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Yang, X., Ingham, D., Ma, L. et al. (2 more authors) (2017) Ash deposition propensity of coals/blends combustion in boilers: a modelling analysis based on multi-slagging routes. Proceedings of the Combustion Institute, 36 (3). pp. 3341-3350. ISSN 1540-7489

https://doi.org/10.1016/j.proci.2016.06.060

Ash deposition propensity of coals/blends combustion in boilers: a modelling analysis based on multi-slagging routes

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Abstract

A method that is based on the initial slagging routes and the sintered/slagging route has been developed and used for predicting the ash deposition propensities of coal combustion in utility boilers supported by the data collected from power stations. Two types of initial slagging routes are considered, namely (i) pyrite-induced initial slagging on the furnace wall, and (ii) fouling caused by the alkaline/alkali components condensation in the convection section. In addition, the sintered/slagging route is considered by the liquids temperature, which represents the melting potential of the main ash composition and is calculated using the chemical equilibrium methods. The partial least square regression (PLSR) technique, coupled with a cross validation method, is employed to obtain the correlation for the ash deposition indice. The method has been successfully applied to coals/blends combustion in boilers, ranging from low rank coals to bituminous coal. The results obtained show that the developed indice yields a higher success rate in classifying the overall slagging/fouling potential in boilers than some of the typical slagging indices. In addition, only using the SiO_2/Al_2O_3 ratio to predict the melting behaviours and slagging potential is inaccurate since the effect of the SiO_2/Al_2O_3 ratio is dictated by both the original ash composition and the way in which the SiO_2/Al_2O_3 ratio is changed. Finally, the influence of the acid components (SiO_2 and Al_2O_3) on the ash deposition prediction is investigated for guiding the mineral additives. It is noticed that the predicted ash deposition potentials of the three easy slagging coals investigated decrease more rapidly by adding Al_2O_3 than by adding SiO_2.

Keywords: ash deposition indice, thermodynamic modelling, partial least square regression, boilers, SiO_2/Al_2O_3 ratio.

1 Introduction

Considerable progress has been made in the last decades in understanding the ash deposition mechanisms of various coals. For example, Eastern US coals (such as Illinois and Appalachian coals) have higher concentrations of Fe components than Western US coals [1], and the initial slagging caused by the pyrite is one of the main issues related to slagging problems [1-3]. For low rank Western US coals (such as Wyoming and Montana coals) which have higher concentrations of alkaline/alkali components than Eastern US coals, fouling in the convection section is a serious problem [4-6]. Figure 1 shows the main ash deposition mechanisms for US coals in utility boilers [1, 7, 8]. Generally, it is regarded that ash deposition can be mainly dictated by three different routes: (i) Pyrite-induced initial slagging route generates from the pyrite particles due to its large density and low melting temperature under reducing atmosphere on the furnace wall [3, 8, 9]; (ii) Fouling-induced initial slagging route generates from the condensation of alkali vapours and thermophertic deposition of aerosol/fume particles on the superheaters or economizers; (iii) The sintered/slagging route is triggered by the molten matrix generated from the major basic components reacting with clay and quartz, etc., and the reducing atmosphere can promote this process when a high Fe concentration is present in the coal [1, 7]. Furthermore, severe slagging in the furnace chamber could increase the furnace exit gas temperature (FEGT) and hence this may further aggravate the ash deposition in the convection section. Therefore, the severe ash deposition in boilers could be triggered by the three different routes and a successful ash deposition indice should be capable of predicting the deposition formation from these three formation routes.

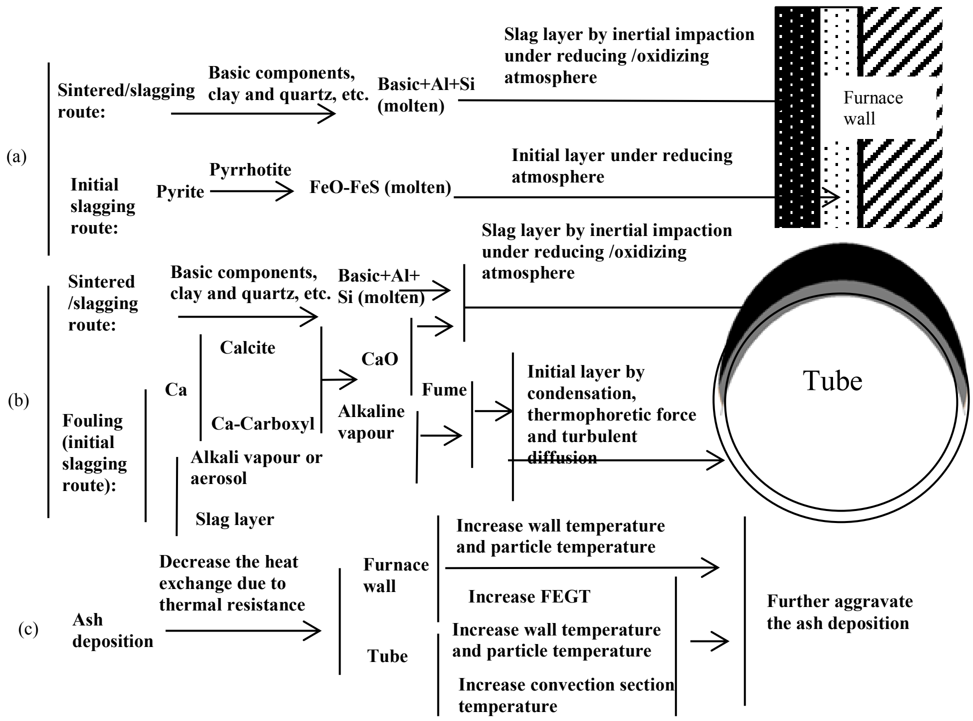

Fig. 1. Schematic of the ash deposition routes in boilers (modified from [1, 7, 8]).

Although there exist several publications on developing a slagging indice for coal combustion, most of these methods were developed either based on slagging observations in entrained flow reactors or by only considering the sintered/slagging route [10-15]. Gibb et al. [12] developed a slagging indice based on the Computer Controlled Scanning Electron Microscopy (CCSEM) based mineral composition in the coal. This indice was developed based on the assumption that the degree of assimilation of iron and calcium into the aluminosilicate glass determines the ash deposition characteristics of the coal. This assumption neglects the influence of the initial slagging routes caused either by pyrite or by condensation. McLennan et al. [11] developed an iron-based slagging indice based on the included and excluded iron related minerals composition in the coal. However, this indice only considers the effect of iron related minerals on the slagging behaviour. Also, both of these two CCSEM slagging indices are yet to be validated with full-scale field observations in boilers [15]. In addition, Barroso et al. [14, 16] employed conventional slagging indices to predict the slagging potential of coals/blends in an entrained flow reactor. It was found that by incorporating the aerodynamic diameter of fly ash particles into the conventional slagging indices one can improve the prediction performance because the aerodynamic diameter is proportional to the particle Stokes number which determines the particle impaction efficiency [1, 15]. It should be noted that the fluid velocity in the EFR is as low as approximately 0.5 m/s [14, 16], which means that particles may not have enough kinetic energy to rebound from the deposition surface after impaction and hence deposition accumulation could increase with an increase in the aerodynamic diameter under this low velocity condition in EFR [17]. However, the fluid velocity could be as high as 10-25 m/s in pulverised coal boilers and, for the particles with similar aerodynamic diameter, it is possible to have high enough kinetic energy (proportional to the square of the velocity, possible 20^2-50^2 times higher than in the EFR) to rebound from the deposition surface after impaction [17, 18]. Therefore, the conclusions from the low velocity conditions of the EFR may not be suitable for the real conditions in boilers. Moreover, for some of the existing typical slagging indices (B/A, B/A*Sulfur, Si value, etc.), the slagging prediction for the sintered/slagging route directly employs the mass fractions of ash components and assumes the same contribution of each basic or acid component to the slagging prediction. However, the sintered/slagging layer is not linearly related to the mass fraction of the basic or acid components [19-21]. Further, fuel ash content and heating values are important factors of ash deposition formation. A numerical slagging indice (NSI) has been developed to reflect these factors for both single coals and blends of coal and biomass [10, 22, 23]. The NSI has shown reasonable success in ranking the slagging potentials of some of the world trade coals. Nevertheless, in general uncertainty still exists in the understanding of the contributions from different slagging routes and correlations between the existing coal slagging indices and the actual observations made in conventional boilers.

This paper takes a new approach to build an ash deposition indice for fuel slagging propensity analysis. The ash deposition indice takes into considerations the multi-ash deposition routes which exist in industrial boilers and the indice is developed with support from the actual observations made in a range of industrial boilers. The sintered/slagging route is predicted by using the overall melting potential of the major ash components through the chemical equilibrium calculations; the initial slagging route caused by either the pyrite or the alkaline/alkali components is predicted by using the amount of the related basic ash components; the known slagging observations for coal combustion in boilers are used as the training data to acquire the correlation of the slagging indice. The partial least square regression (PLSR) method, coupled with cross-validation, is employed to develop the slagging indice. The study reported in this paper is mainly based on the available data for typical US coal, and the results are compared with the field observations for 30 sets of coals/blends combustion in boilers.

2 Mathematical models

2.1 Model assumptions

(i) Both the Fe_2O_3 content and total sulphur content are employed to represent the pyrite content in the US coals, which can be used to represent the severity of the initial slagging route [9, 11]. Therefore, it is assumed that the pyrite-induced initial slagging route can be accounted for by the amount of the Fe_2O_3 content and the total sulphur content.

(ii) The alkaline/alkali content is used to represent the initial slagging route (or fouling route) caused by condensation of the vapour species because the alkaline/alkali content is directly related to the accumulation of the fouling potential [13] and the alkali content is proportional to the content of the alkali phases in the flue gases [24, 25].

(iii) The SiO_2+Al_2O_3 content is considered in the model. This is because the acid components could have dual effects on the slag formation: (a) The high amount of acid components could increase the melting point and the viscosity of the ash [26], which can decrease the sintered/slagging propensity; (b) The acid components could possibly capture the alkali/alkaline components to decrease the alkali evaporation into flue gas [24, 25] as well as pyrite to decrease the formation of high molten Fe^{2+}-slag and Fe^{3+}-slag [27, 28], that can in turn decrease the initial slagging routes.

(iv) The melting capabilities of the major ash composition under oxidizing/reducing atmosphere are employed to represent the sintered/slagging route [29, 30]. This assumption is employed for all types of coals. In order to evaluate the melting capability, liquidus temperature (LT) is employed and predicted by using the chemical equilibrium calculations.

(v) For those coals with Fe_2O_3 as the major basic oxide, the deposition is formed mainly in the radiant section with the slag rich in the iron content [8]. However, for the coals with alkaline/alkali constituents as the major fluxing mineral, serious ash deposition (fouling) is observed in the convection section [31]. Hence coal ash can be classified into two types, the lignitic and bituminous types of ash [14, 32]. For lignitic type ash defined as the amount of either alkaline or alkali components being greater than the amount of Fe_2O_3, only the initial slagging route caused by the alkaline/alkali condensation is considered as the major initial slagging route. For bituminous type ash defined as the amount of Fe_2O_3 being greater than the amount of alkaline and alkali components, only the initial slagging route caused by the pyrite is considered as the major initial slagging route.

Therefore, based on the above assumptions, the proposed method to build the ash deposition indice is developed as follows: for bituminous type coal, the liquidus temperatures under the oxidizing atmosphere and the reducing atmosphere (LT_o and LT_r), the SiO_2+Al_2O_3 content, the Fe_2O_3 content and the total sulphur content can be employed as the independent variables; for lignitic type coal, the liquidus temperatures under oxidizing atmosphere and reducing atmosphere, the SiO_2+Al_2O_3 content, and the alkaline/alkali content can be employed as the independent variables. The overall slagging/fouling observations can be employed as the dependent variable. The partial least square regression (PLSR) technique, coupled with a cross validation method, is employed to obtain the correlation for the indice. This is because (a) in this work, the data of slagging observations is limited and the independent variables in the method to build the ash deposition indice are highly correlated, and (b) the PLSR method is specifically designed to deal with multiple regression problems where the number of observations is limited and the correlations between the independent variables are high [33].

2.2. Prediction of the liquidus temperature

The liquidus temperature is the temperature at which the first solid phase just starts to precipitate on the cooling of a slag-liquid oxide melt [21]. The temperature is predicted based on the major ash composition (Al_2O_3, SiO_2, Fe_2O_3, CaO, and MgO) by using the chemical thermodynamics software FactSage 6.4 [21]. The software is based on the minimization of the Gibbs free energy from the system subject to the mass balance constraints [34, 35].

The calculations were performed by using the equilibrium module together with the databases ELEM, FToxid, FTsalt and FACTPS. The slag model chosen in the calculations was the 'SLAGA' with possible 2-phase immiscibility [21]. Five major ash components (Al_2O_3, SiO_2, Fe_2O_3, CaO, and MgO) were included in the calculations; for lignite, Na_2O is also included due to its high amount; K_2O is excluded due to its low amount in the ash; however, the other components (SO_3 and P_2O_5) were also neglected due to the fact that S and P are volatile under high temperatures observed near the liquidus temperature [21]. It was assumed that all Fe was in the Fe^{3+} state under the oxidizing atmosphere because a large portion of iron is in the Fe^{3+} state for oxidizing conditions [36] and both the Fe^{2+} and Fe^{3+} states were considered under the reducing atmosphere.

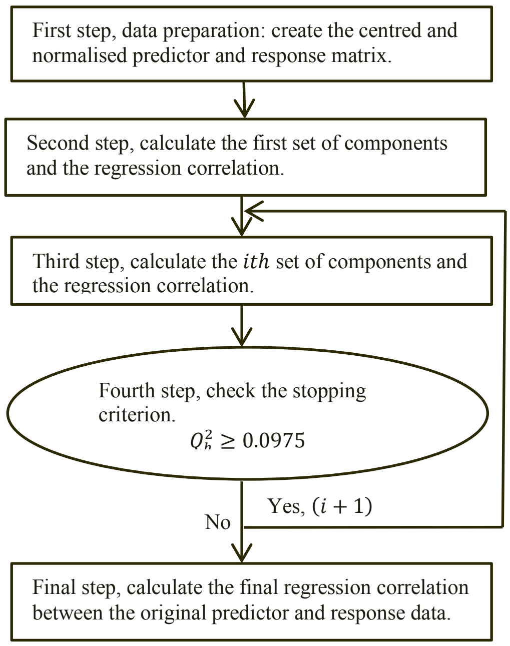

Fig. 2. The algorithm for the PLSR coupled with cross-validation.

2.3 PLSR and Cross-Validation

The Partial Least-Squares Regression (PLSR) technique is a mathematical technique that generalizes and combines features from a principal component analysis and multiple regression [37, 38]. Therefore, PLSR is able to analyse data of larger and highly correlated multivariate systems and it has a higher prediction ability than those obtained with multiple regression [38, 39], which is suitable for the present work because of the high correlation coefficients among the independent variables (liquidus temperature, Fe_2O_3, and alkaline/alkali components). The one-at-a-time form of cross-validation method, which is a criterion to calculate the predicted error sum of squares when leaving out a single observation, is often employed to determine the stopping criterion and the number of latent variables in the PLSR method [33, 37-39]. In this work, the algorithm of the PLSR, coupled with the cross-validation, is analysed and developed based on the Matlab platform as shown in Fig. 2. For more details about the PLSR and cross-validation method, see [33, 37-42].

3 Results and discussion

3.1 Application to boilers

Two representative cases of utility coals have been investigated: (i) Case 1 is the Eastern US bituminous coals/blends combusted in T-fired boilers; (ii) Case 2 is the Western US sub-bituminous or lignite coals/blends combusted in opposed-wall boilers. In this section, the results of the newly developed slagging indice predictions for the two cases are analysed.

Case 1 contains 13 sets of coal combustion data (including data for 6 sets of coal blends); Case 2 contains 17 sets of coal combustion data (including data for 10 sets of coal blends). The range of coals and ash properties for the 30 sets of US coals/blends studies are presented in Table 1. Bituminous coals have a higher Fe_2O_3, SiO_2 and Al_2O_3 contents compared to low rank coals but a lower content CaO and MgO contents. Both bituminous and sub-bituminous coals have low Na_2O and K_2O contents contrary to lignites that have higher levels of Na_2O. Slagging observations in boilers are evaluated by using not only the field performance data in the radiation and convection sections based on FEGT, soot blowing frequency increase, heat transfer rate, etc., but also periodic visual examinations of the deposit strength/ease of removal. The degrees of the slagging observations, ranging from no slagging to severe slagging, are represented using the values from 0 to 1. Also the field slagging observations can be classified into four groups: low slagging < 0.4; 0.4 ≤ medium slagging ≤ 0.6; 0.6 < high slagging ≤ 0.9; severe slagging >0.9.

Table 1.

Ash composition ranges for some US coals.

	Bituminous		Low rank coal			
			Sub-bituminous		lignite	
	Minimum	Maximum	Minimum	Maximum	Minimum	Maximum
SiO_2	44.8	55.9	32.2	41.8	34.3	37.7
Al_2O_3	20.5	28.7	16.4	22.5	16.7	18.2
Fe_2O_3	6.2	22.1	4.0	14.7	5.3	5.6
CaO	1.4	5.6	13.8	21.9	16.7	18.6
MgO	0.7	1.4	2.8	6.5	3.7	4.0
K_2O	1.2	2.6	0.5	1.5	0.3	0.5
Na_2O	0.3	1.3	1.0	1.3	6.3	6.7

Ash content	7.5	10.6	4.9	6.6	3.9	4.6
Sulfur	0.4	2.7	0.3	1.1	0.3	0.4
LHV (MJ/kg)	26.4	30.3	20.6	24.3	20.6	21.6

Based on the ash compositions listed in Table 1, the ash deposition indice for the bituminous type is calculated in Case 1 and the ash deposition indice for the lignitic type is calculated in Case 2. The training data, which cover fuels of low, medium and high slagging propensities, contain less than half of the total data set and therefore the testing data contain more than half of the total data set; see the Supporting Information for details. After performing the PLSR and Cross-Validation calculations, the correlations for calculating the ash deposition indice, I_d for these cases are as follows:

$$\text{Case 1: } I\_d = 4.75 + 10^{-4} \times (-11.1 * LT_o - 7.85 * LT_r) - 2.06 \times 10^{-2} * (SiO_2 + Al_2O_3) + 10^{-2} \times (2.06 * Fe_2O_3 + 10.2 * Sulfur) \quad (1)$$

$$\text{Case 2: } I\_d = 2.19 + 10^{-4} \times (-5.79 * LT_o - 3.42 * LT_r) - 6.31 \times 10^{-3} * (SiO_2 + Al_2O_3) + 3.53 \times 10^{-3} * (CaO + MgO) + 7 \times 10^{-3} * (Na_2O + K_2O) \quad (2)$$

For both cases, the liquidus temperature and $SiO_2 + Al_2O_3$ have negative coefficients, which implies that the predicted slagging observation will decrease with an increase in the liquidus temperature and $SiO_2 + Al_2O_3$. However, the parameters related to the initial slagging routes (Fe_2O_3, $Sulfur$, CaO+MgO and Na_2O+K_2O) have a positive coefficient which means that the predicted slagging/fouling observation increases with a higher content of these four parameters.

Figure 3 shows a comparison of the predicted and experimental slagging observations and the prediction errors. It can be found that, (i) the predicted results are close to the experimental results for both the training data and testing data, and (ii) the slagging predictions of the coal blends do not largely deviate from the slagging observations. In addition, the uncertainty of the predictions may be attributed to the number of the training data set. In our calculations, we tried the number from 5 to 9. The predicted average relative errors range from 16.8% to 19.3% for Case 1 and from 9.0% to 9.4% for Case 2, which indicates that the prediction performance may not be greatly affected by the number of the training data. Figure 4 illustrates a comparison between the predicted performance of the ash deposition indice, I_d in this study and some of the conventional slagging indices based on the ranked slagging observations. It can be observed that the ranking for the accuracy of the prediction performance from high to low is $I\_d > I\_Fe_2O_3 > I\_Si = I\_B/A > I\_B/A \times S > I\_Si/Al$ for Case 1 and $I\_d > I\_Si > I\_Si/$

$Al > I\_Fe_2O_3 > I\_B/A > I\_B/A \times S$ for Case 2, where $I\_Fe_2O_3$, I_Si, I_B/A, $I\_B/A \times S$ and I_Si/Al represent the slagging indice of Fe_2O_3 content, $SiO_2/(SiO_2 + Fe_2O_3 + CaO + MgO)$, $Basic\ content\ /Acid\ content$, $I\_B/A \times\ sulfur\ content$ and SiO_2/Al_2O_3 [14, 16]. It was found that 11 out of 13 coals and 15 out of 17 coals evaluated in Cases 1 & 2 respectively, were accurately predicted for slagging propensity by the proposed indice, I_d. In contrast, conventional slagging indices had limited success rates, ranging from 1 to 7 for case 1 (out of 13) and 0 to 12 for case 2 (out of 17). Therefore, the indice built by considering multi-slagging routes yields a higher success rate in classifying the overall slagging/fouling potential in boilers than that of the typical slagging indices.

In addition, Fig. 5 shows the predicted values using the new indice for Case 1 and Case 2 defined in Eq. (1) and Eq. (2) earlier versus the field slagging observations. It can be observed that the predicted value in the proposed ash deposition indice increases with the increasing value of the experimental slagging observations, which indicates that both the initial slagging routes and the sintered/slagging route increase with the field slagging/fouling observations classification. This is because the coexistent dual slagging (alkali vapour induced slagging and the overall melting induced slagging) inevitably occurs in boilers and dictates the overall slagging behaviours [43].

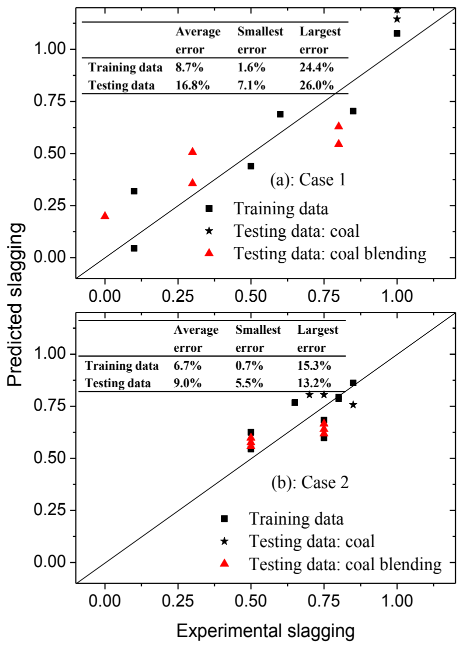

Fig. 3. Comparison of the slagging propensity between the predicted and experimental values and the prediction errors.

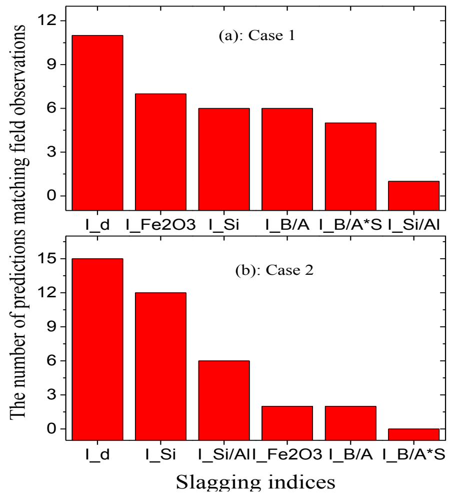

Fig. 4. Comparison of the prediction performance among the *I_d* and five slagging indices: the number of predictions matching field observations.

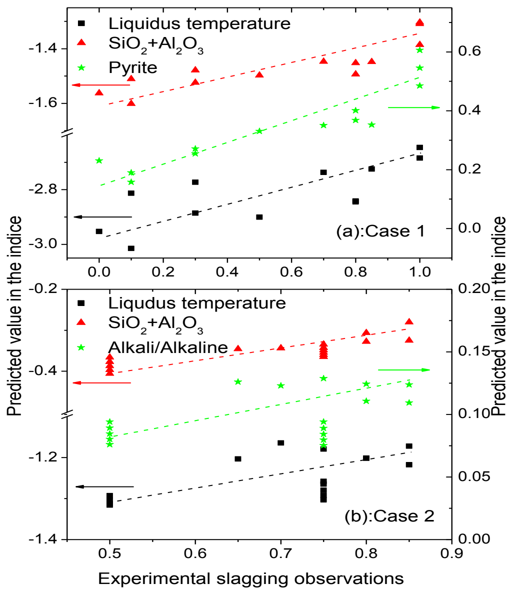

Fig. 5. The predicted values in the proposed indice by Liquidus temperature, SiO_2+Al_2O_3, pyrite for Case 1, and alkali+alkaline for Case 2 versus the field slagging observations.

3.2 Sensitivity of the method

Adding mineral additives is common practice in order to control the slagging and fouling problems in boilers. Therefore, the influence of adding acid components to coals that show higher deposition potential was investigated to test the sensitivity of the developed method.

Either SiO_2 or Al_2O_3 was added as an additive to three easy slagging/fouling US coals and the predicted values of the indice are plotted against the added SiO_2 or Al_2O_3 content of the fuel and the SiO_2/Al_2O_3 ratio as shown in Fig. 6. The sensitivity study indicates that by adding either SiO_2 or Al_2O_3 can reduce the predicted slagging potential. This is because the added acid components could reduce the melting potential due to the increase in the liquidus temperature. In addition, the acid components could capture the alkali/alkaline vapour phase to decrease the condensation potential. Also the analysis shows that the value of the predicted slagging potential decreases more rapidly by using Al_2O_3 than when adding SiO_2. Van Dyk et al. [44] and Li et al. [45] also found that Al_2O_3 is more effective than SiO_2 due to its higher ability to increase the ash fusion temperature than that of SiO_2. However, the analysis shown in the right section of Fig. 7, indicates an opposite trend corresponding to the SiO_2/Al_2O_3 ratio when adding SiO_2 compared to adding Al_2O_3. It is noticed that Song et al. [20] found that ash fusion temperatures (AFTs) are increased with increasing the SiO_2/Al_2O_3 ratio from the fusion experiments and chemical equilibrium calculations. However, Liu et al. [46] found that AFTs are decreased with increasing the SiO_2/Al_2O_3 ratio from the fusion experiments. This is because, see Ref. [20], the SiO_2 was added into the ash with a relatively low CaO content (approximately 15%) and adding the SiO_2 can lead AFTs to move from the low temperature region into the high temperature region [20]; However, see Ref. [46], when the SiO_2 is added into the ash with relatively high CaO content (approximately 40%) the added SiO_2 can react with CaO to generate the low-melting anorthite and gehlenite and this leads the AFTs to move from a high temperature region to a low temperature region [46]. In this study, all the three coals with higher slagging propensity have relatively low/medium CaO content (ranging from 2.9% to 21.8%) and adding either SiO_2 or Al_2O_3 could increase the liquidus temperature from the chemical equilibrium calculations. In addition, further calculations, using chemical equilibrium methods, were undertaken to investigate the influence of the SiO_2/Al_2O_3 ratio on the melting potential. In the calculations: (i) In addition to the three coals tested in this study, coal ashes from Ref. [20] and [46] were chosen; (ii) the SiO_2/Al_2O_3 ratio is considered by changing the individual amounts of SiO_2 and Al_2O_3 simultaneously, holding the total sum (SiO_2 + Al_2O_3) as constant. Figure 7 shows the effect of the SiO_2/Al_2O_3 ratio on the liqudius temperature. It can be observed that, basically, the liqudius temperature decreases with increasing the SiO_2/Al_2O_3 ratio for all coal ashes, which means that ash fusion and slagging potential are increased with an increase in the SiO_2/Al_2O_3 ratio. This is because the Al_2O_3 content increases with a decrease in the SiO_2/Al_2O_3 ratio when the total amount of SiO_2 and Al_2O_3 is not changed. Careful consideration of all scenarios is required when using the parameter (SiO_2/Al_2O_3 ratio) to predict the melting behaviours and slagging potential. Both the ash composition of the original coal and the way in which the SiO_2/Al_2O_3 ratio changes can influence the effect of the SiO_2/Al_2O_3 ratio on the fusion and slagging potential.

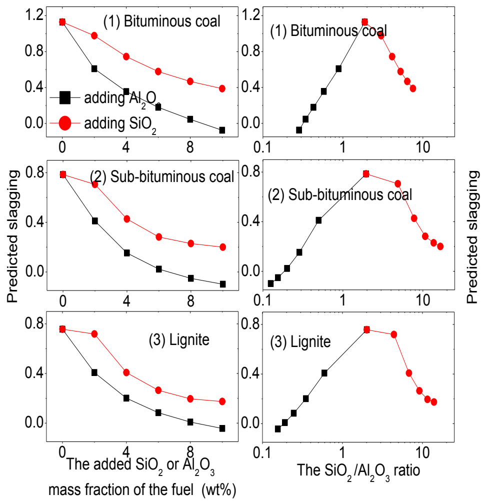

Fig. 6. Values of the proposed indice as a function of the added SiO_2 or Al_2O_3 mass fraction of the fuel and as a function of the SiO_2/Al_2O_3 ratio.

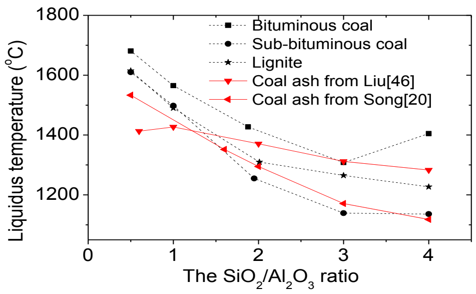

Fig. 7. Effect of the SiO_2/Al_2O_3 ratio on the liqudius temperature.

3.3 Remarks on the implementation of the method

In this paper a new method is developed based on the ash chemistry, without considering the complex particle transport and rebounding mechanisms, to build an ash deposition indice for firing US coals and their blends in boilers. The predicted results of the developed indice and five other existing slagging indices have been compared with the slagging observations for the 30 US coals/blends with a history of ash deposition issues. The indice built by using the proposed method yields a higher success rate in classifying the overall slagging/fouling potential in boilers than those existing slagging indices. It is postulated that this method has a potential to be used as an alternative tool to build an ash deposition indice for industrial use with a better prediction performance compared to existing slagging indices. In addition, an advantage of this method is that the newly developed indice based on the known slagging/fouling history from multiple boiler units makes it more suitable for different boiler configurations and coal types, although some of the aspects regarding the ash chemistry need to be further investigated in order to improve the accuracy and extend the application range of the proposed method. Without addressing the specific conditions in a boiler, the performance of a predictive method could be less accurate [47]. The index reported in this study does not consider the combustion conditions explicitly in its formulation and this may be limited to the conditions observed in the units used to validate the index. Incorporating changes in combustion conditions could be an ideal path moving ahead to further improve the accuracy of this index.

It should be noted that the initial slagging route caused by the pyrite is represented by the contents of Fe_2O_3 and sulphur for US coals since they are known to contain iron, predominantly in the form of pyrite [11]. The distribution of pyrite within the coal samples is important to predict the ash deposition behaviour. Excluded pyrite could generate molten phases under lower temperature and under a reducing atmosphere [3, 7-9]. High density and spherical shape of the molten phases facilitate their arriving at the furnace wall surface [9]. The included pyrite may react with the clay or quartz minerals to generate the aluminosilicate slag [3, 11]. However, siderite may be the dominant iron-bearing mineral for many other coals, such as South African and Australian coals. Although some researchers considered that in addition to pyrite, its contribution to deposition formation [11, 12] needs further investigation. Furthermore, it should be noted that, this study accounts for all of the alkaline/alkali species as active contributors to condensation formation and this is primarily for low rank coals where the alkaline/alkali species are organically-bound [7, 47]. However, not all of the alkaline/alkali components are considered as active forms, except for those leachable by water and weak acids [43, 47, 48]. Taking into consideration these factors could increase the accuracy of predicting deposit formation from alkali condensation. Also, it should be noted that the ash loading, which can affect the deposit accumulation in boilers [10], is not considered in the proposed slagging indice because there is no significant difference in the ash loading for the tested US coals. However, if there exists a great difference in the ash loading, the parameter should be considered in the prediction model and this can be done by using the value of the ash compositions/ ash loading to replace the existing value of ash compositions [1, 10].

4 Conclusions

A novel method to build an indice is developed and used for predicting the overall slagging/fouling potential of coal/blends combustion in boilers. The method couples the initial slagging route caused either by pyrite or by alkaline/alkali components and the sintered/slagging route. The initial slagging route is predicted based on the corresponding ash components and the sintered/slagging route is predicted based on the overall melting potential using the liquidus temperature calculated from chemical equilibrium methods. Utilizing the available slagging observation data from US coal fired boilers, PLSR coupled with the cross validation method was employed to develop the new ash deposition indice.

It should be noted that both SiO_2 and Al_2O_3 can reduce the slagging potential, but the drop in slagging propensity is more significant by adding Al_2O_3 compared to SiO_2 as confirmed by chemical equilibrium calculations. Finally, using the SiO_2/Al_2O_3 ratio alone to predict the melting behaviours and slagging potential of coals is inaccurate owing that the SiO_2/Al_2O_3 ratio alone cannot dictate the overall melting behaviour. The proposed method has been validated against the field performance of slagging observations on 30 sets of US coals/blends combusted in utility boilers. The results obtained indicate that the developed indice shows a much higher success rate for ranking the overall slagging potential in boilers than the other five conventional slagging indices.

Acknowledgment

The authors wish to thank Jaspal Saini (Electric Power Research Institute) for the helpful discussions on the deposition behaviors in boilers. Also X. Yang would like to acknowledge the China Scholarship Council, the University of Sheffield and the University of Leeds, for funding his research studies. The authors also acknowledge the support from the EPSRC grants (EP/M015351/1, Opening New Fuels for UK Generation; EP/K02115X/1, Development and Evaluation of Sustainable Technologies for Flexible Operation of Conventional Power Plants).

Appendix A. Supplementary data

References

[1] R.M. Hatt, Prog. Energ. Combust. 16 (4) (1990) 235-241.

[2] H. Bilirgen, Fuel 115 (2014) 618-624.

[3] R.W. Bryers, Prog. Energ. Combust. 22 (1) (1996) 29-120.

[4] J.P. Hurley, S.A. Benson, Energy Fuels 9 (5) (1995) 775-781.

[5] E.A. Sondreal, P.H. Tufte, W. Beckering, Combust. Sci. Technol. 16 (3-6) (1977) 95-110.

[6] P.M. Walsh, A.F. Sarofim, J.M. Beer, Energy Fuels 6 (6) (1992) 709-715.

[7] T.F. Wall, Proc. Combust. Inst. 24 (1) (1992) 1119-1126.

[8] G.P. Huffman, F.E. Huggins, N. Shah, A. Shah, Prog. Energ. Combust. 16 (4) (1990) 243-251.

[9] R.W. Borio, J.R.R. Narciso, J. Eng. Power 101 (4) (1979) 500-505.

[10] M.U. Degereji, D.B. Ingham, L. Ma, M. Pourkashanian, A. Williams, Fuel 102 (2012) 345-353.

[11] A.R. McLennan, G.W. Bryant, C.W. Bailey, B.R. Stanmore, T.F. Wall, Energy Fuels 14 (2) (2000) 349-354.

[12] W.H. Gibb. The UK Collaborative Research Programme on Slagging Pulverised Coal-Fired Boilers: Summary of Findings. In: Baxter L, DeSollar R, editors. Applications of Advanced Technology to Ash-Related Problems in Boilers, 1996, p. 41-65.

[13] H. Namkung, L.-H. Xu, T.-J. Kang, D.S. Kim, H.-B. Kwon, H.-T. Kim, Appl. Energy 102 (2013) 1246-1255.

[14] J. Barroso, J. Ballester, A. Pina, Fuel Process. Technol. 88 (9) (2007) 865-876.

[15] A.M. Beckmann, M. Mancini, R. Weber, S. Seebold, M. Müller, Fuel 167 (2016) 168-179.

[16] J. Barroso, J. Ballester, L.M. Ferrer, S. Jiménez, Fuel Process. Technol. 87 (8) (2006) 737-752.

[17] C. Mueller, M. Selenius, M. Theis, B.-J. Skrifvars, R. Backman, M. Hupa, et al., Proc. Combust. Inst. 30 (2) (2005) 2991-2998.

[18] E. Raask, Mineral impurities in coal combustion: behavior, problems, and remedial measures, Hemisphere Publishing Corporation, New York, USA, 1985, p. 196-197.

[19] S. Su, J.H. Pohl, D. Holcombe, J.A. Hart, Fuel 80 (9) (2001) 1351-1360.

[20] W.J. Song, L.H. Tang, X.D. Zhu, Y.Q. Wu, Z.B. Zhu, S. Koyama, Energy Fuels 24 (1) (2010) 182-189.

[21] E. Jak, Fuel 81 (13) (2002) 1655-1668.

[22] M.U. Degereji, S.R. Gubba, D.B. Ingham, L. Ma, M. Pourkashanian, A. Williams, J. Williamson, Fuel 108 (2013) 550-556.

[23] M.U. Garba, D.B. Ingham, L. Ma, M.U. Degereji, M. Pourkashanian, A. Williams, Fuel 113 (2013) 863-872.

[24] L. Xu, J. Liu, Y. Kang, Y. Miao, W. Ren, T. Wang, Energy Fuels 28 (9) (2014) 5640-5648.

[25] H.B. Vuthaluru, Fuel 78 (15) (1999) 1789-1803.

[26] K.S. Vorres, J. Eng. Power 101 (4) (1979) 497-499.

[27] B. Q. Dai, X. Wu, A. De Girolamo, L. Zhang, Fuel 139 (2015) 720-732.

[28] B. Q. Dai, X. Wu, A. De Girolamo, J. Cashion, L. Zhang, Fuel 139 (2015) 733-745.

[29] X. Yang, D. Ingham, L. Ma, A. Williams, M. Pourkashanian, Fuel 165 (2016) 41-49.

[30] C. Wieland, B. Kreutzkam, G. Balan, H. Spliethoff, Appl. Energy 93 (2012) 184-192.

[31] S.A. Benson, J.P. Hurley, C.J. Zygarlicke, E.N. Steadman, T.A. Erickson, Energy Fuels 7 (6) (1993) 746-754.

[32] G. F. Moore, R. F. Ehrler, J. Eng. Power 98 (1) (1976) 97-102.

[33] M. Zhang, H. Mu, G. Li, Y. Ning, Energy 34 (9) (2009) 1396-1400.

[34] C.W. Bale, E. Bélisle, P. Chartrand, S.A. Decterov, G. Eriksson, K. Hack, et al., Calphad 33 (2) (2009) 295-311.

[35] L. Fryda, C. Sobrino, M. Cieplik, W.L. van de Kamp, Fuel 89 (8) (2010) 1889-1902.

[36] A.R. McLennan, G.W. Bryant, B.R. Stanmore, T.F. Wall, Energy Fuels 14 (1) (2000) 150-159.

[37] H. Abdi, Partial least square regression (PLS regression), in: M. Lewis-Beck, A. Bryman, T. Futing, Encyclopedia of Social Sciences Research Methods, Sage, Thousand Oaks, CA, 2003, p.792-795.

[38] H.W. Wang, Partial least-squares regression-method and applications, National Defense Industry Press, Beijing, China, 1999, p. 97-104.

[39] M. Seggiani, G. Pannocchia, Ind. Eng. Chem. Res. 42 (20) (2003) 4919-4926.

[40] S. Wold, M. Sjöström, L. Eriksson, Chemometr. Intell. Lab. 58 (2) (2001) 109-130.

[41] A. Lorber, L.E. Wangen, B.R. Kowalski, J Chemometr. 1 (1) (1987) 19-31.

[42] X.Q. Wen. *Predicting the Regularity of the Fouling Characteristics of Heat Exchanger Equipments*, PhD thesis, North China Electric Power University, Beijing, China, 2013.

[43] Y. Niu, Y. Zhu, H. Tan, X. Wang, S.e. Hui, W. Du, Proc. Combust. Inst. 35 (2) (2015) 2405-2413.

[44] J.C. van Dyk, F.B. Waanders, Fuel 86 (17–18) (2007) 2728-2735.

[45] Q.H. Li, Y.G. Zhang, A.H. Meng, L. Li, G.X. Li, Fuel Process. Technol. 107 (2013) 107-112.

[46] B. Liu, Q. He, Z. Jiang, R. Xu, B. Hu, Fuel 105 (2013) 293-300.

[47] R.W. Borio, A.A. Levasseur. Coal Ash Deposition in Boilers. In: editors. Mineral Matter and Ash in Coal, 1986, p. 288-302.

[48] D. Nutalapati, R. Gupta, B. Moghtaderi, T.F. Wall, Fuel Process. Technol. 88 (11–12) (2007) 1044-1052.

Figure Captions

Fig. 1. Schematic of the ash deposition routes in boilers (modified from [1, 7, 8]).

Fig. 2. The algorithm for the PLSR coupled with cross-validation.

Fig. 3. Comparison of slagging propensity between the predicted and experimental values and the prediction errors.

Fig. 4. Comparison of the prediction performance among the I_d and five slagging indices: the number of predictions matching field observations.

Fig. 5. The predicted values in the proposed indice by Liquidus temperature, SiO_2+Al_2O_3, pyrite for Case 1, and alkali+alkaline for Case 2 versus the field slagging observations.

Fig. 6. Values of the proposed indice as a function of the added SiO_2 or Al_2O_3 mass fraction of the fuel and as a function of the SiO_2/Al_2O_3 ratio.

Fig. 7. Effect of the SiO_2/Al_2O_3 ratio on the liqudius temperature.