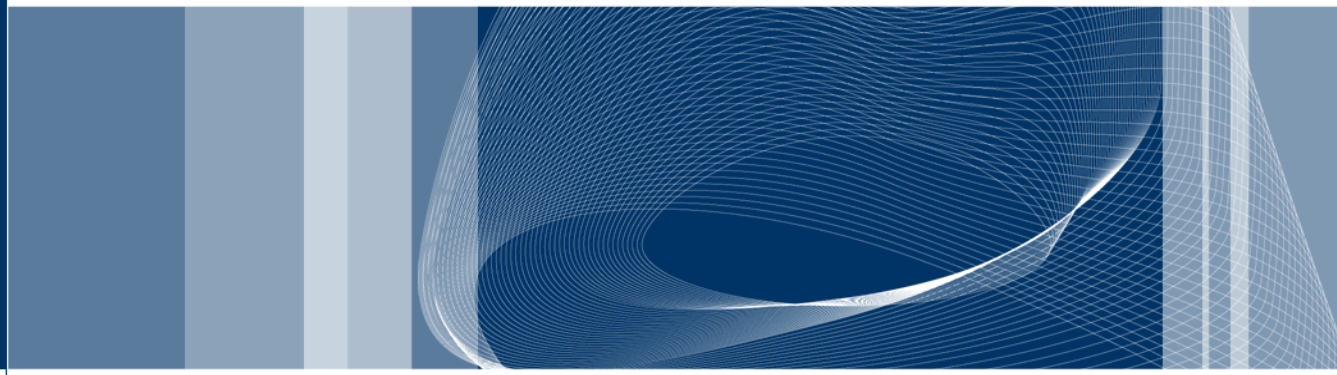
POLITECNICO DI MILANO



2D Modeling - Gas Phase

Maurizio Rondanini, Carlo Cavallotti

Dip. Chimica, Materiali e Ingegneria Chimica “G. Natta” – Politecnico di Milano

Outline

- Model structure
- Summary of previous results and problems
- Plasma Model improvements
- Results

Features of the Model

2 D plasma discharge model

2D Electronic density, electric field

Gas phase composition

Ions + radicals

2 D model of gas phase and surface chemistry model

Surface fluxes

Growth Rates

Literature + Polimi

Reaction rates

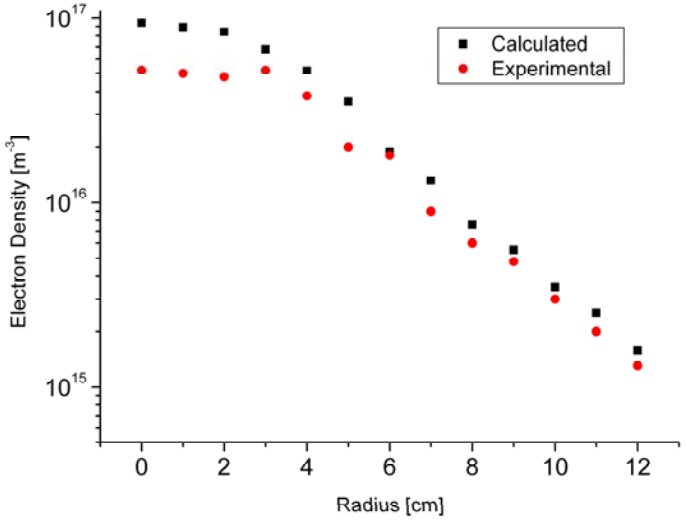
UniMib

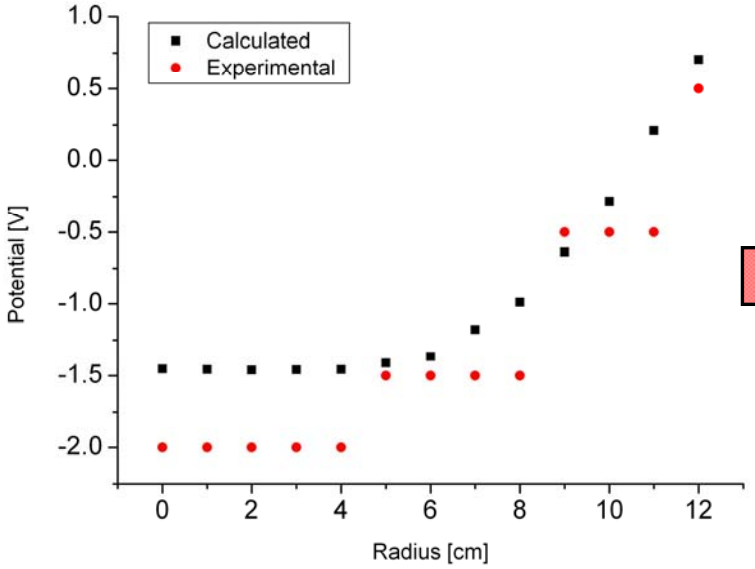
Gas phase and surface

kinetic mechanism of elementary reactions

Plasma Discharge

Model validated on pure Ar plasma discharge





2D Gas Model

Problem: comparison with ion experimental concentrations

Features implemented for Aix

- Introduction of new reactions:

SiH_3, SiH_2, SiH and H ionization and dissociation

e.g.

$SiH_3 + e \rightarrow SiH_3^+ + 2e$ $\quad$ $SiH_3 + e \rightarrow SiH_2 + H$

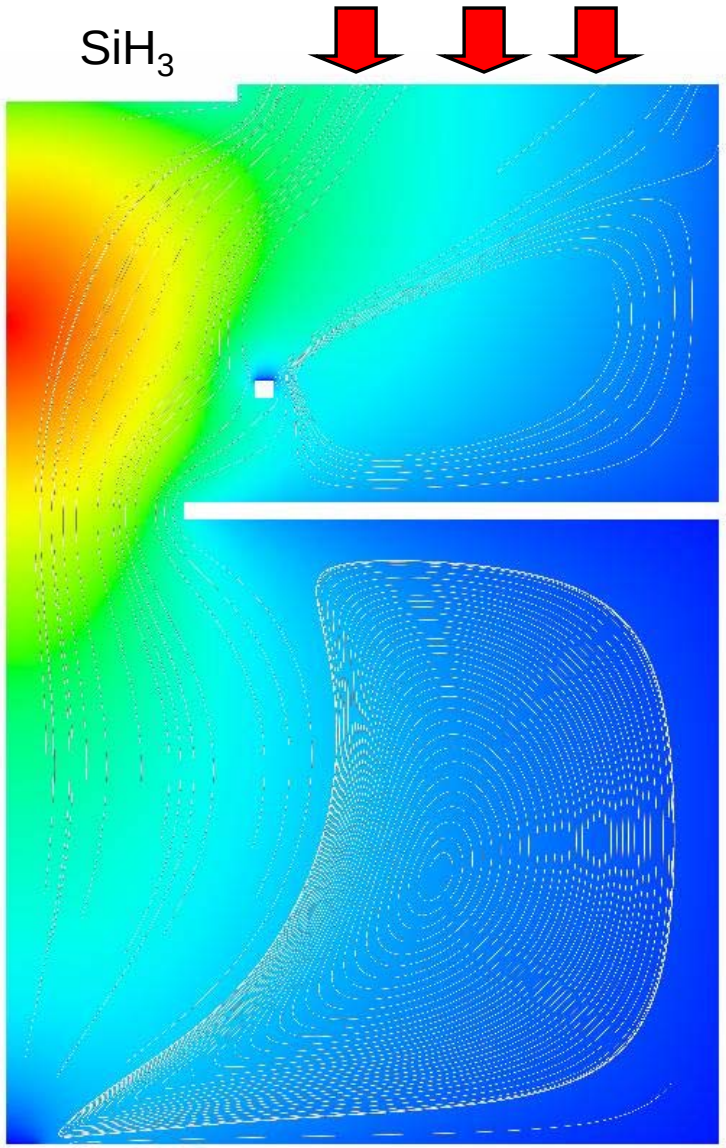
$SiH_3 + e \rightarrow SiH_2^+ + 2e$ $\quad$ $SiH_3 + e \rightarrow SiH + H_2$

$SiH_3 + e \rightarrow SiH^+ + 2e$ $\quad$ $SiH_3 + e \rightarrow Si + H_2 + H$

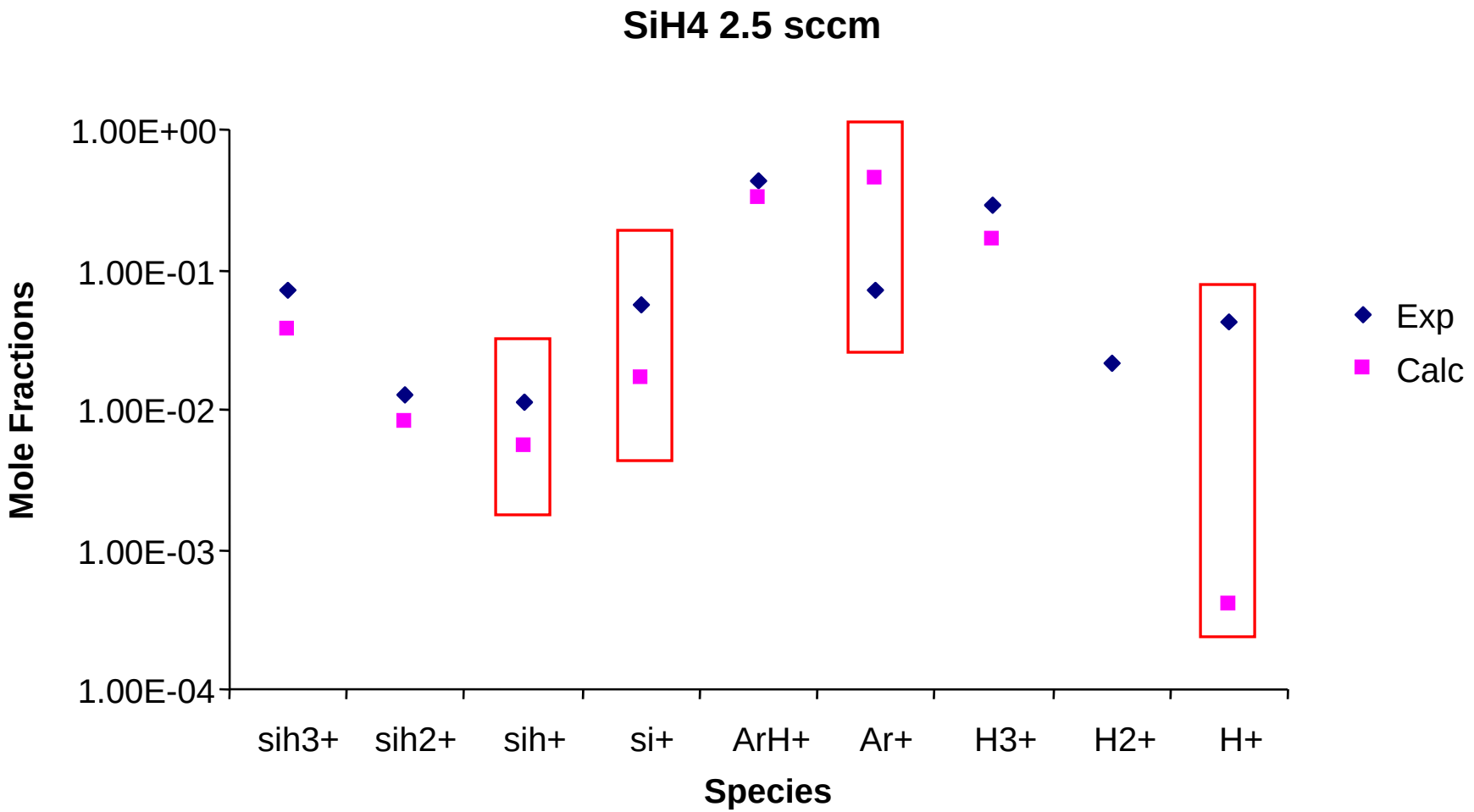
$SiH_3 + e \rightarrow Si^+ + + 2e$

New Boundary conditions at inlets

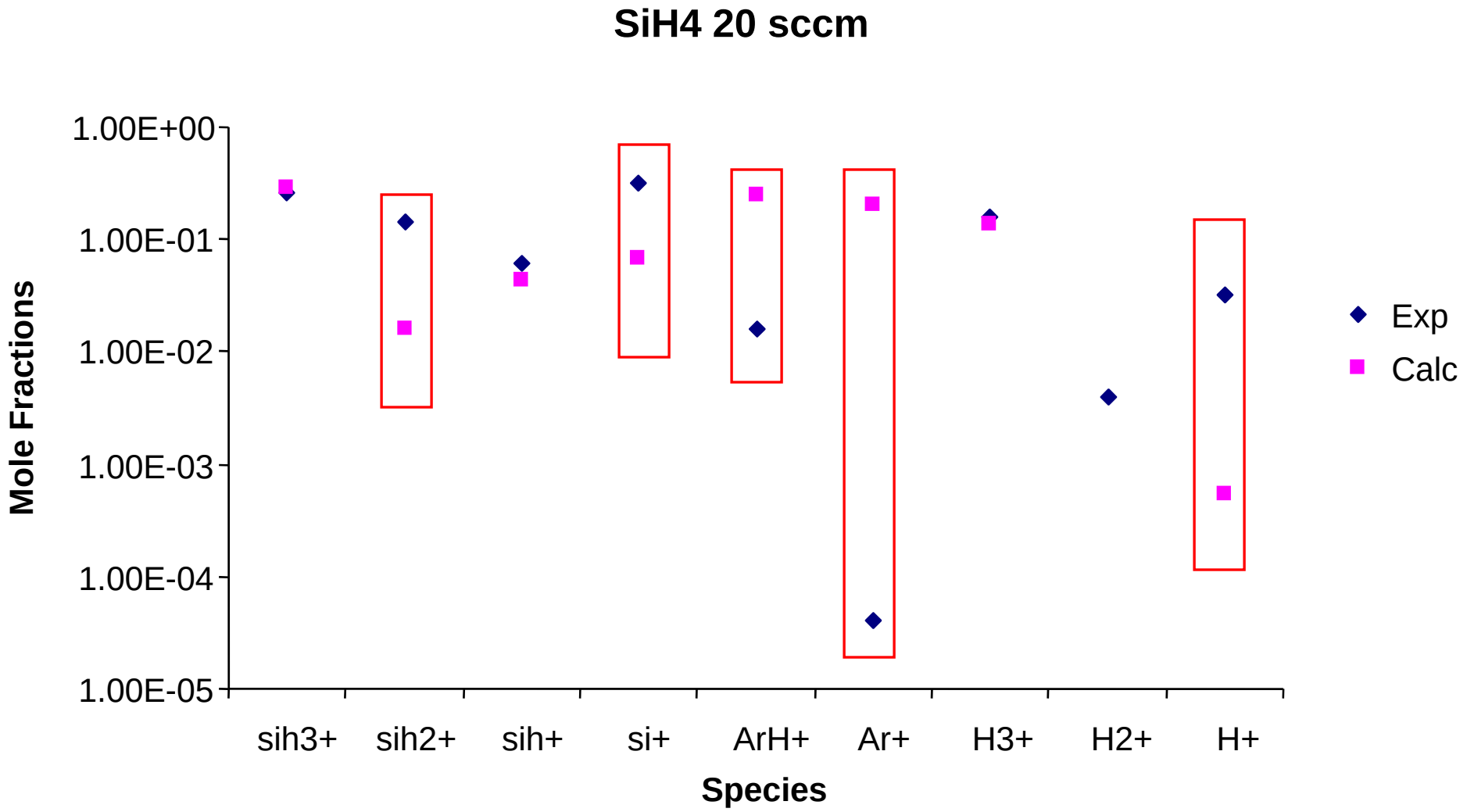
- Flux boundary condition for inlet 2: $D_i \nabla C_i = Flux\ in$
- inlet 1 ($\rightarrow$ Dankwerts BC: $v_i C_i^+ + D_i \nabla C_i = v_i C_i$



Results: ion concentrations – 2.5 sccm SiH4 pos B



Results: ion concentrations 20 sccm pos B



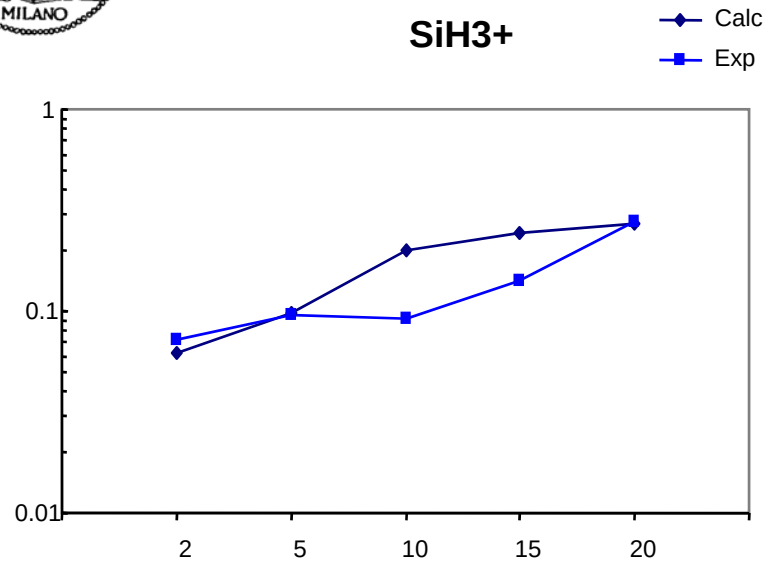
Improvement of model after AIX

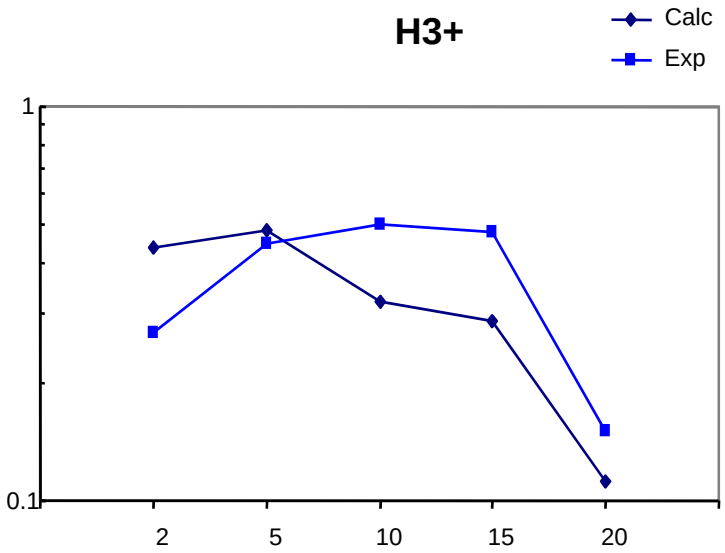
- Elimination of reactions at plasma reactor walls
- Assumption that the mass spectrometer perturbs the eedf in front of the orifice so that there is a volume where electronic reactions are not active. Non reactive volume fitted over exp ArH+ / H_3+ ratio measured for Ar/H2 plasma (only one fitting)
- Introduction of new reactions involving H induced decomposition of SiHx and SiH_3+ species:

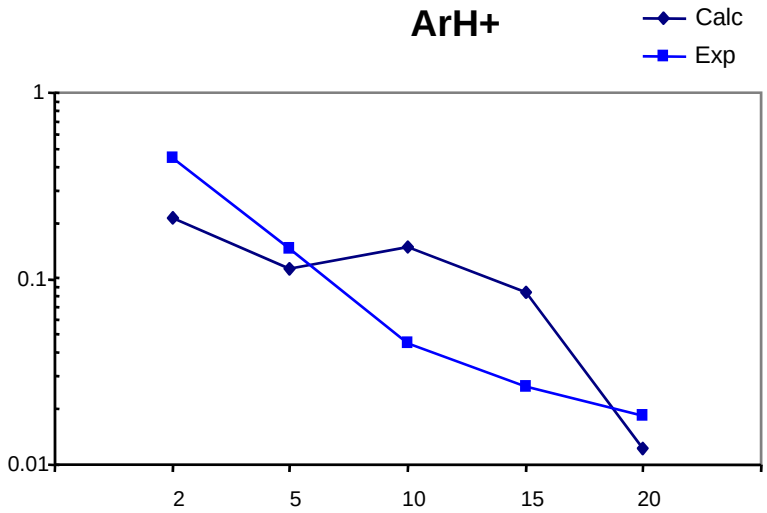
  e.g. $SiH_3 + H \rightarrow SiH_2 + H_2$

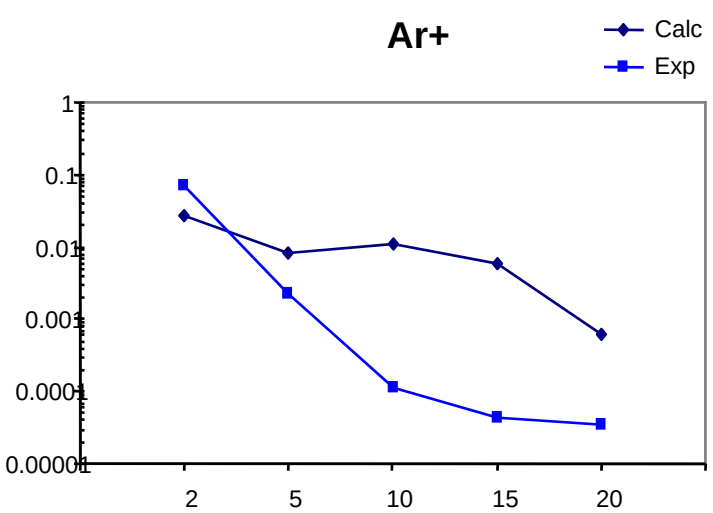
  Low pressure kinetic constant calculated with RRKM/ME approach on high level ab initio data

Last Results – position B

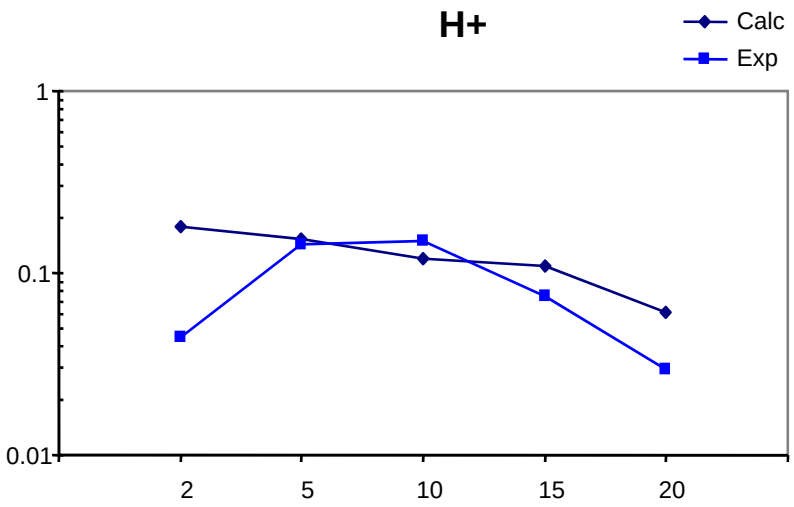


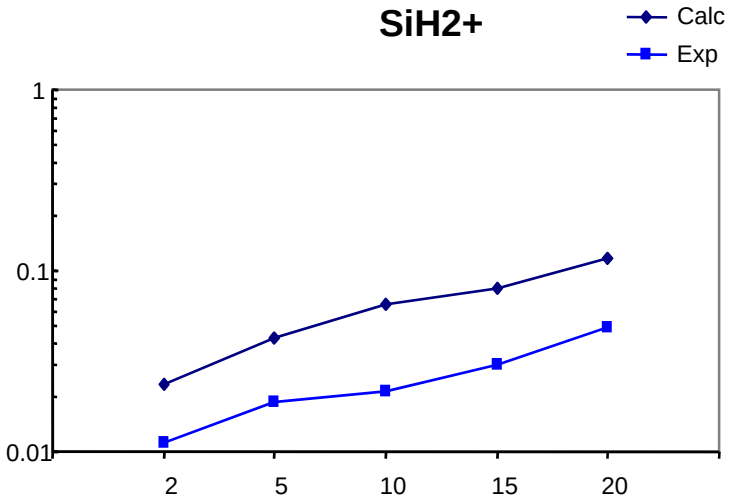


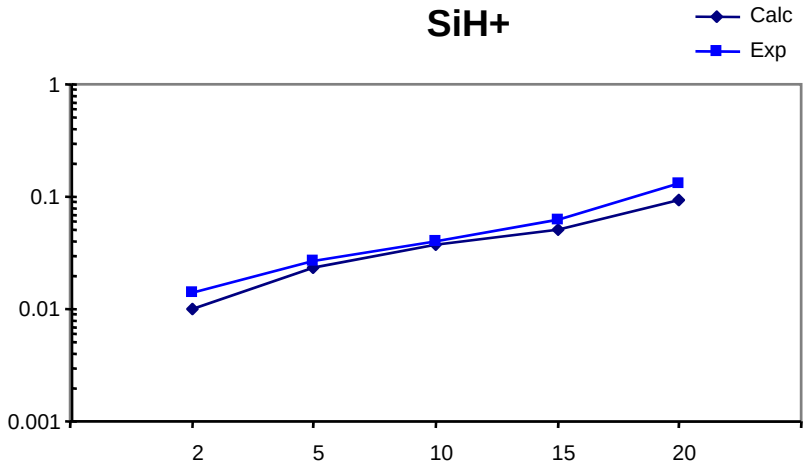


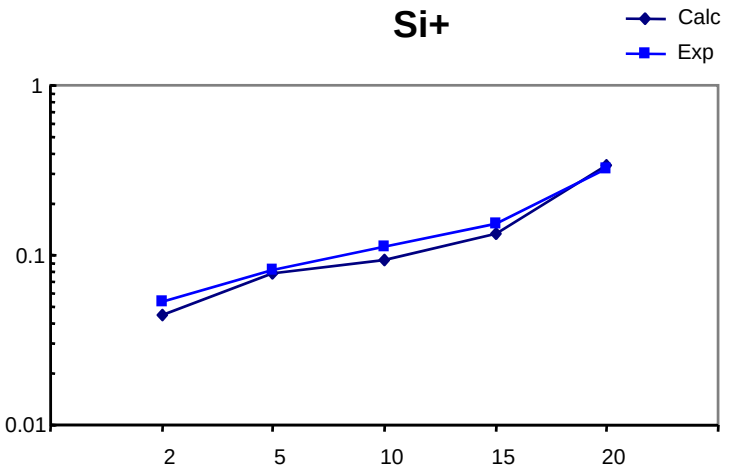


Last Results – position B

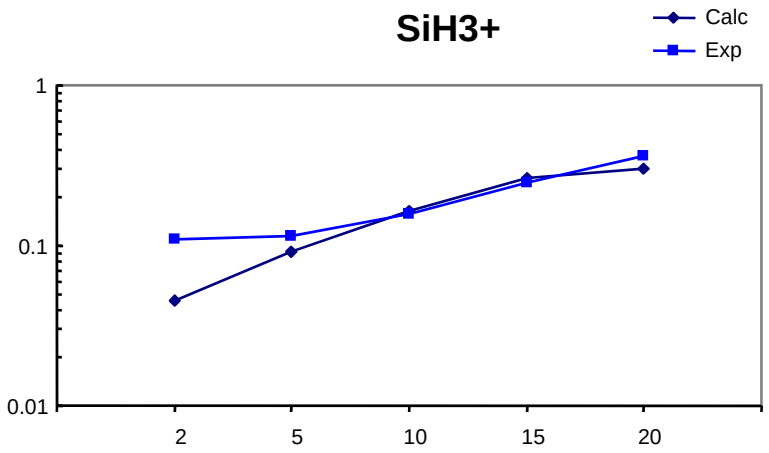


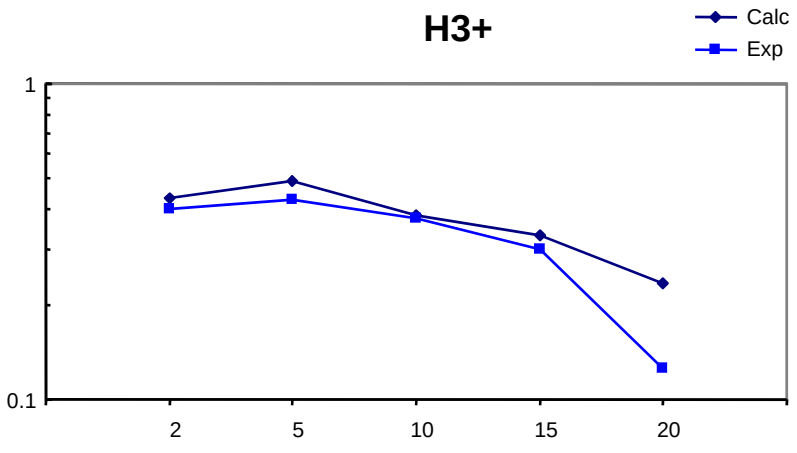


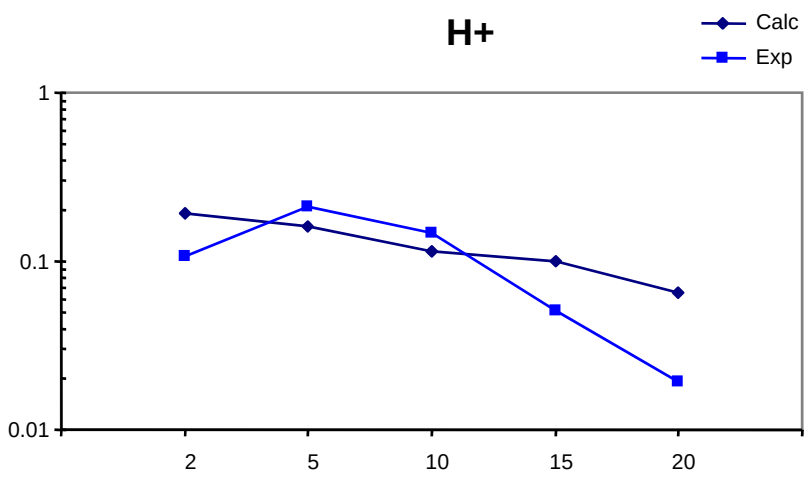


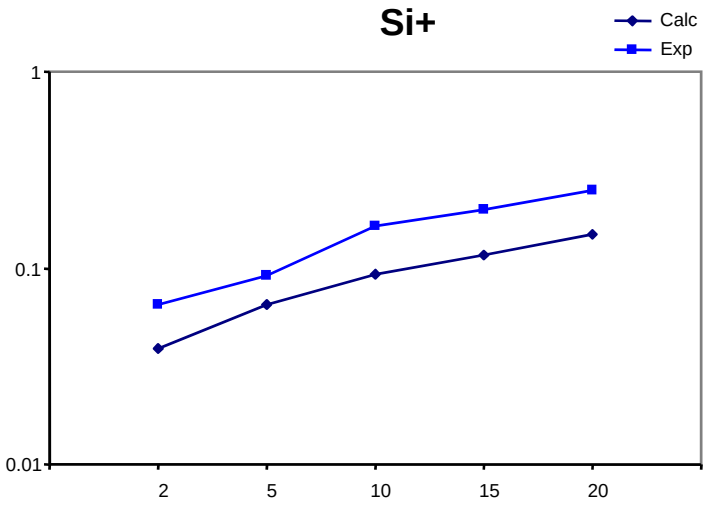


Last Results – position C









Conclusions

- Ion concentrations in very good agreement with experiments
- Radical concentration in qualitative agreement with Tamara results