Plasma Catalysis at the nanoscale: Model development for diffusion and chemical reactions in catalyst pores

Yannick Engelmann

Prof. dr. Annemie Bogaerts

Prof. dr. Erik Neyts

Research group PLASMANT

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University of Antwerp

Introduction

$$CO_2 + 3H_2 \longrightarrow CH_3OH + H_2O$$

<u>Problem 1</u>: CO_2 is relatively inert
processes require high Temp

<u>Problem 2</u>: Poor selectivity
lots of side products

Introduction

Solution: Plasma catalysis

Combining

high reactivity in a plasma

with

high selectivity in chemical catalysis

1. Chiang, W.-H. et al. *ACSNano* **3**, 12, 4023-4032 (2011).
2. Silvearv, F. et al. *J. Mater. Chem. C* **3**, 3422-3427 (2015).
3. Magnin, Y. et al. *Phys. Rev. Lett.* **115,** 205502 (2015).

Two questions…

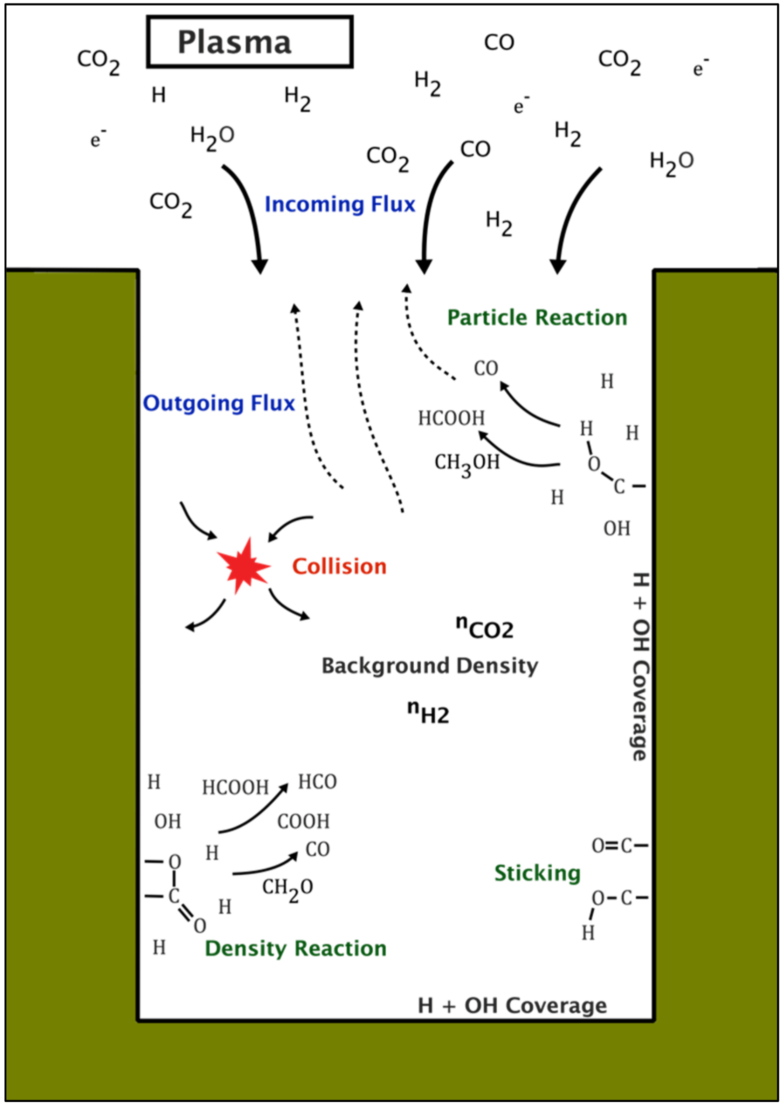
Question 1: How does Plasma catalysis improve on thermal catalysis?

⟶ Study **impact of plasma species** on total yield

Question 2: Can porous surfaces generate higher yields?

⟶ Study the **production rate in catalyst pores**

Kinetic Monte Carlo Model



1. Movement of particles via Newton dynamics

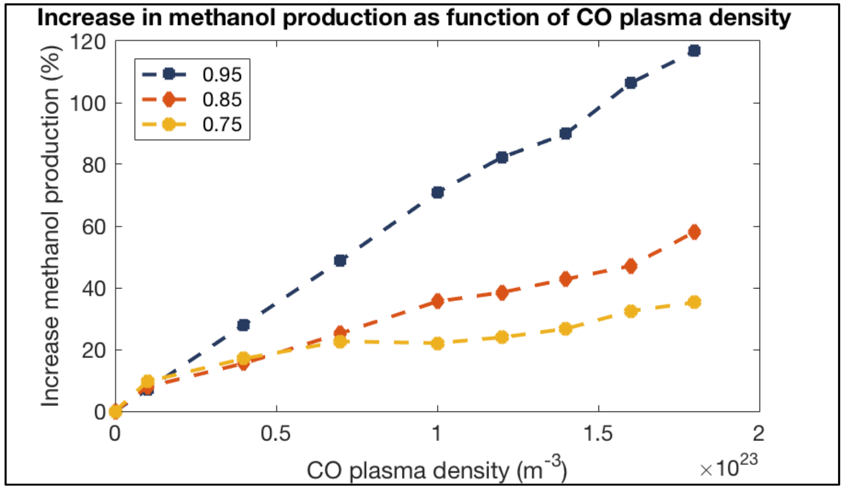
2. Collisions and reactions determined stochastically

3. Sticking coefficients and reaction rate coefficients

Currently: Estimate values

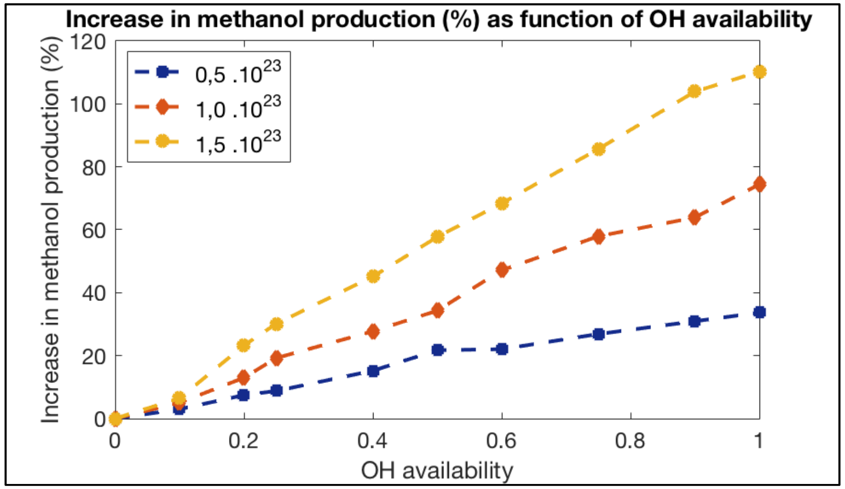
Future: from DFT calc.

Results



Blue curve:
Typical CO density of 10^{23} m^{-3}

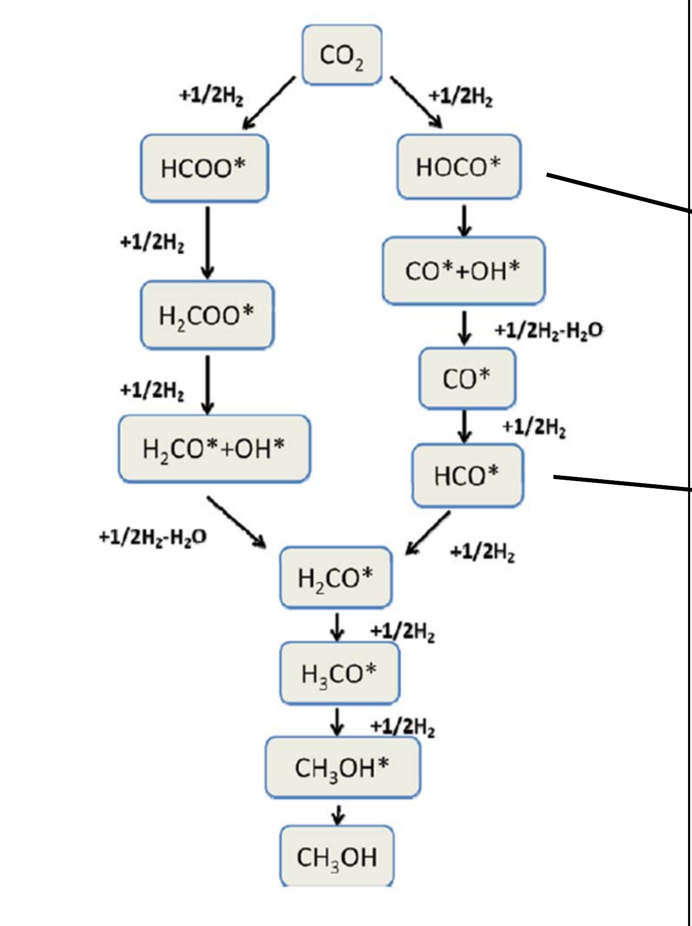
methanol production can **increase up to 71%**

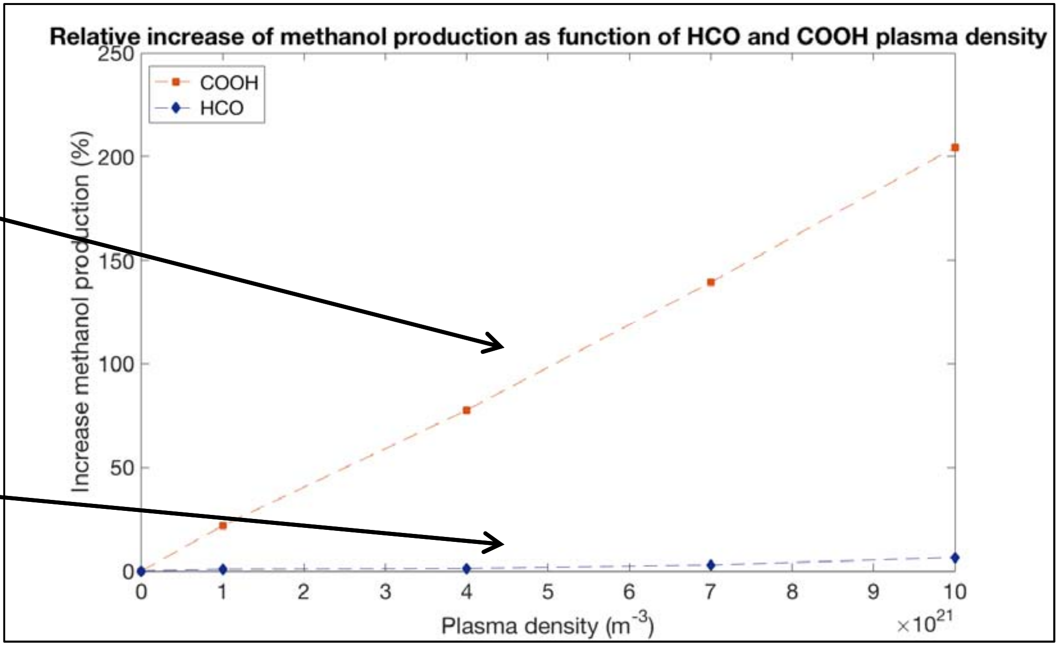


Red curve:
Typical CO density of 10^{23} m^{-3}

methanol production can **increase up to 75%**

Results





Conclusion: Wrong reaction mechanism

Instead: COOH ⟶ $C(OH)_2$ ⟶ CH_3OH

Thank you for your attention

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PLASMANT Plasma, Laser Ablation & Surface Modelling Antwerp

Vlaams Supercomputer Centrum

University of Antwerp