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近红外技术快速测定裂解焦油芳烃含量

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Determination of aromatics in naphtha-cracked tar by near infrared spectroscopy

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摘要 针对常用的气相色谱 (GC) 分析法进行焦油芳烃检测分析周期较长的问题, 本文用傅里叶变换型近红外光谱仪及相关软件对石脑油蒸汽裂解焦油芳烃的含量进行了测定和实验研究。考虑焦油样品颜色差异大、芳烃含量变化大, 实验通过对样品管改进、异常值判断、建模波段及光谱预处理方法优选等优化了碳六、碳七、碳八、碳九、碳十及总芳烃含量6组预测模型性能, 建立了石脑油蒸汽裂解焦油样品中芳烃含量的快速分析方法, 使得单个样品的分析时间缩短到2 min以内。优化后6组模型的相关系数 (R) 分别为0.995 20, 0.993 08, 0.946 33, 0.978 99, 0.948 46, 0.998 63, 交叉验证均方差 (RMSECV) 分别为1.07, 0.806, 2.17, 0.979, 0.665, 1.15。未知样6组芳烃含量的近红外光谱及气相色谱 (GC) 分析数据吻合良好, t -检验绝对值均小于其临界值 ($t_{0.05}(17) = 2.11$)。另外, 近红外分析数据相对标准偏差 (RSD) 均小于2%, 显示提出的方法具有较好的重复性。

关键词 : 近红外光谱术, 预测模型, 芳烃, 裂解焦油, 含量测量

Abstract : Gas Chromatography (GC) is usually used in analysis of aromatic contents of naphtha-cracked tar, however, it costs a longer analytical period. For solve this problem mentioned above, this paper applies Fourier Near-infrared Spectroscopy (NIRS) and corresponding software to the determination of aromatic contents of naphtha-cracked tar to shorten the analytical time and improve the analytical efficiency. Since cracked tars have a wide difference in both color and aromatic contents, modified sample tubes, outlier judgment, selective wave numbers and optimal preprocessing methods for NIR spectra were proposed to optimize 6 predict models of aromatics, by which the five models with carbon numbers from 6 to 10 and one for total aromatics were improved. Then, a rapid analysis method based on NIRS for determining aromatics in naphtha-cracked tar of stream cracking was established. With the method, the analytical time for per sample was shorten within 2 min. Experimental results show that the 6 optimized predict models can offer the correlation coefficients (R) of 0.995 20, 0.993 08, 0.946 33, 0.978 99, 0.948 46 and 0.998 63 respectively, and the Root Mean Square Errors of Cross Validation (RMSECV) of 1.07, 0.806, 2.17, 0.979, 0.665 and 1.15, respectively. The aromatic amounts analyzed by NIRS for random samples are fitted well with those determined by GC and the absolute values of t -test are all smaller than the critical value ($t_{0.05}(17) = 2.11$). Moreover, the NIRS analysis also indicates that the Relative Standard Deviation (RSD) is smaller than 2%, which means the established NIRS method has good repeatability.

Key words : Near Infrared Spectroscopy (NIRS) predict model aromatics cracked tar content measurement

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