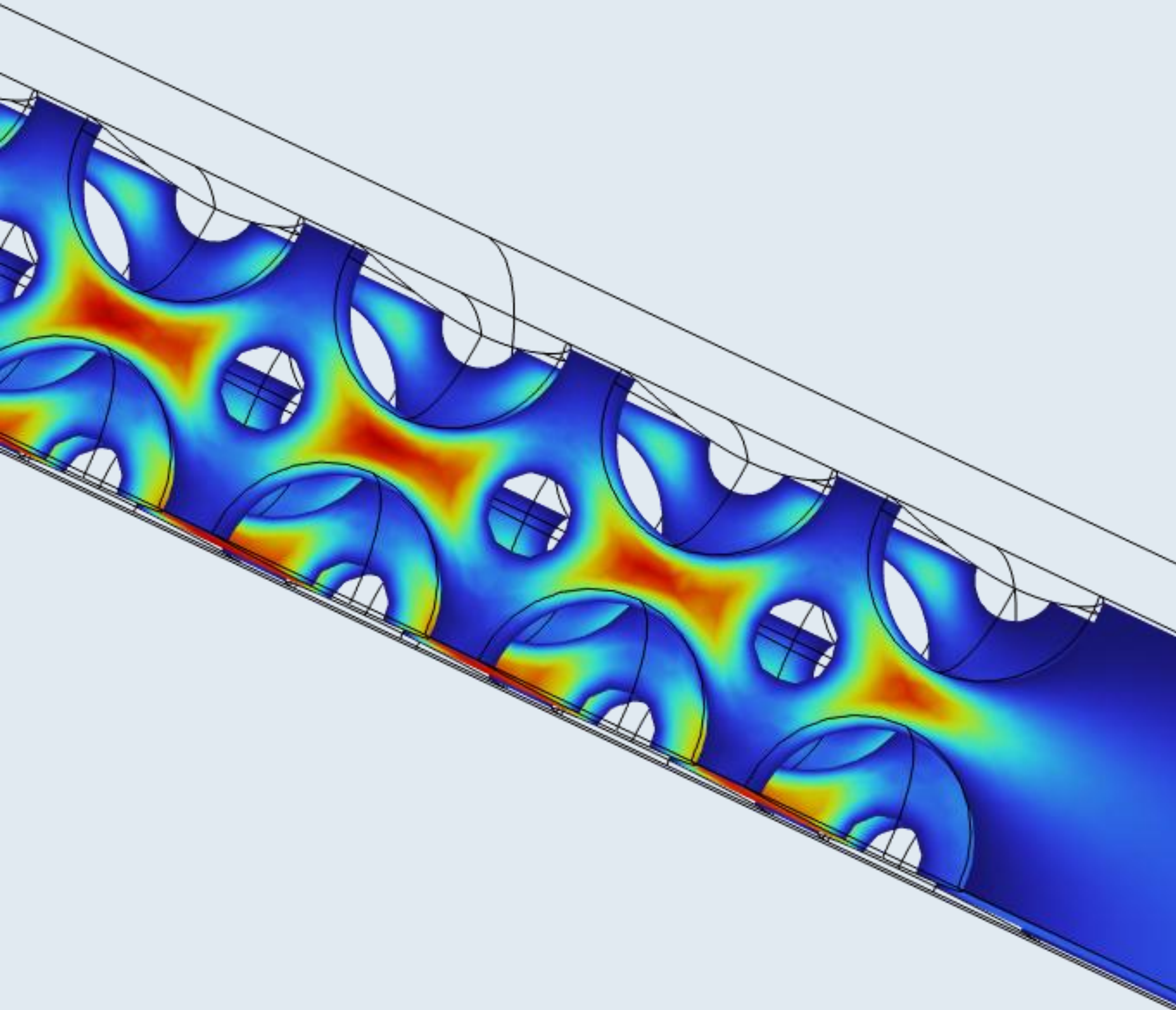




Non-Linear Global Optimization of a Two Zone Ammonia Reactor

A global optimization approach (PSO) was used to find the best ammonia reactor geometry. The approach minimizes costs (CAPEX and OPEX) and maximizes the hydrogen production of the ammonia reactor.

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Introduction & Goals

The goal is to develop a novel two-zone ammonia reactor for efficient and cost-effective hydrogen production. Ammonia reactors are used to convert or “crack” ammonia (NH_3) into nitrogen (N_2) and mainly hydrogen (H_2).

A first zone is used to convert the main amount of ammonia at 400 °C using a ruthenium catalyst. The remaining ammonia is then reduced in a second zone at approximately 650 °C using a nickel

catalyst. By this principle very low residual ammonia concentrations can be achieved, which are required for PEM fuel cell applications. (Usually <100 ppm of residual ammonia)

In order to minimize the amount of costly catalysts while maintaining high conversion, the reactor geometry is optimized using experimentally validated CFD simulations and optimization methods (particle swarm optimization).

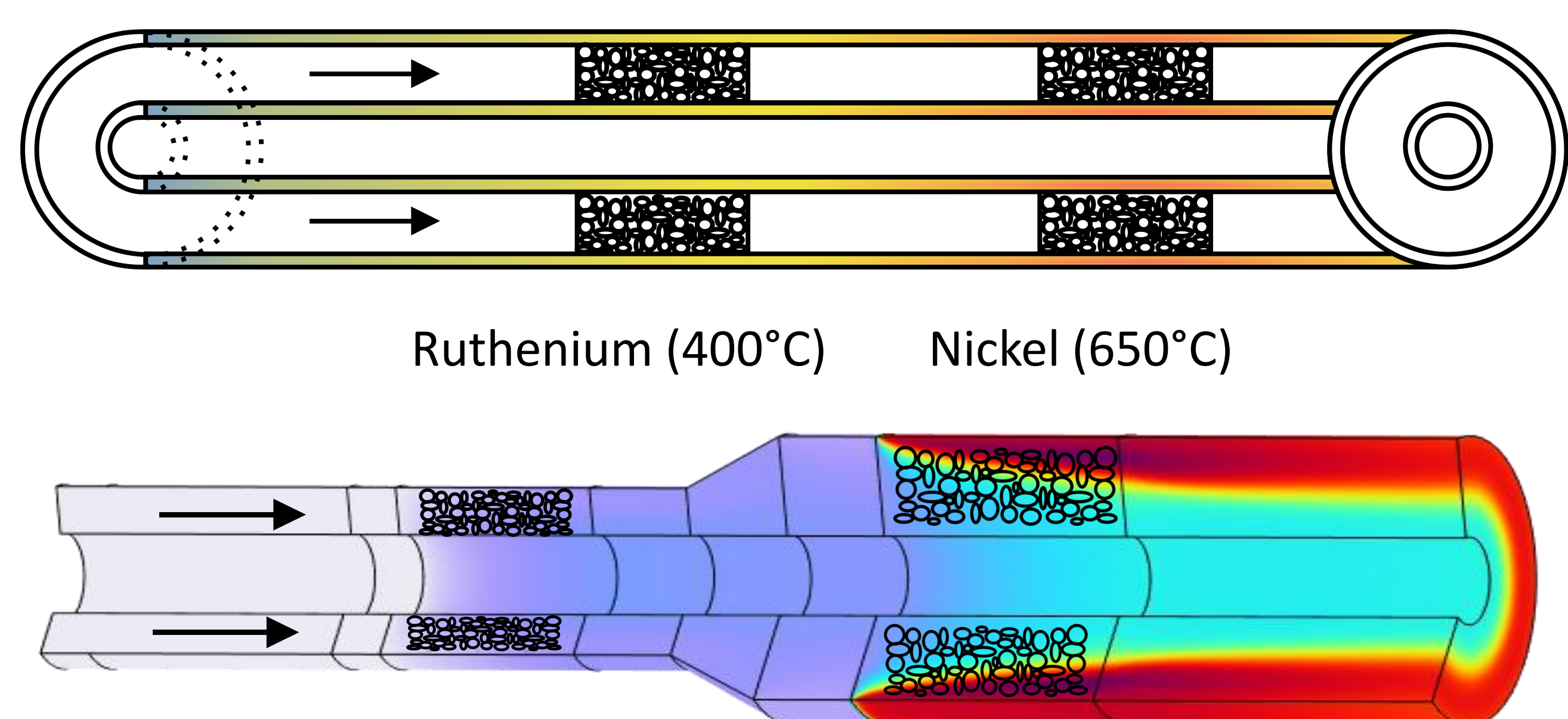


FIGURE 1 : Two Zone Ammonia Cracker (Top: Concept, Bottom: Simplified Simulation Model)

Cracking and Simulation Process

The initial electrical reactor concept considers the gas flow through an annular gap between two concentric pipes. The concept of the two-zone ammonia reactor can be seen on the left.

The optimization approach minimizes the CAPEX costs of the catalysts geometries as well as the OPEX costs resulting from the ammonia flow. The optimization parameters for the ammonia reactor are both the annular gaps of the catalysts as well as both of the catalysts’ lengths.

Because CFD-Simulations of ammonia reactors can be computationally demanding, first a simplified CFD-Simulation was created and validated with experimental data. This simplified CFD-Simulation was then used for the optimization approach.

Reactor Optimization:

By combining the validated/simplified CFD-Simulation in COMSOL with a global optimization strategy in MATLAB® an ideal cracker constellation was found. The coupling of the optimization solver and the CFD-Simulation was done via the COMSOL LiveLink™ for MATLAB®. The optimization approach minimized the resulting LCOH of the reactor geometry:

$$\min(LCOH) = \frac{I_0 + \sum_{t=1}^n \frac{\sum OPEX_t}{(1+i)^t}}{\sum_{t=1}^n \frac{m_{t,H2}}{(1+i)^t}}$$

Current results indicate that the OPEX costs (electrical power for the heating) are the main driving parameters for a minimal LCOH.

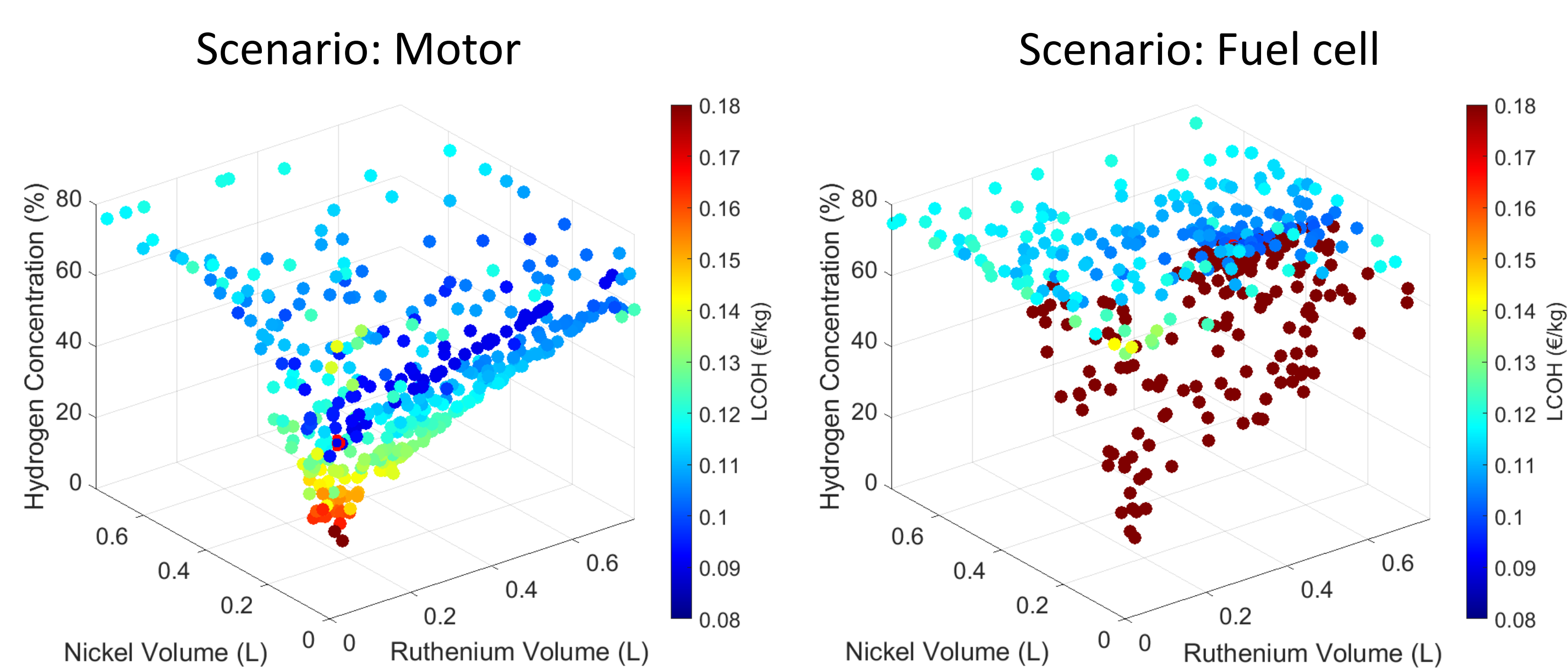


FIGURE 2: Visualization of the Search Field of the Optimized Reactor (Red Circle = Optimum)

REFERENCES

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