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Hydrogen Generation via Steam Methanol Reforming for Sustainable IC Engine Transportation- A Simulative Investigation

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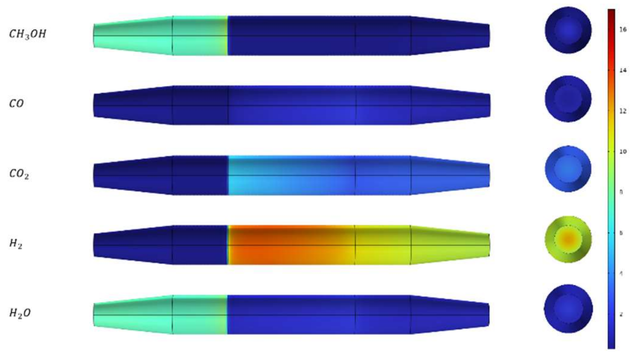
This work investigates the feasibility of onboard hydrogen generation for internal combustion engine applications through methanol steam reforming (MSR) with exhaust-gas-driven thermal integration. The study is motivated by the need to reduce dependence on conventional fossil fuels while developing cleaner transitional energy systems without requiring dedicated hydrogen storage and distribution infrastructure. Among liquid hydrogen carriers, methanol is especially attractive because of its high hydrogen-to-carbon ratio, sulfur-free nature, relatively low reforming temperature, and ease of storage and transport. These properties make methanol a strong candidate for compact reformers integrated with spark-ignition engines, where hydrogen-rich reformate can improve combustion and reduce harmful emissions.

A three-dimensional computational fluid dynamics (CFD) model was developed in COMSOL Multiphysics to analyze a compact methanol steam reformer under steady-state laminar-flow conditions. The model couples fluid flow, heat transfer, multicomponent species transport, and heterogeneous surface reaction kinetics over a $Cu/ZnO/Al_2O_3$ catalyst. Both the overall methanol steam reforming reaction and the reverse water-gas shift reaction were included to capture hydrogen production and carbon monoxide formation. The model also accounts for porous catalytic transport, effective diffusivity, and the endothermic heat demand within the catalytic domain.

A baseline channel geometry was studied in this work. Model validation was carried out against published literature results, showing good agreement in methanol conversion and hydrogen production trends over a range of wall temperatures. This agreement supports the validity of the implemented reaction kinetics, transport model, and thermal coupling, indicating that the model captures the dominant physicochemical processes governing methanol steam reforming. The validated model was then used to investigate reactor behavior under engine-relevant operating conditions. The results show that methanol concentration decreases progressively along the reactor length, while hydrogen concentration rises correspondingly as the reforming reaction proceeds. For the representative case of S/C = 1, the reactor achieves about 87% methanol conversion under favorable conditions, producing a hydrogen-rich reformate with low carbon monoxide concentration. The low CO levels indicate that the reverse water-gas shift reaction remains limited within the selected operating window, which is beneficial for engine reformate utilization.

Axial profiles reveal that the reactor does not operate uniformly along its full length. Instead, there is a weak entrance region followed by a distinct active reforming zone where methanol depletion, hydrogen generation, and temperature variation become much stronger. Temperature and feed velocity were found to be particularly important. Increasing temperature from 640 K to 880 K improved methanol conversion and hydrogen formation by accelerating reforming kinetics, while increasing feed velocity reduced conversion by shortening gas residence time. Thus, the best performance was achieved at high temperature and low feed velocity. Temperature profiles displayed an initial heat-up region, a pronounced temperature dip caused by the endothermic reforming reaction, and a downstream recovery zone. Spatial contour analysis shown in Figure 1 further showed non-uniform reactive fields in both axial and radial directions, highlighting local transport limitations and heat-distribution effects. Overall, this study confirms the technical feasibility of exhaust-driven methanol steam reformers as compact onboard hydrogen generators and provides a useful CFD framework for future optimization of catalyst arrangement, channel geometry, and thermal integration strategy.



Fgure 1: Spatial distributions at S/C = 1, 880 K, and feed velocity.

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