



# Application of uncertainty quantification methods for coal devolatilization kinetics in gasifier modeling



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## ABSTRACT

The focus of this research is to study sensitivity of input parameters in terms of chemical reaction kinetics of coal devolatilization using non-intrusive uncertainty quantification (UQ) methods. The effects of heating rate, pressure, and temperature on coal devolatilization have been considered. Variations in coal devolatilization kinetics and product yields were captured via Carbonaceous Chemistry for Computational Modeling (C3M) for operating conditions similar to the transport gasifier using PC Coal Lab (PCCL) kinetic package. Temperature, pressure and heating rate were considered as three input parameters, while the quantities of interest or response variables were mass fractions of CO, CO<sub>2</sub>, H<sub>2</sub>, tar, H<sub>2</sub>O, and CH<sub>4</sub> along with total volatile yield. A direct Monte Carlo-simulation-based approach was employed to perform the UQ analysis. The correlations among the response variables were investigated by computing a correlation matrix that supports the findings of yield of devolatilization reported by various experiments in the literature. Sensitivity study of the input parameters was analyzed by using the Sobol Total Indices methodology implemented in PSUADE, an open source UQ toolbox. These findings clearly demonstrate the pronounced effect of temperature on coal devolatilization product yields, and hence will be considered as a key parameter in future studies. The preliminary study presented in this paper paves a path for incorporating uncertainty caused by chemical reaction kinetics in computational fluid dynamics based modeling of coal gasifier systems and scale-up studies.

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## 1. Introduction

Non-intrusive parametric input uncertainty propagation is one of the uncertainty quantification techniques employed in numerical or mathematical models to predict the effect of the uncertainty on output due to variations in input parameters. Many assumptions are made by the user when simulating a physical problem as it is very difficult to model exactly all the complex phenomena taking place. Some of these assumptions are directly related to the model parameters or inputs, and the remaining are embedded with the selected model (e.g., the drag model used in multiphase flows). These assumptions can make a significant difference between the model predictions and reality. The discrepancy between the result of the model and the true physical scenario is referred to as predictive uncertainty, and the degree of this uncertainty is often a function of the ability of the model to capture the phenomena in the physical scenario of interest [28]. Therefore, as part of any uncertainty quantification activity it becomes necessary to understand the change in model predictions based on the variations in the user prescribed parameters (e.g., boundary conditions) employed in the set-up of the problem, which is also known as input uncertainty

propagation. In a previous UQ study, the uncertainty issues relating to the hydrodynamics model in a computational fluid dynamics code for gasifiers were addressed [11]. The current study addresses the input parameter uncertainties affecting the chemical reactions taking place during coal conversion by employing non-intrusive input parameter uncertainty propagation techniques. Other sources of uncertainties such as model form uncertainty and numerical approximation uncertainty are disregarded for the scope of the current work.

The uncertainty quantification (UQ) for coal gasification processes can be used to predict the variations in product yields and reaction rates given the uncertainties/variations in operating conditions and fuel properties. The gasification of coal at moderate temperatures goes through 4 stages: (1) primary devolatilization; (2) pyrolysis of secondary volatiles; (3) homogeneous reforming of non-condensables, and (4) char conversion via oxidation and gasification [23]. Among all of the reactions in coal conversion, coal devolatilization can account for up to 70% of the loss in weight of the coal [33]. This process depends on the organic properties of the coal. The quantity of volatiles released during pyrolysis impacts the char's heterogenous and gas phase homogeneous reaction chemistry. Various studies [5,18,21] have reported that operating conditions such as temperature, pressure, heating rate, particle diameter, residence time, and coal rank can affect the coal devolatilization reaction kinetics. Hence, it is crucial to obtain kinetics

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and product yields for devolatilization by considering the effects of these parameters. Kinetic software packages such as PC Coal Lab (PCCL), Chemical Percolation Model for Coal Devolatilization (CPD), Solomon's Functional-Group, Depolymerization, Vaporization, and Cross-linking (FGDVC) predict the effect of operating conditions on coal devolatilization kinetics and product yields, so they have been considered for this UQ study. These kinetic packages are accessed via the recently developed Graphical User Interface (GUI) known as Carbonaceous Chemistry for Computational Modeling (C3M) [47]. This study focuses on predicting the effect of operating conditions on coal devolatilization kinetics and product yields predicted by PCCL. Based on the results of various experiments available in the literature, effects of heating rate, pressure, and temperature on coal devolatilization have been considered in this study.

### 1.1. Effect of heating rate on coal devolatilization

Heating rate has a significant effect on coal pyrolysis such that primary devolatilization reaction rate and yield increase with an increasing heating rate [10,14]. Various experimental and analytical studies have reported that an increase in heating rate during coal devolatilization can lead to a decrease in coal particle swelling ratio, an increase in the amount of tar produced, an increase in total volatile yield released causing a decrease in char yield, and an increase in particle size along with an increase in devolatilization rate [5,7,40,41]. In the literature, different coal types were tested showing the effects of heating rate on coal devolatilization.

Work performed by Gibbins and Kandiyoti [12] on coal samples of Pittsburgh No.8, Illinois No. 6, Wyodak-Anderson, and Pocahontas No.3 used heating rates from 1 to 1000 °C. Experiments were performed by Griffin et al. [13] on samples of Pittsburgh No.8 at heating rates between 10 to 20,000 K/s and data reported by Freihaut and Seery [9] on Ben and Utah bituminous coal samples at heating rates ranging from 1.0 to 10<sup>5</sup> K/s. These studies for coal devolatilization provided the evidence for an increase in the tar and total volatile yield at higher heating rates. Hayashi et al. [15] reported that when brown coal was pyrolyzed at slow and high heating rates, it affected the selectivity to tar, CO, CO<sub>2</sub>, and gaseous hydrocarbons (GHC) on a carbon basis.

Fletcher and Shurtz in their studies [10,34] observed an increase in swelling ratio when Pittsburgh No. 8 and Illinois No.6 coal were pyrolyzed at heating rates between 1 to 10<sup>6</sup> K/s. Findings of studies carried out by Roberts et al. [29] on Australian coal and by Serio et al. [33] on North Dakota (Zap) lignite, Gillette and Montana Rosebud subbituminous coals, and Pittsburgh No. 8, Kentucky No. 9, and Illinois No. 6 bituminous coals, report an increase in devolatilization rate with respect to heating rates. These findings confirm the importance of heating rate as an input parameter in this study.

### 1.2. Effect of temperature on coal devolatilization

Temperature has a similar effect as heating rate on coal devolatilization. Reaction rate of primary pyrolysis/devolatilization along with total volatile yield increases with an increase in temperatures [33,37]. Total tar yield depletes when temperature is increased beyond 650 °C because of the onset of secondary tar cracking reactions [9,24,46]. Ismail [17] reported that the particle swelling ratio increases with temperature during coal devolatilization for plastic coals such as bituminous and sub-bituminous coals but does not change significantly for non-plastic coals such as lignite and anthracite. In a similar way, the study performed by Zhong et al. [46] on bituminous coal showed the effect of changing temperature (700–950 °C) on devolatilization yield and rate along with experiments done by Matsuoka et al. [22] on Taiheiyu coal at temperatures 600–850 °C. The latter reported an increase in H<sub>2</sub>, CH<sub>4</sub>, CO and CO<sub>2</sub> yields, while the yields of H<sub>2</sub>O and tar decreased with respect to increasing temperature. The results of these studies confirm the significant effect that temperature has on volatile

yields and reaction rates for devolatilization and that temperature is a key input parameter for this study.

### 1.3. Effect of pressure on coal devolatilization

The effects of pressure on coal devolatilization have been observed for different coal ranks over a wide range of operating conditions. Multiple studies have reported that the devolatilization rate decreases as pressure increases [20,25,27,39,43]. Increasing pressure inhibits tar release that ultimately reduces the total volatile gas yield and promotes secondary tar reactions [10,20,22]. Serio et al. [33] observed the reduction in tar yield with increase in pressure and the reduction in char reactivity when pyrolysis experiments were carried out on three subbituminous and one lignite coal at pressures between 3 and 13 atm. The reduction in tar and total volatile yields appear to be most significant for bituminous coals and less pronounced for lignite. However, according to Zeng and Fletcher [45], the effect of pressure on the tar and total volatile yields appears to be less pronounced at high pressure.

Sun et al. [36] examined the pyrolysis of two Chinese coals (0.4–4 mm) as a function of pressure (1 to 13 atm), their results showed that the yield of total volatiles decreased with increasing pressure when temperature was above a certain temperature (560 °C for a Chinese bituminous coal and 680 °C for a Chinese anthracite coal). Arendt and van Heek [2], Griffin et al. [13], Anthony and Howard [1], and Bautista et al. [4] confirmed this trend while studying a variety of coals. The Matsuoka et al. [22] study, mentioned earlier, reported increases in yields of CH<sub>4</sub> and CO<sub>2</sub> with increasing pressure, whereas C<sub>2</sub>–C<sub>6</sub> product yields monotonically decreased with increasing pressure. Fletcher and Shurtz in two different studies [10,35] reported a decrease in particle swelling ratio with an increase in pressure. The sensitivity of pressure on coal devolatilization makes it a suitable choice for an input parameter for this study.

## 2. Software packages

### 2.1. Carbonaceous chemistry for computational modeling (C3M)

The Department of Energy's National Energy Technology Laboratory (NETL) has developed a Graphical User Interface (GUI) known as Carbonaceous Chemistry for Computational Modeling (C3M) that creates a seamless connection between the computational fluid dynamic (CFD) software codes such as Multiphase Flow with Interphase Exchanges (MFI) developed at NETL, ANSYS-FLUENT by ANSYS Inc., and BARRACUDA by CPFD and available kinetic packages such as, METC Gasifier Advanced Simulation (MGAS), PC Coal Lab (PCCL), Chemical Percolation Model for Coal Devolatilization (CPD), Solomon's Functional-Group, Depolymerization, Vaporization, Cross-linking (FGDVC). Fig. 1 shows the basic framework of C3M.

C3M is used to access and analyze a variety of kinetic processes and reaction mechanisms typically found in coal/biomass/petcoke gasification, gas clean-up, and carbon capture processes [47]. The GUI provides a platform for the user to conduct virtual kinetic experiments to evaluate kinetic predictions as a function of fuel and sorbent type and/or operating conditions before using it in a CFD code of interest for simulating a process. C3M's unique features provide a way to compare simultaneously the graphical outputs of all kinetic packages (in terms of reaction rate constants and product yields). C3M can export the reaction kinetics of interest in the acceptable input-file format for the chosen CFD code.

Currently, several UQ analysis methods are being implemented within C3M through a direct integration with an open source UQ toolbox as part of the effort to offer basic UQ analyses capability within C3M. Because of the low computational cost of all the kinetic packages, C3M can be utilized for multiple operating conditions and fuel types very cheaply and quickly, which also enables direct Monte Carlo simulation without the need for a surrogate model during UQ analysis.

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