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Estimation of combustion flue gas acid dew point during heat recovery and efficiency gain

Alireza Bahadori*

Curtin University, School of Chemical and Petroleum Engineering, GPO Box U1987, Perth, WA 6845, Australia

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ABSTRACT

When cooling combustion flue gas for heat recovery and efficiency gain, the temperature must not be allowed to drop below the sulfur trioxide dew point. Below the SO_3 dew point, very corrosive sulfuric acid forms and leads to operational hazards on metal surfaces. In the present work, simple-to-use predictive tool, which is easier than existing approaches, less complicated with fewer computations is formulated to arrive at an appropriate estimation of acid dew point during combustion flue gas cooling which depends on fuel type, sulfur content in fuel, and excess air levels. The resulting information can then be applied to estimate the acid dew point, for sulfur in various fuels up to 0.10 volume fraction in gas (0.10 mass fraction in liquid), excess air fractions up to 0.25, and elemental concentrations of carbon up to 3. The proposed predictive tool shows a very good agreement with the reported data wherein the average absolute deviation percent was found to be around 3.18%. This approach can be of immense practical value for engineers and scientists for a quick estimation of acid dew point during combustion flue gas cooling for heat recovery and efficiency gain for wide range of operating conditions without the necessity of any pilot plant setup and tedious experimental trials. In particular, process and combustion engineers would find the tool to be user friendly involving transparent calculations with no complex expressions for their applications.

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1. Introduction

During combustion, sulfur present in hydrocarbons and coke generates sulfur dioxide (SO_2) in flue gas. Many coke calciners have waste heat boilers to recover energy from the hot flue gas. Some of the coke dust in flue gas accumulates on boiler tubes. Vanadium and other metals in the dust catalyze the oxidation of SO_2 to SO_3, especially in the convection section where a temperature of approximately 750 °F is sufficiently hot to promote the kinetics of the oxidation reaction, yet cool enough to allow SO_3 formation. At higher temperatures, SO_2 is the favored species of oxidized sulfur [1,2].

Whenever fossil fuels containing sulfur are fired in heaters or boilers, sulfur dioxide, and to a small extent sulfur trioxide, are formed in addition to water vapor [3]. The SO_3 combines with water vapor present in the flue gas to form sulfuric acid and condenses on heat transfer surfaces, leading to corrosion and destruction of the surfaces [1,4]

Given these consequences, significant efforts have been devoted for establishing methods to predict sulfuric acid dew point of flue gases. Thermodynamic approach has been used by few researchers for the prediction of sulfuric acid vapor/liquid equilibrium conditions [5,6]. However, the predicted results are proved to be quite sensitive to the accuracy of data. Similar approaches have been presented [7–9] to describe complex vapor–liquid equilibrium behaviour of aqueous sulfuric acid mixtures. Unfortunately these models have made some simplifications and covered limited conditions. The available thermodynamic models [10] are not accurate enough for prediction of flue gas sulfuric acid dew points for industrial applications. Verhoff and Banchero [11] provided an empirical fit of available experimental data as a more accurate method for estimating dew point conditions. However, there are some disagreements between the experimental data and their correlation especially at low SO_3 concentrations. An artificial neural network model [3,12] has been recently presented for the prediction of sulfuric acid dew point at the operating conditions relevant to stack and heat recovery systems. Existing methods are suitable for predicting acid dew points as a function of sulfur trioxide and water vapor concentrations at the operating conditions of stack. However, there is no simple-to-use predictive tool to date for the estimation of the acid dew point for cooling combustion flue gas which takes into account fuel type, sulfur fraction in fuel, and excess air.

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* Tel.: +61 8 9266 1782; fax: +61 8 9266 2681.
E-mail address: alireza.bahadori@postgrad.curtin.edu.au.

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In view of the above-mentioned critical issues which are of paramount importance for cooling combustion flue gas for heat recovery and efficiency gain, it is necessary to develop an accurate and simple method which is easier than existing approaches less complicated with fewer computations for predicting the acid dew point for cooling of combustion flue gas. The paper discusses the formulation of such a predictive tool in a systematic manner along with sample example to show the simplicity of the model and usefulness of such tools.

2. Development of predictive tool

In this work a simple-to-use predictive tool is developed using Vandermonde matrix to predict the acid dew point temperature, as a function of elemental concentrations of carbon, excess air fraction and sulfur mass fraction in liquid fuel (sulfur volume fraction for gaseous fuel).

2.1. Vandermonde matrix

Vandermonde matrix is a matrix with the terms of a geometric progression in each row, i.e., an $m \times n$ matrix [13].

$$V = \begin{bmatrix} 1 & \alpha_1 & \alpha_1^2 & \dots & \alpha_1^{n-1} \\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^{n-1} \\ 1 & \alpha_3 & \alpha_3^2 & \dots & \alpha_3^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha_m & \alpha_m^2 & \dots & \alpha_m^{n-1} \end{bmatrix} \tag{1}$$

or

$$V_{i,j} = \alpha_i^{j-1} \tag{2}$$

For all indices i and j. The determinant of a square Vandermonde matrix (where $m = n$) can be expressed as [13]:

$$\det(V) = \prod_{1 \le i < j \le n} (\alpha_j - \alpha_i) \tag{3}$$

The Vandermonde matrix *evaluates* a polynomial at a set of points; formally, it transforms *coefficients* of a polynomial $a_0 + a_1 x + a_2 x^2 + \ldots + a_{n-1} x^{n-1}$ to the *values* the polynomial takes at the points α_i. The non-vanishing of the Vandermonde determinant for distinct points α_i shows that, for distinct points, the map from coefficients to values at those points is a one-to-one correspondence, and thus that the polynomial interpolation problem is solvable with unique solution; this result is called the unisolvence theorem [14]. They are thus useful in polynomial interpolation, since solving the system of linear equations $Vu = y$ for u with V an $m \times n$ Vandermonde matrix is equivalent to finding the coefficients u_j of the polynomial(s) [13,14]

$$P(x) = \sum_{j=0}^{n-1} u_j x^j \tag{4}$$

For degree $\le n-1$ which has (have) the property:

$$P(\alpha_i) = y_i \quad \text{for } i = 1, \ldots m. \tag{5}$$

The Vandermonde matrix can easily be inverted in terms of Lagrange basis polynomials: each *column* is the coefficients of the Lagrange basis polynomial, with terms in increasing order going down. The resulting solution to the interpolation problem is called the Lagrange polynomial [13,14].

2.2. Methodology to develop predictive tool

In this work, the acid dew point temperature is predicted rapidly by proposing a simple tool and the following methodology has been applied to develop the predictive tool. In this study $F1$ and $F2$ are empirical correction factors to correlate acid dew point temperature of combustion flue gas with elemental concentration of carbon in fuel and excess air fraction. The required data to develop this predictive tool includes the acid dew point temperature, as a function of elemental concentrations of carbon, excess air fraction and sulfur mass fraction in liquid fuel (sulfur volume fraction for gaseous fuel). Firstly, the elemental concentration of carbon correction factors ($F1$) is correlated using Vandermonde matrix as a function of sulfur mass fraction in liquid fuel (sulfur volume fraction for gaseous fuel) for different elemental concentrations of carbon. Then calculated coefficients for the polynomials are correlated as a function of elemental concentrations of carbon. The derived polynomials are applied to calculate new coefficients for Eq. (6) to predict, the elemental concentration of carbon correction factors ($F1$). Table 1 shows the tuned coefficients for Eqs. (7)–(10) for the elemental concentration of carbon correction factors ($F1$) according to the available data [15].

In brief, the following steps [16–21] using Matlab [22] are repeated to tune the coefficients of predictive tool.

1. Correlate the elemental concentration of carbon correction factors ($F1$) as a function of sulfur mass fraction in liquid fuel (sulfur volume fraction for gaseous fuel) for a given elemental concentration of carbon.
2. Repeat step 1 for other elemental concentrations of carbon.

Table 1
Tuned coefficients for equations.

Coefficient	Tuned coefficients values for Eqs. (7)–(10)	Tuned coefficients values for Eqs. (12)–(15)	Tuned coefficients values for Eqs. (17)–(20)
A_1	1.6169452391383	0	5.952258088966
B_1	$6.177669313207 \times 10^{-1}$	1.216819390081	$3.743552731891 \times 10^{-2}$
C_1	$-3.9653315193609 \times 10^{-1}$	$-1.2791492533202 \times 10^{-1}$	$-2.974543370669 \times 10^{-2}$
D_1	$8.9951003043175 \times 10^{-2}$	$3.7468691518322 \times 10^{-3}$	$8.012058874906 \times 10^{-3}$
A_2	$-7.3040211893195 \times 10^{-3}$	0	$1.4895974060729 \times 10^{-2}$
B_2	$6.9240838237836 \times 10^{-3}$	−3.503800354635	$-2.544717126420 \times 10^{-2}$
C_2	$-5.8556137033616 \times 10^{-3}$	$3.535258397881 \times 10^{-1}$	$2.8643928068906 \times 10^{-2}$
D_2	$1.5959152734857 \times 10^{-3}$	$-1.0220477526401 \times 10^{-2}$	$-8.5637681681247 \times 10^{-3}$
A_3	$1.0870177961324 \times 10^{-5}$	0	$6.451897071864 \times 10^{-5}$
B_3	$-8.5890701137873 \times 10^{-6}$	4.2457067211595	$9.793132697859 \times 10^{-3}$
C_3	$8.1950413834671 \times 10^{-6}$	$-4.2048282453109 \times 10^{-1}$	$-1.110888172768 \times 10^{-2}$
D_3	$-2.434315454803 \times 10^{-6}$	$1.2049410160293 \times 10^{-2}$	$3.330438432415 \times 10^{-3}$
A_4	$-6.1128433683661 \times 10^{-9}$	0	$5.095744544013 \times 10^{-5}$
B_4	$4.61199570025008 \times 10^{-9}$	−1.9582714147904	$-9.303357512632 \times 10^{-4}$
C_4	$-4.4972769064777 \times 10^{-9}$	$1.8294597536652 \times 10^{-1}$	$1.057513224690 \times 10^{-3}$
D_4	$1.3588028937503 \times 10^{-9}$	$-5.1643724550433 \times 10^{-3}$	$-3.172695022725 \times 10^{-4}$

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