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Equilibrium stage based model of a vegetable oil based wet packed bed scrubbing system for removing producer gas tar compounds

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ABSTRACT

This study was aimed to develop and validate equilibrium stage based absorption model to investigate the removal of model producer gas tar compounds using vegetable oil as a solvent. The absorption model was developed using split (φ/γ) approach and a "RadFrac" block in Aspen Plus™. The model used Peng–Robinson equation of state (EOS) and non-random two-liquid (NRTL) activity coefficient model to predict the fugacity coefficients (φ) for vapor phase and activity coefficients (γ) for liquid phase. The developed model was validated using the extreme conditions of the experimental test range. The model predictions showed best fits with the experimental data within 6% for benzene, 4% for toluene, and 2% for ethylbenzene at the solvent temperature of 30 °C. Packing specific constants of Billet and Schultes (1999) correlation ($C_h = 2.52$ and $C_{P,0} = 2.93$) were found experimentally. These constants can be used to predict pressure drop across the column for vegetable oil based wet packed bed scrubbing systems. The average deviation of predicted pressure drop across the column compared to experimental data was within 5%. The developed absorption model and packing specific constants would be beneficial in the design, optimization, and economic evaluation of vegetable oil based wet packed bed scrubbing systems.

1. Introduction

The bioeconomy is emerging rapidly in the USA in an effort to reduce the dependence on the imported oil. One of the focused areas of the bioeconomy is meeting the raising energy demands through renewable biomass [1]. Sustainable fuels, chemicals and biobased products can be produced using several different pathways, including thermochemical conversion. Gasification, one of the thermochemical technologies, is a process of decomposing biomass in the presence of heat and partial oxygen or air. The gasification process can convert most any type of carbonaceous feedstock such as dedicated energy crops, agricultural waste and industrial waste to producer gas which can be converted into fuels, chemicals, products, heat and power. In the generation of producer gas, the gasification process also produces undesirable impurities such as tars [2,3]. A mitigation of tars is the major technical obstacle for the advancement of the gasification technology [4,5].

Biomass producer gas tar is a complex compound consisting of more than two hundred hydrocarbon compositions [6] which are classified as heavy and light tars. Condensation behavior of tar compounds depends mainly on type and associated concentration and resultant dew-point temperature of the tar compounds. Tar compounds start condensing when the producer gas temperature drops below tar dew-point temperature. This is often problematic in most downstream processes and applications. Wet scrubbing processes are widely reported as an effective method for the removal of tar compounds. Bhoi [7] showed that vegetable oil based wet packed bed scrubbing system is a promising technology for removing biomass producer gas tar compounds.

For economical design and optimization of wet packed bed scrubbing system, an accurate and reliable prediction of the system performance as a function of operating conditions is essential. Only a few studies have been reported on modeling of tar removal processes [8,9]. Tisdale [8] described a process model of the spray chamber type water based scrubber system for tar removal. The scrubbing system used two scrubbers in series. Flash 3 [8] (flash drum with vapor and two liquid products) was used to model

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the first scrubber, i.e., spray chamber, and Flash 2 [8] (flash drum with vapor and liquid products) for modeling the second scrubber, i.e., spray chamber. To estimate the amount of saturated tars in water, Flash 3 was modeled through liquid–liquid–vapor equilibrium. Tisdale used Redlich–Kwong–Soave (RK–SOAVE) property method for the process model, and observed that Peng Robinson (PENG–ROB) is comparable to RK–SOAVE property method.

Seethamraju et al. [9] reported simulating a high pressure absorption system using diesel, canola oil, and biodiesel as a solvent. The simulation used non-random two-liquid (NRTL) as a vapor–liquid equilibrium model. UNIQUAC functional-group activity coefficients (UNIFAC) method was used to determine the missing binary interaction parameters of the NRTL model.

Bhoi [7] stated that a wet packed bed scrubbing system is a good choice due to its highest absorption efficiency and a low pressure drop. The solvent selected plays a major role in the design and operation of the system. Based on the preliminary experiments and literature review, it was observed that vegetable oil is a potential solvent for the absorption of tar compounds [10,11]. Potential advantages of vegetable oils as solvents are: readily available, plant-based, renewable, and low vaporization loss due to its low vapor pressure.

As stated above, a little information is available on the process modeling of vegetable oil based wet packed bed wet scrubbing system for tar removal. The objectives of this study were to develop an equilibrium stage based absorption model to study removal of model tar compounds in vegetable oil based wet packed bed scrubbing system and to validate the model using experimental data.

2. Materials and methods

2.1. Wet packed bed scrubbing system model

The absorption of producer gas model tar compounds, i.e., benzene, toluene and ethylbenzene in vegetable oil was studied using a bench scale wet packed bed scrubbing column of 0.5 m diameter by 1.1 m height (Fig. 1). Design and construction details of the scrubbing system and experimental performance results were presented by Bhoi [7].

Table 1
Characteristics of raschig rings [7].

Parameters	Values
Size (diameter × length × thickness), mm	6 × 6 × 0.3
Density, kg/m^3	900
Surface area, m^2/m^3	900
Packing factor, 1/m	2297
Void fraction, %	89

Table 2
Properties of soybean oil [7].

Parameters	Value
Palmitic acid (16:0), %	9
Steric acid (18:0), %	4.4
Oleic acid (18:1), %	26.4
Linoleic acid (18:2), %	51.6
Linolenic acid (18:3), %	6.8
Density, kg/m^3	922.5
Viscosity, mm^2/s	65.4
Heating value, MJ/kg	37
Flash point, °C	>288

Absorption of tars was carried out in a counter–current (gas flows upward while liquid flows downward) wet packed bed scrubbing column. The packed bed consisted of 6-mm raschig rings. The characteristics of raschig rings provided by the supplier are given in Table 1.

2.1.1. Selection of chemical compounds

Aspen Plus™ contains a large database of chemical compounds that are typically used in industry. The database mainly contains organic, inorganic, aqueous, electrolytic and salt compounds. In this study, the compounds selected from the in-built database were air, model tar compounds (benzene, toluene and ethylbenzene) and soybean oil which was represented using supplier's composition of fatty acids (palmitic, steric, linoleic, linolenic and oleic acids) as given in Table 2.

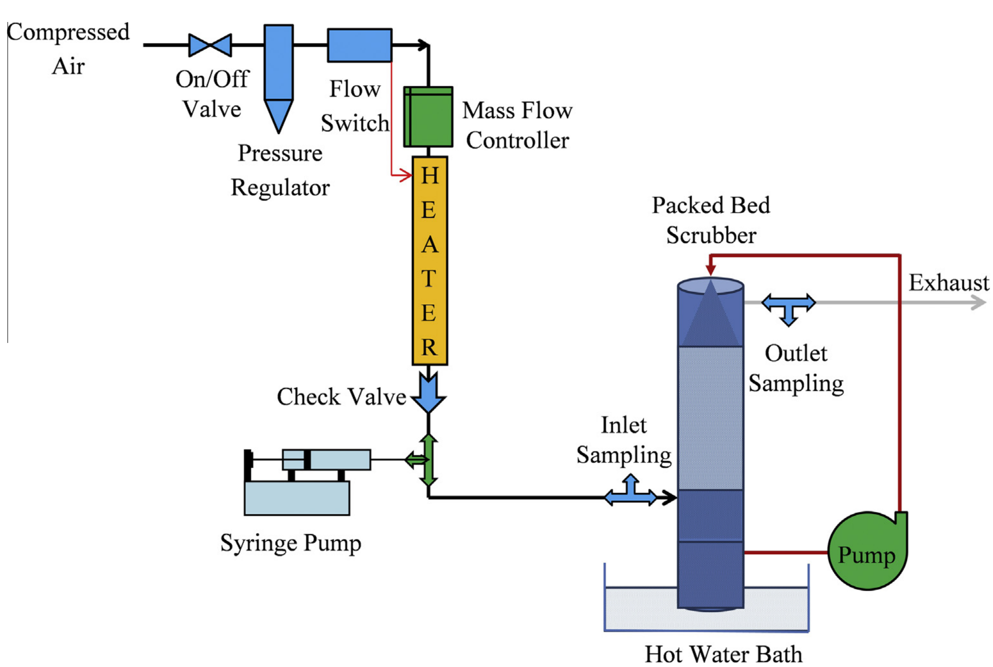

Fig. 1. Schematic diagram of bench-scale wet packed bed scrubbing set-up [7].