



## An expert system for monitoring and diagnosis of ammonia emissions from the post-combustion carbon dioxide capture process system



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### ABSTRACT

The amine-based carbon dioxide (CO<sub>2</sub>) capture technology has become an important method for ensuring reduction of greenhouse gas emissions from electricity generation plants. While the amine is a comprehensive solvent that has been used in the post-combustion carbon capture process, the amine-based CO<sub>2</sub> capture process emits the primary gas of ammonia (NH<sub>3</sub>). Since ammonia emissions are hazardous to human health and contribute to acidification of air, soil and water, it is critical that the ammonia from the amine-based carbon capture process be closely monitored.

The research objective is to investigate monitoring and diagnosis of ammonia emissions from an amine-based carbon capture process system using an automation approach. This paper presents design and construction of an expert system for monitoring and diagnosis of ammonia emissions from a carbon dioxide capture system. The expert system can conduct automated monitoring and diagnosis of ammonia emissions from the post-combustion CO<sub>2</sub> capture process system at the International Test Centre for CO<sub>2</sub> Capture (ITC) located at the University of Regina in Saskatchewan, Canada. The system is called the Expert System for Monitoring and Diagnosis of AMmonia emissions (ESMDAM), and application of the system in three case scenarios demonstrates validity of the system recommendations.

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### 1. Introduction

Emissions of carbon dioxide (CO<sub>2</sub>) derived from human activities are known to have contributed to climate change and global warming. The major greenhouse gas (GHG) of CO<sub>2</sub> is often generated from fossil-fueled power generation systems, which remain to be one of our main sources of energy. According to Suebsiri (2010), fossil fuels are likely to be continuously used as one of our main energy sources for at least the next few decades. As a consequence of this reliance on fossil fuels, there will likely be an increase in CO<sub>2</sub> emissions to the atmosphere if no proper control technology is in place. Hence, application of an effective CO<sub>2</sub> capture technology, which can ensure reduction of CO<sub>2</sub> emissions to the atmosphere, is urgently needed. There are three major CO<sub>2</sub> capture methodologies, which include the pre-combustion, post-combustion, and oxy-fuel combustion technologies. In this paper, we focus on the post-combustion carbon capture technology and the modeled data

were generated at the implemented CO<sub>2</sub> capture system of the International Test Centre for CO<sub>2</sub> Capture (ITC).

The research objective is to investigate how ammonia emissions from a post-combustion carbon capture plant can be detected and monitored using an expert system. First, a brief introduction to the problem of ammonia emissions from the post-combustion carbon capture process is given. While many solvents such as chilled ammonia and potassium carbonate can be used for capturing CO<sub>2</sub> from the post combustion flue gases, the amine is often chosen due to its high reactivity, high CO<sub>2</sub> absorbing capacity on a mass basis, and low cost (Davidson, 2007). However, while the amine has been considered as the benchmark solvent for the post-combustion capture process, the weakness is that using amine can possibly result in solvent loss due to: (i) degradation, (ii) vaporization, (iii) mechanical losses, and (iv) aerosol (mist) formation (Mertens et al., 2013).

Among the four causes of solvent loss, the losses, degradation and vaporization of amine can cause unwanted contaminations in the treated off-gas, which leaves the absorber column and escapes to the air. The contaminations can be significant when the capture plant is not operated properly. The off-gas that is discharged from the process is often lean in CO<sub>2</sub>, but it can also contain more toxic substances such as sulfur oxide (SO<sub>x</sub>), nitrogen oxide NO<sub>x</sub>, particulate matter (PM), and aerosol formation (i.e.

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entrained monoethanolamine (MEA)). In addition, various products from amine degradation, in particular those that are easily volatile such as ammonia (NH<sub>3</sub>), aldehydes, and ketones, can also be carried over to contaminate the off-gas stream and pose immediate hazard to human health and the environment (Thitakamol et al., 2007). Among these, the three substances of SO<sub>x</sub>, NO<sub>x</sub>, and PM can be managed respectively by installing a flue gas desulphurization unit (FGD), low-NO<sub>x</sub> burners, and an electrostatic precipitator (ESP) prior to operation of the capture plant. However, the volatile products from amine degradation are harder to manage and there are no control units to specifically deal with their emissions (Morris, 2011). In particular, the oxidative degradation of most amines can produce NH<sub>3</sub>, which is the primary gas emitted from the CO<sub>2</sub> capture plant. Since a large amount of ammonia in the atmosphere is hazardous to human health, monitoring the NH<sub>3</sub> emissions is essential. According to the American Industrial Hygiene Association (AIHA), the American Conference of Governmental Industrial Hygienists (ACGIH), and the National Institute for Occupational Safety and Health (NIOSH), the Threshold Limit Value (TLV) of NH<sub>3</sub> is 25 parts per million (ppm) (based on an 8-h average time-interval) (Alberta Environment, 2004). The existing emission limit on NH<sub>3</sub> varies depending on the province in Canada and only three provinces provide jurisdictional information. The existing limit on NH<sub>3</sub> emissions for the provinces of Alberta and Manitoba is 2 ppm in an 1-h average time-interval, while in Ontario it is 5.17 ppm in a 30-min average time-interval (Alberta Environment, 2004). To ensure the NH<sub>3</sub> emissions stay within the allowable limits, constant monitoring of the NH<sub>3</sub> emissions is necessary so that the plant operators can be informed on: (i) integrity of the solvent, and (ii) whether it is necessary to adjust process parameters in order to make up solvent loss and ensure effective CO<sub>2</sub> capture operations.

Therefore, the objective of this study is to build an expert system for monitoring and diagnosis of NH<sub>3</sub> emissions in the post-combustion CO<sub>2</sub> capture system, the system is called ESMDAM. The system ensures that when the NH<sub>3</sub> concentration discharged from the CO<sub>2</sub> plant exceeds the allowable or normal level, the operator will be informed and the system parameters will be adjusted to reduce the level of NH<sub>3</sub> emissions. In other words, the expert system provides decision support in the task of process system monitoring; its recommendations help the plant operator keep the harmful NH<sub>3</sub> emitted from the carbon capture process within a level acceptable according to regulatory standards. The expert system was developed on G2 (trademark of Gensym Corp, USA), which is a powerful expert system development platform that allows users create and deploy rule-based systems.

This paper is organized as follows. Section 2 provides some background on the problem of NH<sub>3</sub> emissions from the carbon dioxide process system. Section 3 describes development of the ESMDAM. Section 4 discusses implementation of ESMDAM in G2. Section 5 describes three application case studies that illustrate how the ESMDAM can provide decision support to the plant operator, and Section 6 presents the conclusion and some suggestions for future work.

## 2. Background

Koornneef et al. (2009) evaluated NH<sub>3</sub> emissions from different carbon capture and storage technologies (CCS), and found that pre-combustion CO<sub>2</sub> capture could produce zero NH<sub>3</sub> emissions while post-combustion CO<sub>2</sub> capture resulted in a significant increase in the emissions. Also, Thitakamol et al. (2007) identified four major products that are most often emitted from the post combustion process, and these include the treated gas, waste from the process solvents, fugitive emissions, and some accidental releases. Among these products, NH<sub>3</sub> in the treated gas was also identified as a

$$r_{NH_3\text{ emission}} = \frac{\{1.75 \times 10^{-6} e^{-(0.62/RT)} [MEA]^{0.38} [O]^{3.41}\}}{\{1 + 0.86[CO_2]^{0.57} + 0.46[H_2SO_3]^{0.16} + 1.45[HNO_3]^{0.08}\}}$$

Fig. 1. NH<sub>3</sub> rate equation.

fairly toxic substance, which could adversely affect human health through skin burns and irritation.

A review of the relevant literature reveals that there are only a few studies that provide quantitative data of NH<sub>3</sub> emissions. For example, Chanchey et al. (2011) showed that the presence of sulfuric acid (H<sub>2</sub>SO<sub>3</sub>), nitric acid (HNO<sub>3</sub>), and CO<sub>2</sub> in the carbon capture process all decreased NH<sub>3</sub> emissions while a rise in temperature in the system would increase them. Saiwan et al. (2013) provided kinetic rate information of NH<sub>3</sub> emissions in the CO<sub>2</sub> absorption process. The study found that an increase of MEA, oxygen (O<sub>2</sub>) concentrations, and temperature increased the NH<sub>3</sub> emissions rate, and increases in the H<sub>2</sub>SO<sub>3</sub>, HNO<sub>3</sub>, and CO<sub>2</sub> concentrations decreased the rate. A useful NH<sub>3</sub> rate equation proposed in this work is given in Fig. 1. Mertens et al. (2012) proposed a Fourier transform infrared (FTIR) system for on-line monitoring and control of amine emissions from a post combustion carbon capture plant. The system can measure both inorganic and organic components and a zirconium analyzer was also used to measure the concentration of O<sub>2</sub>. The analysis was conducted for investigating the effect of the plant's operational settings, so that its amine emissions can be reduced to a very low level. Zhou et al. (2012) developed a knowledge-based system for the CO<sub>2</sub> capture process using the Inferential Modeling Technique (IMT); the system was able to support detailed specification of knowledge elements of the amine-based carbon capture process.

The literature review reveals that little work has been done on monitoring and diagnosis of amine plant emissions, and nothing has been done that addresses specifically NH<sub>3</sub> emissions. To fill the research gap, this study aims to test feasibility of building an automated system for monitoring, diagnosis, and control of NH<sub>3</sub> emissions in the CO<sub>2</sub> absorption process. The assumption adopted is that including such a system in the capture process system would help ensure safe and efficient operation of the post-combustion carbon dioxide capture process system.

## 3. Development of the ESMDAM system

### 3.1. Rationale for the expert system approach

The expert system approach has been adopted in this study because it has definite advantages over conventional information technologies, which often involve algorithmic programs for providing numeric solutions. By contrast, the main component of an expert system is the knowledge base, which can represent both algorithmic and heuristic information. Since human expertise is needed to solve the NH<sub>3</sub> emissions problem, this knowledge is represented as rules in the knowledge base. The knowledge represented enables the expert system to perform reasoning and make recommendations to the process system operator when an NH<sub>3</sub> emission problem arises. In addition, the represented knowledge enables the system to provide explanations to the user, so that the rationale for making the recommendation can be clarified to the user. Both capabilities of (i) representing heuristics or human expertise and (ii) providing explanations on how a particular solution is derived are absent in conventional information technologies (Gupta and Singhal, 2013; Negnevitsky, 2002).

### 3.2. Knowledge acquisition

The knowledge acquisition (KA) process involved extracting, structuring, and organizing knowledge about the post-combustion

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