329a Optimization of Batch Processes Using Data Driven Latent Variable Models

Salvador Garcia-Munoz, Debashis Neogi, Sanjay Mehta, John MacGregor, and Theodora Kourti

Jaeckle and MacGregor (AICHE J. 1998, 44 (5), 1105-1118) introduced a technique to estimate operating conditions in order for a process to yield a final product with a desired set of quality characteristics. Their proposed technique involves the used of empirical latent variable models which are fitted with historical data from the process. This talk provides a detailed study of the application of such technique when the operating conditions include a set of time varying profiles for the manipulated variables as in the case of a batch. The effect of including constraints in the objective function to minimize in order to estimate the desired score vector is analyzed. The multiple solutions contained in the null space are studied to select the final variable trajectories. An industrial case from the pulp and paper industry is considered throughout the paper to explain and illustrate the key concepts. This methodology is further extended to include constraints in the process operation itself. The proposed new formulation considers explicit initial conditions which variables can be different in nature from those followed throughout the run. This new formulation allows the inclusion of additional optimal criteria in the design. The methodology is illustrated with an industrial batch emulsion polymerization process where the batch trajectories are designed to satisfy certain customer requirements in the final properties of the polymer while using the minimal amount of time for the batch run.