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Assessing Intrusion by the Capillary During Spatially Resolved Mass Spectrometry Measurement

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Abstract

The impact of the capillary probe of a spatially-resolved mass spectrometer system (SpaciMS) on the measured reactant conversion is reported using propylene oxidation over Pt/Al₂O₃ washcoated monoliths. The findings suggest that the invasive nature of SpaciMS depends on its configuration and application. Using monoliths with a range of cell densities (100 to 600 cells per square inch, CPSI), the concentration profiles of propylene sampled with probes of two different outer diameters (170 and 363 μm) are compared with the temperature measured using coherent optical frequency domain reflectometry (c-OFDR). The comparison indicates that flow blockage has a negligible effect if the limiting propylene is depleted in the downstream reactor section. Suction by the probe compensates for the blockage for certain combinations of the channel diameter and probe size. In such cases the profile measured by a probe with the larger outer diameter (363 μm) is similar to that measured by a smaller capillary (170 μm). The experiments reveal that the axial position of the probe does not influence the flow profile in a 100 CPSI monolith channel, nor does it affect the amount of flow deflected to surrounding channels for a 600 CPSI monolith. Under some conditions the results are impacted by transverse concentration gradients. Their existence complicates the interpretation of the SpaciMS data. The difference between the location of propylene depletion and temperature maximum provides a useful metric for capturing the collective impacts of flow deflection and transverse gradients. The complexity of the flow, transport and reaction suggests that at least three dimensionless groups are needed to bound the operating regions in which the presence of the probe has minimal impact on the measured concentration.

Keywords: propylene; oxidation; monolith; mass spectrometry; SpaciMS, c-OFDR

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