Topology Optimization of Ammonia Synthesis in Microfluidic Reactors

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In order to produce food for the world's population, around 160 million tonnes of ammonia is synthesized annually solely for production of fertilizers, with an additional 30 million tonnes produced annually for other purposes.

The ammonia synthesis is very energy consuming, and in fact 1 % of the total energy consumption worldwide is used for ammonia synthesis alone. Based on this, even small improvements in the energy efficiency of this synthesis will result in significant energy reduction and thereby decrease its environmental impact.

In our new innovative approach, where the reaction takes place within a micro scale system, we aim at improving the process by highlighting the importance of the geometric distribution of the catalytic material.
This is in contrast to the classical approach, which has mainly focused on adjusting the different operating conditions or catalysts.

By taking advantage of state-of-the-art optimization method – topology optimization – we intend to utilize the catalytic material in the best possible way, and thus enhance the efficiency of the synthesis reactor.

The synthesis reactor has been modelled by taking into account the mass, momentum and energy balance, and the model is solved numerically using the commercial software Comsol.

To the best of our knowledge this is the first time the ammonia synthesis, and indeed any synthesis of this complexity, has been improved by the use of topology optimization.

Finally, we will investigate if the combined yield from several million optimized microfluidic reactors can match or even exceed that of an industrial chemical plant.

It is our hope that microreactors, and specifically topology optimizations thereof, in the future will replace many classical chemical reactors.