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过程系统工程

# 基于MLFN-PLSR的PX氧化反应组合建模方法

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摘要 针对对二甲苯（p-xylene，PX）氧化反应过程中影响主要副产物对羧基苯甲醛（4-carboxybenzaldehyde，4-CBA）含量的因素众多且呈高度非线性的特征，提出了多层前向型神经网络（multi-layer feedforward network，MLFN）与偏最小二乘回归（partial least squares regression，PLSR）相结合的建模方法，建立反应产物中4-CBA含量关联模型。MLFN-PLSR采用三层网络结构和尽量多的隐节点，通过MLFN充分提取样本数据信息；然后采用PLSR消除隐含层输出冗余信息，建立具有良好预测精度的模型。与MLFN相比，最佳性能模型的预测偏差平方和均值下降了12.11%、模型平均预测偏差平方和均值下降了8.37%。与PLSR相比，最佳性能模型的预测偏差平方和均值下降了70.62%。

关键词 神经网络 偏最小二乘回归 对二甲苯 对羧基苯甲醛

分类号



# Develop p-xylene oxidation reaction model based on MLFN-PLSR

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**Abstract**

Due to the fact that there exist many factors having highly-nonlinear and complex effects on the concentration of 4-carboxybenzaldehyde (4-CBA),the most important intermediate product of p-xylene (PX) oxidation reaction, a novel approach integrating multi-layer feedforward network (MLFN) with partial least squares regression (PLSR) was proposed to develop a model of 4-CBA concentration in the PX oxidation product.A three-layer network consisting of an input layer, a single hidden layer and an output layer was selected by MLFN-PLSR and the number of the hidden layer nodes was as large as possible.Firstly, MLFN learned from the training sample.Secondly, PLSR was used to identify PLS components from the hidden-layer node output and remove the correlation among them.And, an optimal prediction ability model with the optimal number of the latent variables was obtained according to the prediction ability of the model for the verified sample.The comparison results showed that the prediction ability of the optimal MLFN-PLSR was 12.11% higher than that of the optimal MLFN and 70.62% higher than that of the optimal PLSR, and the mean prediction ability of MLFN-PLSR was 8.37% higher than that of MLFN.

**Key words** artificial neural network partial least square regression p-xylene 4-carboxybenzaldehyde

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