Influence of molecular and turbulent diffusion on CO_2 conversion in thermal plasma reactors

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Abstract: In this contribution we report the results of a thermo-chemical multidimensional computational fluid dynamics model, validated by experimental data. We discuss the effects of radial transport, and especially radial diffusion, for various thermal plasma reactors aimed at converting CO_2. Our findings demonstrate that radial diffusion is the main driver of conversion in CO_2 thermal plasmas.

1. Introduction

Thermal plasmas offer a promising avenue for energy-efficient carbon dioxide (CO_2) utilization by converting CO_2 into carbon monoxide (CO) and oxygen (O_2) using renewable energies, effectively reducing greenhouse gasses. While the plasma chemistry of CO_2 conversion can be quite complex [1], in atmospheric pressure thermal CO_2 plasmas, it can be reduced to thermal chemistry, which is experimentally found to determine the conversion [2].

2. Methods

To reveal the influence of the flow pattern and species transport inside the plasma and effluent (i.e., afterglow), we developed 2D axisymmetric reacting flow models that calculate gas flow velocity, temperature profiles, transport of species, electric currents and chemistry, all self-consistently, for two different thermal plasma reactors within COMSOL Multiphysics 6.2. The models are validated against results from literature for a microwave reactor and our own experiments for a newly designed plasma torch for CO_2 conversion, an upscale in both input power and flow rate from previous reactors.

3. Results and Discussion

The model captures both the experimental trends and absolute values for the measured conversion, as well as temperature profiles reasonably well. We demonstrate that LTE is not obtained in the plasma core of thermal CO_2 plasmas. Furthermore, we show that diffusion is the main driver of conversion, and radial diffusion effectively prevents the back-reaction of CO into CO_2, as it is transported to the reactor edge and leaves the reactor.

Figure 1 presents the difference in axial temperature profile along a microwave reactor, when accounting for turbulence or neglecting turbulent diffusion and turbulent heat transfer. It is clear that turbulence leads to a much lower afterglow temperature. Moreover, turbulent heat transport is the main mechanism of transporting energy out of the simulation domain. Importantly, our computational results indicate that increasing turbulence in plasma reactors may improve conversion by efficiently transporting CO into the cold gas stream.

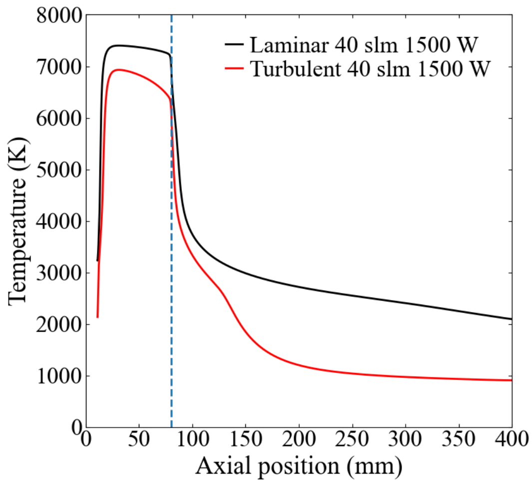

Fig. 1. Comparison of temperature profile along the symmetry axis, for laminar (black) and turbulent (SST; red) flows, at 1 atm. The start of the afterglow is indicated by the vertical dashed line.

4. Conclusion

Thermo-chemical models of CO_2 plasma can quite accurately predict conversion provided diffusion is accounted for. Moreover, especially at higher flow rates, turbulence becomes important in determining temperature profiles. Last but not least, stronger turbulence in a reactor may lead to higher conversions in CO_2 plasmas. Especially in high SEI, high flow rate reactors like the plasma torch.

References

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