DEVELOPMENT OF A COMPUTER PROGRAM FOR PREDICTING THE PROPERTIES OF COAL

Ву

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DEVELOPMENT OF A COMPUTER PROGRAM FOR PREDICTING THE PROPERTIES OF COAL

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PREFACE

The purpose of this research was to construct a computer program capable of calculating slagging and fouling behavior and viscosity of coals at various temperatures. The calculations in the program were based on ash composition and existing models.

I would like to express my sincere gratitude to all the people who assisted me in my studies. I wish to express my deepest gratitude to my major advisor, Dr. Arland H. Johannes, for his expertise and valuable assistance. I am also thankful to my other committee members, Dr. R. C. Erbar and Dr. K. A. Gasem for their advice and cooperation.

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CHAPTER I

INTRODUCTION

The proven reserves of coal in the world are more than those of any other fossil fuel. Coal is not only important as a fuel but also as a precursor for producing metallurgical coke. But coal utilization for power generation requires huge storage areas for coal and for temporarily storing the ash. It also needs additional auxiliary equipment like conveyers, unique burners, fuel supply systems, accessory support equipment such as soot blowers, ash disposal units, F.D/I.D fans and control systems. In addition to this problem, most coals are not of good quality in that their combustion results in emission of large amounts of sulfur dioxide gas, slagging in the radiant section and fouling in the convective section of a furnace. The outcome of slagging and fouling in boilers can be disastrous in many ways such as reduction of heat transfer and impedance of the gas flow as well as corrosion, erosion and physical damage to boiler tubes.

A possible solution to the problems associated with the use of coal is the blending of coals of good and adverse

qualities and then using them for producing energy. By doing this the operating capital costs can be reduced and the resulting coal of constant heating value can minimize the fluctuations in the operation of the furnace. This is also necessitated by the limits imposed by the Environmental Protection Agency (EPA) for sulfur dioxide emissions for new facilities (1.2 pounds SO₂ per million Btu fired). Another restriction is imposed by the state of Oklahoma. This regulation requires that power plants in the state of Oklahoma use at least 10% Oklahoma coal. Power companies are motivated to use blended coal due to the fact that the purchase of additional coal on the spot market is usually advantageous to them.

Coal blending also has some disadvantages. For example, serious slagging and fouling can result as compared with that resulting from combustion of pure coals. Another problem is the lack of ability to predict operational properties such as slagging and fouling potential. The possibility of coal blending depends on whether the two (or more) coals are compatible or not. Properties of both the coals and their ashes must be determined carefully in order to examine this possibility.

The properties of coals which must be considered before blending are coal rank, moisture levels, heating values, pulverizing properties, composition of ashes produced, their slagging and fouling properties and fusibility temperatures. Many models have been developed to predict the slagging and

fouling potentials of coals but all of them apply to specific cases only. None of them can be generalized for all types of coal. The confidence level of these predictive models for the behavior of mineral matter during coal combustion is very low even for individual coals. This necessitates the future development of models for predicting the behavior of ash at high temperatures which are flexible for various fuels having different mineral matter contents. By doing this the time and cost involved in acquiring experimental information for each individual fuel can be avoided. The purpose of this research is to construct a computer program capable of calculating slagging and fouling behavior of coals based on ash composition and existing models.

CHAPTER II

LITERATURE REVIEW

Composition Effects on Properties of Coal and Ash

The difficulty or ease of boiler operation can be related to specific mineral species in coal. The design of a coal combustion plant must be consistent with the type of coal it handles. For example, high-sulfur coals with ironrich ash are likely to cause severe boiler slagging in pulverized-coal-fired boilers. In cyclone-fired boilers iron-rich ash does not require an excessively high temperature for a satisfactory slag flow (Raask).

The principal elemental composition of ash consists of sodium, calcium, magnesium, potassium, aluminium, silicon, iron, sulfur, titanium and phosphorous (which generally occurs in minor amounts in most coals). Ash analysis results are generally reported as oxides; for example, sodium is reported as the percent of sodium oxide, and iron is reported as the percent of ferric oxide. This convention is followed although virtually none of the elements are present in the ash as their respective oxides. This is

because several empirical equations have sometimes successfully predicted ash behavior from ash composition in this form. The lower melting components are the ones that can separate and cause problems.

The elements which are considered as most influential in the fireside deposition process are sodium and iron. If sodium is present in amounts exceeding 4 percent, fusibility temperatures will be lowered (Bogot and Heusel, 1978). As the sodium content increases, both the rate and density of the buildup increases, and at sodium levels above 4 percent, the deposit becomes dense, more tightly bonded and difficult to remove. However, Honea, et al. (1981) suggests that the upper limit for sodium percent to cause fouling should be related to the percent of ash in the coal and with few exceptions, a sodium level below 1% and a high ash indicates a low fouling potential. For ash levels above 8%, coals are likely to have low fouling potentials for sodium levels below 1%, medium fouling potentials at 1 to 5% and high fouling above 5%. For a low-ash coal with about 4% ash, the fouling potential may be low to medium at sodium levels above 5%.

Iron has frequently been known to separate from the bulk ash and create slagging problems. Iron is mostly present in the form of pyrites (FeS₂), which on combustion, reduce to FeS or lower oxides, Fe_3O_4 , Fe_2O_3 , FeO or even metallic iron, Fe. These lower substances have very low melting temperatures and hence they increase the slagging and

fouling propensity. Iron is usually considered in the form of its ratio with calcium, i.e, Fe_2O_3/CaO . The interrelationship between the two may produce a eutectic with a lower melting temperature than that produced by either acting alone. Extreme effects of lowered fusibility temperatures are evident between ratios of 0.3 and 3.

For slagging and fouling it is not just the overall ash composition that is important, but also the distribution of the elements within the mineral matter associated with the coal. One element that has a strong influence on both the slagging and fouling propensity of a coal is calcium. Lignitic coals generally contain more calcium than bituminous coals. Calcium combines with sulfur compounds to form calcium sulfate. It also acts as a "flux" to promote melting of other ash components. The combination of alumina (Al_2O_3) and lime (CaO) is reported to form a eutectic mixture having a melting point of 1600 ^OC which is much lower than the melting temperature of the two individual oxides (Macdonald, 1984). Gibb (1986) states that the viscosity/temperature curves are increasingly steep for coals of increasing calcium content. Analysis of superheater deposits from the boilers shows that the inner layer adjacent to the tubes is always rich in anhydrite, $CaSO_4$, indicating that formation is probably initiated by deposition of fine particles of CaO which then react in situ with SO_2 and O_2 from the flue gas to form $CaSO_4$. A dual role of calcium in fouling was observed by Gibb (1986). He

argues that on the one hand increasing calcium may exacerbate the initiation process of CaSO₄ buildup owing to CaO deposition, while on the other hand, calcium tends to inhibit the development of sintered strength in the bulk deposit by forming a solid solution called plagioclase.

The oxides, SiO_2 , Al_2O_3 , TiO_2 , are the acidic oxides in the ash while Fe₂O₃, CaO, MgO, Na₂O and K₂O are the basic oxides. As a rule, ash high in silica, alumina or TiO_2 has a high softening temperature, and this temperature is not greatly affected by a reducing atmosphere. The alkali metal compounds Na₂O and K₂O, as well as the alkaline earth, MgO, tend to lower the softening temperature of the ash. The tendency of the other basic compounds, Fe₂O₃ and CaO, is also to lower the softening temperature. The sum of the acidic components can range from 20 to 90 percent of the Generally, highly acidic ashes have high slag ash. viscosities. On the other hand, basic components can be 5 to 80 percent of the ash. Either high or low basic values can result in high fusion temperatures (Singer, 1981). About 30 to 40 percent basic components result in minimum fusion temperatures.

Prediction of Ash properties

A knowledge of the properties of coal is useful in the design of furnaces and ash-handling systems. The behavior of the ash, as it influences the fouling of the convection-

type surfaces, affects the amount of such surfaces, their spacing, and the quantity of sootblowers required to clean these heat transfer surfaces. Similarly, ash behavior in the radiant section of the furnace influences the slagging reactions during the combustion process and, so, is a significant factor in furnace sizing in terms of volume, plan area, and fuel burning zone. Ash in the form of tenacious deposits on waterwall surfaces insulates the heattransfer portions of the furnace, thus affecting the cleaning requirements of both radiant and convective heating surfaces. Further, the rate of wear of pulverizer parts and the mechanism and rate of fire-side metal loss by corrosion or erosion or both is influenced by the properties of coal ash.

In order to assess the fouling and slagging propensity, coal ash samples are prepared in the laboratory for analysis. Ash preparation in the laboratory can take one of the two forms: Low temperature ash (LTA) or High temperature ash (HTA). Low temperature ash is prepared in a low pressure, low temperature, oxygen plasma reactor and gives a better representation of the constituents of mineral matter in the coal prior to combustion. High temperature ash is prepared according to existing standards such as ASTM (1968) or the British standard (1970). Laboratory prepared ash samples are analyzed for the most abundant constituent elements and expressed in terms of the weight percents of the corresponding oxides: SiO₂, Al₂O₃, Fe₂O₃, CaO, MgO, K₂O,

 Na_2O and TiO_2 . Amounts of sulfur and ash in the coal are also reported and sometimes water soluble Na_2O is also determined. Once the ash samples are analyzed, evaluation of slagging and fouling indices can be conducted.

A number of empirical correlations have been developed by researchers for predicting the slagging and fouling behavior of coal ashes. One of the earliest calculation of slagging and fouling potential has been done by Sedor et. al. (1960) and Griffin and Profitta (1965). Their index is based on the calculation of Na₂O-equivalent in the ash according to the relation:

$$Na_2O_{eq} = (Na_2O + 0.659 * K_2O) * Ash/100$$
 (2.1)

where Na_2O and K_2O are the percentages by weight of sodium oxide and potassium oxide in the ash. The quantity of ash is expressed as weight percent in the coal. The relationship of this index with the amount of slagging is presented in table 2.1.

A major index having some theoretical background is the base to acid ratio (Rba). This involves the eight most common metallic constituents of coal ash broken down into two distinct categories: acidic oxides (SiO_2 , Al_2O_3 , TiO_2), and basic oxides (Fe_2O_3 , MgO, CaO, Na_2O, and K_2O). The index is defined as:

$$Rba = (Na_{2}O+K_{2}O+MgO+CaO+Fe_{2}O_{3})/(SiO_{2}+TiO_{2}+Al_{2}O_{3})$$
 (2.2)

whereas each oxide in equation 2.2 is expressed as
percentage by weight in the ash. Singer (1981) suggests
that for most of the coal ashes, an Rba in the range of 0.4
- 0.7 manifests low ash-fusibility temperatures and a high
slagging potential.

Attig and Duzy (1969) modified the base to acid ratio index in the following manner:

$$Fy = Rba * Na_2O \tag{2.3}$$

The range of slagging potential values for this index is presented in table 2.2. The above index is exclusively for bituminous coals and it emphasizes the effects of Na₂O in the ash.

Attig and Duzy (1969) also developed an index based on the weight percent of sulfur in the dry coal. This index is defined as:

$$Fs = Rba * S \tag{2.4}$$

whereas S represents the weight percent of sulfur in the coal. The relationship between the values of Fs and the amount of slagging is presented in table 2.3.

Winegartner (1974) performed experiments on lignitic type ashes and suggested the following modifications in the Attig and Duzy equation:

TABLE 2.1

SLAGGING PROPENSITY OF COAL BASED ON EQUIVALENT SODIUM IN THE ASH (SEDOR ET. AL., 1960, GRIFFIN & PROFITTA, 1965)

Slagging index	Boiler slagging
< 0.3	Low
0.3 - 0.45	Medium
0.45 - 0.6	High
> 0.6	Severe

TABLE 2.2

FOULING PROPENSITY OF COAL BASED ON SODIUM CONTENT AND BASE-TO-ACID RATIO (ATTIG & DUZY, 1969)

Fouling index Boiler foul	
< 0.2	Low
0.2 - 0.5	Medium
0.5 - 1.0	High
> 1.0	Severe

$$Fy' = Rba * Na_2O_{WS}$$
(2.5)

where Na_2O_{WS} is the water soluble fraction of Na_2O in the ash. This index is exclusively for lignitic type ash and the relation between slagging propensities and the values of Fy' is presented in table 2.4.

The criteria for determination of whether an ash is lignitic or bituminous is also defined by Winegartner as:

Bituminous ash: $SiO_2 > (Na_2O + Fe_2O_3 + CaO)$ (2.6) Lignitic ash: $SiO_2 < (Na_2O + Fe_2O_3 + CaO)$ (2.7)

An index depending on the initial deformation temperature and the hemispherical temperature of the ash has been developed by Gray and Moore (1974). The experimental values of these temperatures for a pyramidal shape ash sample are determined in a reducing atmosphere, which frequently exists in boilers. Also, it has been pointed out by Raask (1985) that temperatures determined in a reducing atmosphere can be up to 200 ^OK less than those in an oxidizing atmosphere. The equation for the slagging index, Fs, is:

$$Fs = (4 * IT + HT) / 5$$
 (2.8)

where IT is the initial deformation temperature at which the

TABLE 2.3

SLAGGING PROPENSITY OF COAL BASED ON SULFUR IN THE ASH (ATTIG & DUZY, 1969)

Slagging index	Boiler slagging
< 0.6	Low
0.6 - 2.0	Medium
2.0 - 2.6	High
> 2.6	Severe

TABLE 2.4

SLAGGING PROPENSITY OF COAL BASED ON WATER SOLUBLE SODIUM CONTENT AND BASE-TO-ACID RATIO (WINEGARTNER, 1974)

Slagging index	Boiler slagging
< 0.1	Low
0.1 - 0.25	Medium
0.25 - 0.7	High
> 0.7	Severe

top of the sample shows evidence of deformation and HT is the hemispherical temperature at which the sample assumes a hemispherical shape and its height equals one half of its width. The relation between the amount of slagging and the values of Fs is presented in table 2.5. Since this index relies heavily on physical observations, the results are often unrealistic.

Studies on low-rank Western coals by Soundreal, et. al. (1978) resulted in the development of a slagging index which takes into account the fact that additional silica enhances deposition in coals with high CaO content. This index, Fx, is given by:

 $Fx = 0.38 Na_20+0.006 SiO_2-0.008 CaO+0.062 ash+0.0037$ (2.9)

Raask (1985) developed an index based on the silica ratio of the ash, which is defined as:

 $Fsilica = SiO_2 / (MgO+CaO+Fe_2O_3+SiO_2) * 100$ (2.10)

whereas the slagging propensities are related to Fsilica according to table 2.6. This index considers the effects of silica, iron oxide, calcium oxide and magnesium oxide content of ash but ignores the effect of sodium oxide.

In addition to the above index, Raask (1985) developed two more indexes for predicting the slagging propensities of ashes. One index is based solely on the sodium oxide

TABLE 2.5

SLAGGING PROPENSITY OF COAL BASED ON PHYSICAL OBSERVATION IN AN ASH SAMPLE (GRAY & MOORE, 1974)

Slagging index	Boiler slagging
1505 - 1615	Low or Medium
1325 - 1505	High
< 1325	Severe

TABLE 2.6

SLAGGING PROPENSITY OF COAL BASED ON SILICA RATIO (FSILICA) (RAASK, 1985)

Slagging index	Boiler slagging	
72 - 80	Low	
65 - 72	Medium	
50 - 65	High or Severe	

content and another on iron oxide content. The index based on Fe_2O_3 content is related to the amount of slagging according to table 2.7. The index based on sodium oxide content have different prediction criteria for bituminous and lignitic coals. This criteria is listed in table 2.8.

TABLE 2.7

SLAGGING PROPENSITY OF COAL BASED ON IRON OXIDE IN THE ASH (RAASK, 1985)

Slagging index	Boiler slagging	
< 9.0	Low	
< 16.0	Medium	
> 16.0	High or Severe	

TABLE 2.8

SLAGGING PROPENSITY OF COAL BASED ON SODIUM OXIDE IN THE ASH (RAASK, 1985)

Slagging index		Boiler slagging	
Bituminous	ash L	ignitic ash	
< 0.5		< 2	Low
0.5 - 1.1		2 - 7	Medium
1.1 - 2.6		7 - 9	High
> 2.6		> 9	Severe

CHAPTER III

MODEL DESCRIPTION

The program developed in this study is capable of calculating the various fouling and slagging indexes of a coal based on its composition, physical properties and operating temperature. It is also capable of estimating the temperature of critical viscosity, viscosities at various temperatures and the percentage of mineral matter in the original coal prior to the combustion process.

The input data to this program includes the percentages of the eight most common oxide constituents of the coal ash which are silica, alumina, iron oxide, lime, magnesia, sodium oxide, potassium oxide and titanium dioxide. The percentage of the water soluble portion of sodium oxide is also provided. Other input parameters include the percentages of sulfur and ash in the coal; physical properties like calorific value of the coal, initial deformation and hemispherical temperatures of the ash sample; and an appropriate value of temperature for the calculation of ash viscosity. Each input parameter is taken on a screen developed for that parameter which also shows

the range in which the parameter usually occurs. For example, the percentage of any of the oxide constituents of ash cannot be below zero or above hundred, so the screen does not vanish if a negative number or a number above hundred is punched. After taking the input data, the program corrects the values if some of them are out of the normal range. This correlation is made by subtracting from hundred the sum of the oxides other than that for which the correction is made. In this way, the program is able to correct the value of only one oxide. However, there is no limitation on the correction of other parameters.

The usual range for the oxides is given in table 3.1. In addition to this, the program warns the user if the sum of the percentages of the eight oxide constituents of ash is far from hundred. Before any actual calculation begins, the program presents the input data on screen for perusal by the user and then starts the calculations if it is found okay. However, the user can re-enter the input data if he thinks that some of it has been entered incorrectly.

The program uses Winegartner's criteria for determining whether the ash is lignitic or bituminous. This criteria is as follows:

Bituminous ash: $SiO_2 > (Na_2O + Fe_2O_3 + CaO)$ (3.1)

Lignitic ash: $SiO_2 < (Na_2O + Fe_2O_3 + CaO)$ (3.2)

The program starts the calculations with the estimation

Tab	le	з.	1

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COAL-ASH CHEMICAL COMPOSITION RANGES

of the fouling index by the method of Attig and Duzy (1969). In this method the eight most common metallic constituents of coal ash are broken down into two distinct categories: ACID representing the acidic oxides (SiO_2 , Al_2O_3 , TiO_2), and BASE representing the basic oxides (Fe_2O_3 , MgO, CaO, Na_2O , K_2O). The index is then calculated as:

$$Fy = Rba * Na_2O \tag{3.3}$$

The program also writes the qualitative meaning of the above index according to table 2.2.

The calculations continues for the slagging index by Attig and Duzy (1969) which is given by the equation:

$$Fs = Rba * S \tag{3.4}$$

where S represents the percentage of sulfur in the coal. The relation between the values of Fs and the amount of slagging is presented in table 2.3.

Gray and Moore's index depending on the initial deformation temperature (IT) and the hemispherical temperature (HT) of the ash is calculated by the equation:

$$Fs = (4 * IT + HT) / 5$$
 (3.5)

The qualitative result is presented in table 2.5. As was mentioned in the last chapter this index relies heavily on physical observations, so the results are often unrealistic.

Raask's index is presented which is a direct measure of the sodium oxide content in the ash. For bituminous coals , it suggests low slagging at relatively lower sodium oxide contents than what it suggests for lignitic coals. The criteria for deciding the amount of slagging is presented in table 2.8.

A slagging index exclusively developed for bituminous coals by Sedor et. al. (1960), Griffin and Profitta (1965) is calculated by the equation:

$$Na_2O_{eq} = (Na_2O+0.659*K_2O) * Ash/100$$
 (3.6)

If the input data is for a lignitic coal, the program comments that this index is not valid. The relation of the above index with the amount of slagging in furnace is presented in table 2.1.

Another index by Raask (1985) is presented which is a direct measure of the percentage of iron oxide in the ash. The relation between the values of this index and the amount of slagging is presented in table 2.7.

Raask developed a third index also which is based on the percentage of silica in the ash. This index is calculated by the equation:

$$Fsilica = SiO_{2} / (MgO+CaO+Fe_{2}O_{3}+SiO_{2})*100$$
 (3.7)

whereas the slagging propensities are defined according to table 2.6.

Next calculation is for the slagging index by Soundreal, et. al. (1978) which takes into account the fact that additional silica enhances deposition in coals with high CaO content. This index, Fx, is calculated by:

$$Fx = 0.38*Na_2O + 0.006*SiO_2 - 0.008*CaO + 0.062*Ash + 0.0037$$
(3.8)

The calculations of slagging indices ends with the slagging index by Winegartner which is developed exclusively for lignitic ashes. This index is actually a modification of the index by Attig and Duzy and considers only the water-soluble fraction of the sodium oxide content (Na_2O_{WS}) . The index is calculated according to the equation:

$$Fy' = Rba * Na_2O_{WS}$$
(3.9)

The relation between Fy' and the slagging propensities is presented in table 2.4.

The next calculation is for the temperature of critical viscosity by the method of Hoy et. al. (1965). The temperature of critical viscosity is defined as that temperature at which the viscosity properties of molten slag change, on cooling, from those of a Newtonian fluid to those of a Bingham plastic. Once it is calculated, it becomes possible to predict the temperature at which molten slag will run freely from the furnace wall tubes. The maximum viscosity at which molten slag can readily be trapped from a boiler is 250 poise. The first step in the calculation of the temperature of critical viscosity is to normalize the sum of SiO_2 , Al_2O_3 , Fe_2O_3 , CaO and MgO to 100, which means ignoring the other oxides in the ash. Each of five oxides is normalized by dividing its actual percentage in the ash by the sum of the percentages of the five oxides and then multiplying the ratio by hundred. Temperature of critical viscosity is then calculated by the relation:

$$Tcv = 2990 - 1470 * SiO_2n/Al_2O_3n + 360 * (SiO_2n/Al_2O_3n)^2$$

-14.7*(Fe₂O₃n+CaOn+MgOn)
+ 0.15*(Fe₂O₃+CaOn+MgOn)² (3.10)

whereas the symbol `n' at the end of each oxide indicates its normalized value.

Viscosity is calculated by the method of Reid and Cohen (1944) and reported at forty different temperatures. The first temperature selected is 200 degree celcius below the temperature provided by the user. The second temperature is 10 degree above the first one and the same increment in temperature continues each time for viscosity calculations until the final calculation at 200 degrees above the temperature provided. The model used for viscosity

$$Eata = 10^{A}$$
(3.11)

$$A = 4.468 * (Fsilica/100)^{2} + 1.265 * (10^{4}/Tk) - 7.44$$
(3.12)

whereas Fsilica is the silica ratio calculated by Raask's method, Tk is the temperature in degree kelvin and Eata is the viscosity in poise.

Viscosity is also calculated by the method of Watt and Faraday (1969). This method is based on SiO_2 , Al_2O_3 , Fe_2O_3 , CaO and MgO normalized to 100%. The model for viscosity calculations is:

$$Eata = 10^{A}$$
(3.13)

 $A = 10^7 * Am/(T-150)^2 + C$ (3.14)

 $Am = 0.00835 * SiO_2n + 0.00601 * Al_2O_3n - 0.109$ (3.15)

```
C = 0.0415 * SiO_2n + 0.0192 * Al_2O_3n + 0.0276 * Fe_2O_3n + 0.016 * CaOn - 3.92 (3.16)
```

whereas trailing `n' indicates the normalized values of the oxides, T is the temperature in degree celcius and Eata is the viscosity in poise. Again, the viscosities are reported at forty different temperatures starting from 200 degree below, and ending at 200 degrees above the temperature provided. However, certain parameters are checked before any actual calculations begin. If these parameters are not within the range of accurate prediction by this method, the user is warned of this fact. These ranges are presented in table 3.2.

Mineral matter is estimated by Parr's method (1928) according to the equation:

Mineral Matter =
$$1.08 * Ash + 0.55 * S$$
 (3.17)

The last of all the calculations is mineral matter by Thiessen's model (1919):

Mineral Matter =
$$1.08 * Ash + K * S$$
 (3.18)
 $K = 0.55 - 5000/CV$ (3.19)

whereas CV is the calorific value of coal on a dry, mineralmatter-free basis and S and Ash are the respective percentages of sulfur and ash in the coal.

After completing the predictions for one ash composition the user has the option to continue with another composition or to stop.

TABLE 3.2

RANGE OF PARAMETERS FOR VISCOSITY CALCULATION BY WATT AND FARADAY'S METHOD

Parameter	Range (%)
Fsilica (silica ratio)	40 - 80
sio ₂ /Al ₂ o ₃	1.4 - 2.4
Fe ₂ 0 ₃	3 - 30
CaO	2 - 30
МдО	1 - 10

CHAPTER IV

RESULTS AND DISCUSSIONS

High temperature ash analyses of the two Wyoming coals, Jacobs Ranch and Clovis Point, were used as input to the program developed in this study. Zecchini (1986) lists the composition of Jacob Ranch and Clovis Point coal ashes along with the composition of their various blends. Before using these compositions as input to the program, they are normalized on the basis of the sum of the eight most common oxides, SiO₂, Al₂O₃, Fe₂O₃, CaO, MgO, Na₂O, K₂O and TiO₂ equalling hundred. The input data is summarized in table The program was also run with different blends of 4.1. these two coals in order to assess the ability of these correlations to predict slagging due to blending. The blends selected were 75% JR -25% CP, 50% JR -50% CP and 25% JR -75% CP whose compositions are listed in table 4.2.

In actual practice, neither Jacobs Ranch nor Clovis Point presents excess fireside deposition but when the two coals are blended, severe fireside deposition occurs. The worst case was observed with the blend of 75% Jacob Ranch and 25% Clovis Point, although all blends created more

TABLE 4.1

Parameter	Jacobs Ranch	Clovis Point
Iron as Fe ₂ 0 ₃ %	6.47	4.24
calcium as CaO %	21.19	23.59
Magnesium as MgO %	5.18	6.0
Sodium as Na ₂ 0 %	0.83	1.79
Potassium as K ₂ 0 %	0.36	0.11
Silicon as SiO ₂ %	49.57	48.1
Aluminum as Al ₂ 0 ₃ %	16.4	16.18
Titanium as TiO ₂ %	0.0	0.0
Sulfur % in the coal	0.64	0.43
Ash % in the coal	6.81	6.14
Temperature in (c) for viscosity calculation	1,200	1,200
Calorific value in Btu/lbm (dry m.m.free)	10,800	10,000
Initial deformation temperature (k)	1,394	1,372
Hemispherical temperature (k)	1,439	1,416

HIGH TEMPERATURE ASH COMPOSITION OF PURE COALS

TABLE 4.2

Parameter	75%JR-25%CP	50%JR-50%CP	25%JR-75%CP
Iron as Fe ₂ 0 ₃ %	5.11	4.86	4.26
calcium as CaO %	21.82	22.34	22.87
Magnesium as MgO %	5.58	5.69	5.79
Sodium as Na ₂ 0 %	1.13	1.28	1.56
Potassium as K ₂ 0 %	0.29	0.24	0.17
Silicon as SiO ₂ %	50.07	49.31	49.09
Aluminum as Al ₂ O ₃ %	15.99	16.29	16.25
Titanium as TiO ₂ %	0.0	0.0	0.0
Sulfur % in the coal	0.57	0.53	0.47
Ash % in the coal	6.64	6.4	6.24
Temperature in (c) for viscosity calculation	1,200	1,200	1,200
Calorific value in Btu/lbm (dry m.m.free)	10,800	10,500	10,300
Initial deformation temperature (k)	1,411	1,389	1,383
Hemispherical temperature (k)	1,439	1,427	1,439

HIGH TEMPERATURE ASH COMPOSITION OF BLENDED COALS

deposition than either pure coals. These results were observed by the engineers at the Public Service of Oklahoma's (PSO's) power plant located at Oolagah, Oklahoma, the site were these coals were used. However, the results of the program indicates that the correlations are far from consistent even for the pure coals. Some of them predict that neither coal should cause slagging problem while others predict that both should cause severe slagging problems. A similar variation in predictions is observed in the results for the various blends of coals. The results are listed in table 4.3.

The first index is the Attig and Duzy's prediction of fouling in the boiler tubes. Their index is calculated by the equation:

$$Rf = Rba * Na_2 0 \tag{2.3}$$

This index suggests medium fouling for Jacobs Ranch coal. Such a result is actually observed at the power plants using coal. Similarly, the prediction of high fouling potential in all the blends of these two coals is consistent with the practical observations. However, the prediction of high fouling for Clovis Point coal is contradicted by the observations in the power plants. The reason for this inconsistency is that this index is directly proportional to only the sodium content in the ash which increases continuously as we gradually move from 100% JR to

TABLE 4.3

Method of prediction	JR	75% JR- -25% CP	50% JR- -50% CP	25% JR- -75% CP	CP
Attig & Duzy! Attig & Duzy	М	Н	Н	Н	Н
(based on %sulfur)	L	${f L}$	L	L	L
Gray & Moore	Н	Н	Н	Н	Н
Raask (based on %Na ₂ 0)	М	н	Н	Н	н
Sedor, Griffin & Profitta	L	L	L	L	L
Raask (based on %Fe ₂ 0 ₃)	L	L	L	L	L
Raask (based on silica)	H/S	H/S	H/S	H/S	H/S
Base-to-acid ratio index	H/S	H/S	H/S	H/S	H/S
Winegartner	NV	NV	NV	NV	NV

PREDICTIONS OF FOULING AND SLAGGING IN FURNACE

! -Fouling index L -Low slagging M -Medium slagging H -High slagging S -Severe slagging NV -Not valid blends with increasing percentage of Clovis Point and finally to 100% CP. Hence, this index presents reasonable predictions for the Jacobs Ranch and the blended coals but is a failure in predicting the behavior of Clovis Point coal.

Attig and Duzy's slagging index is calculated by the relation:

$$Fs' = Rba * S \tag{2.4}$$

For pure coals, the predictions of Attig and Duzy's slagging index is consistent with the actual observation. However, this correlation is a complete failure in predicting the behavior of blended coals. This index is based on the sulfur content in the ash which does not play the main role in the slagging problem.

Gray and Moore's index is calculated by the following equation:

$$Fs = (4 * IT + HT)/5.0$$
 (2.8)

Gray and Moore's index predict high slagging for the pure coals as well as for the blended coals. The prediction is incorrect for the former case but correct for the latter one.

This index is based on the temperatures determined during the ash fusion tests and relies only on the observed behavior of ash samples. Hence this method have failed to predict the problem as it actually occurs.

The slagging index by Raask is a direct measure of the sodium oxide content in the ash. It predicts medium slagging for the Jacobs Ranch coal and high slagging for the Clovis Point and the blended coals. The results are reasonable for Jacobs Ranch coal but are erroneous for Clovis Point and the blended coals.

Sedor, et. al. (1960), Griffin and Profitta (1965) have based their index on equivalent sodium oxide in the ash:

 $Na_2O_{eg} = (Na_2O + 0.659 * K_2O) * Ash / 100$ (2.1)

This index predicts low slagging potential for the pure as well as the blended coals. Again, the results are unsatisfactory.

Raask has developed an index based on the iron oxide content in the ash. The results show low slagging potential for all the coals under consideration. The error in the results is due to the fact that the index depends solely on one constituent, i.e, iron oxide and completely ignores the interactions of other oxides.

Contrary to the first two, the third index by Raask predicts high or severe slagging for the pure as well as the blended coals. This index is calculated by the relation:

Fsilica = SiO_2 / (MgO + CaO + Fe₂O₃ + SiO₂) * 100 (2.10)

Obviously, the results are not correct for the pure coals but are correct for the blended coals.

The slagging index based on the base-to-acid ratio suggests high or severe slagging for both the coals and their blends. Hence, the results of this index are inaccurate for the pure coals. However, the results are found true for the blended coals.

Incidentally, the slagging index by Winegartner (1974) does not print any result because this index has been developed for lignitic coals only while the coals selected for this study are all bituminous coals.

In general, we see that none of the slagging indices gave reasonable results. If the predictions for any index were correct for the pure coals, they were incorrect for blended coals and vice versa.

The next calculation is for the temperature of critical viscosity, Tcv, by method of Hoy et. al. (1965). The temperature of critical viscosity gives an indication of the minimum temperature at which molten slag will run freely down the furnace walls. The results are listed in table 4.4. It is evident from the results that Tcv is generally smaller for the pure coals than for the blended coals. However, the difference in the values is very small. The maximum value of Tcv is obtained for 75% JR - 25% CP blend which predicts that the ash will adhere to the surface and grow even at a very high temperature. Hence the blend of 75% JR - 25% CP is likely to cause more slagging and fouling

TABLE 4.4

PREDICTIONS FOR THE TEMPERATURE OF CRITICAL VISCOSITY FOR PURE AND BLENDED COALS

Coal type	Temperature of critical viscosity (c)
Jacobs Ranch	1512.9
75% JR - 25% CP	1595.7
50% JR - 50% CP	1514.8
25% JR - 75% CP	1510.9
Clovis Point	1472.5

than the others. This is in accordance with the practical observation reported by the engineers at PSO's Oolagah power plant. However, the results for the other blends do not coincide with the experimental results.

Viscosity of molten slag is calculated by two methods, i.e, the Reid's and the Watt's method and the results are presented in figures 4.1 through 4.5. For all the types of coals studied, Reid's method predicted lower values of viscosity than Watt's method. The results are almost identical for all the coals under investigation. Therefore, it can be concluded that these methods are not sensitive to variations in the composition of coal.

During the combustion process, some of the mineral matter in the original coal escapes as part of the flue gas while the rest is converted into ash. So the percentage of mineral matter in the coal should be slightly greater than that of the ash. The estimation of the mineral matter is first performed according to Parr's method and then according to Thiessen's method. The results are summarized in table 4.5 and are found to be reasonable because, for each coal, the percentage of mineral matter is slightly greater than that of ash in the coal.



Figure 4.1



Figure 4.2



Figure 4.3



Figure 4.4



Figure 4.5

TABLE 4.5

Mineral Matter (%) Coal type Ash (%) Parr's Method Thiessen's Method Jacobs Ranch 6.81 7.707 7.411 75% JR - 25% CP 6.64 7.485 7.218 50% JR - 50% CP 6.40 7.204 6.951 25% JR - 75% CP 6.770 6.24 6.998 Clovis Point 6.14 6.868 6.653

ESTIMATION OF MINERAL MATTER IN COAL PRIOR TO THE COMBUSTION PROCESS

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

Evaluation of the various slagging indices reveals that they are unable to predict realistic results. This failure is observed, not only for the blended coals, but for pure coals as well. Each of these correlations was developed after experimentation on a particular type of coal and was found good for that coal and for a similar coal. However, when applied to other types of coals, these correlations gave misleading results. Unfortunately, some of the correlations were developed for coals found in a certain geographical region which failed very often when applied to coals of other regions. Therefore, these correlations need to be tested with many different types of coal and then the results be used in developing the criteria for the range of applicability of each of these correlations. This procedure needs analyses of different coals as well as experiments to obtain data against which the predictions can be assessed.

Another line of research is to develop a versatile index which would accurately predict the behavior of all types of coal. Such an index might take into account the

mutual interactions and transformations of the various constituents of mineral matter and the actual mechanism of deposition and slagging in furnaces. It might also consider the design features of the furnace, the environment (reducing or oxidizing) and the temperature.

In a furnace, the composition of ash at one location differs from the composition at other locations. Some computer models predict the distribution of ash components in various parts of the furnace. The program developed in this study should be coupled with these models, so that the slagging and fouling behavior in every part of the furnace could be assessed.

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APPENDIX

PROGRAM FOR PREDICTING THE PROPERTIES OF COAL

\$debug \$storage:2 С C C This program can calculate the various fouling and Ċ C slagging indexes of a coal based on its composition, С С C physical properties and operating temperature. It is С C also capable of estimating the temperature of critical C viscosity, viscosities at various temperatures and the С C percentage of mineral matter in the original coal prior С С C to the combustion process. С С C ACID: Sum of the percentages of acidic oxides in the ash С C AIT: Initial deformation temperature (k) С С C AK20: Wt % of potassium oxide in the ash С C AL203: Wt % of alumina in the ash С C AL2O3n: Wt % of Al2O3 such that: С С SiO2+A12O3+Fe2O3+CaO+MqO=100 C AMgO: Wt % of magnesium oxide in the ash С С C AMgOn: Wt % of MgO such that: С С SiO2+A12O3+Fe2O3+CaO+MgO=100 С C AMIN: Wt % of mineral matter in the coal С C ANa20: Wt % of sodium oxide in the ash С C ANa20eq: Equivalent sodium oxide in the ash С C ANa20ws: Wt % of water soluble sodium oxide in the ash С C ASH: Wt % of ash in the coal С C BAS: Sum of the percentages of basic oxides in the ash С C CaO: Wt % of calcium oxide in the ash С C CaOn: Wt % of CaO such that: С SiO2+A12O3+Fe2O3+CaO+MqO=100 С С C CV: Calorific value of coal (dry m.m.free basis) С in Btu/lbm С С C EATA: Viscosity of ash in poise С C FCMN: Sum of Fe2O3n, CaOn and AMgOn С C FCN: Sum of the percentages of Na20, Fe203 and CaO in С the ash С С C Fe2O3: Wt % of iron oxide in the ash С C Fe2O3n: Wt % of Fe2O3 such that:

С SiO2+Al2O3+Fe2O3+CaO+MgO=100 С C Fs: Slagging index by method of Gray and Moore С C FSILICA: Silica ratio, i.e, С С SiO2/(MgO+CaO+Fe2O3+SiO2)*100 С C Fx: Slagging index by method of Soundreal et. al. С C Fy: Slagging index by method of Winegartner С C HT: Hemispherical temperature (k) С C Rba: Slagging index based on ratio of basic to acidic С С oxides С C Rf: Fouling index by method of Attig and Duzy С C Rs: Slagging index by method of Attig and Duzy С C S: Wt % of sulfur in the ash С C SAFCM: Sum of SiO2, Al2O3, Fe2O3, CaO & MgO percentages С C SAN: SiO2/Al2O3 on the basis of С SiO2+Al2O3+Fe2O3+CaO+MgO=100 С С C SiO2: Wt % of silica in the ash С C SiO2n: Wt % of SiO2 such that: С С SiO2+Al2O3+Fe2O3+CaO+MgO=100 С C T: Temperature at which the viscosity is to be С С calculated С C Tcv: Temperature of critical viscosity (c) С C TiO2: Wt % of TiO2 in the ash С C Tk: Operating temperature (k) С PROGRAM COAL С С C CALL SCRN?? are default information screens С С С INTEGER*2 pattr, page, ier INTEGER*2 attr, rattr, xattr, dattr, ZATTR INTEGER*2 mode, ncols, battr INTEGER*2 wid2, wids INTEGER*2 White, Yellow, Black, Blue, Red, Green, cyan, * magen,brown,Gray INTEGER*2 lblue,lcyan,lred,lmagen,whit INTEGER*2 fattr С С Ċ CLEAR SCREEN AND GET ADAPTER TYPE C SET SCREEN COLORS C С С call setvm(3) call getmod(mode, ncols, page) IF(mode .eq. 3) THEN Black = 0Blue = 1GREEN = 2CYAN = 3RED = 4MAGEN = 5BROWN = 6WHIT = 7GRAY = 8LBLUE = 9LGREEN=10 LCYAN = 11LRED =12LMAGen=13 YELLOW=14

```
WHITE =15
           CALL SETAB(ATTR, WHITE, BLUE, 0, 0)
           call setab(dattr,lcyan,blue,0,0)
           call revab(dattr,battr)
           call setab(pattr,RED,WHITE,0,1)
           call revab(attr,rattr)
           call setab(fattr,12,blue,0,1)
           call setab(xattr,White,Blue,0,0)
           call setab(Zattr,WHITE,RED,0,0)
           call revab(xattr,rattr)
        else
          PRINT *, 'AN EGA OR VGA COLOR GRAPHICS ADAPTER'
          print *, 'IS REQUIRED TO RUN THIS PROGRAM'
          PRINT *, ' PROGRAM STOPPED'
          stop
     END IF
С
C CALL SETVM(3) changes to 80x25, 16 color text mode EGA
C EMODE(16) Changes to 640x350, 16 color graphics
C This also clears the screen.
C CALL LOCAT(r,c) moves cursor to the desired row
C and column
C CALL CURON() Turns on cursor
C CALL CUROFF() Turns off cursor
С
C make borderless backdrop window
С
C
       call wopen(wids, attr, attr, 0, 0, 23, 78, char(0), 0, 0, 0)
С
100
     CONTINUE
     call cls()
122
     call wopen(widS, dattr, dattr, 0, 0, 23, 78, char(0), 0, 0, 0)
     CALL FE
     call wopen(wid2, battr, attr, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
124
     CALL WCLS(WID2)
     CALL WPRINT (WID2, ' \% =  ')
     FE2O3=WGETR4 (WID2, IER)
     IF(FE2O3 .lt. 0 .OR. FE2O3 .GE. 100)GOTO 124
     CALL WCLOSE(WID2)
     CALL WCLOSE(WIDS)
     call wopen(widS, dattr, dattr, 0, 0, 23, 78, char(0), 0, 0, 0)
     CALL CAOSCRN
     call wopen(wid2, battr, attr, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
128
     CALL WCLS(WID2)
     CALL WPRINT(WID2, \% = \%)
     CAO=WGETR4 (WID2, IER)
     IF(CAO .lt.
                   0 .OR. CAO .GE. 100)GO TO 128
      CALL WCLOSE(WID2)
      CALL WCLOSE(WIDS)
     call wopen(widS, dattr, dattr, 0, 0, 23, 78, char(0), 0, 0, 0)
      CALL MG
     call wopen(wid2, battr, attr, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
 132 CALL WCLS(WID2)
     CALL WPRINT(WID2, ' % = `')
```

```
AMGO=WGETR4 (WID2, IER)
    IF(AMGO .lt.
                  0 .OR. AMGO .GE. 100)GOTO 132
     CALL WCLOSE(WID2)
    CALL WCLOSE(WIDS)
    call wopen(widS, dattr, dattr, 0, 0, 23, 78, char(0), 0, 0, 0)
    CALL NA
    call wopen(wid2, battr, attr, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
136 CALL WCLS(WID2)
     CALL WPRINT(WID2, ' % = `')
     ANA2O=WGETR4 (WID2, IER)
     IF(ANA20 .lt. 0 .OR. ANA20 .GE. 100)GOTO 136
     CALL WCLOSE(WID2)
     CALL WCLOSE(WIDS)
     call wopen(widS,dattr,dattr,0,0,23,78,char(0),0,0,0)
       CALL K
     call wopen(wid2, battr, attr, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
140 CALL WCLS(WID2)
     AK2O=WGETR4 (WID2, IER)
      IF(AK20 .lt. 0 .OR.
                             AK20 .GE. 100)GOTO 140
      CALL WCLOSE(WID2)
      CALL WCLOSE(WIDS)
      call wopen(widS, dattr, dattr, 0, 0, 23, 78, char(0), 0, 0, 0)
      CALL SI
      call wopen(wid2,battr,attr,10,34,1,10,CHAR(0),2,1,2)
144 CALL WCLS(WID2)
      CALL WPRINT(WID2, ' % = `')
      SIO2=WGETR4(WID2, IER)
      IF(SIO2 .lt. 0 .OR. SIO2 .GE. 100)GOTO 144
      CALL WCLOSE(WID2)
      CALL WCLOSE(WIDS)
      call wopen(widS, dattr, dattr, 0, 0, 23, 78, char(0), 0, 0, 0)
      CALL AL
      call wopen(wid2, battr, attr, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
148 CALL WCLS(WID2)
     CALL WPRINT(WID2, ' % = `')
     AL2O3=WGETR4 (WID2, IER)
     IF(AL203 .lt. 0 .OR. AL203 .GE. 100) GO TO 148
     CALL WCLOSE(WID2)
      CALL WCLOSE(WIDS)
     call wopen(widS, dattr, dattr, 0, 0, 23, 78, char(0), 0, 0, 0)
      CALL TSCRN
     call wopen(wid2, battr, attr, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
152 CALL WCLS(WID2)
     CALL WPRINT(WID2, ' % = `')
      TIO2=WGETR4 (WID2, IER)
                     0 .OR. TIO2 .GE. 100)GOTO 152
      IF(TIO2 .lt.
     CALL WCLOSE(WID2)
     CALL WCLOSE(WIDS)
     CALL WOPEN(WIDS, DATTR, DATTR, 0, 0, 23, 78, CHAR(0), 0, 0, 0)
     CALL WS
     CALL WOPEN (WID2, BATTR, ATTR, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
     CALL WCLS(WID2 )
154
                CALL WPRINT(WID2, ' % = `')
```

```
ANA2OWS=WGETR4 (WID2, IER)
    IF(ANA2OWS .LT.
                      0 .OR.
   *
                 ANA2OWS .GE. 100) GO TO 154
                 CALL WCLOSE(WID2)
                 CALL WCLOSE(WIDS)
     CALL WOPEN(WIDS, DATTR, DATTR, 0, 0, 23, 78, CHAR(0), 0, 0, 0)
     CALL SU
     CALL WOPEN(WID2, BATTR, ATTR, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
156 CALL WCLS(WID2)
     S=WGETR4 (WID2, IER)
     IF(S .LT.
                 0 .OR. S .GE. 100) GO TO 156
     CALL WCLOSE(WID2)
     CALL WCLOSE(WIDS)
     CALL WOPEN(WIDS, DATTR, DATTR, 0, 0, 23, 78, CHAR(0), 0, 0, 0)
                CALL AS
     CALL WOPEN(WID2, BATTR, ATTR, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
158 CALL WCLS(WID2)
     CALL WPRINT(WID2, ' % = `')
     ASH = WGETR4(WID2, IER)
     IF(ASH .LT.
                            ASH .GE. 100) GO TO 158
                   0 .OR.
       CALL WCLOSE(WID2)
       CALL WCLOSE(WIDS)
     CALL WOPEN(WIDS, DATTR, DATTR, 0, 0, 23, 78, CHAR(0), 0, 0, 0)
     CALL TE
     CALL WOPEN(WID2, BATTR, ATTR, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
160 CALL WCLS(WID2)
                 CALL WPRINT(WID2, ' `')
         T = WGETR4(WID2, IER) IF(T .LT. 0) GO TO 160
     CALL WCLOSE(WID2)
     CALL WCLOSE(WIDS)
     CALL WOPEN(WIDS, DATTR, DATTR, 0, 0, 23, 78, CHAR(0), 0, 0, 0)
     CALL CVALUE
     CALL WOPEN(WID2, BATTR, ATTR, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
162 CALL WCLS(WID2)
                CALL WPRINT(WID2, ' `')
                CV = WGETR4(WID2, IER)
                IF(CV .LT. 0) GO TO 162
                CALL WCLOSE(WID2)
                CALL WCLOSE(WIDS)
    CALL WOPEN(WIDS, DATTR, DATTR, 0, 0, 23, 78, CHAR(0), 0, 0, 0)
                CALL AI
     CALL WOPEN(WID2, BATTR, ATTR, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
164 CALL WCLS(WID2) CALL WPRINT(WID2, ' `')
    AIT = WGETR4(WID2, IER)
    IF(AIT .LT. 0) GO TO 164
     CALL WCLOSE(WID2)
     CALL WCLOSE(WIDS)
     CALL WOPEN(WIDS, DATTR, DATTR, 0, 0, 23, 78, CHAR(0), 0, 0, 0)
     CALL H
     CALL WOPEN(WID2, BATTR, ATTR, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
166 CALL WCLS(WID2) CALL WPRINT(WID2, '`')
     HT = WGETR4(WID2, IER)
     IF(HT .LT. 0) GO TO 166
```

```
CALL WCLOSE(WID2)
        CALL WCLOSE(WIDS)
C -Providing default values-----
     If (SiO2 .LT. 10.0 .OR. SiO2 .GT. 70.0) then
     SiO2=100-Al2O3-Fe2O3-CaO-AMgO-ANa2O-AK2O-TiO2
     Elseif (Al2O3.LT.8.0 .OR. Al2O3.GT.38.0) then
     Al203=100-Si02-Fe203-Ca0-AMg0-ANa20-AK20-Ti02
     Elseif (Fe203.LT.2.0 .OR. FE203.GT.50.0) then
     Fe203=100-CaO-AMgO-ANa20-AK20-Al203-Ti02-Si02
     Elseif (CaO.LT.0.5 .OR. CAO.GT.30.0) then
     CaO=100-Fe2O3-AMgO-ANa2O-AK2O-Al2O3-TiO2-SiO2
     Elseif(AMgO.LT.0.3 .OR. AMGO.GT.8.0) then
     AMg0=100-Fe2O3-Ca0-ANa20-AK20-Al2O3-TiO2-SiO2
     Elseif(ANa20.LT.0.1 .OR. ANA20.GT.8.0) then
     ANa20=100-Fe203-Ca0-AMg0-AK20-Al203-Ti02-Si02
     Elseif(AK20 .LT. 0.1 .OR. AK20 .GT. 3.0) then
     AK20=100-Fe203-Ca0-AMg0-ANa20-Al203-Ti02-Si02
     Else
     TiO2=100-Fe2O3-CaO-AMgO-ANa2O-AK2O-Al2O3-SiO2
     END IF
      IF (ANa2Ows.LT.0.001 .OR. ANa2Ows.GT.ANA2O)
     ANa2Ows=ANa2O/2.0
      If (S .LT. 0.001 .OR. S .GT. 40)
      S = 3.3
      If (Ash .LT. 0.01 .OR. Ash .GT. 40) Ash = 7
      If (t .LT. 700 .OR. t .GT. 7000) t = 1100
      If (CV .LT. 9090.91 .OR. CV .GT.
                                         100000) CV = 9091
      If (Ait .LT. 600 .OR. Ait .GT.
                                        100000) Ait = 600
      If (Ht .LT. 800 .OR. Ht .GT. 100000) then
          Ht = -7.17 * (FE203 + CAO + AMGO) + 1460.0
     END IF
C -Deciding the type of Ash (k1=1 for Bituminous ash)
C -
                            (k1=2 for Lignitic Ash)
     SUM=FE203+CA0+AMG0+ANA20+AK20+SI02+AL203+TI02
     FCN = ANa20 + Fe203 + Ca0
     If (SiO2 .GT. FCN) then
               k1 = 1
            Else
               K1 = 2
     End If
      С
      WRITE(*,*) '-----Ash Analysis-----'
      WRITE(*,1) ASH, S
      WRITE(*,10) FE2O3, CAO, AMGO, ANA2O
      WRITE(*,12) AK20, SI02, AL203, TI02
      WRITE(*,*) 'Fe203+CaO+MgO+Na2O+K2O+SiO2+Al2O3+TiO2=',
    * SUM
     WRITE(*,*) 'NOTE: The value of the above summation'
     WRITE(*,*)'should be near hundred. If it is far from'
     WRITE(*,*) 'hundred the results will be inaccurate.'
      WRITE(*,13) CV
      WRITE(*,11) AIT
      WRITE(*, 15) HT
      WRITE(*,5) T
```

```
IF (K1 .EQ. 1) THEN
   WRITE(*,*) ' Ash type: Bituminous'
   ELSE WRITE(*,*) ' Ash type: Lignitic'
   END IF
   WRITE(*,*)'Is this data okay? If yes, enter 1'
   WRITE(*,*)'otherwise enter 0'
   READ(*,*) OK
   IF (OK .EQ. 0) GO TO 100
   OPEN(8, FILE='COAL.DAT', STATUS='UNKNOWN')
   WRITE(8,*) 'PROGRAM FOR CALCULATING COAL PROPERTIES'
   WRITE(8,*) '-----'Ash Analysis-----'
   WRITE(8,1) ASH, S
 1 FORMAT(1X,7H ASH =,F7.3,6H S =,F7.3,10H % of coal)
   WRITE(8,10) Fe2O3, CaO, AMGO, ANA2O
10 FORMAT(1X,7H FE2O3=,F7.3,6H CAO =,F7.3,7H MGO =,F7.3,
  * 6H NA2O=,F7.3)
   WRITE(8,12) AK2O, SiO2, AL2O3, TIO2
12 FORMAT(1X,7H K2O =, F7.3,6H SIO2=, F7.3,7H Al2O3=, F7.3,
  * 6H TiO2=,F7.3)
     WRITE(8,13) CV
     WRITE(8,11) AIT
     WRITE(8,15) HT
13 FORMAT(20H Calorific Value =, F10.3,8H Btu/lbm)
11 FORMAT(34H Initial deformation temperature=,F10.3,1HC)
15 FORMAT(1X,28H Hemispherical temperaure =,F10.3,2H C)
   WRITE(8,5) T
   FORMAT(1X, 3H T=, F10.3)
5
   If (k1 .EQ. 1) then
         WRITE(8,*) ' Ash type: Bituminous'
    Else
         WRITE(8,*) ' Ash type: Lignitic'
   End If
    WRITE(*,*)' ---Results of Calculations -----'
    WRITE(8,*)' -----Results of Calculations-----'
    WRITE(*,*) ' Fouling index by method of Attig & Duzy'
    WRITE(8,*) ' Fouling Index by method of Attig & Duzy'
    BAS = FE2O3 + CAO + AMGO + ANA2O + AK2O
    ACID = SIO2 + AL2O3 + TIO2 RF = BAS / ACID * ANA2O
    WRITE(*,14) Rf
    WRITE(8,14) Rf
    FORMAT(1X, 4H Rf=, F10.3)
14
    If (Rf .LT. 0.2) then
          WRITE(*,*) ' Low Fouling'
          WRITE(8,*) ' Low Fouling'
       Elseif (Rf .LT. 0.5) then
          WRITE(*,*) ' Medium Fouling'
          WRITE(8,*) ' Medium Fouling'
       ELSEIF (Rf .LT.
                       1.0) then
          WRITE(*,*) ' High Fouling'
          WRITE(8,*) ' High Fouling'
       Else
          WRITE(*,*) ' Severe Fouling'
          WRITE(8,*) ' Severe Fouling'
    End If
```

```
C -Calculating Slagging Index by method of Attig &
C -Duzy(1969)
    Rs = Bas/Acid * S
    WRITE(8,*) ' -----'
    WRITE(*, 17) S
    WRITE(8,17) S
 17 FORMAT(1X, 16H Sulfur in Coal=, F7.3)
   WRITE(*,*) ' Slagging Index by method of Attig & Duzy'
   WRITE(8,*) ' Slagging Index by method of Attig & Duzy'
    WRITE(*,20) Rs
    WRITE(8,20) Rs
 20 FORMAT(1X, 4H RS=,F10.3) If (Rs .LT. 0.6) then
       WRITE(*,*) ' Low Slagging'
       WRITE(8,*) ' Low Slagging'
    Elseif (RS .LE. 2.0) then
    WRITE(*,*) ' Medium Slagging'
    WRITE(8,*) ' Medium Slagging'
    Elseif (Rs .LE. 2.6) then
    WRITE(*,*) ' High Slagging'
    WRITE(8,*) ' High Slagging'
    Else
       WRITE(*,*) ' Severe Slagging'
       WRITE(8,*) ' Severe Slagging'
    End If
   WRITE(*,*) ' -------'
   WRITE(8,*) ' ------'
C -Calculating Slagging Index by Method of Gray & Moore--
    Fs = (4 * Ait + Ht) / 5.0
    WRITE(*,*)'Slagging Index by method of Gray & Moore'
    WRITE(8,*)'Slagging Index by method of Gray & Moore'
    WRITE(*,23) Fs
    WRITE(8,23) Fs
 23 FORMAT(1X, 4H Fs=,F10.3)
   If (Fs .LT. 1325) then
        WRITE(*,*) ' Severe Slagging'
       WRITE(8,*) ' Severe Slagging'
      Elseif (Fs .LT. 1506) then
       WRITE(*,*) ' High Slagging'
       WRITE(8,*) ' High Slagging'
      Else
       WRITE(*,*) ' Low or Medium Slagging'
       WRITE(8,*) ' Low or Medium Slagging'
      End If
    WRITE(*,*) ' -----'
    WRITE(8,*) ' ------'
C -Calculating Slagging Index By method of Raask (1985) --
    WRITE(*,*)' Slagging Index by Raask (based on Na20)
  * content) '
    WRITE(8,*)' Slagging Index by Raask (based on Na20
  * content) '
    WRITE(*,25) ANa20
    WRITE(8,25) ANa20
 25 FORMAT(1X, 6H NA2O=, F7.3)
```

```
If (k1 .EQ. 2) GO TO 26
    IF (ANa20 .LT. 0.5) then
             WRITE(*,*) ' Low Slagging'
             WRITE(8,*) ' Low Slagging'
        Elseif (ANa20 .LE. 1.1) then
             WRITE(*,*) ' Medium Slagging'
             WRITE(8,*) ' Medium Slagging'
        Elseif (ANa20 .LE. 2.6) then
             WRITE(*,*) ' High Slagging'
             WRITE(8,*) ' High Slagging'
        Else
             WRITE(*,*) ' Severe Slagging'
             WRITE(8,*) ' Severe Slagging'
    END IF
       GO TO 27
 26 continue
    IF (ANa20 .LT. 2.0) then
             WRITE(*,*) ' Low Slagging'
             WRITE(8,*) ' Low Slagging'
         Elseif (ANa20 .LT. 7) then
             WRITE(*,*) ' Medium Slagging'
             WRITE(8,*) ' Medium Slagging'
         Elseif (ANa20 .LT. 9) then
         WRITE(*,*) ' High Slagging'
         WRITE(8,*) ' High Slagging'
         Else
         WRITE(*,*) ' Severe Slagging'
         WRITE(8,*) ' Severe Slagging'
         End If
 27 CONTINUE
         WRITE(*,*) ' -----'
         WRITE(8,*) ' -----'
C-Slagging Index By Sedor et. al.(1960) and Griffin and
C-Profitta (1965)
C -For Bituminous coal ashes only------
    WRITE(*,*) ' Slagging Index by Sedor, Griffin &
    * Profitta (ba-sed on Na20-equivalent in ash) '
    WRITE(8,*) ' Slagging Index by Sedor, Griffin &
    * Profitta (ba-sed on Na20-equivalent in ash) '
    IF (K1 .EQ. 2) GO TO 32
        ANA2OEQ = (ANA2O + 0.659 * AK2O) * ASH / 100.0
        WRITE(*,29) ANa2Oeq
        WRITE(8,29) ANa2Oeq
  29 FORMAT(1X, 9H NA2OEQ=, F10.3)
        If (ANa2Oeq .LT. 0.3) then
        WRITE(*,*) ' Low Slagging'
        WRITE(8,*) ' Low Slagging'
        Elseif (ANa2Oeq .LT. 0.46) then
        WRITE(*,*) ' Medium Slagging'
        WRITE(8,*) ' Medium Slagging'
        Elseif (ANa2Oeq .LT. 0.6) then
        WRITE(*,*) ' High Slagging'
        WRITE(8,*) ' High Slagging'
```

```
Else
        WRITE(*,*) ' Severe Slagging'
        WRITE(8,*) ' Severe Slagging'
        END IF
        GO TO 35
 32
        CONTINUE
        WRITE(*,*) ' Not valid for Lignitic coals'
        WRITE(8,*) ' Not valid for Lignitic coals'
 35
       CONTINUE
        WRITE(*,*) ' -----'
        WRITE(*,*) ' Please enter 1 to proceed'
        READ(*,*) ENTER
C -Slagging Index By Raask (1985) --
    WRITE(*,*)'Slagging Index by Raask (based on Fe203
   * content) '
    WRITE(8,*)'Slagging Index by Raask (based on Fe203
   * content) '
        WRITE(*,38) Fe2O3
        WRITE(8,38) Fe2O3
38
    FORMAT(1X, 7H FE203=, F7.3)
    If (Fe2O3 .LT. 9.0) then
        WRITE(*,*) ' Low Slagging'
        WRITE(8,*) ' Low Slagging'
    Elseif (Fe2O3 .LT. 16) then
        WRITE(*,*) ' Medium Slagging'
        WRITE(8,*) ' Medium Slagging'
    Else
        WRITE(*,*) ' High or Severe Slagging'
        WRITE(8,*) ' High or Severe Slagging'
    End If
        WRITE(*,*) ' -----'
        WRITE (8,*) ' -----'
C --Slagging Index By Raask (1985) Based On SiO2-----
    Fsilica = SiO2 / (AMgO + CaO + Fe2O3 + SiO2) * 100.0
    WRITE(*,*)'Slagging Index by Rassk on silica basis '
    WRITE(8,*)'Slagging Index by Raask on silica basis'
    WRITE(*,44) Fsilica
    WRITE(8,44) Fsilica
44
    FORMAT(1X, 9H FSILICA=,F10.3)
    If (Fsilica .LT. 66) then
        WRITE(*,*) ' High or Severe Slagging'
        WRITE(8,*) ' High or Severe Slagging'
    Elseif (Fsilica .LT. 73) then
        WRITE(*,*) ' Medium Slagging'
        WRITE(8,*) ' Medium Slagging'
    Else
        WRITE(*,*) ' Low Slagging'
        WRITE(8,*) ' Low Slagging'
    End If
    WRITE(*,*) ' ------'
    WRITE(8,*) ' -----'
C -Slagging Index Based On Base/Acid Ratio-
    Rba = BAS / ACID
    WRITE(8,*) ' Base-to-acid ratio index--'
```

```
WRITE(*,50) Rba
    WRITE(8,50) Rba
  50 FORMAT(1X, 5H Rba=, F10.3)
     IF (RBA .LT. 0.4 .OR. RBA .GT. 0.7) THEN
WRITE(*,*) ' Low or Medium Slagging'
               WRITE(8,*) ' Low or Medium Slagging'
       ELSE
               WRITE(*,*) ' High or Severe Slagging'
               WRITE(8,*) ' High or Severe Slagging'
           END IF
      WRITE(*,*) ' ------'
      WRITE(8,*) ' -----'
C-Slagging Index For Lignitic Ashes By Winegartner (1974)-
      WRITE(*,*) ' Slagging Index by Winegartner----'
     WRITE(8,*) ' Slagging Index by Winegartner----'
           IF(K1 .EQ. 1) GO TO 55
           Fy = Rba * ANa2Ows
           WRITE(*, 53) Fy
               WRITE(8,53) Fy
  53 FORMAT(1X, 4H Fy=, F10.3)
     If (Fy .LT. 0.1) then
               WRITE(*,*) ' Low Slagging'
WRITE(8,*) ' Low Slagging'
           Elseif (Fy .LT. 0.26) then
WRITE(*,*) ' Medium Slagging'
WRITE(8,*) ' Medium Slagging'
           Elseif (Fy .LE. 0.7) then
               WRITE(*,*) ' High Slagging'
WRITE(8,*) ' High Slagging'
           Else
               WRITE(*,*) ' Severe Slagging'
WRITE(8,*) ' Severe Slagging'
     End If
     GO TO 57
  55 CONTINUE
           WRITE(*,*) ' Not valid for Bituminous ashes'
           WRITE(8,*) ' Not valid for Bituminous ashes'
  57 CONTINUE
      WRITE(*,*) '-----'
      WRITE(8,*) ' -----'
      WRITE(*,*) ' Do you want to calculate viscosity? '
      WRITE(*,*) ' If yes, enter 1 otherwise enter 0'
      Read(*,*) ENTER
           IF (ENTER .NE. 1) GO TO 76
  C -Calculating temperature of critical viscosity-----
  C Method of Hoy, Roberts and Wilkins-----
  C -Normalize SiO2 + Al2O3 + Fe2O3 + CaO + MgO to 100--
      Safcm = SiO2 + Al2O3 + Fe2O3 + CaO + AMgO
      SiO2n = SiO2 / Safcm * 100
      Al203n = Al203 / Safcm * 100
      Fe2O3n = Fe2O3 / Safcm * 100
      CaOn = CaO / Safcm * 100
      AMgOn = AMgO / Safcm * 100
      San = SiO2n / Al2o3n
```

```
Fcmn = Fe2O3n + CaOn + AMqOn
     Tcv = 2990 -1470*San + 360*San**2 - 14.7 * Fcmn +
    * 0.15 * Fcmn**2
     WRITE(*,*) ' Temperature of critical viscosity by
    * method of Hoy ,Roberts and Wilkins'
     WRITE(8,*) ' Temperature of critical viscosity by
    * method of Hoy, Roberts and Wilkins '
          WRITE(*,60) TCV
          WRITE(8,60) TCV
  60 FORMAT(1X, 5H TCV=, F10.3, 2H C)
    WRITE(*,*) ' ------'
    WRITE(8,*) ' -----'
C-Calculating viscosity By Method of Reid and Cohen-----
      TK = T + 273.0
    WRITE(*,*) ' Viscosity by method of Reid and Cohen---'
WRITE(8,*) ' Viscosity by method of Reid and Cohen---'
     TK = TK - 200
     TI = T - 200
     DO 63 I = 1,41
        A=4.468 * (FSILICA / 100.)**2. + 1.265 * (10.**4.
    * /TK)-7.44
          EATA = 10.**A
          WRITE(*,62) EATA , TI
          WRITE(8,62) EATA , TI
  62 FORMAT(1X,11H Viscosity=,F10.3,12H Poise at t=,F10.3
    * ,2H C)
    IF(I .EQ. 19) THEN
          WRITE(*,*) ' Please enter 1 to proceed'
          READ(*,*) ENTER
          ELSE
          CONTINUE
     END IF
          TK = TK + 10.0
          TI = TI + 10.0
  63 CONTINUE
     WRITE(*,*) '-----'
     WRITE(8,*) ' -----'
          WRITE(*,*) ' Please enter 1 to proceed'
          READ(*,*) ENTER
C-Calculating viscosity in poise by Method of J.D.Watt and
       Faraday using SiO2 + Al2O3 + Fe2O3 + CaO + MgO
С
С
      normallized to 100
      WRITE(*,*) ' Viscosity by method of Watt and
    * Faraday-----'
      WRITE(8,*) ' Viscosity by method of Watt and
    * Faraday-----'
      IF (FSILICA .LT. 40.0 .OR. SAN .LT. 1.4)GOTO 80
      IF(FE2O3N.LT.3.OR.CAON.LT.2.OR.AMGON.LT.1)GOTO 80
      IF (FSILICA .GT. 80.0 .OR. SAN .GT. 2.4) GO TO 80
      IF(FE203N.GT.30.OR.CAON.GT.30.OR.AMGON.GT.10)GO TO 80
      GO TO 85
  80 WRITE(*,*)' These predictions may be inaccurate because
    * the composition lies outside the applicable range'
     WRITE(8,*) ' These predictions may be inaccurate because
```

```
* the composition lies outside the applicable range
 85 CONTINUE
          T = T - 200.0
    DO 70 J = 1,41
        AM = 0.00835 * SIO2N + 0.00601 * AL2O3N - 0.109
        C = .0415*SIO2N +0.0192*AL2O3N +0.0276*FE2O3N
   *
     +0.016*CAON -* 3.92
        A = 10.**7. * AM / (T-150)**2.0 + C
        EATA = 10.**A
        WRITE(*,65) EATA, T
        WRITE(8,65) EATA, T
 65 FORMAT(1X, 16H Viscosity Eata=,F10.3,12H Poise at
   * t=,F10.3, * 2H c)
      IF (J.EQ. 20) THEN
          WRITE(*,*) ' Please enter 1 to proceed'
          READ(*,*) ENTER
          ELSE
          CONTINUE
      END IF
          T = T + 10.0
 70 CONTINUE
          WRITE(*,*) ' -----'
          WRITE(8,*) ' -----'
    WRITE(*,*) 'Do you want to estimate the percentage of'
    WRITE(*,*)'mineral matter in the coal? Mineral matter'
    WRITE(*,*) 'represents the inert portion of the coal
   * prior to the combustion process.'
    WRITE(*,*)' If yes, enter 1 otherwise enter 0'
    READ(*,*) ENTER
    IF (ENTER .EQ. 0) GO TO 76
C -Estimating mineral matter by the method of Parr-----'
    AMin = 1.08 * Ash + 0.55 * S
    WRITE(*,*) ' Mineral matter -----'
    WRITE(8,*) ' Mineral matter -----'
    WRITE(*,71) AMIN
    WRITE(8,71) AMIN
 71 FORMAT(21H Mineral matter AMin=,F10.3,17H % by Parr
   * method)
C -Estimating mineral matter by the method of Thiessen----
    Ak = 0.55 - 5000/CV
    AMin = 1.08 * Ash + Ak * S
    WRITE(*,75) AMIN
    WRITE(8,75) AMIN
 75 FORMAT(17H Mineral matter =, F10.3, 21H % by Thiessen
   * method)
           WRITE(*,*) ' -----'
           WRITE(8,*) ' -----'
            WRITE(*,*) ' Please enter 1 to proceed'
            READ(*,*) ENTER
  76 CONTINUE
    Call wopen(widS, dattr, dattr, 0, 0, 23, 78, char(0), 0, 0, 0)
    CALL DECISION
    CALL WOPEN (WID2, BATTR, ATTR, 10, 34, 1, 10, CHAR(0), 2, 1, 2)
    CALL WCLS(WID2)
```

```
CALL WPRINT(WID2, 'NUM = `')
ANOTHER = WGETR4(WID2,IER)
CALL WCLOSE(WID2)
CALL WCLOSE(WID3)
500 FORMAT(/////,25H RESULTS FOR ANOTHER COAL)
IF (ANOTHER .EQ. 1.0) THEN
WRITE(8,500)
GO TO 100
ELSE
CLOSE(8)
STOP
```

STOP END

NADIR KAMAL

VITA

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Masters of Science

Thesis: DEVELOPMENT OF A COMPUTER PROGRAM FOR PREDICTING THE PROPERTIES OF COAL

Major Field: Chemical Engineering

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