Trans Indian Inst Met (2020) 73(1):207–214
https://doi.org/10.1007/s12666-019-01823-9

TECHNICAL PAPER

Viscosity Analysis of Indian Origin Coal by Using FactSage at Different Temperatures

Priya Ranjan Mishra[1] · Rina Sahu[1] · Sanchita Chakravarty[2]

Received: 2 July 2019 / Accepted: 11 October 2019 / Published online: 24 October 2019
© The Indian Institute of Metals - IIM 2019

Abstract Slagging of the ash inside the furnace boiler causes operational problems such as furnace shutdowns and low heat exchange efficiency. To avoid this problem, ash fusion temperature (AFT) parameter has been well accepted for determining the ash fusion characteristics since many years. In this paper, an extensive study has been conducted on the deposition characteristics of ash particles based on the viscosity and phase transformation properties in boiler operation. The FactSage thermodynamic software package is utilized for the phase transformations and viscosity predictions of coal ash in furnace operating temperatures. The effect of solid or crystalline fractions in slag phase on the viscosity is calculated by using the Roscoe equation. Calculations show that an increase in solid fractions increases the viscosity of the slag phase. AFT analysis of coal samples for the present study shows that their IDT and FT values are higher than 1340 °C and 1470 °C, respectively. The reason for the high IDT and FT in Indian origin coals is the formation of high-temperature-stable phases—tridymite and sillimanite. Furthermore, the numerical viscosity models developed by using the Roscoe viscosity equation are correlated with the experimental AFT results.

Keywords Viscosity · FactSage · AFT · Crystalline phases · Phase transformations

✉ Priya Ranjan Mishra
mishranit90@gmail.com

[1] Metallurgical and Materials Engineering, National Institute of Technology, Jamshedpur, India

[2] CSIR-NML-ANC Division, Jamshedpur, India

1 Introduction

In India, electricity production has expanded dramatically to ease the energy shortages throughout the country. Most of the newly established power generation plants will be fueled by Indigenous coal resources to reduce the overall cost burden of imported coals. However, Indian coals are characterized by high ash content (20–40 wt%) as compared to imported coals (7.5–15 wt%), while in the case of sulfur content, this scenario is opposite because Indian origin coal has very less sulfur content which is advantageous in low greenhouse gaseous emissions [1].

High ash content in the Indian coal causes problems such as furnace shutdowns and low efficiency in the heat exchangers. It is important to understand the ash characteristics in the boilers for efficient operation. Many researchers have stated that ash fusion temperature (AFT) parameter gives a good idea on the stability and fusion characteristics of ash in boilers and gasifiers. However, this parameter is useful only in finding fusion temperatures and flow properties. AFT does not give any information about phase transitions and first slag melt temperature characteristics of coal ash. AFT of the coal ash is dependent on the composition, heating rates and several other factors [2]. A lot of work has been done on the dependency of AFT on the ash composition of coal. Gupta et al. [3] studied the progressive changes in chemical characteristics and ash fusion mechanisms on the shrinkage of coal ash when it is heated. It can be seen that the temperature corresponds to 50% of the shrinkage in the thermomechanical analysis test which is related to extensive melting of phase. Various authors expressed the ash fusibility with respect to the acid-to-base ratio in the coal ash and the effect of different oxide compounds in coal ash on the fusion temperatures and viscosity [4, 5].

Many researchers had reported the applications of the FactSage thermodynamic software for a better understanding of mineral composition effect on the AFT of the coal ash [6–8]. Hanxu et al. [9] used the FactSage thermodynamic software for estimating the ash behavior and fusion temperatures of Huainan coal ash samples. They observed that experimental AFT results are in good agreement with the thermodynamic analysis of slag phase formation temperature using FactSage software. Song et al. [2] worked on the thermodynamic study of liquidus temperature of different coal ash contents and observed the variations in the liquidus temperature and viscosity with respect to CaO, MgO, SiO_2, Al_2O_3 and Fe_2O_3 content in coal ash using the FactSage thermodynamic software.

1.1 Objective

Coal ash fluxing is used for the cleaning of ash deposits in boiler and gasifiers. The limiting requirement for slag viscosity and temperature can vary from 5 to 25 Pa and 1100 °C to 1500 °C, respectively, based on the boiler type [10]. The present study helps in resolving the different kinds of issues related to selection of coals to achieve the required characteristics and to know the appropriate fluxing temperatures for a particular boiler. The objective of the present study is to develop a general viscosity model which can be used to find the appropriate slagging or fluxing temperatures in boilers for respective coals based on their viscosities. The experimental AFT analysis and thermodynamic calculations using FactSage software are correlated with the effect of composition on the first melt slag temperature, liquidus temperature and viscosity of the coal ashes.

2 Experimental Work

2.1 Materials and Methods

Five Indian origin coal ash samples were collected for the study. MSRB1(M1), MSRB2(M2), MSRB3(M3), MDNR12(M12) and MDNR24(M24) samples belonged to Salanpur, Raniganj coalfield region. As-received coal samples were crushed to (−)72 mesh size for the AFT and XRF analysis. Ash fusion temperature of the samples was analyzed according to ASTM D1857 standard [8, 11, 12].

Ash fusion temperature analysis for the ash samples was correlated by using the basicity index (B) of the samples. Chemical composition of the ash was determined by using X-ray fluorescence. Thermodynamic analysis of the compounds and the liquidus phase formation during ash preparation was performed through the CALPHAD approach.

2.2 FactSage Modeling

FactSage is a thermodynamic software package, which is a merger of two well-known computational thermochemical packages: Fact-Win and ChemSage. It is well known for predicting metallurgical processes, multi-phase equilibria, liquidus temperature and chemical and metallurgical process modeling. FactSage consists of several thermodynamic calculation modules such as (1) Reaction, (2) Equilibria, (3) Predom, (4) Phase Dia and (5) E-Ph. Multiphase equilibrium and liquidus temperatures in the present study are calculated by using the 'Equilibria' and 'Phase Dia' modules [13, 14]. Gibbs free energy minimization and the modified non-ideal associate species models are used for the phase equilibrium and liquidus temperature calculations, respectively. Gibbs free energy of the pure substances and solution phases is modeled by using the Meyer and Kelley and Redlich–Kister polynomial equations, respectively [15, 16]. FTOxid database is used for the present thermodynamic calculations.

2.3 Viscosity Modeling

2.3.1 *Viscosity Calculations Using FactSage*

Viscosity model in the FactSage 6.4 has been used to calculate viscosity. Molecular theory and Arrhenius equation were used for measuring viscosity of the slags.

$$\eta = A\exp\left(\frac{E}{RT}\right) \quad (1)$$

2.3.2 *Viscosity Calculations Using Modified Urbain Model*

The viscosity of the coal ash is calculated using the Kalmanovitch or modified Urbain model [17–20]. The advantage of the modified Urbain model is that, it can be effective for predicting the viscosity of both raw coal ash composition and simple slag phase or oxide glass phase melt. In the Urbain model, the entire composition of the ash is assumed to be in a liquid or molten state. For these calculations, all the Fe_2O_3 in the raw coal sample is taken into FeO form. The equations related to the viscosity calculations by using the Urbain model are given in Fig. 1.

2.3.3 *Roscoe Equation of Viscosity*

The Urbain model does not give any idea about the viscosity of solid–slag colloidal mixtures. There are numerous equations proposed for determining the viscosity of these kind of mixtures. In this study, the Roscoe equation has been used to calculate the effect of fraction of solid particles on the viscosity of slag mixtures.

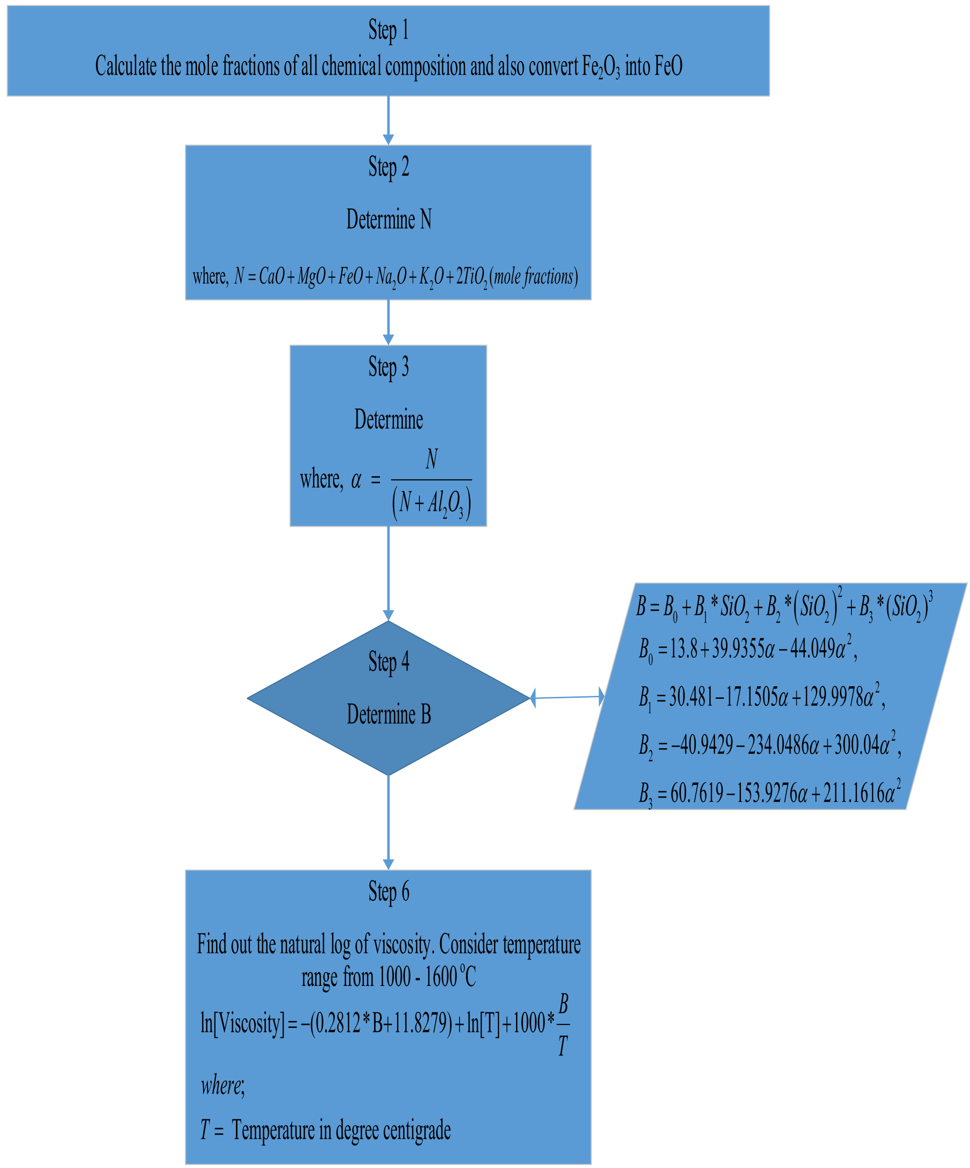


Fig. 1 Urbain model viscosity process

$$(V_{is})_S = (V_{is})_L (1 - f_s)^{-2.5} \quad (2)$$

where $(V_{is})_S$ is the viscosity of slag-solid suspension, $(V_{is})_L$ is the viscosity of slag liquid and (f_s) is the fraction of liquid.

The fraction of solid phases and composition of the slag phase at different temperatures have been calculated by using FactSage software.

3 Results and Discussion

3.1 Elemental Analysis of the Samples

Elemental composition of coal is an indicator of mineral species present in coal samples and also predicts the behavior of AFT. Chemical composition of ash samples is given in Table 1. It shows that silicon, aluminum, iron, titanium and calcium are the major elements present in MSRB1, MSRB2 and MSRB3 ash samples. MDNR12 and MDNR24 samples contain major elements silicon, aluminum and iron. Potassium, sodium, phosphorus and sulfur are the minor elements present in MSRB1, MSRB2 and MSRB3 samples. SiO_2 content (60.02–70.7%) and Al_2O_3 content (23.6–27.12%) are the most predominant phases for the coal seam samples. The overall quality of all coal seams of Talcher and Salan coalfields studied in the work is identical.

3.2 AFT Analysis

The behavior of ash fusibility is an important factor for the calculation of efficiency of the boiler plant. Table 2 shows

Table 1 Chemical composition of coal ash

Sample ID	SiO_2%	Al_2O_3%	Fe_2O_3%	K_2O%	TiO_2%	CaO%	MgO%	Na_2O%	P_2O_5%	SO_3%
MSRB1	60.02	25.25	4.5	0.87	3.34	3.13	1.86	0.15	0.35	0.53
MSRB2	60.5	27.12	3.96	0.99	2.13	3.06	0.97	0.06	0.38	0.24
MSRB3	61.7	25.56	2.96	0.78	2.6	3.63	1.15	0.14	0.84	0.64
MDNR12	66.9	24.8	2.4	0.38	1.5	1.0	0.5	0.26	0.03	0.08
MDNR24	70.7	23.6	1.2	0.39	1.3	0.2	0.5	0.29	0.06	0.09

Table 2 Fusion temperature of coal ashes

Sample ID	IDT (°C)	ST (°C)	HT (°C)	FT (°C)
MSRB1	1340	1370	1390	1470
MSRB2	1350	1380	1460	> 1500
MSRB3	1390	1410	1470	> 1500
MDNR12	1360	1390	1470	> 1500
MDNR24	1370	1390	> 1500	> 1500

the ash fusion temperature analysis of the respective coal ash samples. It shows that fusion temperature has increased with an increase in silica content. The presence of high silica content in ash increases the AFT temperature along with P_2O_5 and other acidic oxides. The content of calcium and iron is believed to be an indicator of ash fusion properties. The initial deformation temperature (IDT) for the five ash samples is higher than 1340 °C. The major reason for higher AFT value is the existence of acidic compounds in the coal ash ($SiO_2 + Al_2O_3 + TiO_2$). The S/A (SiO_2/Al_2O_3) ratio of coal samples are higher than 2.0 (2.377, 2.230, 2.41, 2.697 and 2.995), respectively, which is accountable for FT => 1470 °C [21]. Table 2 shows a similar range of AFTs for all the samples, which suggests similar mineral phase composition in all coal samples studied. Furthermore, basicity in coal ash (Fe_2O_3, CaO and MgO) and alkalis (Na_2O and K_2O) has a fluxing effect on SiO_2 and Al_2O_3, thereby reducing the fusion point of ash.

3.3 Thermodynamic Modeling

Phase equilibrium calculation has been done by FactSage 6.4 software 'Equilib' module. FToxid and FactPS databases are selected for the calculations. The weight percentage of the components obtained from the XRF analysis of coal ash sample is fed into the Equilibria module input. FT-SlagA is selected for the liquid phase or slag phase calculation. Equilibrium calculations are done by varying the temperature from 25 to 1600 °C and maintaining the pressure at 1 atm.

Figures 2, 3, 4, 5 and 6 show the variation of coal composition with temperature. At lower temperature, quartz is a major phase. It also shows that tridymite and sillimanite are the major phases in all coal samples. At 825 °C, quartz is transformed into tridymite phase. The samples, which contain higher Al_2O_3 content, show andalusite and sillimanite phases in the equilibrium calculation. The presence of sillimanite phase increases the final liquidus temperature of slag constituent. MgO forms a low-temperature fusion phase cordierite by combining with Al_2O_3 and SiO_2, which reduces the final liquidus temperature. Fusion temperature can be labeled as the 50% of the slag phase formation, and our study depicts that fusion temperature for all the samples is above 1400 °C.

3.4 Viscosity

Figure 7 represents $\ln(\eta)$ values of different coal ash samples by using FactSage calculation, and Fig. 8 represents the process used for viscosity calculation by using the Urban model. From both the calculations, it is evident that viscosity value decreases rapidly with an increase in temperature. MSRB1, MSRB2 and MSRB3 coal ash samples show high viscosity at all temperatures by using the Urbain model, while in the FactSage calculations, M24 sample shows high viscosities. This difference is may be due to the consideration of composition effect in the Urbain model. Equilibrium plots for the coal ash samples also show that M24 ash sample has a maximum amount of solids at all temperatures compared to other samples. AFT calculations also predict that the M24 sample has higher HT and AFT temperatures compared to other samples. From these calculations, we can say that FactSage software can be a very effective tool for predicting the phase changes and fusion behavior for ash samples.

In general, the average viscosity calculations by using the Urbain model with the initial coal composition give no idea of the actual viscosities of slag proportions, because the Urbain model calculations does not consider the solid fractions in slag phase, which leads to large deviations from the actual values. In order to determine the effect of

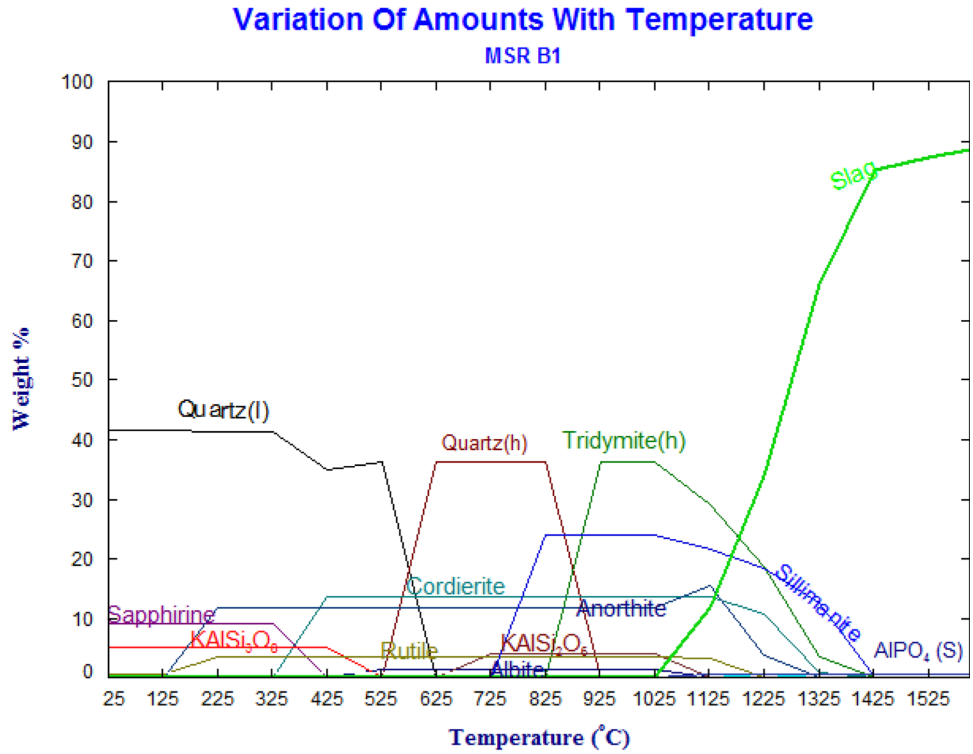


Fig. 2 Decomposition of coal with temperature for MSRB1

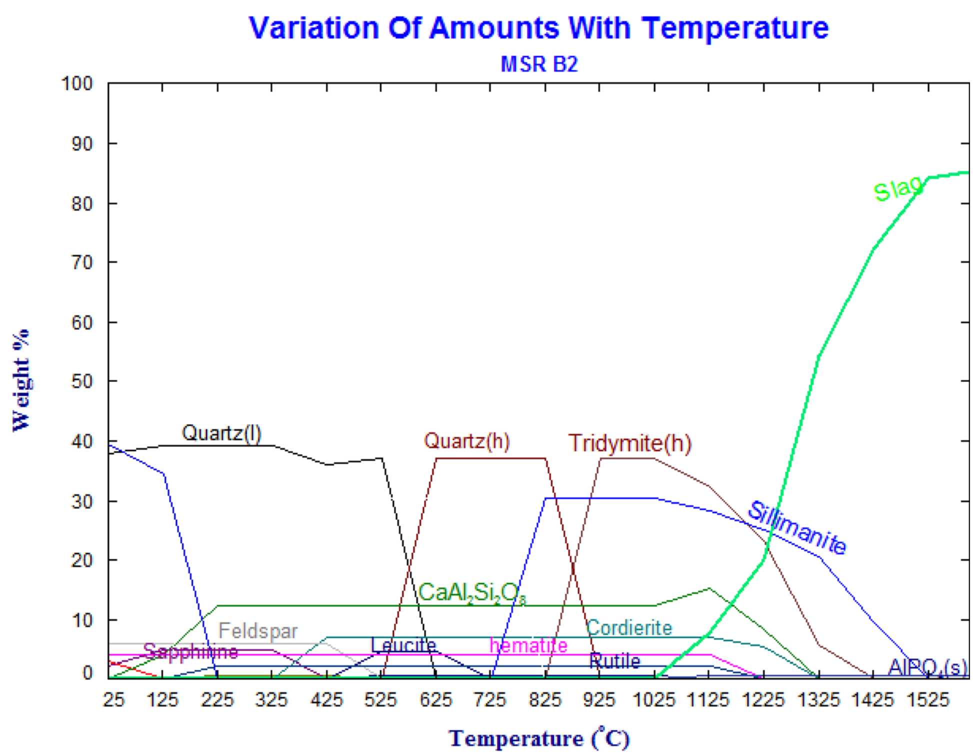


Fig. 3 Decomposition of coal ash with temperature for MSRB2

solid fractions, as well as the basicity of slags, the composition of the slag phase and amount of solid fractions obtained from the FactSage calculations are used. The variations of solid fractions with respect to temperature are shown in Table 3. The effect of solid fractions on the viscosity is calculated by using the Roscoe equation. Figures 8 and 9 indicate the log viscosity calculations by using the Urbain model and Roscoe model. It is clear from the figures that the viscosities determined by specific slag compositions and solid fractions differ largely from the

Fig. 4 Decomposition of coal with temperature for MSRB3

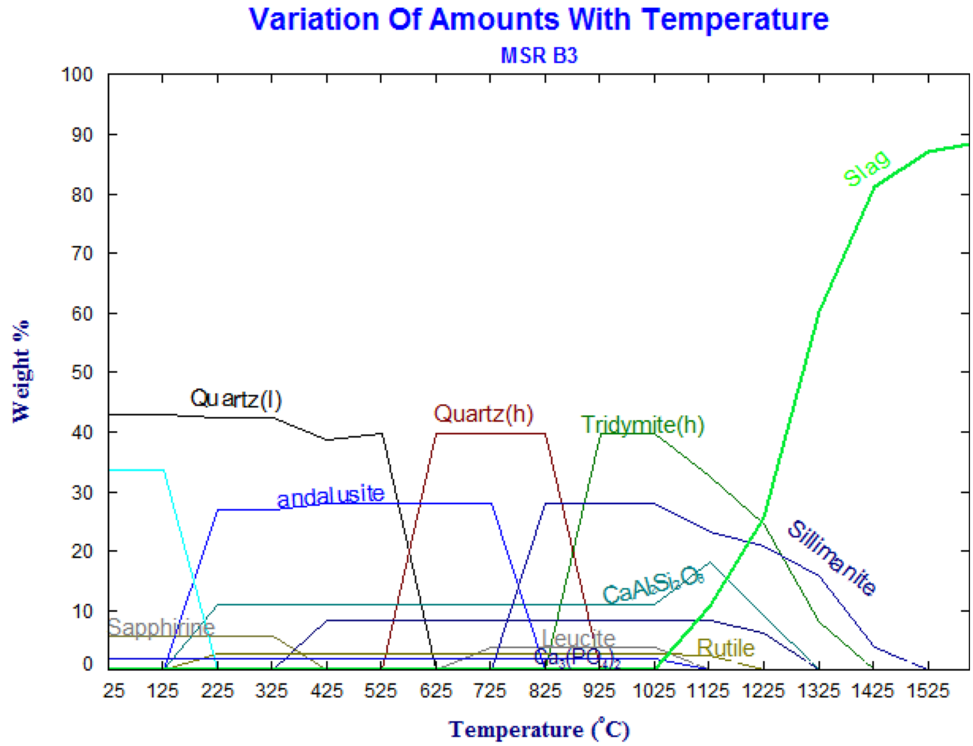
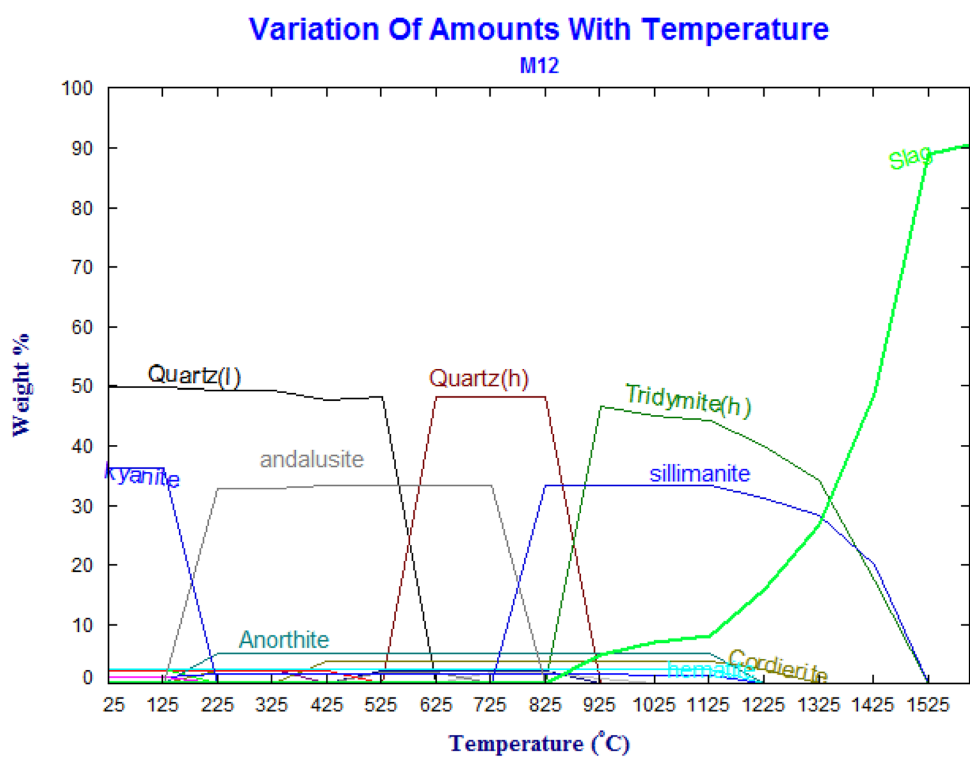


Fig. 5 Decomposition of coal with temperature for MDNR12



Urbain model viscosities at a specific temperature. In the Urbain model, coal ashes lie in the molten zone at temperatures below the AFT, while, in the case of the Roscoe model, all the ash samples turn into strong deposits above 1300 °C, which is comparable with the IDT temperatures for all samples. Molten state exhibits for all the slag samples after 1600 °C, which is related to the fusion temperature calculations in actual AFT analysis. Actual AFT calculations also show that IDT temperatures are low for MSRB1 and MSRB2 samples as compared to others.

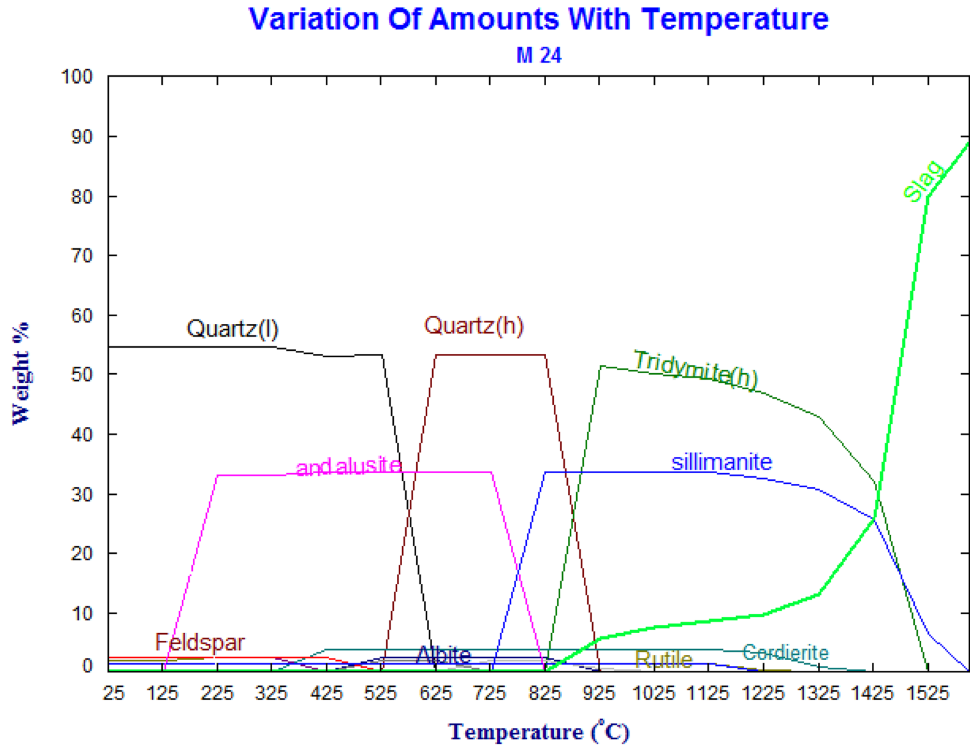


Fig. 6 Decomposition of coal with temperature for MDNR24

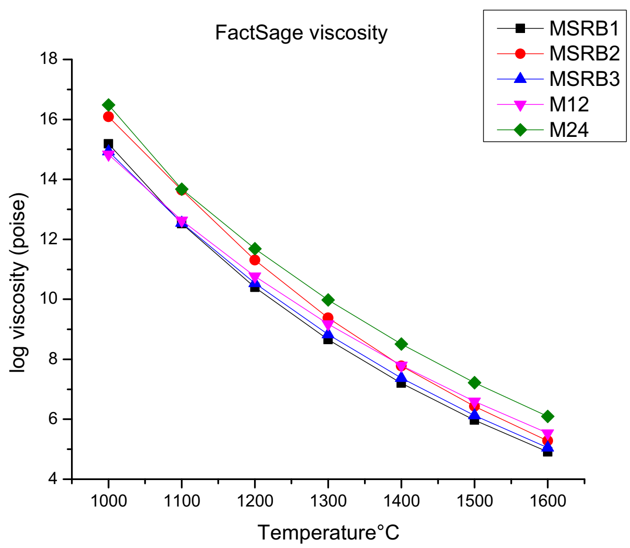


Fig. 7 ln (viscosity) of FactSage

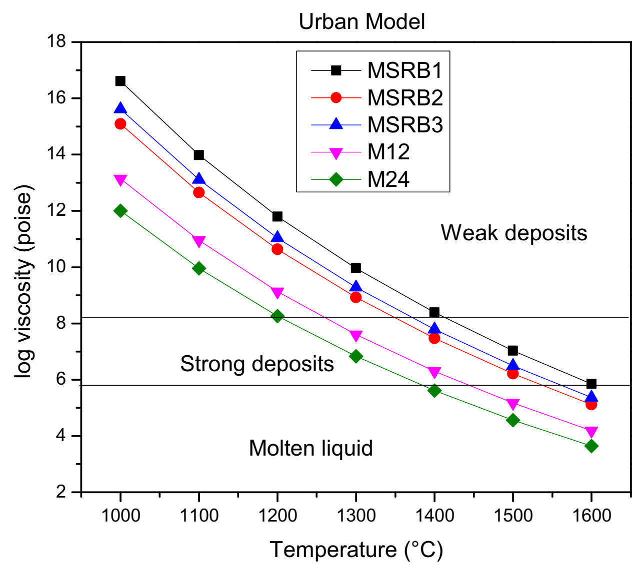


Fig. 8 ln (viscosity) by using Urbain model

From Table 3, it is evident that the solid fraction decreases with an increase in temperature for each coal. The calculated viscosities are high compared to the normal Urbain model. The major reason for the stability of solid fractions at high temperature is the sillimanite phase, which is shown in thermodynamic curves. Actual AFT calculation also shows that IDT temperatures are low for MSRB1 and MSRB2 samples.

4 Conclusion

A viscosity model that correlates the real-time AFT analysis values and thermodynamic calculations has been developed for boiler operating temperatures. The AFT analysis and thermodynamic viscosity values incorporated in the Roscoe equation are found to be in good match compared to the viscosities calculated by using the Urbain equation. The present model can now be implemented to

Table 3 Solid fractions of coal ashes

Temp (°C)	Solid fraction				
	MSRB1	MSRB2	MSRB3	M12	M24
1050	0.946051	0.97842	0.949647302	0.92841	0.956565
1100	0.902269	0.960907	0.908784086	0.922969	0.917697
1200	0.64641	0.85393	0.708693822	0.807683	0.870781
1300	0.284913	0.345704	0.323872731	0.675919	0.785809
1400	0.043677	0.143301	0.094337721	0.491824	0.653621
1500	0.015018	0.01809	0.23339059	0.082583	0.147699
1600	0.015306	0.01809	0.023504072	0.025009	0.019743

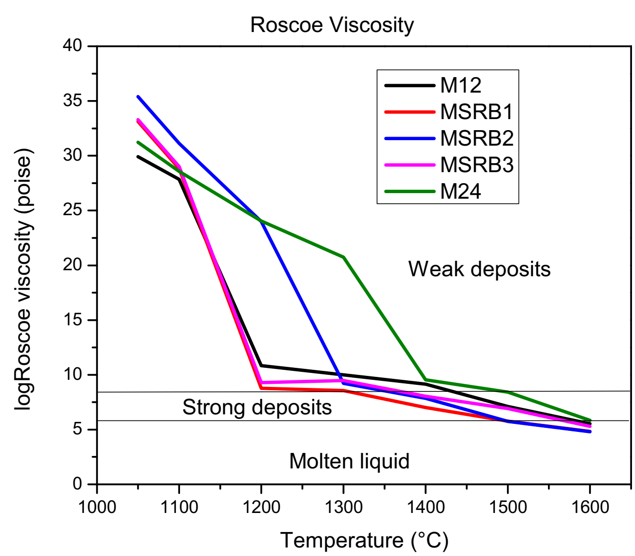


Fig. 9 log viscosity by using Roscoe viscosity

predict the coal ash chemistry and fluxing temperatures of a particular coal. Thermodynamic calculations of ash characteristics of present coals show that the slag phase formation starts at around 1100 °C and is complete at slag liquidus temperatures of above 1400 °C. In between these temperatures, the slag phase coexists with the solid particles. Solid fractions present in the slag phase increase the viscosity of usual liquid slag viscosity. The order of stability of slag deposits from low to high is MSRB1 < MSRB2 < MSRB3 < M24 < M12. An increase in the basicity of the slag lowers the solid fractions as well as the viscosity for respective coal. The reason for this is the formation of low-melting cordierite-like phases with the addition of basic oxides. AFT analysis of all five ash samples indicate that IDT for all five ash samples is greater than 1340 °C and fusion temperatures are greater than 1470 °C which can be good for industrial usage.

Acknowledgements The authors acknowledge and extend their sincere gratitude to the significant contribution and moral support provided by NIT Jamshedpur and CSIR-NML (Jamshedpur).

References

1. Chandra A, and Chandra H, *J Scient Industry Res* **63** (2004) 156.
2. Song W J, Tang L H, Zhu X D, Wu Y Q, Zhu Z B, and Koyama S, *Energy Fuels* **24** (2009) 182.
3. Gupta S K, Wall T F, Creelman R A, and Gupta R P, *Fuel Process Technol* **56** (1998) 33.
4. Alpern B, Nahuys J, and Martinez L, in *Symposium on Gondwana Coals*, Lisbon (1983), p 299.
5. Seggiani M, *Fuel* **78** (1999) 1121.
6. Mishra V, Bhowmick T, Chakravarty S, Varma A K, and Sharma M, *Fuel* **186** (2016) 443.
7. Chakravarty S, Mohanty A, Banerjee A, Tripathy R, Mandal, G K, Basariya M R, and Sharma M, *Fuel* **150** (2015) 96.
8. Banerjee A, Mishra P R, Mohanty A, Chakravarty K, Biswas R D, Sahu R, and Chakravarty S, *Int J Coal Sci Technol* **3** (2016) 97.
9. Hanxu L I, Yoshihiko N, Zhongbing D, and Zhang M, *Chin J Chem Eng* **14** (2006) 784.
10. Harris D J, and Patterson J H, *Aust Inst Energy News J* **13** (1995) 22.
11. ASTM D1857–87, *Standard Test Method for Fusibility of Coal and Coke Ash*, American Society for Testing and Materials, Philadelphia (1987).
12. Gray V R, *Fuel* **66** (1987) 1230.
13. Bale C W, Bélisle E, Chartrand P, Decterov S A, Eriksson G, Gheribi A E, Hack K, Jung I H, Kang Y B, Melançon J, and Pelton A D, *Calphad* **55** (2016) 1.
14. Gheribi A E, Audet C, Le Digabel S, Bélisle E, Bale C W, and Pelton A D, *Calphad* **36** (2012) 135.
15. Besmann T M, and Spear K E, *J Am Ceram Soc* **85** (2002) 2887.
16. Koukkari P, and Pajarre R, *Calphad* **30** (2006) 18.
17. Van Dyk J C, Waanders F B, Benson S A, Laumb M L, and Hack K, *Fuel* **88** (2009) 67.
18. Mills K C, and Sridhar S, *Ironmak Steelmak* **26** (1999) 262.
19. Kondratiev A, Jak E, and Hayes P C, *JOM* **54** (2002) 41.
20. Pati A, Sahoo S K, Mishra B, and Mohanty U K, *Trans Indian Inst Met* (2018) 1.
21. Liu B, He Q, Jiang Z, Xu R, and Hu B, *Fuel* **105** (2013) 293.

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.