

Dow Polyols near Infrared Chemometric Model Reduction Based on Clustering: Reducing Thirty Global Hydroxyl Number (OH) Models to Less Than Five

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Abstract : Polyurethane Materials are present in a wide range of industrial segments such as Furniture, Building and Construction, Composites, Automotive, Electronics, and more. Dow is one of the leaders for the manufacture of the two main raw materials, Isocyanates and Polyols used to produce polyurethane products. Dow is also a key player for the manufacture of Polyurethane Systems/Formulations designed for targeted applications. In 1990, the first analytical chemometric models were developed and deployed for use in the Dow QC labs of the polyols business for the quantification of OH, water, cloud point, and viscosity. Over the years many models have been added; there are now over 140 models for quantification and hundreds for product identification, too many to be reasonable for support. There are 29 global models alone for the quantification of OH across > 70 products at many sites. An attempt was made to consolidate these into a single model. While the consolidated model proved good statistics across the entire range of OH, several products had a bias by ASTM E1655 with individual product validation. This project summary will show the strategy for global model updates for OH, to reduce the number of models for quantification from over 140 to 5 or less using chemometric methods. In order to gain an understanding of the best product groupings, we identify clusters by reducing spectra to a few dimensions via Principal Component Analysis (PCA) and Uniform Manifold Approximation and Projection (UMAP). Results from these cluster analyses and a separate validation set allowed dow to reduce the number of models for predicting OH from 29 to 3 without loss of accuracy.

Keywords : hydroxyl, global model, model maintenance, near infrared, polyol

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