

DISCUSSION

G. F. Moore⁸

The discussor would like to commend Ed Winegartner and B. T. Rhodes for an outstanding paper. The stepwise regression analysis of the effect of the chemical constituents of a coal ash on its ash fusability is a powerful tool. The discussor is impressed by the large number of samples used in the correlation. It would have provided a greater scope, though, if coal from more than two areas had been used—notably Ohio, West Virginia, Pennsylvania, and New Mexico, as well as Illinois and the Fort Union area of the Great Plains states. When using empirical data, the results are valid only when the input is similar to the data used to develop the correlation. Sometimes erroneous and misleading results can be attained when the input is much different than those data. We used a linear regression analysis to correlate the viscosity-temperature relationship of a coal ash with its ash constituents and we tried to calculate the viscosity of a glass furnace slag that contained similar constituents as coal ash but differed in that it contained 10 percent TiO₂. The results we obtained showed the viscosity temperature relationship with a positive slope instead of a negative one which was obviously wrong.

Recently, we have been using a stepwise regression analysis to correlate the viscosity-temperature relationship of a coal ash with its ash constituents which involves the study of the same basic principals described in this paper with very good results.

It is true, as the authors have stated, that if all is needed are

simple fusion temperatures, that it is probably better and just as easy to determine them directly. The real value of this program is that basic studies of the variance of different coal ash constituents can be studied: what effect will blending two coals have on the slugging characteristics? In what proportion should they be blended to give the best slugging potential? What is the effect of changing the concentration of various ash constituents on the slugging characteristics of a coal.

There is one thing the authors have done that the discussor questions. They have used only FeO in their correlation. It is true that the effect of FeO on fusion temperatures is greater than that of Fe₂O₃. There is both FeO and Fe₂O₃ in furnace slag. We have used ferric percent which is the ratio of FeO to Fe₂O₃. We have gotten good correlation when using ferric percent. Ferric percent is determined by the oxidation state of the slag and is controlled by the percent total iron in the slag and by the temperature. This can be very significant for coal ashes containing large amounts of iron oxide.

The spread between reducing and oxidizing fusion temperatures is important because for coals that contain large amounts of iron oxide in its ash the furnace should be designed to minimize areas where reducing conditions could occur. This spread might influence fan size, furnace size, etc. It has been a practice of boiler operators for many years when slugging conditions occurred, due to reducing areas in the boiler, to increase total excess air. Often times, this cannot be tolerated because increasing excess air also increases NO_x. Special consideration should be given to the boiler design because of this.

R. W. Bryers,⁹ B. K. Biswas,⁹ and T. E. Taylor⁹

The discussors have reviewed Messrs. Winegartner's and Rhodes' paper with considerable interest as we have been pursuing a very similar investigation, using a slightly different approach. A correlation relating ash chemistry to a fouling index such as ash fusion temperature, is highly desirable. Hopefully, this work will lead to an empirical relationship which will relate ash chemistry to a degree of fouling or slugging providing a more direct assessment of the risks involved in firing certain coals and a means by which the risks can be reduced through a change in boiler design operation or fuel preparation.

We began our program with the development of a relationship between ash chemistry and the softening temperature using a single variable linear regression analysis. The data used were generated from the various size and gravity fractions of a single coal with a moderately acidic ash. The percent basic constituents were chosen as the independent variable. We realized, from the beginning, the value of a linear expression was limited, and had no physical meaning. This step was taken merely as a means of examining the quality of the data and the mechanics of the computer program in an area where the data were known to have a linear relationship.

Prior literature has indicated that a plot of the basic constituents in the ash against the softening temperature provides a pseudo-phase diagram for the liquidous line of the Al₂O₃SiO₂-Fe₂O₃ system or the Al₃O₃SiO₂-CaO system depending upon whether one is dealing with an Eastern or Western fuel. The curve formed takes on the shape of a parabola as illustrated in Fig. 3 of the paper. Further development of a meaningful relationship with a significant physical interpretation required using a second order

single variable regression analysis. This technique was used first for examining individual coals analyzed by size and gravity fraction and then for large groups of coal by rank and geographic location. Fig. 3 illustrates a typical fit of data taken from a single coal subdivided by size and gravity. As we expected, the accuracy of the fit decreased as the analysis was extended to more than one coal. In executing our study, we did not confine our results to one laboratory.

To improve upon the fit, the program was extended again to include a multiple variable second order regression analysis with the capability of examining one variable at a time in the order of their contribution. Although the fit of the data improved, the expressions developed became too complex to handle. Obviously, the data could not be plotted to illustrate the results, and this approach appeared impractical.

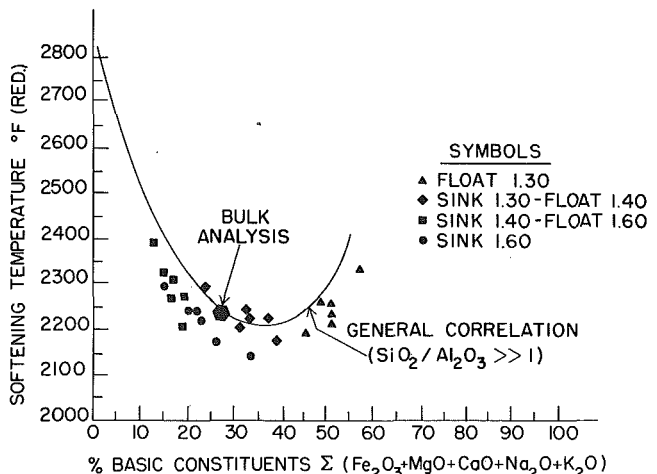


Fig. 3 Change in ash softening temperature with the percent basic constituents in the ash for a Wyoming subbituminous

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REFERENCES

1. Lignites and Wyoming Subbituminous, $SiO_2/Al_2O_3 \gg 1$
2. Wyoming Subbituminous $SiO_2/Al_2O_3 \gg 1$
3. Wyoming Subbituminous $SiO_2/Al_2O_3 \approx 1$
4. Eastern Bituminous

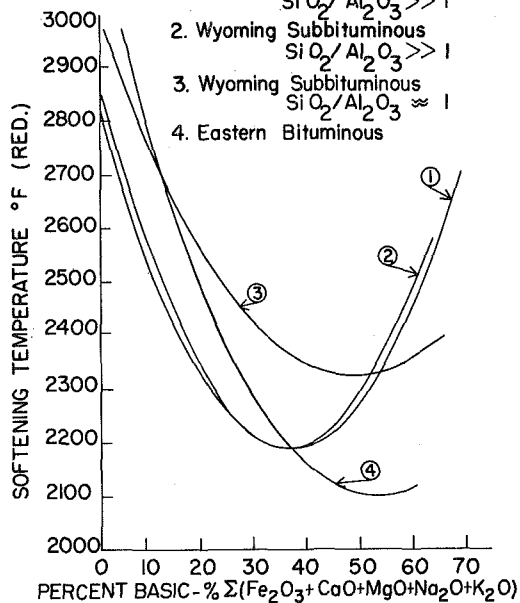


Fig. 4 Influence of percent basic constituents in the ash on ash softening temperatures under reducing conditions for different ranks of coal

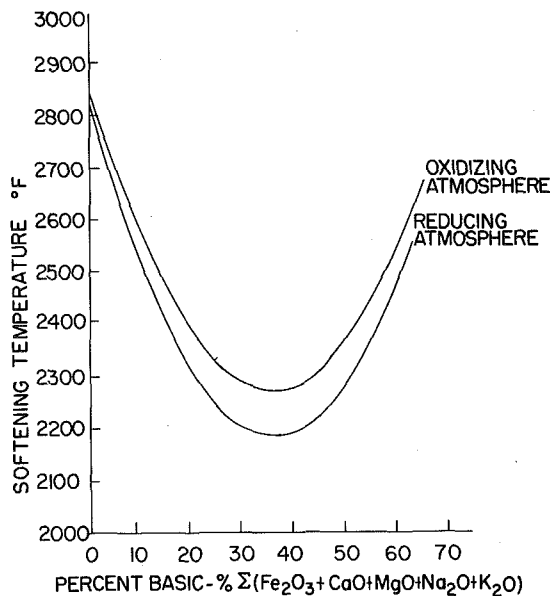


Fig. 5 Comparison of softening temperatures under reducing and oxidizing atmospheres for various percentages of basic constituents in Wyoming subbituminous coal ash

Despite this feeling, it was decided to explore a bit further by increasing the order of the regression analysis. As the order was increased, the fit of the expression to the data became progressively better and the resulting expression progressively more difficult to cope with. No doubt we were converging on the same results obtained by Messrs. Winegartner and Rhodes in going to 51 variables.

Rather than fit the data with a good deal of precision, we decided to sacrifice accuracy and return to a single variable second order regression analysis. The influence of coal rank and mineral content on the resulting expression was examined by careful selection of the data input. The influence of ash chemistry on the fluid tem-

perature and the initial deformation temperature was also examined along with the effect of oxidizing and reducing environment in the ash softening temperature of coal of a given rank.

By using size and gravity analysis of the ash, the analysis becomes a useful tool in predicting the merits of coal preparation as a means of improving on the potential fireside problems of the coal.

Figs. 4 and 5 are typical of the results that have been generated to date. Fig. 4 illustrates the influence of rank, i.e., iron and calcium, and silica to alumina ratios on the ash softening temperature with environment for one specific rank of coal. In our multiple variable second order regression analysis, the computer reported that calcium was the most important single variable for Western fuels and iron for Eastern fuels. Neither was a surprising conclusion. The curves developed provide a quick and simple means for predicting the effect of fuel preparation on a potentially fouling fuel, the main advantage being that a computer does not have to be used once the curve is generated.

It is our feeling that Messrs. Winegartner and Rhodes have done a fine job in breaking ground in the systematic investigation of a correlation for ash chemistry in terms of a fouling problem. We feel, however, that they have over-complicated the analysis by including so many variables. Although the number of analyses used appears to be quite large, the data have apparently been restricted to two coals. This makes the analysis highly customized and quite restrictive, prohibiting extrapolation beyond the limits of the immediate data. This is particularly true if a multiple variable first order regression analysis is used and the variables chosen do not include data taken to the second power. Extrapolation of the data without laboratory confirmation could be extremely dangerous.

Considering the number of variables selected to improve the fit of the data, we feel the differences in fit that result may be so slight as to be explainable only in terms of experimental error. We feel, also, that the number of variables selected is not justified in terms of the limited number of data used, namely, two coals. Finally, we question the merit of extending the 10 original variables to 51, when 41 are combinations of the 10 original.

Although we do not understand how the authors arrived at the justification of reporting the ash composition in mole percent by means of the expression of softening temperature in terms of the base-to-acid ratio, we do agree that this may be the best way to express the ash chemistry as a matter of unifying nomenclature.

We hope the authors will continue their program on a less sophisticated plane and extend their investigation to include other fuels as well as distribution of mineral matter within a given coal.

W. T. Reid¹⁰

For about the last half century, fuels technologists concerned with burning coal have faced up to problems with the fusibility of ash using what can best be described as intelligently guided empirical approaches. The concept of "silica percentage" in the early 1940's was a case in point; a large number of experimental measurements of coal-ash slag viscosity when correlated with chemical composition showed that the dominant parameter was the percentage of silica in the melt. No fundamental prediction based on complex silicate chemistry led to this conclusion. It came as a simple result of relating cause and effect. But although this correlation has been widely useful for predicting the flow characteristics of most coal-ash slags in the Newtonian-flow region, it is almost completely useless in estimating the rate and the extent at which particles of mineral matter in coal interact during combustion

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leading to extensive fouling, massive deposits, and objectionable slagging on heat-receiving surfaces.

It was inevitable that sooner or later someone would apply today's advances in computer technology to extending our abilities to relate ash composition to ash behavior. The authors here have done just that with their calculation of correlation coefficients which lead them to generalized conclusions. Probably the most significant of these is the recognition that mole percentage is preferred to weight percentage when seeking correlations, and that ferrous oxide (FeO) interacting with other ash constituents is much more significant than ferric oxide (Fe₂O₃). The "ferric percentage" concept of 30 years ago recognized the importance of FeO, but the calculations described here are much more convincing.

A disappointing point in this paper is the generally poor correlation between fouling tendency and the amount of sodium in coal ash. It is generally conceded that high-sodium ashes are badly fouling ashes, but nothing found here permits a better way of predicting fouling based on sodium content. Is this a basic problem in this sort of analysis, and must we seek better analytical procedures to determine the true role of sodium in furnace fouling? Is the form in which sodium occurs in coal—as carboxylic salts for example, or as halite, or as feldspars—the most important factor, and should these sodium forms be taken into account in a further search for correlation coefficients? The comments about potassium are interesting but sketchy.

The authors have made one important point here that may be overlooked by a casual reader—that correlations should be based on SO₃-free ash analyses. Sulfur is *not* retained in coal-ash slags, and its presence in deposits is a function of the maximum temperature at which the deposit is held. Because the ASTM ashing temperature is below the dissociation temperature of the sulfates, CaSO₄ for example, the amount of SO₃ reported in an analysis of ASTM ash is not representative of slag or of sintered forms of that ash at furnace temperatures. Many investigations ignore this point.

Finally, these correlations are bound to be useful in the years ahead, if not so much for the results they report as for a description of a powerful tool for assessing coal-ash characteristics. The next step, of course, will be in extending these same techniques to the relationship between the forms of mineral matter in coal and the behavior of those minerals when the coal is burned. Considerable efforts along these lines are being planned presently.

Author's Closure

The authors wish to thank all of the discussers for their many helpful comments. We realized at the time the paper was written that others were attempting similar computer correlations of ash properties. All of us have similar problems trying to decide which and how many variables to use and what interactions to consider. It is hoped that publication of our results will encourage others to present their data so that eventually we may develop the simple correlations which we all seek. We are especially anxious to see the correlations with the viscosity-temperature relationships referred to by Fred Moore since these parameters should be more accurate than the cone fusion tests used in our work.

It appears to us that Bill Reid got to the heart of the paper when he pointed out that the most significant point was the recognition that mole percentage on an SO₃ free basis should be used rather than weight percentage on a whole ash basis. We strongly suspect that if Dick Bryers would replot Fig. 2 from his discussion on this basis, all of the minimum points on his "U" shaped curves would fall at 50 mole percent base.

Fred Moore and Bill Reid both mention the fact that we calculate all of the iron as FeO rather than Fe₂O₃ whereas in fact Bill Reid introduced the concept of "ferric percentage" thirty years ago. We consider ferric percentage to be a furnace parameter rather than an ash parameter. With knowledge only of the coal and ash analysis one cannot say what the ferric percentage will be. One way this might be handled would be to assign a nominal percentage, i.e., 20 percent, as the portion of the iron present as Fe₂O₃ and the balance FeO. Since our work was based on laboratory ash fusion cones it would be interesting to determine the ferric percentage in these cones at the time that the readings are made. As mentioned in our paper, however, our correlation of B/A with ash fusion temperatures did suggest very strongly the use of FeO rather than Fe₂O₃.

Sodium in coal ash did not correlate well with fouling tendency because we had no measure of fouling tendency to correlate it with. We measured only cone fusion temperatures which may correlate with slagging tendency in the furnace. A low ash fusion temperature would only cause superheater deposits if the furnace slagged up so badly that the exit gas temperature increased to greater than the ash fusion temperature so that molten particles carry over into the convection passes. Alkali bonded deposits in the superheater are probably totally unrelated to ash fusion temperatures.

We regret that the mass of the data available for this study was primarily from only two coal provinces. We would point out, however, that several seams were included from each province and that the range of analyses was fairly broad. The last two columns of the tables in Appendix B give the mean values for each of the parameters and the standard deviations. We have had good success in using the formulas presented in the paper so long as the values of the parameters are within plus or minus one standard deviation of the mean. If the values are outside of two standard deviations the results are generally meaningless. Between one and two standard deviations proceed with caution.

We would like to point out that stepwise regression is a procedure to select a "small" number of variables from a "large" set. We used 50–60 variables in the large set but the final equations never contained more than 15 variables. In all cases there was statistical evidence that these parameters were significant and not due to experimental error. The intermediate equations obtained in stepwise regression (Appendix C available from the authors) can be used if equations with only a few terms are desired.

The computer program we used permitted us to include any variables which were functions of the ten elemental variables which are not intrinsically non-linear. Thus, we did include the entire "multiple variable, second order equations" with all terms to the second power including cross products. What proved more important was the terms like the (B/A-1)² on mole basis. This type of study appears "over-complicated" at first, but this is relative to our experience. Actually it is much simpler than trying to build equations for the GNP or other problems which can now be attacked with the tools and the data which are available.