

ASSESSING COAL QUALITY IMPACT ON P.C. COMBUSTION BEHAVIOR

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ABSTRACT

This paper demonstrates a computational approach for assessing coal quality impacts that achieves the accuracy of laboratory testing for a fraction of the expense. It is based on FLASHCHAIN, the world's most extensively evaluated model for the thermal decomposition of coal. Two applications are considered here. First, the model is used to identify the parameter values in the simple devolatilization rate expressions used in coal combustor simulators that mimic the FLASHCHAIN predictions. In the second application, predicted yields for rapid heating conditions and coal-nitrogen release are used as regression variables in engineering correlations to relate coal quality to NO_x emissions and unburned carbon in ash (as LOI) from full-scale furnaces.

INTRODUCTION

With the advent of so-called coal network depolymerization models, it is now possible to predict how the different properties of various coals will affect the initial stages of pulverized coal combustion. Three phenomenological network models are available [1-3]. All represent devolatilization as a depolymerization that disintegrates coal's macromolecular structure into smaller volatiles fragments with subsequent reintegration of larger intermediates into char. Whereas FLASHCHAIN and the CPD model are based on the same concise set of rate mechanisms, the FG-DVC model is all-encompassing. Each can generate predictions for yields, transient evolution rates, and various product characteristics based on coal-specific characterization data.

Although these models' underlying mechanisms share much in common, there are also tangible performance aspects to consider. To date, FLASHCHAIN has been used to predict the devolatilization behavior of more than 400 different coals from every geographical region worldwide. No other model comes close to this level of performance, simply because only FLASHCHAIN simulations can be performed without specialized and expensive laboratory tests. The only sample-specific information needed is the proximate and ultimate analyses of the coal. And full simulations require only a few seconds on modern personal microcomputers.

FLASHCHAIN predicts the yields, release rates, and compositions of all major products of coal devolatilization, including nitrogen species and all major gas species, from any coal at any operating conditions. Some 70 coals have been included in published performance evaluations [1]. Here we focus on applications.

One immediate application of FLASHCHAIN is to use it as a replacement for the rudimentary rate expressions currently used in coal combustor simulators. While conceptually straightforward, this option entails extensive re-coding, and provides more detailed information on product compositions than can be used within current limitations on modeling turbulence-chemistry interactions in large-scale systems. A more expedient strategy delivers the benefits of FLASHCHAIN without the development costs of modifying the large-scale combustor code. Instead of installing FLASHCHAIN as a new submodel, we use it to identify the parameter values that make the simpler rate expressions currently in use mimic the FLASHCHAIN predictions. For example, nominal devolatilization rates can always be defined from any model predictions according to the following rearrangement of a single first-order reaction rate law:

$$\langle k \rangle = (dV/dt)/(V_{\infty} - V(t))$$

where $\langle k \rangle$ is the nominal devolatilization rate constant, $A \exp(-E_a/RT)$, s^{-1} ; $V(t)$ is the instantaneous volatiles yield and V_{∞} is the ultimate weight loss. The volatiles release rate, instantaneous yield and ultimate yield are assigned with the rates and yields for gas and tar release predicted by FLASHCHAIN.

Predicted ultimate weight loss and tar yields are compared to measured values in Fig. 1a. Although all samples in this evaluation are hv bituminous coals and the test conditions were directly comparable, weight loss ranges from 40 to 60 %, and tar yields range from 20 to 40 %. The FLASHCHAIN predictions depict these ranges, and also depict the sample-to-sample variability among individual coals. Yet the predictions are based only on the proximate and ultimate analyses.

In Fig. 1 b, predicted rates during uniform heating at different rates illustrate how the nominal rates change as heating rates are varied. Devolatilization rates increase in direct proportion to increases in heating rate; they increase by a factor of 6 for every order of magnitude increase in heating rate. The apparent activation energies are surprisingly uniform, becoming only slightly larger for faster heating rates

information to assign a particle heating rate, FLASHCHAIN can be used to assign parameters in simple global rate laws for any coal type. Whereas a single first order expression was analyzed here, the same approach can also be applied with competing 2-step or distributed activation energy rate laws. It can also be used to assign rates for the release rates of individual products, including nitrogen species.

Above and beyond applications as a devolatilization submodel in detailed simulations, FLASHCHAIN can also be used as a virtual coal laboratory. In this sense, it provides the same information that would normally be acquired in, for example, drop-tube tests, such as rapid heating volatiles yields, the partitioning between volatile- and char-nitrogen species, soot loadings, and gas compositions and heating values. In turn, these quantities can be used as regression variables in engineering correlations that relate coal properties to macroscopic boiler performance characteristics.

For example, FLASHCHAIN has been incorporated into a PC-Based software package developed by EPRI called the NO_xLOI Predictor that estimates NO_x emissions in the exhausts of full-scale utility boilers. As depicted in Fig. 2a, the structure of the calculation is straightforward. The user provides a few measured values of NO_x emissions and describes the major furnace operating conditions, such as the firing configuration, the type of NO_x control technology, the firing capacity, etc. The user also enters the proximate and ultimate analyses for the coal that was fired while the data was recorded, as well as those for any coals that he or she wants to screen. This computer program then predicts the NO_x emissions for the set of coals being screened when they are burned *under the same firing conditions* as were used when the data was collected.

In this program, FLASHCHAIN is used to predict two critical characteristics that relate coal properties to NO_x emissions: First, it predicts the total amount of volatiles driven off the coal while it is being heated under flame conditions, where heating rates approach 10⁵ K/s and temperatures approach 3000 °F. The weight loss under flame conditions typically exceeds the proximate volatile matter contents by 20 to 100 %, which explains why NO_x emissions do not correlate very well with fuel ratios determined from typical ASTM proximate analyses. The second critical information from FLASHCHAIN is the partitioning of fuel-nitrogen species among gaseous pyrolysis products and char. This partitioning is important because only the chemistry involving gaseous nitrogen compounds can be affected by aerodynamic NO_x abatement strategies that regulate

An evaluation for full-scale coal-fired furnaces appears in Fig. 2b. These predictions are for situations that were not part of the database used to formulate the regressions. The software predict NO_x emissions for coal ranks from subbituminous through lv bituminous within 10 to 15 ppm of observed values. We also expect that the same basic approach would work as well in correlating coal quality impacts on plan area heat release rates, near-burner radiation loads, heat rates, furnace exhaust temperatures, and steam-side temperatures.

REFERENCES

1. Niksa, S., *Combust. Flame* 100:384 (1995).
2. Solomon, P. R., Hamblen, D. G., Serio, M. A., Yu, Z.-Z., and Charpenay, S., *Fuel* 72:469 (1993).
3. Fletcher, T. H., Kerstein, A. R., Pugmire, R. J., Solum, M. S., and Grant, D. M., *Energy Fuels* 6:414 (1992).

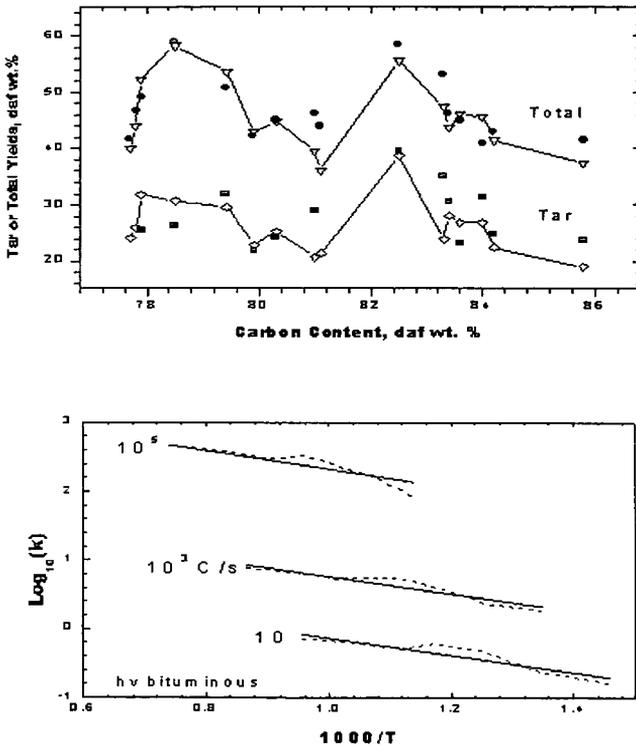


Figure 1. (a, top) Measured weight loss and tar yields from hv bituminous coals compared to FLASHCHAIN predictions (∇). (b, bottom) Nominal devolatilization rates based on the single first-order reaction (solid lines) and FLASHCHAIN (dashed curves) for devolatilization of a high volatile bituminous coal at three heating rates.

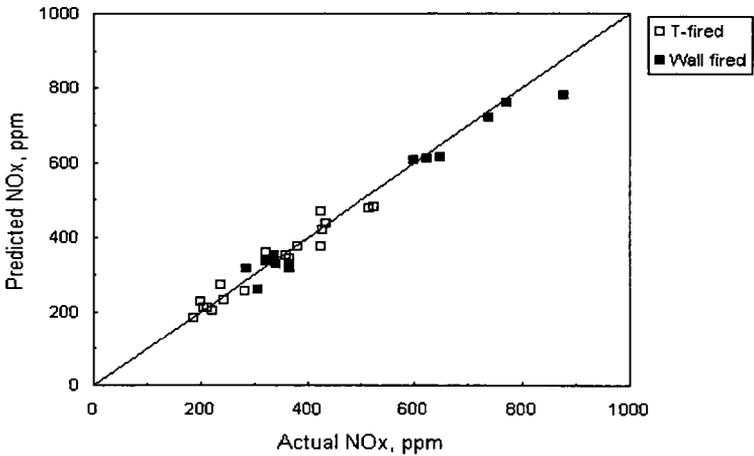
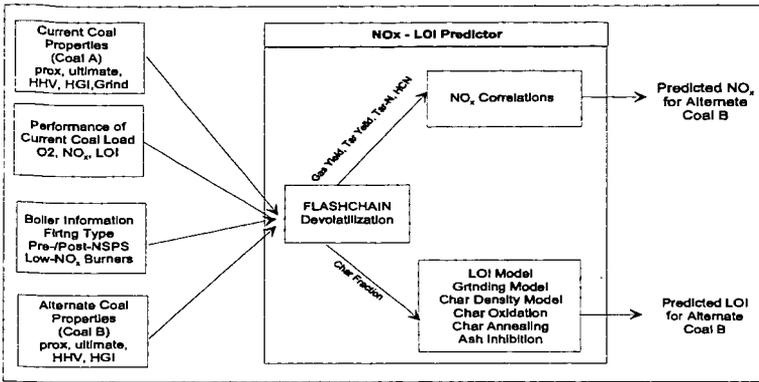


Figure 2. (a, top) Calculation structure for EPRI's NO_x LOI Predictor. (b, bottom) Evaluation of predicted exhaust NO_x levels from full-scale coal-fired utility boilers.