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A hybrid approach for estimating fugitive emission rates in process development and design under incomplete knowledge

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ABSTRACT

Fugitive emissions are one of the most notable contributors to atmospheric releases in chemical process industries affecting not only the economy but also both the environment and workers' health. In order to reduce fugitive emissions released in this process, the assessment of fugitive emissions should be conducted at the early stage of chemical process design when the cost of making changes is the lowest. This is however impeded by the limited knowledge on the leak sources, since the process is still under design. The paper presents a hybrid approach for estimating fugitive emission rates early in the design phase. The method combines a pre-calculated emission database of standard process module based approach with estimation by using generic piping and instrumentation diagrams if a suitable module is not available from the database. Also, both working and breathing emissions are included in the assessment. The emissions' assessment from a case study of hydrodealkylation distillation and storage systems is presented to demonstrate the proposed approach.

1. Introduction

To move toward a globally greener, safer and healthier working environment, it is important to consider safety, health and environment factors in designing more sustainable processes. In line with this, there have been a lot of efforts taken to control emissions in chemical and oil industry. Fugitive emissions (FEs) contribute to a significant portion of problems related to air pollution and climate change. FEs can be defined as *leaks or releases that occur wherever there are discontinuities in the solid barrier that maintains containment* (Hassim, 2010). The fugitive losses may occur on process plants from leaking process components, storage tanks breathing and filling, and wastewater treatment systems (Shine, 1996). Although the amount of FEs released from a single leak point is usually very small, the total accumulative amount of the emissions from thousands of the sources in one plant may be considerably large and cause significant impact to the environment. For example, in Canada, it was estimated that 12% of CO_2 equivalent greenhouse gas emissions of upstream oil and gas industry came from FEs, when all fuel combustion emissions counted 41% of CO_2 equivalent (CAPP, 2004). In addition, FEs can also affect the health of employees and the public. It was found that incidences of certain types of cancers (e.g., in brain, nervous system, etc.) are related to volatile organic compounds (VOCs) emission (Boeglin et al., 2006).

The most cost effective way of reducing or eliminating the sources of FEs is to perform the assessment on the emissions as early as possible, starting from the process development and design phase, when the cost of making changes is still low. Such effort however is hampered by the incomplete knowledge on process details, such as the

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Nomenclature

A	Cross section area
A_f	Total floor area
C_i	Concentration of chemical substance *i*
EPA	United States Environmental Protection Agency
FE	Fugitive emission
$FE_{i,m}$	Fugitive emission of chemical *i* in process module *m*
FE_i^{total}	Total fugitive emission of chemical *i*
FE_m	Fugitive emission in process module *m*
G/V	Gas/vapor
h	Maximum height for the leak points
HDA	Hydrodealkylation
HL	Heavy liquid
LL	Light liquid
P&ID	Process and instrumentation diagram
PFD	Process flow sheet diagram
Q	Air volumetric flowrate
s	Edge width of area
v	Local average wind speed
VOC	Volatile organic compound
W_i	Weight composition of chemical

number of leak sources and their specific type. To make the estimation of FE rates possible to be conducted with a very limited process information, Hassim et al. (2010) developed a method which provides a pre-calculated emissions database for various standard (or typical) process modules in chemical process industries (distillation, reactors, absorber etc.). Since the method has some limitations, in a way that it is not covering types of process modules (also commonly known as unit operations) in process industries, the aim of this paper is to present a hybrid framework to overcome the limitations by utilizing more than one estimation methods and also including other emission types such as tank emissions, based on the information available in the design stage.

2. Literature review

Over the past decades, various methods have been presented for quantifying the amount of FEs. The approaches can be categorized into two main categories; modeling and measurement, which are shown in Table 1. *Modeling approaches* basically employ mathematical methods to estimate the FEs without measurements. The typical sub categories are emission factors and mathematical approaches. The emission factors are empirical approaches for equipment leaks estimation. There are four techniques: average emission factor, screening range, correlation, and unit-specific correlation approaches (EPA, 1995). The emission factors have been developed and compiled from source test data, material balance studies, and engineering estimates. The mathematical approach on the other hand considers models based on physical phenomena. This approach generally gives more accurate result compared to emission factor method because of their rigorous principle. For example filling, heating or purging losses can be calculated based on phase equilibrium models (Shine, 1996). Vasquez-Beggs equation and Peng-Robinson equation of state have been used for calculating tank flashing, working and breathing loses (EPA, 2009). To assist engineers to perform assessment in a faster way, computational tools for estimating FEs based on emission factor and mathematical approaches have been applied in different specific fields.

Different from modeling approach, *measurement approach* can be used for estimating emissions from *existing* plants, detecting leak sources and providing real-time information on the emissions. Different methods have been adopted to perform leak detection and quantify FE in any section of the chemical plants (Table 1). However measurement approach can only be implemented on an existing operation/process.

The combination of both modeling and measurement approaches have also been developed in recent years. Brereton and Johnson (2012) proposed a new approach by using four trajectory statistical methods to locate sources of within a complex geometry representative of an actual petroleum industry gas plant. Foster-Wittig et al. (2015) presented two inverse Gaussian source emission rate estimation approaches based on modeled and reconstructed plumes. These approaches can be used to enhance the effectiveness of fugitive emissions detection and measurement approaches such as the EPA draft method OTM 33A. A multiregional hybrid life cycle assessment (LCA) model was used to investigate the effect of fugitive methane emissions associated with the

Table 1 – Previous works on fugitive emissions.

Category	Authors (year)	Study scopes
Modeling	Cheng et al. (2008)	The emission rates of VOCs in a single wastewater collection and treatment facility was estimated by using Water 9, which was designed by the EPA.
	Gong et al. (2008)	The FEs in C8 alkylates production via solid acid/carbon dioxide process were estimated by using ASPEN HYSYS simulation software.
	Hassim et al. (2010)	The average emission factor approach was adopted to estimate FEs by counting equipment and piping items in the process.
	Horne et al. (2010)	The screening range approach was adopted in calculating VOCs emissions.
	Dadashzadeh et al. (2011)	A new set of emission correlation equations for oil and gas facilities was developed based on the United States Environmental Protection Agency (EPA) correlation equation approach.
	Pawelzik and Zhang (2012)	The FEs in simultaneous saccharification and co-fermentation process were calculated using the Air Emission Calculator from the Environmental Fate and Risk Assessment Tool which linked with ASPEN Plus.
Measurement	Onat (2006)	Flushing or sniffing methods were applied to measure methane by using organic vapor analyzer.
	Pandya et al. (2006)	VOCs emissions were analyzed via bagged equipment coupled with hydrocarbon analyzer.
	Todd et al. (2001)	The uses of open-path Fourier transform infrared spectroscopy and computer-assisted tomography were demonstrated to measure ammonia concentrations from an animal waste lagoon.