

Carbon 2 Chem®

L-0 | Trace Analysis in Carbon2Chem[®]: **Metallurgical Gases and Raw Methanol**

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Max Planck Institute for Chemical Energy Conversion (MPI CEC) analyzes chemical traces in metallurgical gases and raw methanol products by utilizing several infrastructures. The HügaProp-Container monitors the gas composition changes of the raw gases (A). Lab 5 provides the needed infrastructures for the online-analysis of the treated gases (B). Additionally, traces in raw and treated gases are analyzed offline at Carbon2Chem[®] lab (C). The analysis of chemical traces in raw methanol products is also carried out at Carbon2Chem[®] lab as well as at MPI CEC (D).



Figure 1: Overview of chemical trace analysis in Carbon2Chem[®] performed by MPI CEC.

UNRAVELING THE TRACE IMPURITIES IN **METALLURGICAL GASES (A)**



Figure 2: a) Time series of toluene and acrylonitrile in raw coke oven gas using H_3O^+ as primary ion. b) Full mass spectra of coke oven gas and nitrogen 6.0 measured online with PTR-QiTOF.^[1]

REALLY TREATED!? - LAB 5 MONITORS THE GAS TREATMENT CONTINUOUSLY (B)



Figure 3: a) Gas composition of the treated BFG measured via Proton

OFFLINE ANALYSIS OF TRACE IMPURITIES IN RAW AND TREATED GASES (C)

Raw methanol analysis



- Precise dilution ($P_1V = P_2V$)
- Reproducible measurement
- Regulated flow



Figure 4: a) Sketch of pressure aperture for canister samples. Decay in Al-coated Tedlar[®] bags for b) Standard toluene and c) Naphthalene in raw gas.

INVESTIGATING CHEMICAL TRACES IN **RAW METHANOL PRODUCTS (D)**



• Up to 23 compounds in Carbon2Chem[®] raw methanol were identified by MPI CEC.

Transfer Mass Spectremetry (PTR-MS). b) Comparison of an insufficient and a thoroughly sulfur removal via the gas treatment in Carbon2Chem[®].^[2]

Salazar Gómez, J. I., Klucken, C., Sojka, M., Waydbrink, G., Schlögl, R. and Ruland, H. The HüGaProp-Container: Analytical Infrastructure for the Carbon2Chem[®] Challenge. Chem. Ing. Tech. 2020, 92(10), 1514-1524.

Hegen, O., Salazar Gómez, J.I., Grünwald, C., Rettke, A., Sojka, M., Klucken, C., Pickenbrock, J., Filipp, J., Schlögl, R. and Ruland, H. Bridging the Analytical Gap Between Gas Treatment and Reactor Plants in Carbon2Chem[®].

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• Well-separated peaks are required for a better quantification.

Figure 5: GC-MS chromatogram showing detected traces in a Carbon2Chem[®] raw methanol product.

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