National Institute of Technology Rourkela

Departmental Seminar

Seminar Title	: Conference Return Seminar on PCA and fuzzy based clustering of esterification products using electrochemical features: prediction of exit concentration in batch reactor (Presented at CHEMCON 2024, NIT Jalandhar)
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Venue	: New Seminar Hall, Chemical Engg. Department
Date and Time	: 09 Jan 2025 (11.00 A.M.)
Abstract	: Esters are industrially important chemicals which find a broad spectrum of applications. Determination of concentration of unconverted acid/conversion through conventional techniques are cost, time and material consuming. Electrochemical features combined with artificial intelligence provide an alternative for reducing cost and time for detection of species. This study deals with determination of unconverted acid concentration/conversion in esterification reaction in batch reactor. Cyclic voltammetry is used as mapping technique for acid concentration at different sampling time intervals at three reaction temperatures (60 oC, 75 oC, and 90 oC). Principal component analysis (PCA) and fuzzy C-means clustering is used for classification of electrochemical data corresponding to sampling time interval or conversion/concentration. Three sets of data are used for clustering and the remaining are used for validation of clustering model. The results show that 15 min, 60 min and 90 min data are distributed separately for 60 and 75 oC reactor temperature and the models can classify each data separately and satisfactorily while at 90 oC, classification results show less satisfactory results due to arrival of equilibrium conversion at 50 mins. Keywords: esterification; electrochemistry; classification