# Modeling and Simulation of Dielectric Barrier Discharge Plasma Reactor for Nitrogen Fixation Reaction

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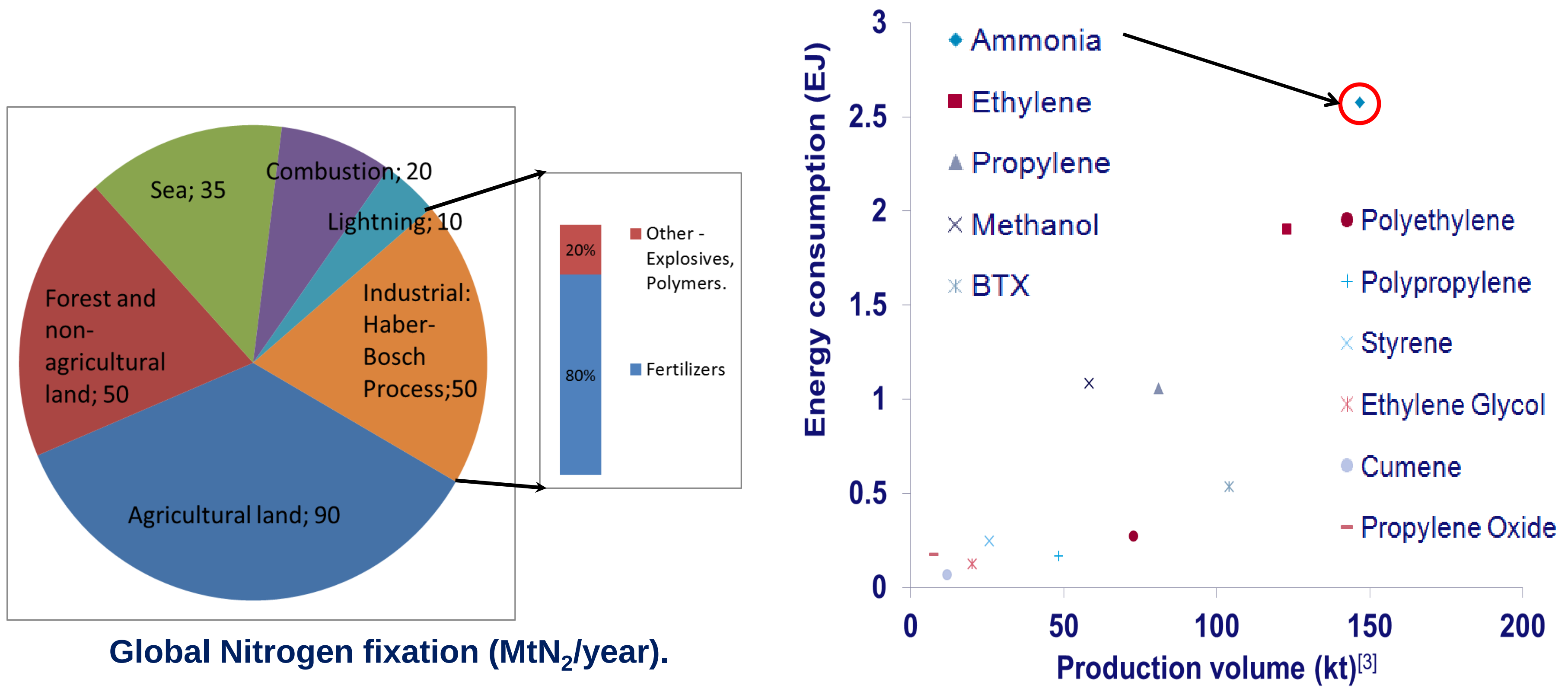
## Introduction



Global Nitrogen fixation ($MtN_2$/year).

**Figure 1**. What and why nitrogen fixation [2]

### *How?*

- Direct reaction of nitrogen and oxygen.
- Investigate using cold plasma reactors with catalytic function [1].
- Challenges: Very high dissociation energy of nitrogen (9.76 eV) and suppress reformation of elements.

## Problem Definition

Nitrogen will be fixed to produce nitric oxide; captivating benefits of plasma and catalysts synergetic effects in dielectric barrier discharge reactor.

$$N_2 + O_2 \xrightarrow{Plasma+Catalyst} 2NO \qquad \Delta H = 90.45 kJ/mol$$

**Basic understanding of the phenomena inside the DBD plasma reactor, e.g., for catalyst placing, micro-discharges, and energy.**

- Argon is used as model fluid.
- 1D model in COMSOL multiphysics using Plasma module.
- Solved following equations;

1. Drift diffusion: $$\frac{\partial}{\partial t}(n_e) + \nabla\cdot\left[-(\mu_e \bullet E)n_e - D_e \bullet \nabla n_e\right] = R_e$$
2. Heavy species transport: $$\frac{\partial}{\partial t}(w_k) + \rho\cdot(u\cdot\nabla)w_k = \nabla\cdot j_k + R_k$$
3. Bulk gas flow transport: $$\frac{\partial \rho}{\partial t} + \nabla\cdot\rho u = 0$$ $$\rho\frac{\partial u}{\partial t} + \rho(u\cdot\nabla)u = -\nabla p + \nabla\cdot\eta\left[\nabla u + (\nabla u)^T\right]$$
4. Plasma chemistry: Rate of reaction; $r = k^f \prod_{k=1}^{Q} c_k^v$
5. Electrostatic field: Poisson's equation; $-\nabla\cdot\varepsilon_0\varepsilon_r\nabla V = \rho$

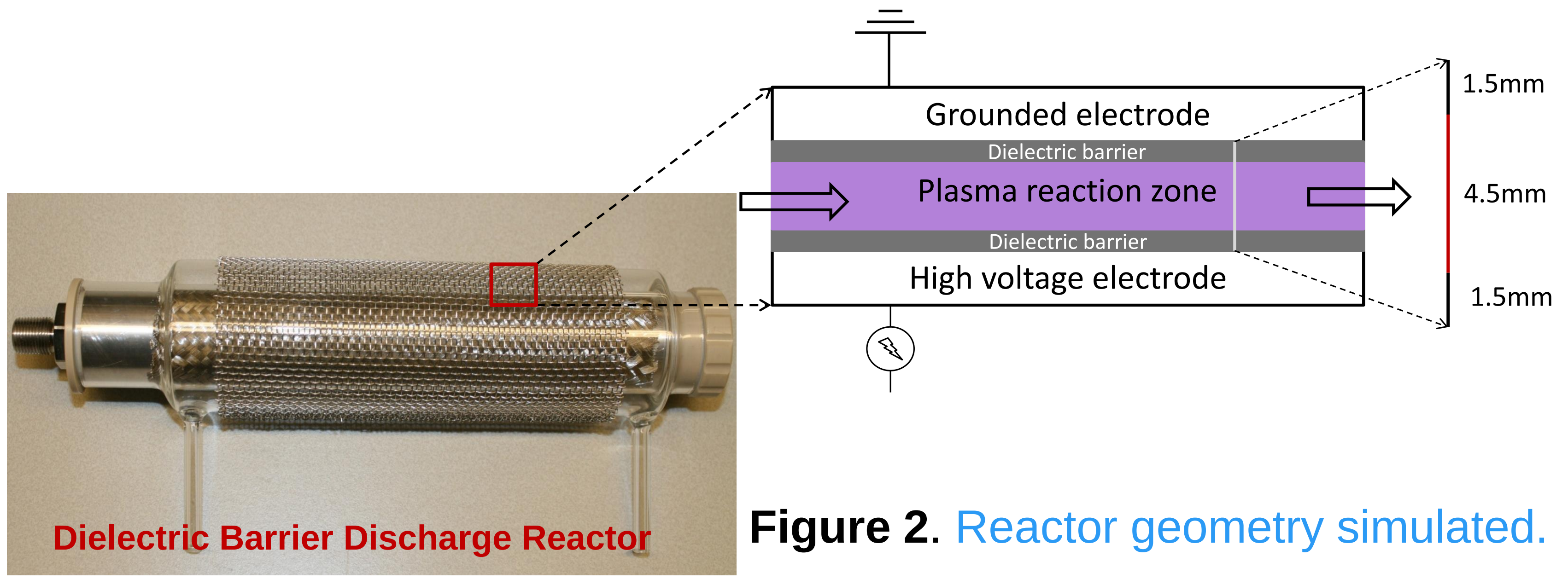


**Figure 2**. Reactor geometry simulated.

## Results

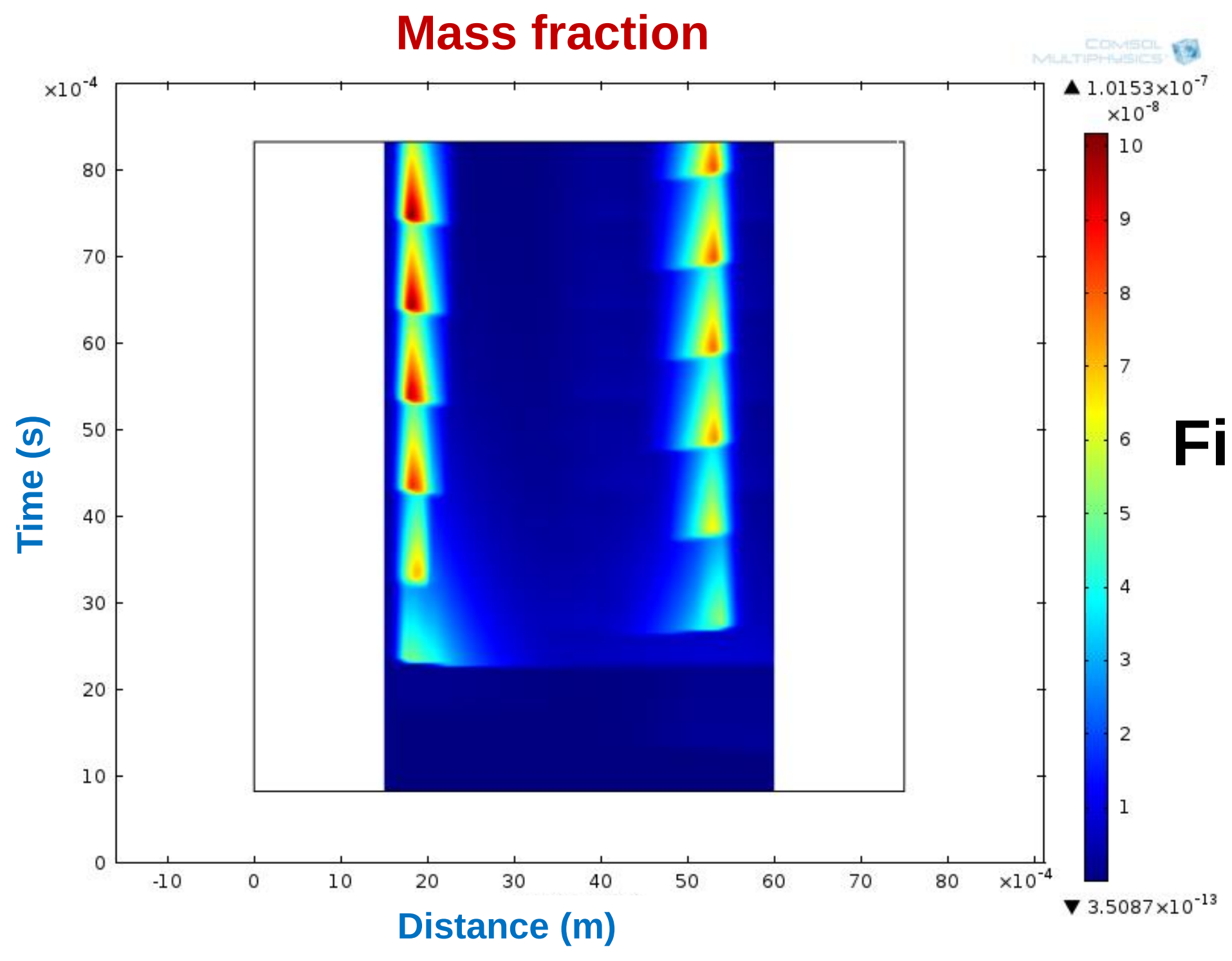


**Figure 3**. Mass fraction of Ars

**Figure 4**. Electron temperature distribution

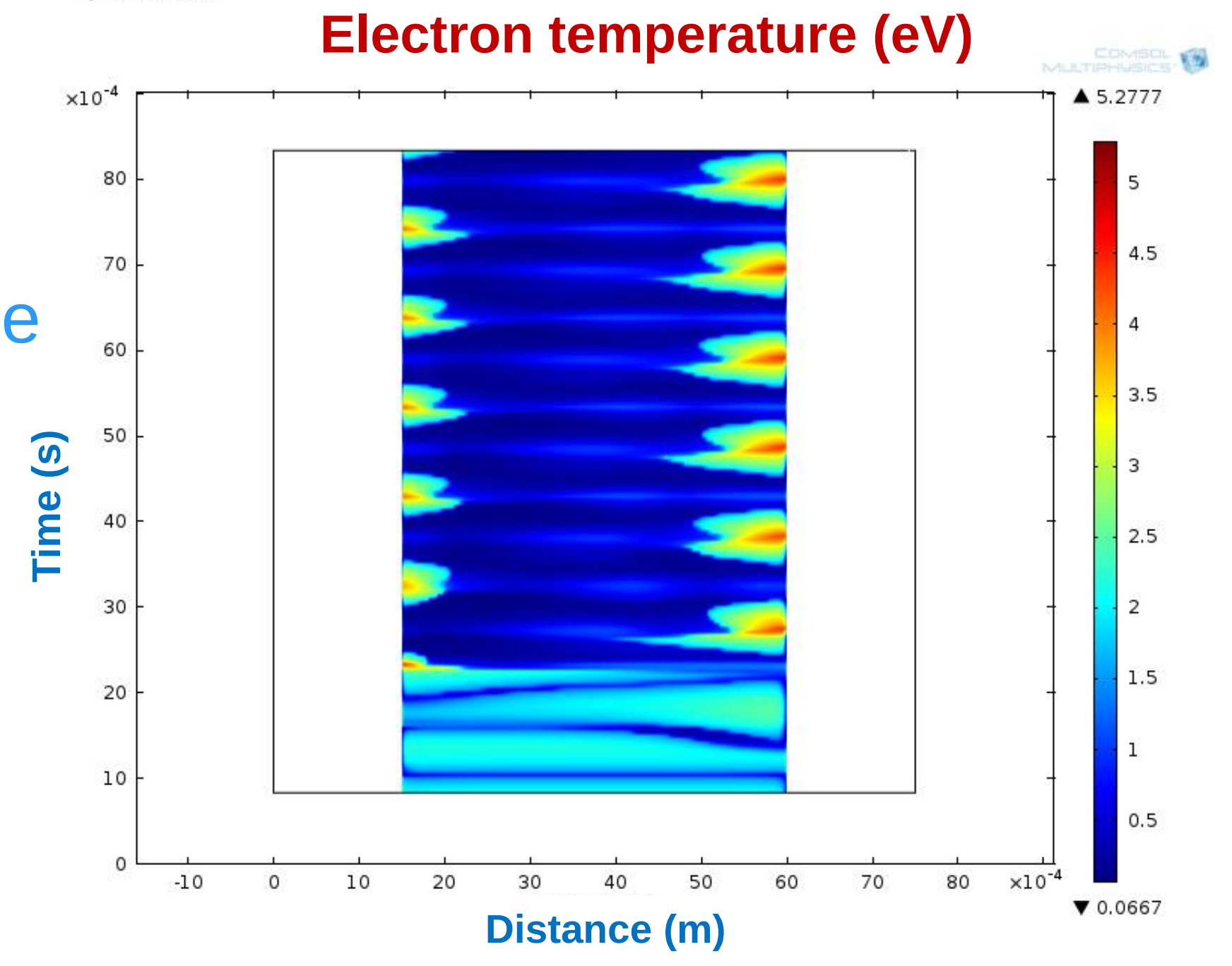


**Table 1**. Input variables

| Variable | Value | Units |
|---|---|---|
| Frequency | 80 | kHz |
| Applied voltage | -750sinwt | V |
| $D_{in}$ | 0.028 | m |
| Length | 0.17 | m |

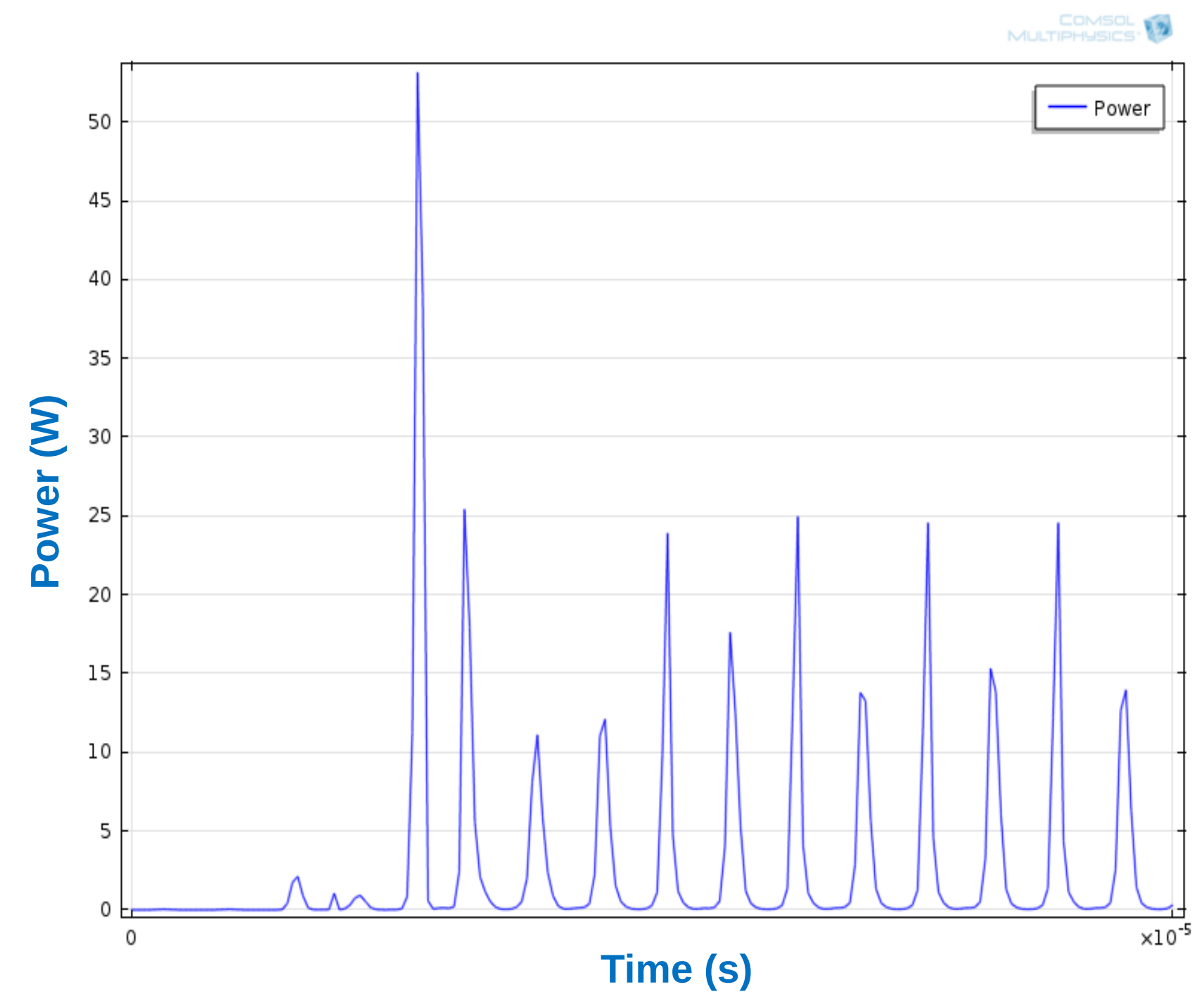


**Figure 5**. Power consumption

## Conclusions

COMSOL simulations can be an effective tool to get useful insights in plasma processes.

- **Best possible catalyst arrangement**: Information on active species concentration distribution inside plasma region to utilized the plasma activated species.
- **Micro-discharge phenomena:** Simulations could capture this in DBD reactor.
- **Energy transferred:** Enabled to calculate the actual energy transferred to plasma region.

*Future direction:*

- Simulating molecular gases ($N_2$ and $O_2$) and reaction between these gases to produce products (NO and $NO_2$)

## References

1. Hessel, V., Cravotto, G., Fitzpatrick, P., Patil, B., Lang, J. & Bonrath, W. (2013). *Chemical Engineering and Processing: Process Intensification*, doi:10.1016/j.cep.2013.02.002.
2. Technology Roadmap – Energy and GHG reduction in the chemical industry via catalytic processes, 2013.

## Acknowledgements

This work is funded by the EU project MAPSYN under grant agreement No. CP-IP 309376 of the EU Seventh Framework Program. In a close collaboration with 12 project partners. For plasma assisted reactions; TU/e will collaborate with Evonik Industries, KPE, UWE, and University of Hull.

Excerpt from the Proceedings of the 2013 COMSOL Conference in Rotterdam