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论文

苯乙烯/丙烯酸正丁酯乳液聚合反应过程中残余单体含量的实时监测

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摘要:

采用近红外光谱分析技术在线测量苯乙烯(St)/丙烯酸正丁酯(BA)乳液聚合体系中残余单体的含量。共设计9个半连续方式的St/BA乳液共聚反应, 在反应过程中实时取样测量其残余单体含量, 并记录取样时刻对应的聚合体系的近红外光谱。采用多元散射校正法(MSC)处理光谱, 有效地克服了乳胶粒子散射效应对近红外光谱分析的影响。采用主成分分析法(PCA)对乳液体系的近红外光谱数据进行了解析。选取6个聚合反应对应不同反应时间的72个样品, 用于建立校正模型, 另外3个聚合反应共取36个样品用于校正模型的验证, 并在反应设计上体现了乳化剂用量的变化, 从而使校正模型对乳化剂用量的变化具有一定的适应性。研究结果表明, 所得模型对残余单体St和BA含量的预测结果标准差(SEP)分别为0.08026和0.05305。

关键词: 在线测量 乳液聚合 多元散射校正 近红外光谱 残余单体 主成分分析

Real-time Monitoring the Residual Monomer in St/BA Emulsion Copolymerization

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Abstract:

The near-infrared(NIR) spectroscopy was used to monitor the residual monomer in the styrene/butyl acrylate emulsion copolymerization reaction. There were nine semi-batch styrene/*n*-butyl acrylate emulsion copolymerization reactions. The samples were gotten in line, and the NIR spectroscopy of the emulsion were measured at the same time. It was shown that the emulsion particles scattered the NIR and affected the result of analysis, through the pretreatment of Multiplicative Scatter Correction(MSC) to the spectra. The NIR data of emulsion was analyzed by the method of Principal Component Analysis (PCA). The calibration model was established with 72 samples of six reactors, and the model was validated with 36 samples of three reactors. The amount of emulsifier was variational in the nine reactors in order that the calibration model could adapt the amount of emulsifier. The result of the research is that the Standard Error of Prediction of the calibration models for St and BA were 0.08026 and 0.05305.

Keywords: In-line measurement Emulsion copolymerization Multiplicative scatter correction Near-infrared spectroscopy Residual monomer Principal component analysis

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