ESRF	**Experiment title:** Multiple-technique Spatial imaging of a working SAPO catalyst for the MTO process	**Experiment number**: **CH- 2965**
Beamline: ID15	**Date of experiment**: from: 24 February 2010 to: 01 March 2010	**Date of report**: 12/8/10
Shifts: 15	**Local contact(s)**: Marco Di Michiel	*Received at ESRF:*

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Report:

This experiment aimed both to improve the mechanistic understanding of the commercially important methanol to olefin (MTO) conversion process by studying the flow of reactants through a large bed of SAPO-34 catalyst, and develop X-ray imaging techniques by constructing imaging data based on real physical parameters extracted from powder XRD data by the Rietveld method. Despite some problems in recovering the data from the ESRF servers we are now in a position to believe that both of our goals are achievable.

12 datasets were collected during the experiment: 6 being full scans of the reactor after reaction for 3D tomographic reconstruction and 6 being series of fast scans up the bed during the course of the reaction. Images were collected with an exposure time of 1 second meaning that a fast scan from bottom to top of the reactor took between 15 and 30 seconds depending on the depth of the catalyst bed.

Data from the latter stages of one of the fast scan experiments using a SAPO-34 catalyst have now been processed using a parallel Rietveld refinement method in the program TOPAS. The data from 12 z-scans (168 powder XRD patterns in all) show some variation in lattice parameters even at this late stage in the deactivation of the catalyst (figure 1). We expect to see more significant variation in the lattice parameters of the catalyst in the early stages of the reaction as observed in earlier studies using a capillary reactor [1].

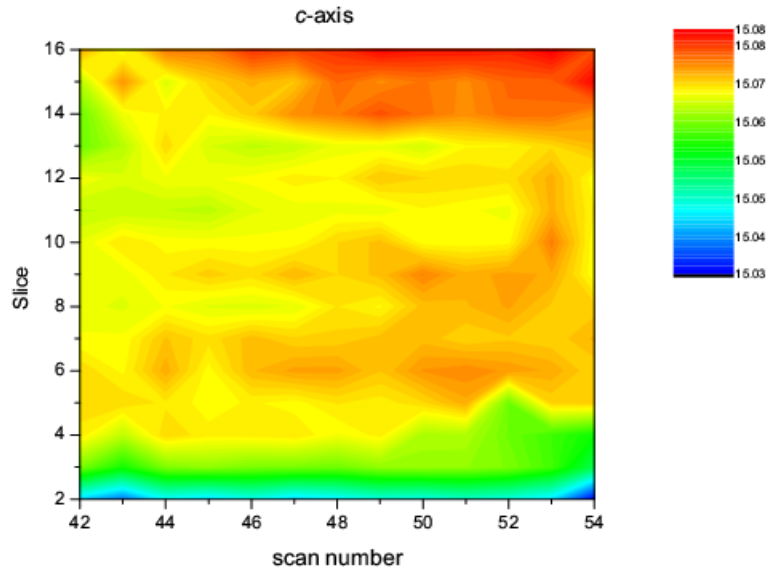

Figure 1. Contour plot showing the variation in the *c*-axis length of SAPO-34 during the latter stages of the MTO reaction.

This shows that we can observe variations in the physical properties of the catalyst from the data and use these to construct images of the reactor. We aim to extend this to a complete tomographic dataset soon. We anticipate this will lead to at least two papers in good quality journals- one documenting the use of full profile reitveld fitting in tomographic reconstruction and another concerning the mechanistic insights from the reaction.

[1] D. S. Wragg, R. E. Johnsen, M. Balasundaram, P. Norby, H. Fjellvåg, A. Grønvold, T. Fuglerud, J. Hafizovic, Ø. B. Vistad, D. Akporiaye, J. Catal., 268, (2009), 290-296.