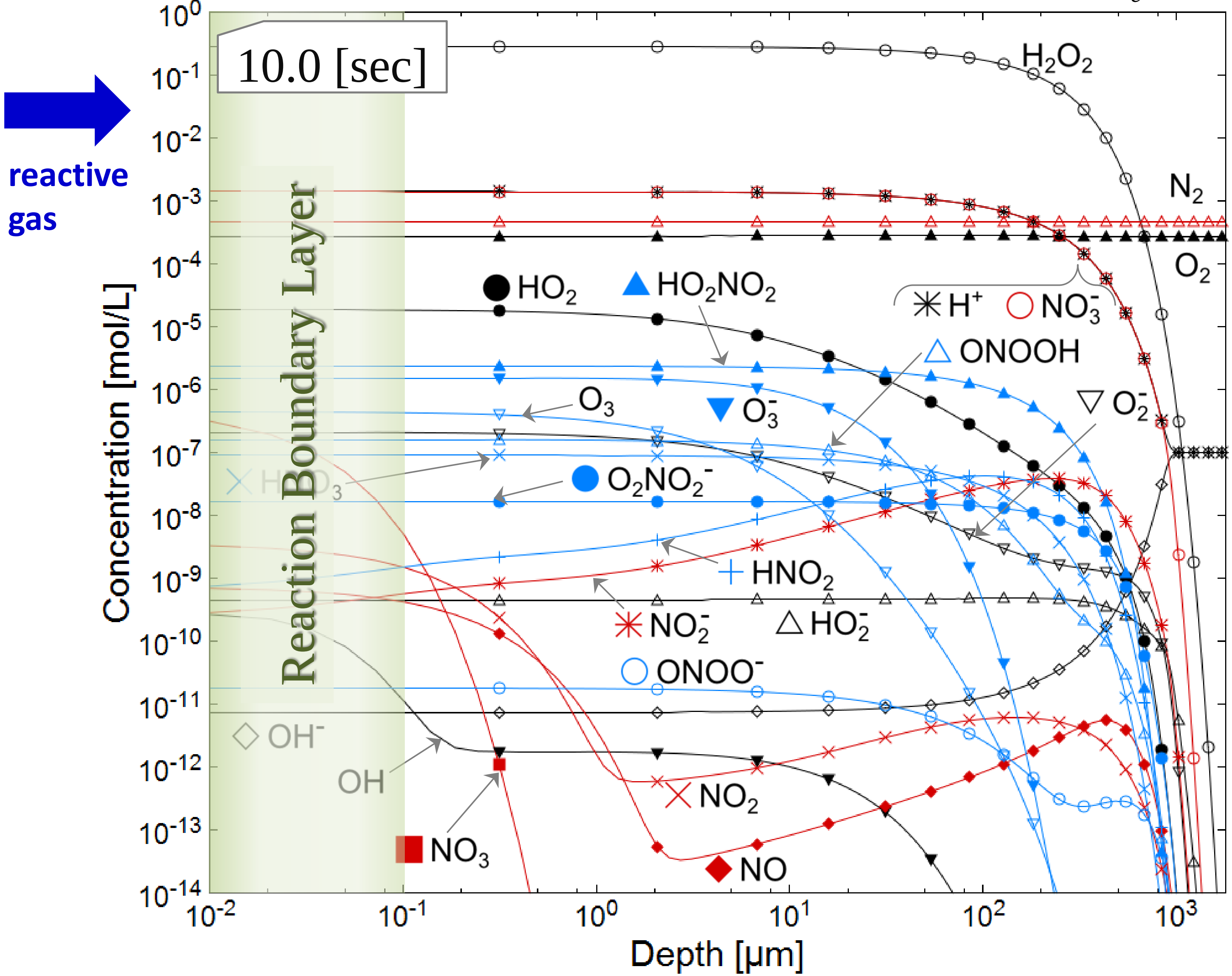
$[A]_{gas}$
$\bar{v}$
$[A]_{liq}$
$[A]_{gas}$
$\bar{v}$
$[A]_{liq}$
depth

Concentration profiles in water

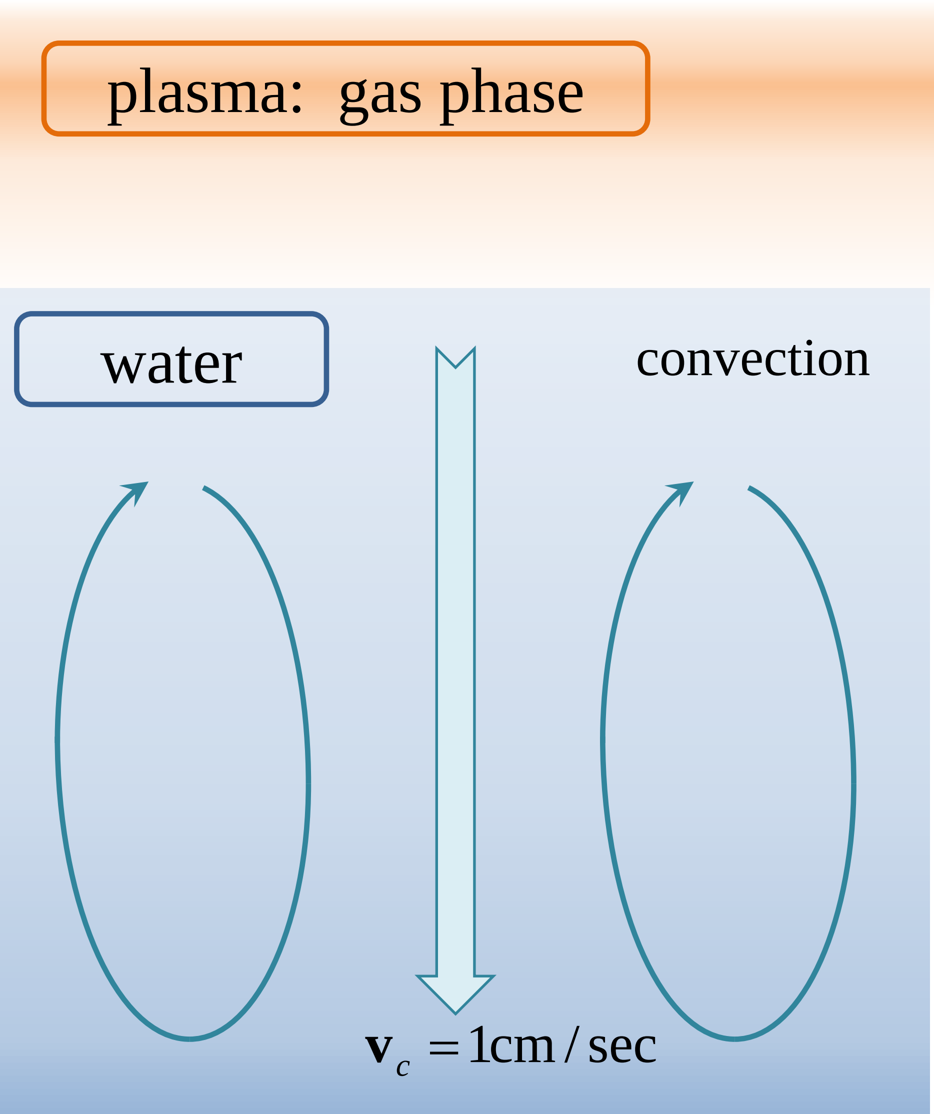


Concentration profiles in water (in log scale)

$\mathbf{v}_c = 0.$



Simulation model with advection

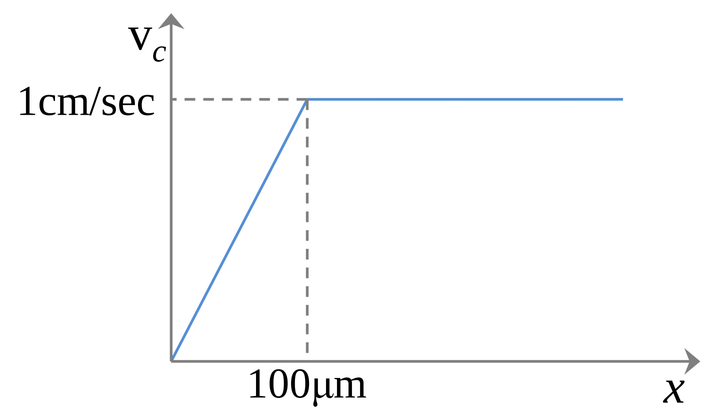


$$\frac{\partial n_i}{\partial t} = \tilde{R}_i - \nabla \cdot \left(-D_i \nabla n_i + \mu_i n_i \mathbf{E} \right) - \mathbf{v}_c \nabla n_i$$

flow velocity

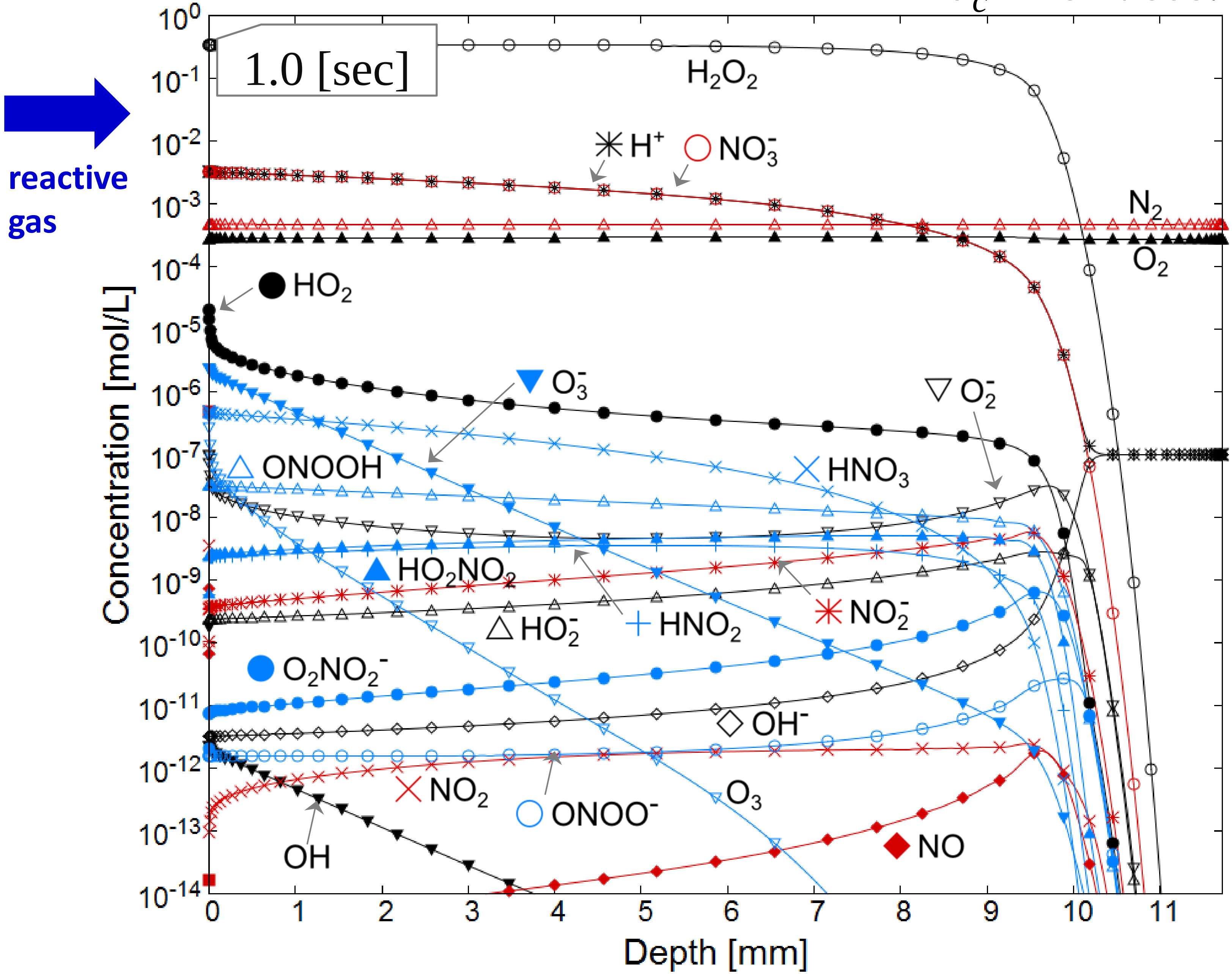
$0 \leq x \leq 100\mu\text{m}$: linear

$100\mu\text{m} < x$: constant (1cm/sec)



Concentration profiles in water

$\mathbf{v}_c = 1\text{cm}/\text{sec}.$



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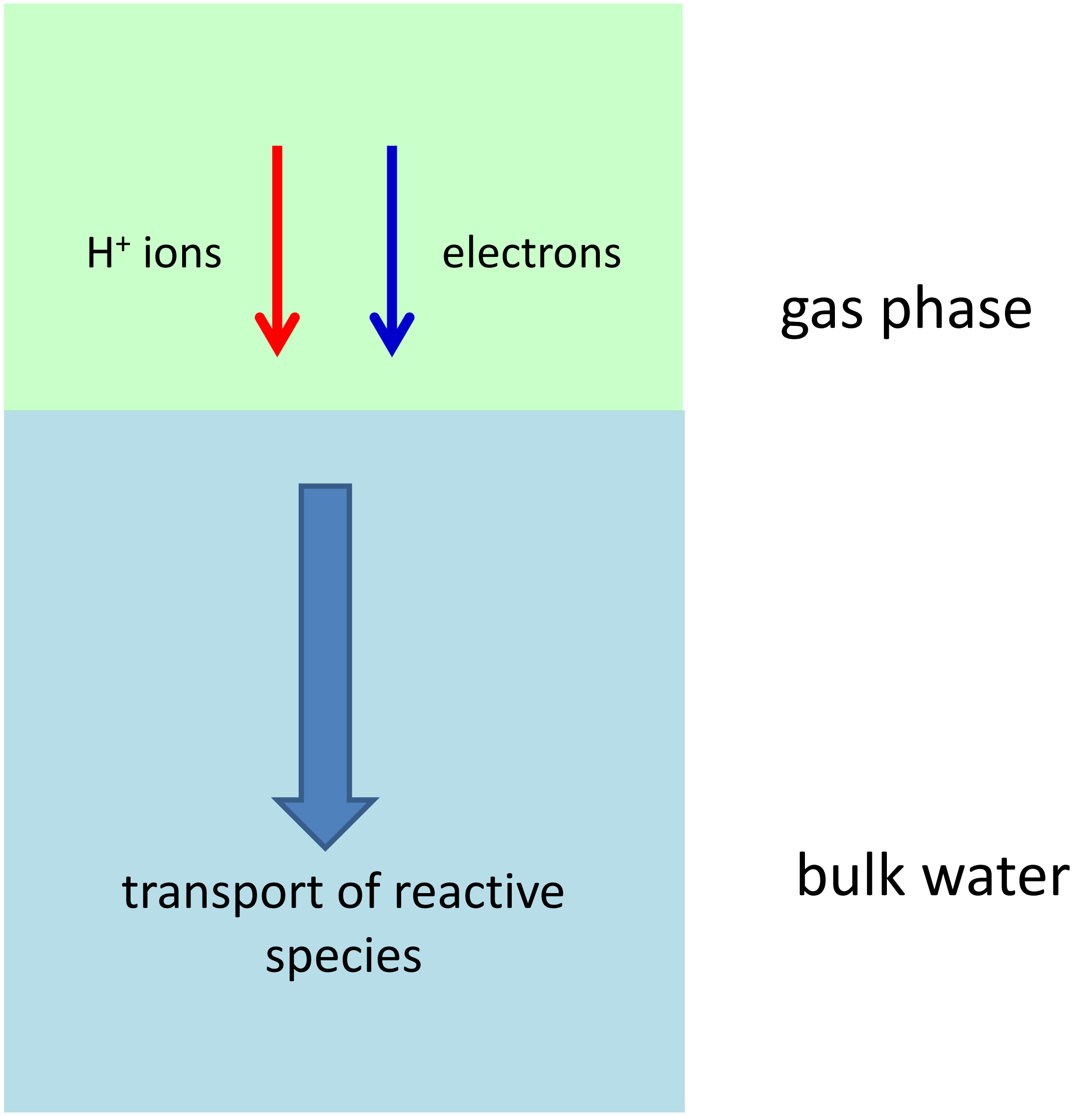
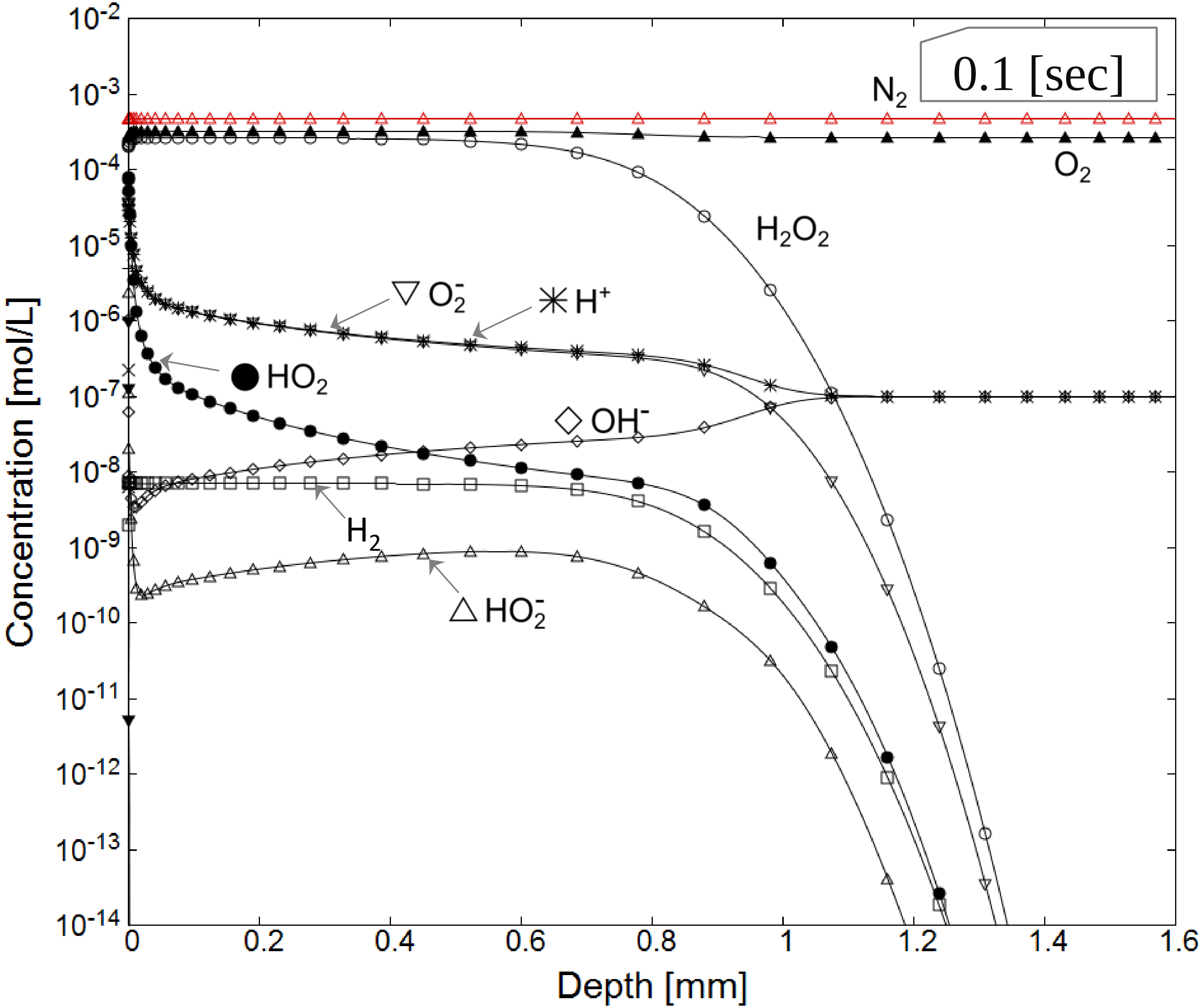
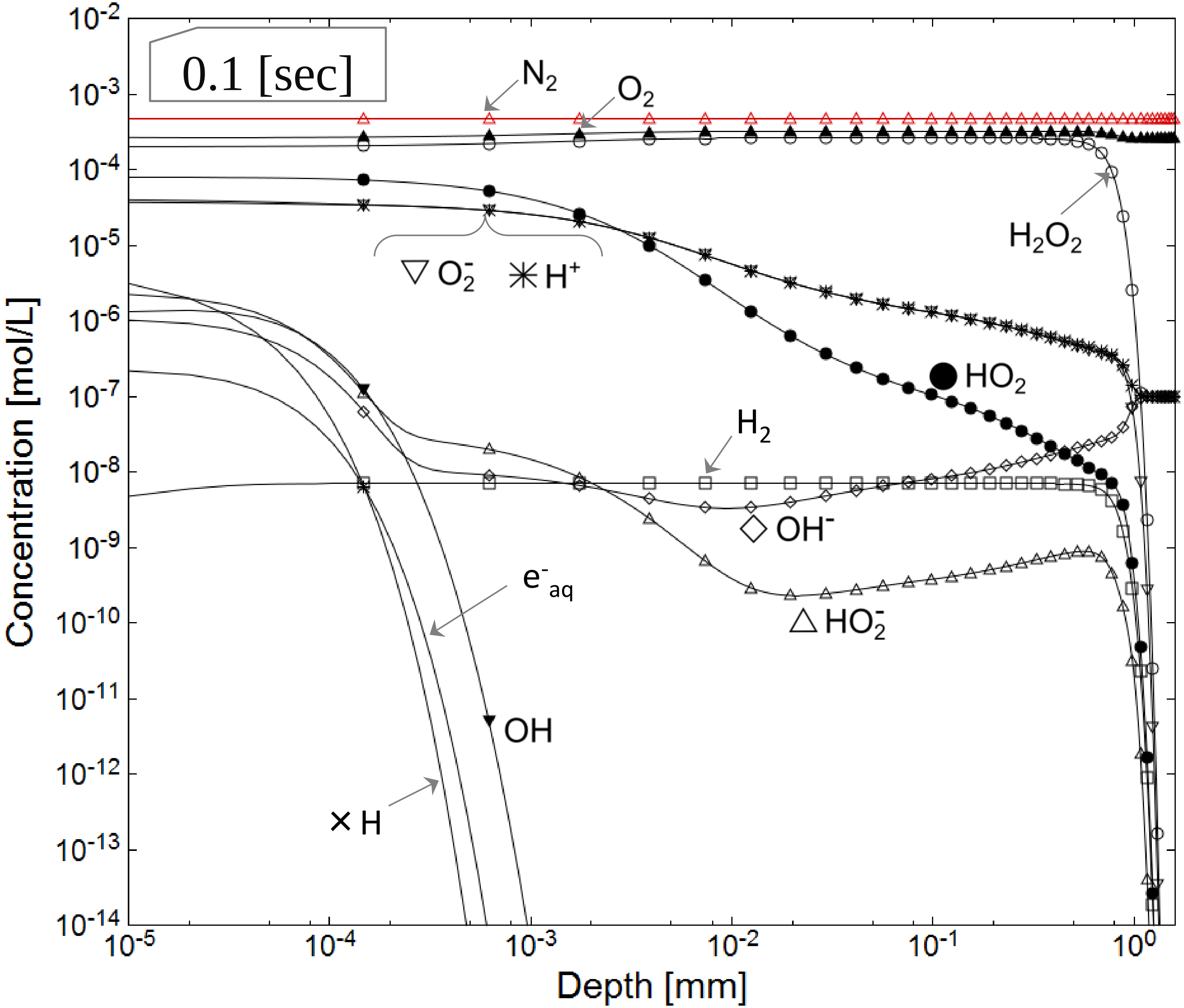
current effects (without net current)



electron and H^+ supply（±0.01mA/cm^2 : no net current)



electron and H^+ supply (±0.01mA/cm^2 : no net current)



Conclusions

1. **Numerical simulators for advection-reaction-diffusion equations for reactive species in liquid has been developed for 1D systems based on available chemical data.**
2. **There is a liquid-phase boundary layer with a thickness of about 100nm~1μm, only in which highly reactive chemical species supplied through the surface exist.**
3. **Current (electrons and H^+ ions) generates H_2O_2 via O_2^-/HO_2 and then also generates OH radicals from**

$$e_{aq} + H_2O_2 \rightarrow OH + OH^-$$