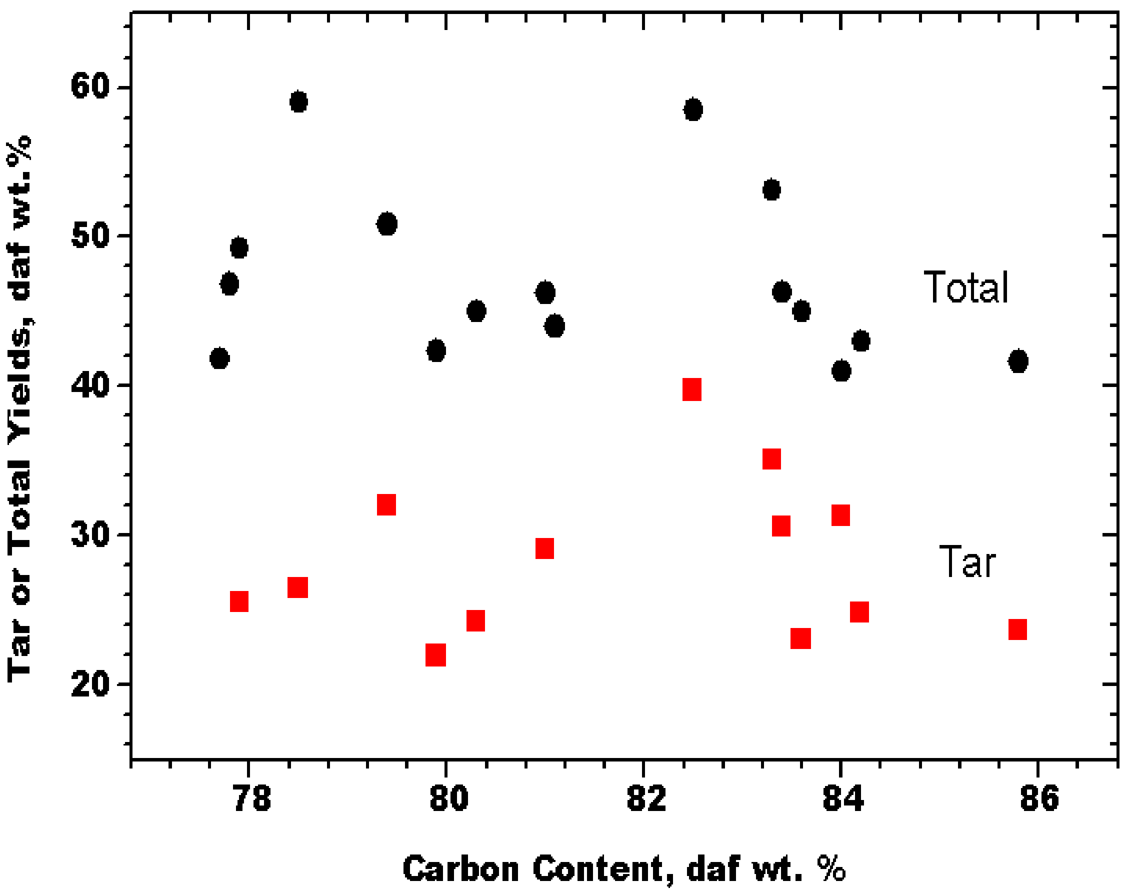
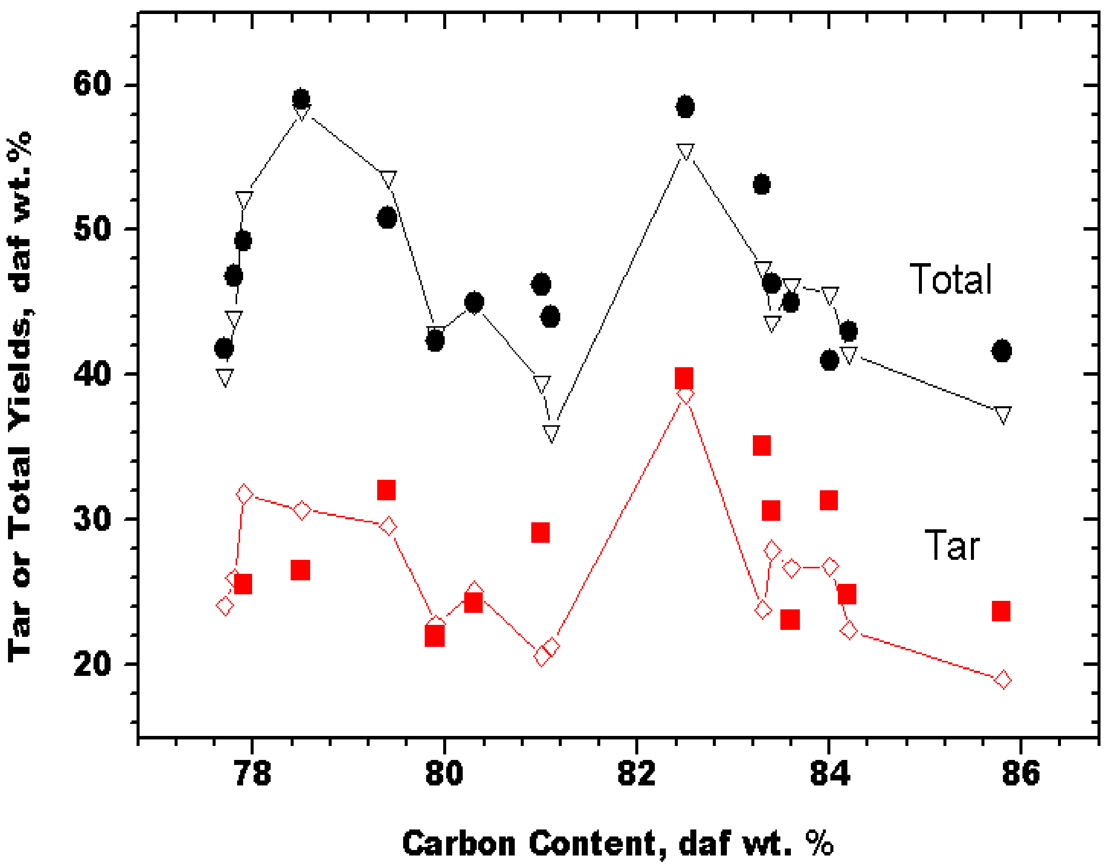
The Imperative For An Accurate Total Volatiles Yield

In any careful review of measured total volatiles yields for devolatilization for coals of even the same rank, the variations are so erratic that it may seem pointless to even try to predict them. The figure below shows the total and tar yields at very similar test conditions – rapid heating rates to high temperatures for long residence times at near-atmospheric pressure – for a collection of very similar high volatile (hv) and medium volatile (mv) bituminous coals from various mines around the world. Note that the carbon content of the samples only varies from 78 to 86 dry-ash-free (daf) wt. %. Yet the total volatiles yields vary by 50 % from 40 to 60 daf wt. %, and the tar yields vary by a factor of two from 20 to 40 wt. %.



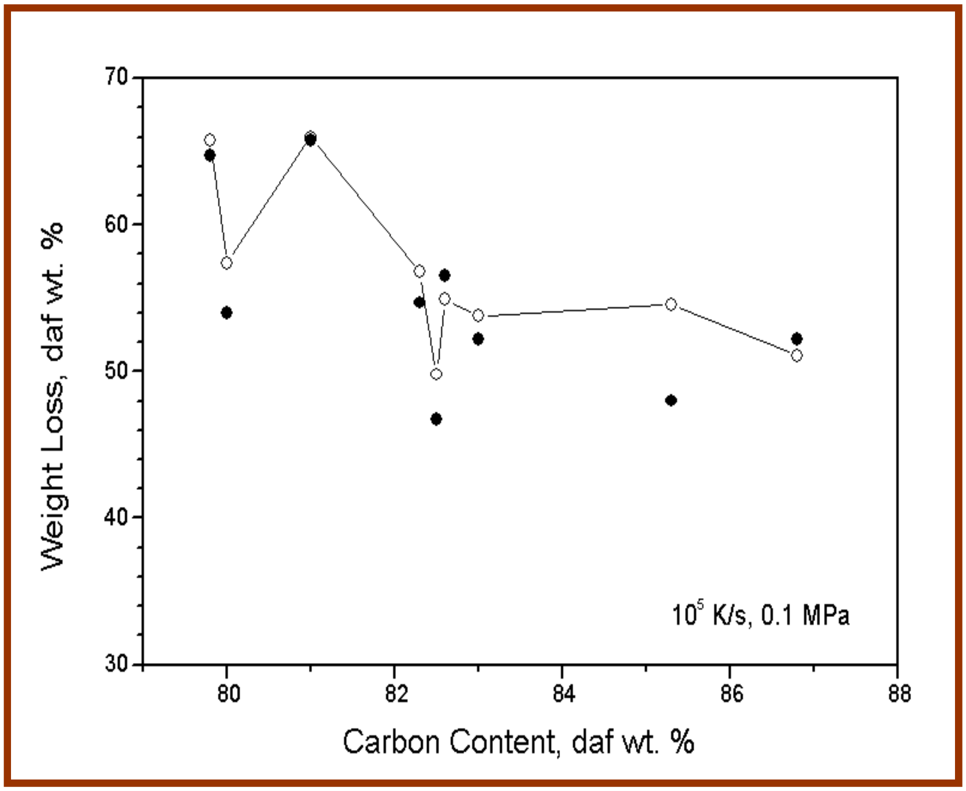
The erratic variations among these data illustrate why prediction schemes based on statistical correlations of the primary coal properties are bound to perform poorly. Indeed, the literature already contains data like these on so many different coals that average yields for different segments of the rank spectrum can simply be evaluated with a calculator. Models that only predict average total yields and omit the sample-to-sample variations are superfluous !

The next figure shows the same data along with the predicted total and tar yields from FLASHCHAIN®. The predictions for each sample are indicated with open symbols; the line segments are included simply to guide the viewing from each sample to the next. The predictions for both total and tar yields accurately show the ranges of the variations in the measured values. Most important, they also depict the sample-to-sample variability with uncanny accuracy. With only a few exceptions, the predictions are within measurement uncertainties, even though the only sample-specific input data in the calculations were the proximate and ultimate analyses of the fuel.



If this performance required monumental laboratory support, then it could be appreciated as a scientific advance. But there would be little practical benefit, because the last task a simulation specialist wants to accept is to run complex fuel analyses every time he or she needs to simulate the behavior of some new solid fuel sample. FLASHCHAIN® delivers the same values with no laboratory support whatsoever, since the proximate and ultimate analyses are the only sample-specific fuel properties in the analysis. Such accuracy is truly unique, and the reason we say, "Simulation specialists who absolutely need an accurate volatiles yield need FLASHCHAIN®.

Of course, one figure cannot possibly convert the many skeptical people who believe that accurate predictions for volatiles yields are a pipedream. So, in 1995, NEA began conducting blind evaluations, in which a testing team provided the test conditions and the proximate and ultimate analyses of the fuel samples to NEA, but not the measured volatiles yields. NEA then prepared FLASHCHAIN® simulations for each individual test in the dataset, and exchanged the results with the testing team. The testing team then disclosed the data to NEA for direct comparison with the model results. Two such evaluations in the figure and table below were performed with similar bituminous coal samples with two different devolatilization reactors.



The data in the figure were obtained with a drop tube furnace and very fine fuel particles, so the estimated heating rates approached 10^5°C/s. The measured total volatiles yields (●) ranged from 46 to 66 daf wt. % for these hv and mv bituminous coals. The predicted yields (O) span a range from 50 to 66 wt. % and, as seen above, depict the sample-to-sample variability with uncanny accuracy. Note particularly the accuracy for the four coals whose carbon contents vary by less than one percent around 83 daf wt. %, and also for the two samples with carbon contents close to 80 % whose yields differ by more than 10 daf wt. %. Considering that almost all the predictions are accurate within the measurement uncertainties, it is hard to attribute the lone discrepancy for the coal with 85 % carbon to the analysis or the testing.

Evaluation of Predicted Ultimate Yields from Bituminous Coals at Two Heating Rates

Sample	Wire Grid		Drop Tube Furnace	
	Predicted	Measured	Predicted	Measured
TyBl	44.7	41.1	57.6	61.6
Atc	40.6	37.4	50.8	51.6
Dryt	46.9	45.8	59.2	62.6
Lcer	45.9	45.8	58.1	62.1
Ashl	45.8	42.6	60.5	68.9
ShCr	35.9	31.6	48.2	48.4
Nriv	47.0	44.7	58.5	64.7

The above table presents blind evaluations for another suite of bituminous coals in another drop tube furnace and in a wire mesh reactor, which imposed a slower heating rate on the order of 10^3°C/s. As expected, the reported volatiles yields from the wire grid are uniformly lower than those from the drop tube due to slower heating. The FLASHCHAIN® predictions depict the yields from the wire grid even more accurately then those from the drop tube with no parameter adjustments whatsoever. Indeed, these predictions are within the measurement uncertainties throughout, except for two of the yields from the drop tube.

Time and time again, in blind evaluations with testing teams from around the world, the FLASHCHAIN® predictions for total volatiles yields are within the measurement uncertainties in 9 of 10 cases, even though they are based on only the proximate and ultimate analyses. Competing approaches may claim the same performance. Just make sure that they actually achieve it by staging your own blind evaluation.