



Full Length Article

A framework for devolatilization breakdown in entrained flow gasification modeling

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ABSTRACT

A new framework for volatile breakdown is developed for entrained flow gasification modeling. The framework is based on an optimized solution of an under-determined system of equations formulated using a two-step Moore-Penrose generalized matrix approach. The approach permits the determination of the volatile composition using just the Proximate-Ultimate analysis data of coal. The method can be utilized for all coal types irrespective of origin. The accuracy and consistency of the framework is demonstrated by direct comparison with available devolatilization breakdown data. The overall performance of the framework is also appraised by incorporating it in a CFD simulation of an actual entrained flow gasifier. The reactor exit syngas composition from the simulation is favorably compared with available experimental data.

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1. Introduction

Devolatilization has a significant impact on coal gasification. The composition of the coal volatile gases and their evolution rates directly affect the heterogeneous char reactions and the homogeneous gasification reactions. The physical process of devolatilization is fairly complex [1]. It involves several reactions with the release of a mixture of organic and inorganic gases and liquids from the coal particle. The volatile evolution rates are primarily influenced by temperature, residence time, pressure, particle size, the type of coal and their heating rates [2]. Various models have been developed to predict the volatile release rate and its composition under different operating conditions.

The important devolatilization models are the single and multi-step global kinetic models, distribution activation (DA) model which assumes a large number of reactions permitting the assumption of a continuous distribution function for the activation energy and structural models like the FG-DVC model [3], the chemical percolation devolatilization (CPD) model [4] and the FLASH CHAIN model [5].

Whereas the kinetic and the distributed activation models are based on empirical rate relationships, the structural models are based on the physical and chemical transformation of the coal molecular structure. In one form or the other, the structural models assume a molecular structure of coal arranged into several func-

tional groups. A network of chemical bridges link the functional groups together.

Although the DA and the structural models have large generality, valid for different coal types, they are inherently complex and difficult to formulate and implement in the overall gasification modeling process. Hence, single or multi-step kinetic devolatilization models are quite appealing due to their simplicity. The simplest mathematical model of coal devolatilization is the single step first order reaction model. This model is often complemented by the introduction of the so called Q-factor to incorporate the effect of temperature on the volatile yield [6]. In the next level of complexity, the Kobayashi model [7] describes devolatilization reaction by a pair of parallel first-order, irreversible reactions. The two reaction paths have different activation energies. This causes one of the reaction paths to become active at low temperatures and the other at high temperatures. Hence the Kobayashi model automatically takes into account the effect of temperature on the volatile yield. Due to the simplicity of the model, it is often used in its original form or modified form in coal gasification modeling studies [8–10].

The devolatilization models only describe the kinetics of volatile release but not the volatile matter composition. Ma and Zitney [10] provide an account of the different approximate approaches available in literature for estimating the composition of the volatiles.

This paper provides a new framework for volatile breakdown formulated on a strict mass balance basis and it allows the

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determination of the volatile composition with the knowledge of just the coal Proximate and Ultimate analysis. The framework is based on a two step least norm solution of an under-determined system of equations representing the volatile breakdown process. A general algorithm is provided to estimate the volatile composition that can be applied to all coal types. The paper is organized as follows. The next section elaborates on the volatile breakdown framework, followed by a brief introduction to entrained flow gasification modeling in Section 3. The results section is divided into two parts. In the first part, the accuracy of the framework is assessed by comparison with available devolatilization breakdown data for five South African coal types [11]. In the 2nd part, the devolatilization framework is applied to model a two-stage gasifier [12] where experimental syngas data is available for direct comparison.

2. Volatile breakdown framework

Following Merrick [13], the volatile matter is defined by a set of the following nine species: CH₄, C₂H₆, CO, CO₂, H₂, H₂O, NH₃, H₂S and TAR. The nine species are the minimum required to provide an accurate description of the volatile matter. It is assumed that higher hydrocarbons if present, can be dealt with as ethane equivalent [13]. Given a coal type, the final yields of the volatile matter can be determined by constructing a mass balance on the elements C, H, N, O and S from the coal proximate and ultimate analysis data. In matrix form, the mass balance equations can be written as:

$$\begin{bmatrix} \frac{M_C}{M_{CH_4}} & \frac{2M_C}{M_{C_2H_6}} & \frac{M_C}{M_{CO}} & \frac{M_C}{M_{CO_2}} & 0 & 0 & 0 & 0 & \frac{M_C}{M_{TAR}} \\ \frac{4M_H}{M_{CH_4}} & \frac{6M_H}{M_{C_2H_6}} & 0 & 0 & \frac{2M_H}{M_{H_2}} & \frac{3M_H}{M_{NH_3}} & \frac{2M_H}{M_{H_2S}} & 0 & \frac{M_H}{M_{TAR}} \\ 0 & 0 & \frac{M_O}{M_{CO}} & \frac{2M_O}{M_{CO_2}} & 0 & 0 & 0 & 0 & \frac{M_O}{M_{TAR}} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{M_N}{M_{NH_3}} & 0 & \frac{M_N}{M_{TAR}} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{M_S}{M_{H_2S}} & \frac{M_S}{M_{TAR}} \end{bmatrix} \begin{bmatrix} y_{CH_4} \\ y_{C_2H_6} \\ y_{CO} \\ y_{CO_2} \\ y_{H_2} \\ y_{H_2O} \\ y_{NH_3} \\ y_{H_2S} \\ y_{TAR} \end{bmatrix} = \begin{bmatrix} C_U - FC_P \\ H_U \\ O_U \\ N_U \\ S_U \end{bmatrix} \quad (1)$$

The symbols M and y on the left hand side of the above equation are the molecular weight and the species mass fraction respectively. On the right hand side, C_U, H_U, O_U, N_U and S_U are the carbon, hydrogen, oxygen, nitrogen and sulfur fractions from the coal ultimate analysis. The symbol FC_P refers to the fixed carbon fraction from the coal proximate analysis. Eq. (1) can be written symbolically as

$$\mathbf{A}\mathbf{y} = \mathbf{b} \quad (2)$$

where **A** is a 5 × 9 coefficient matrix representing the volatile matter species expressed as mass fractions of carbon, hydrogen, oxygen, nitrogen and sulfur. **y** is the unknown vector of volatile species and **b** is the known vector obtained from coal ultimate and proximate analysis.

Eq. (2) is a rectangular under-determined system of equations with more unknowns than equations. One way to close the system is to supplement it with four extra equations obtained through specialized experiments [13] or available correlations [14]. In the absence of any other information, it is useful to consider one solution (among the many) of the above under-determined system of equations by examining the following optimization problem [15] in the composition manifold of the volatile species:

Minimize:

$$F(\mathbf{y}) = \mathbf{y}^T \mathbf{y} = \|\mathbf{y}\| \quad (3)$$

subject to:

$$\mathbf{A}\mathbf{y} - \mathbf{b} = 0 \quad (4)$$

Using a vector λ of Lagrange multipliers [16], the solution of the constrained optimization problem is found to be the same as the extremum of the Lagrangian, $L(\mathbf{y}, \lambda)$

$$L(\mathbf{y}, \lambda) = F(\mathbf{y}) + \lambda^T (\mathbf{A}\mathbf{y} - \mathbf{b}) \quad (5)$$

The first order optimality criteria gives:

$$\nabla_{\mathbf{y}} L = 2\mathbf{y} + \mathbf{A}^T \lambda = 0 \quad (6)$$

and

$$\nabla_{\lambda} L = \mathbf{A}\mathbf{y} - \mathbf{b} = 0 \quad (7)$$

From Eq. (6), we have

$$\mathbf{y} = \frac{-\mathbf{A}^T \lambda}{2} \quad (8)$$

Substituting Eq. (8) in Eq. (7), one obtains

$$\lambda = -2(\mathbf{A}\mathbf{A}^T)^{-1} \mathbf{b} \quad (9)$$

Finally substituting Eq. (9) in Eq. (8), one obtains the volatile species vector **y** as solution of the under-determined system of equation.

$$\mathbf{y} = \mathbf{A}^T (\mathbf{A}\mathbf{A}^T)^{-1} \mathbf{b} \quad (10)$$

The matrix $\mathbf{A}^T (\mathbf{A}\mathbf{A}^T)^{-1}$ in the above equation is called the Moore-Penrose matrix and the solution **y** represents the least norm solution in the volatile composition space. This often provides the best

possible solution [17,18,15]. However, such solutions are not random. They are dominated by certain internal constraints. This is a paradigm shift in how constraints can be incorporated in an analysis. The system of equations are based on fundamental mass balance concepts and the constraints are specific observational attributes to be treated separately from the original system.

Constraints or corrections in one or more of the species can be introduced at this stage to improve predictions. Introducing a parameter $\xi \in (0, 1)$, depicting the application of the correction factor with $\xi = 0$ yielding the least norm solution ($\mathbf{y} = \mathbf{y}_{LN}$) without any correction and $\xi = 1$ yielding the corrected solution ($\mathbf{y} = \mathbf{y}_{LN,C}$), the volatile species vector is determined to be

$$\mathbf{y} = (1 - \xi)\mathbf{y}_{LN} + \xi\mathbf{y}_{LN,C} \quad (11)$$

An algorithm to construct a correction is discussed in Section 4. The correction is made to the least-norm solution obtained from Eq. (10). The modified least-norm species vector ($\tilde{\mathbf{y}}_{LN}$) is perturbed to obtain the final volatile yield $\mathbf{y}_{LN,C} = \tilde{\mathbf{y}}_{LN} + \delta\mathbf{y}$, where the species perturbations $\delta\mathbf{y}$ are obtained by solving a 2nd under-determined perturbed system of equations using the Moore-Penrose method [19].

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