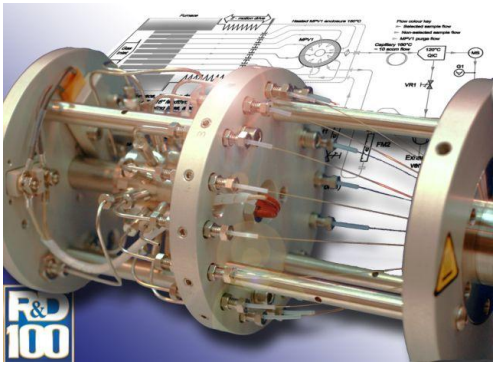
Gas Analysis
Application Note 286

SpaciMS

Mass Spectrometer Inlet for Spatially Resolved Measurements



Winner of a R&D100 award in conjunction with Oak Ridge National Laboratory, Cummins Inc, CenTACat and Y-12 National Security Complex

SpaciMS Overview

Hiden Analytical introduces the first commercially available Spatially Resolved Capillary Inlet MS (SpaciMS). The SpaciMS was originally conceived and developed by researchers at the Oak Ridge National Laboratory and Cummins, Inc. to study diesel catalysis [1].

SpaciMS is an instrument for minimally invasive sampling of transient species distributions inside operating, confined-space, reactors such as the small channels of automotive catalysts, fuel reformers, or fuel cells. Its unique capillary sampling system measures variations in species concentration from point to point within small operating reactors. Conventional analytical instruments only measure the composition of reactor exhaust and thus do not capture the spatially and temporally rich intra-reactor chemistry resolved by the SpaciMS. By resolving this detail, SpaciMS provides a quantum increase in the ability to understand catalyst and reactor chemistry.

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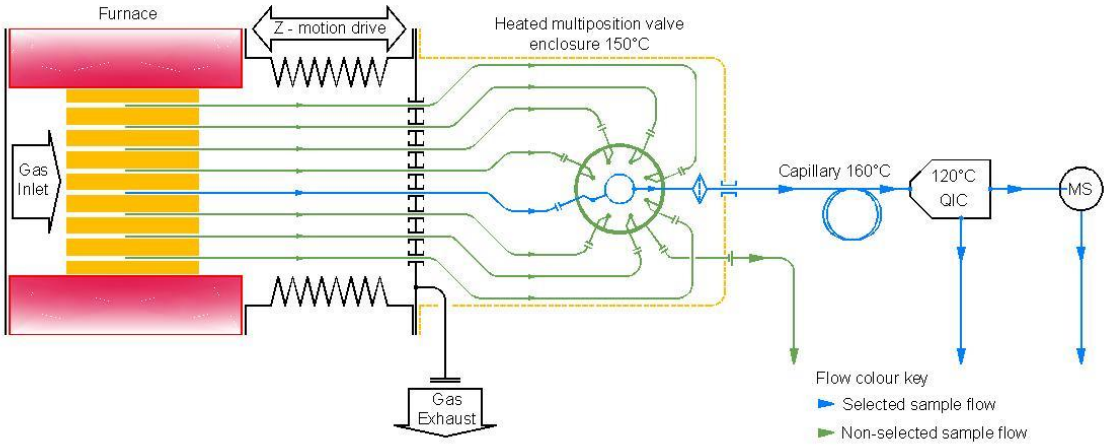


Figure 1 Schematic of the Hiden SpaciMS Interface

Hiden Spaci-MS

A schematic of the Hiden SpaciMS inlet is shown in Figure 1. The inlet consists of a 16 capillary array of inlets with optional z-drive for movement of capillaries through the catalyst monolith sample. In addition the system can also be configured with up to 16 thermocouples for simultaneous temperature and species concentration measurements.

Coupled to the SpaciMS is the Hiden HPR-20 gas analysis system, Figure 2, for fast, continuous sampling of transient species at concentration levels from 100% to ppm levels.

Figure 2. Hiden HPR-20

The SpaciMS determines the transient species distribution in chemical reactors through minimally invasive sampling. Such sampling is critical in accurately determining species distributions within confined-space chemical reactors. Automotive emissions-control catalysts commonly consist of a honeycomb-like array of catalyst-coated channels (Fig. 3). Each catalyst channel is typically 1 to 1.5 mm square by 150mm long. The SpaciMS is the only instrument that allows determination of the transient species distributions within these catalyst channels without affecting species flow and thus catalyst chemistry. This provides unprecedented insights into the detailed catalyst chemistry and therefore catalyst formulation and design, model development, catalyst control, catalyst health, and system integration, all key aspects to successful product development.

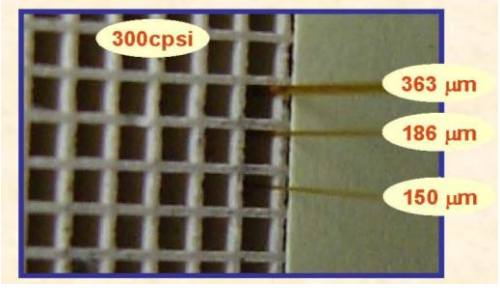


Figure 3. Channelized monolithic catalyst showing SpaciMS capillary sampling probes of various sizes.

Q-Spaci

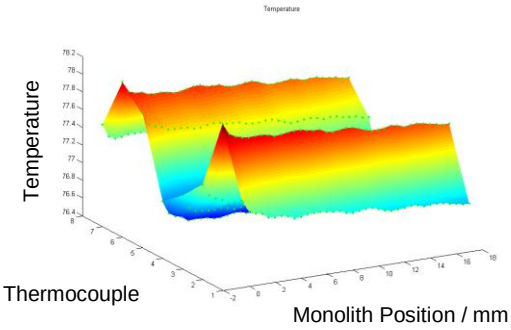
Q-Spaci is a post analysis software package developed by Queens University Belfast [2] for analysis of the large amount of data produced by the 16 inlet SpaciMS system.

Features include:

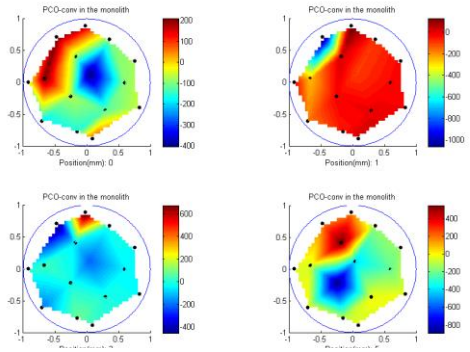
- Direct reading of Hiden Massoft files.
- Auto-correction for blank and pressure fluctuations.
- Conversion of m/z signals into partial pressures.
- Simultaneous calculation and plot representation.
- Interactive display.
- 3D maps representation.

Typical data plots include:

Temperature vs Monolith Position

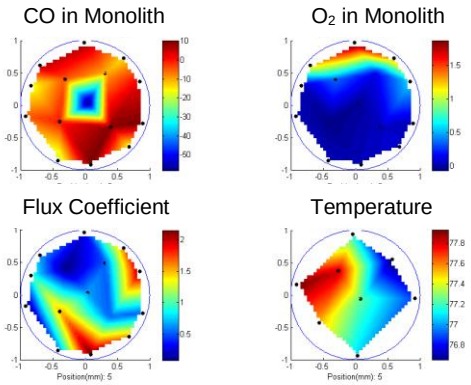


Single Variable Multiple Positions



CO Conversion at different positions of the monolith

Multiple Variable Single Position



1. P Partridge, W.P., Storey, J.M.E., Lewis, S.A., Smithwick, R.W., DeVault, G.L., Cunningham, M.J., Currier, N.W. and Yonushonis, T.M. (2000). SAE Transactions - Journal of Fuels & Lubricants 109, 2992-2999.
2. Data courtesy of Daniel Fernandes (software development), Jacinto De Paiva Sa and Alexandre Goguet of Queens University Belfast, UK.