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The use of sensitivity analysis and genetic algorithms for the management of catalyst emissions from oil refineries

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Abstract

Excessive catalyst emissions from Fluidized Catalytic Cracking Units (FCCU) during start-up situations are common, and have been deemed 'normal', with little research conducted on determining their causes. A MATLAB model found to predict trends in emission rates under normal conditions has been expanded to better represent the actual processes inside a FCCU. First and second order sensitivity analysis techniques are used to assess the interactions between various operational parameters, with a genetic algorithm used to optimize the operating conditions to minimize air emissions. These 'key' parameters may then be altered to help manage both normal and start-up emissions through operational changes. It was also found that significant scale-up issues arise with the use of the attrition models found in the literature.

keywords: Sensitivity analysis; Genetic algorithm; Air pollution; Modelling

1. Introduction

The petroleum industry currently employs Fluidizing Catalytic Cracking Units (FCCUs) as the major tool in producing gasoline from crude oil. FCCUs typically consist of a rising main where the chemical reactions between catalyst and hydrocarbons occur; a reactor to separate the product and catalyst; and a regenerator to re-charge the used catalyst. The regenerator is a fluidized bed used to combust coke from the used catalyst, with cyclones to remove particles from the flue gas stream before venting to the atmosphere. The recharged catalyst then re-circulates through the rising main and the process is repeated [1].

Catalyst emissions from FCCUs have the potential to impact significantly on the environmental efficiency of the overall refining operation [2]. Currently, FCCUs are designed and operated in such a way as to maximize output and profitability of the refinery [3]. In recent years, fine particle emissions from industry have been identified as important

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contributors to poor environmental and health standards across the United States [4]. With increasing demands for cleaner air, and the lack of literature dealing with FCCU emissions, there is a need for the relationships between current operational strategies and air pollution to be better understood.

In an attempt to better understand emission modeling, an emission model was developed using MATLAB and tested on FCCU emissions [5,6]. The model was based on the essential processes inside the FCCU including fluidization, elutriation, entrainment and attrition, with model equations sourced from the literature. Emission results were then compared with observations from an operating FCCU, where the FCCU particle emissions during a start-up period were identified. This allows the complete range of emissions to be compared with modelled results [7].

The aim of this paper is to further develop the model into a more realistic package, for use in modelling industrial emissions. Genetic algorithms and sensitivity analysis are used to identify the key input parameters required to best predict emissions from an operating FCCU. This will provide a simulation package of the FCCU, where the simulated emission can be studied in terms of system parameters.

2. Background

2.1. Model background

The original model from the literature [5] is of the form $y = f(x)$ where x is a vector of 11 input parameters, which are listed in Table 1. The output of the model, y, is the emission level in mg/m^3 of catalyst particles from the cyclones, and the function $f(x)$ is essentially algebraic. The model accepts the input parameters, and steps through a series of subroutines to calculate specific process outcomes in the regenerator. The nonlinear equation representing each process uses a combination of operating parameters and the solution of previous routines, to implement its particular process. This model was tested extensively using published examples as well as sensitivity analysis and was found to be approximately 95% accurate when predicting emission rates from small scale worked examples from the literature [5,6].

This original model was updated and expanded to take into account particle attrition rates and a particle feedback loop from the cyclone into the fluidized bed, providing a more realistic model of the FCCU process. The attrition term selected was comprised of three independent components developed using FCCU catalyst particles to predict cyclone attrition, bubble attrition and jet attrition separately [8].

The three-part attrition model uses three different attrition coefficients, one for each of the attrition sources. These three coefficients are: cyclone attrition, jet attrition and a particle attrition factor which is used to determine bubbling attrition. Coefficients were determined experimentally by Werther and Reppenhagen [8] using FCC catalyst in a small scale fluidized bed. As the attrition coefficients were based on appropriate catalyst, all values were deemed reasonable for use in this paper as it is nearly impossible to obtain accurate industrial attrition coefficients from a large scale operational FCCU. It is important to note that no reference has been found in the literature warning of scale-up problems associated with the use of attrition terms based on small scale systems (as is the Werther and Reppenhagen model [8]) when used to model industrial systems.

The new emission model which forms the basis of this research paper again consists of the form $y = f(x)$, but is extended to include the attrition processes, where x is a vector of 11 input parameters (listed in Table 1), and the attrition constants. The input parameters define the operational conditions of the FCCU through a series of equations stepping through the physical processes in the FCC, taking into account particle attrition and particle feedback in the system. The model provides the output parameter (emissions in mg/m^3) based on the operational input parameters (see Fig. 1).

2.2. Sensitivity analysis

The New Morris Method, as developed by Campolongo and Braddock [9] and corrected by Cropp and Braddock [10], was selected and used to test the sensitivity of the model to uncertainty in the input parameters. The original Morris method is a "one-factor-at-a-time" (OAT) screening method which was selected as it allows first order sensitivity to be determined by alternating each of the parameters individually and then estimating the overall sensitivity measure of that parameter to the output. The sensitivity is assessed as an average over the range of the parameter space, where the parameters are allowed to vary across the range of admissible values, such as those given in Table 1.