Numerical Simulation of Vibrationally Active Ar-H2 Microwave Plasma

Franco Bosi[1], Mirko Magarotto[2], Paola de Carlo[2], Marco Manente[2], Fabio Trezzolani[2], Daniele Pavarin[2] , Davide Melazzi[2] , Piergiorgio Alotto[1] , Roberta Bertani[1]

1. Department of Industrial Engineering, University of Padova, Via Marzolo 9, Padova, 35132 Italy;
2. CISAS G.Colombo Space Activities Research Center, Via Venezia 59/4, Padova, 35132 Italy.

Introduction: Microwave discharges provide an efficient way for dissociating molecular gases [1]. Non-equilibrium conditions are attained, where *electron*, *vibrational* and *translational temperatures* differ from each other. The condition Tv>T results in catalytic promotion of endothermic dissociating reactions. In this work we simulate this non-equilibrium condition choosing as test case the Ar-H2 plasma.

Computational Methods:
2.45 GHz microwave irradiate a Ar:H2 (9:1) plasma in a 2D rectangular domain.

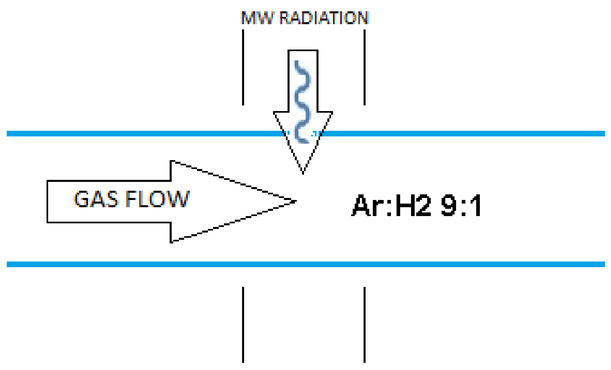

Figure 1. Discharge Schematic

Species: Ar, Ar(4s), Ar+, H2, H , H2+, H3+.
Modules: Microwave plasma + Laminar Flow + PDE vibrational energy equation + PDE total energy equation

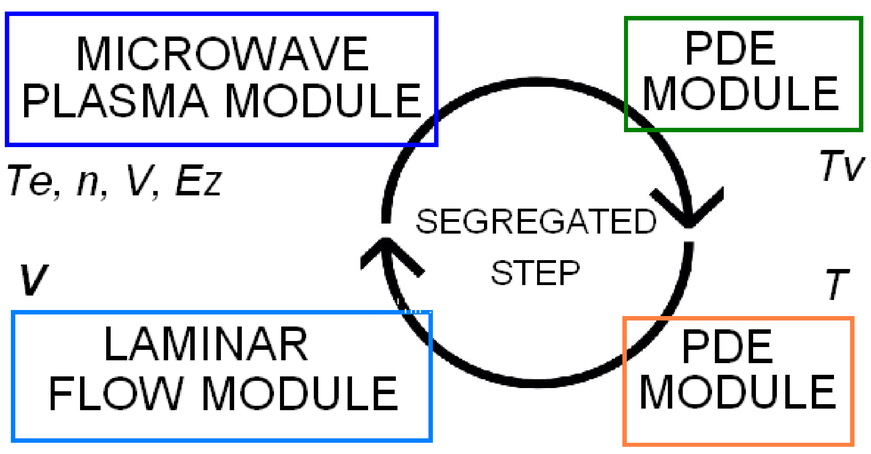

Figure 2. Solution scheme

- $\frac{\partial e_v}{\partial t} + \nabla \cdot (e_v \mathbf{v}) = \frac{S_{n_{H_2}}}{n_{H_2}} + S_{eV} - P_{VT}$
- $\frac{\partial e_t}{\partial t} + \nabla \cdot (e_t \mathbf{v}) = \frac{1}{\rho} [S_{eV} + S_{eR} + S_{el} + S_{eD}]$
- $K(T, T_v) = \Phi(T, T_v) \cdot K(T)$

Kuznetsov formula [2] for vibrational enhanced unimolecular dissociation rate

Results: Two simulations at 1 Torr pressure with feeding gas in "*cold*" 300 K and *"pre-heated"* 1400 K conditions

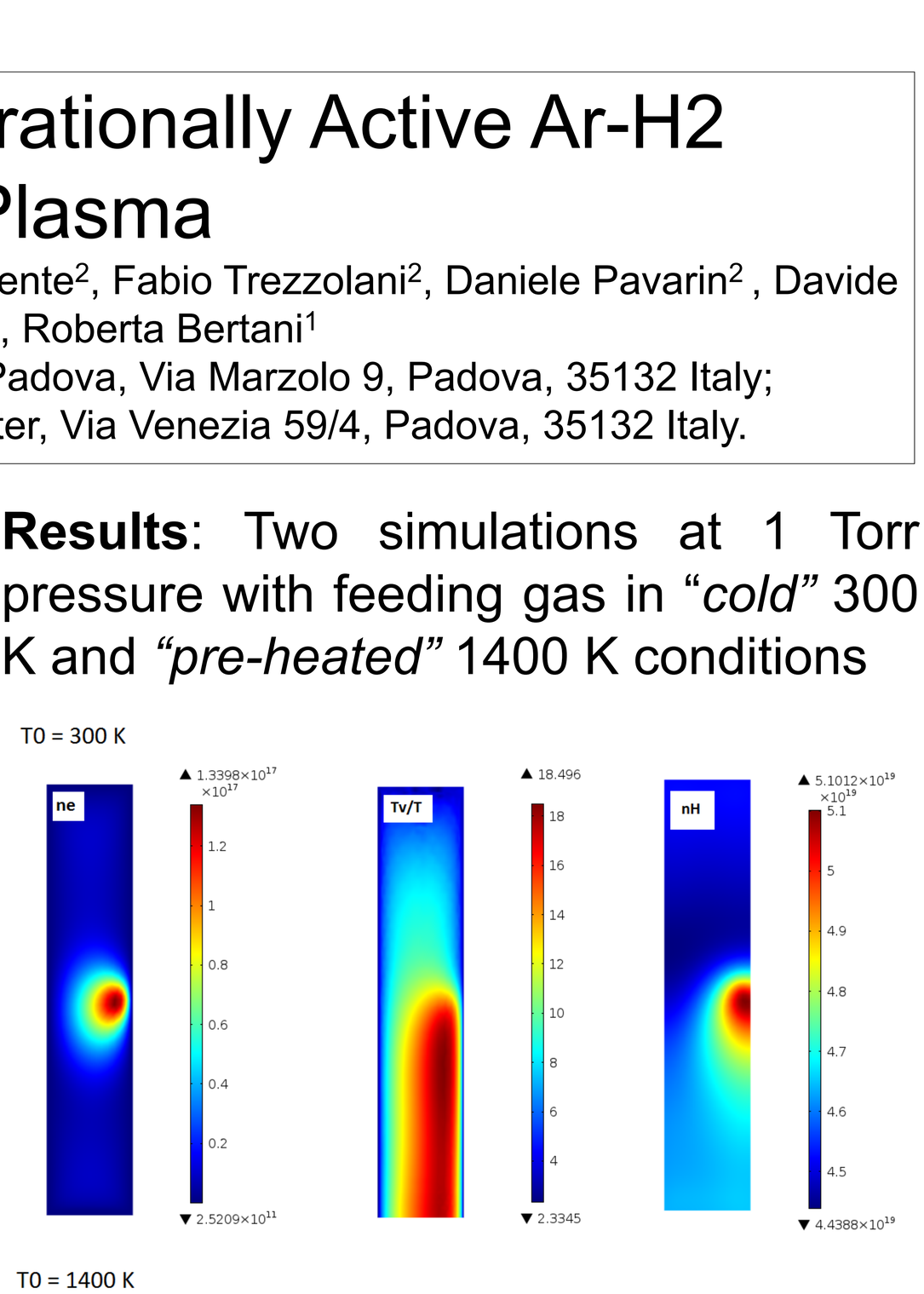

Figure 3. Electron density, Tv/T ratio and H density for the two discharge regimes

Conclusions: Conversion efficiency of the first case is 0.7%; efficiency of the second case is 5% with consistent contribution of vibrational catalysis

References:

1. VD Rusanov et al, The physic of chemically active plasma with non-equilibrium vibrational excitation of molecules, Soviet Physics Uspekhi, **24**(6):447, 1981.
2. G Chernyi, et al. Physical and Chemical Processes in Gas Dynamics: Cross sections and rate constants. Volume I, AIAA, 2002.