

Slag Management of Carbon Feedstock Used in Gasification

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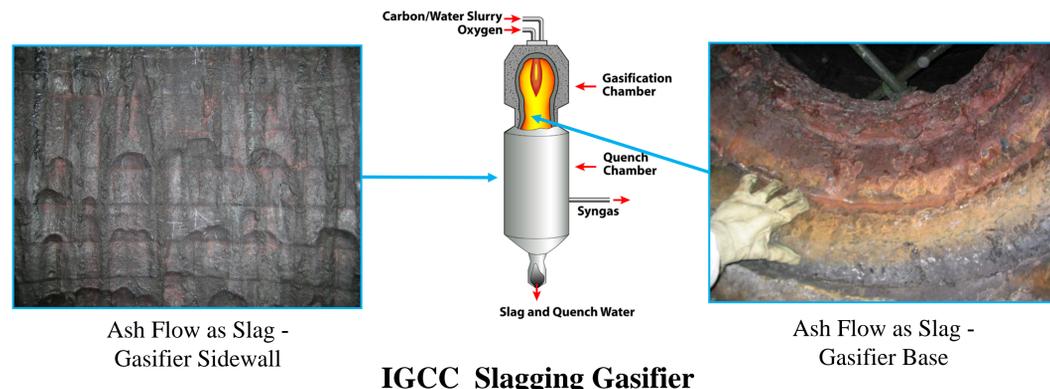
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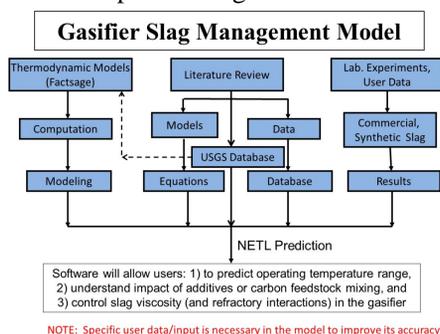
BACKGROUND

Gasification is used to convert carbon feedstock (primarily coal and/or petcoke) into synthesis gas, a mix of carbon monoxide (CO) and hydrogen (H₂), for use in power generation or chemical production. In high temperature gasification processes, the mineral impurities in coal and petcoke melt and coalesce to form a liquid (slag) that must flow from the gasifier. If slag does not flow from a gasifier, its buildup will cause process shutdown and 1) the need for physical entry into the gasifier to remove the buildup (consuming time and damaging the refractory lining), and/or 2) the gasification temperature must be increased to lower slag viscosity so it will flow from the gasifier. Temperature increases, however, lead to greater refractory wear/corrosion (resulting in a shorter refractory service life), as well as an increase in gasifier fouling and downstream component wear.



NEED

The ability to accurately predict coal ash viscosity in advance of its gasification is important to gasifier operators so they know in advance how to control slag flow from a gasifier at a desired gasification temperature, and so they can predict interactions with refractory liners based on slag composition. NETL developed a first generation computer program to predict slag viscosity using an expandable database of coal slag viscosities, allowing a user to predict coal ash viscosity before use and to determine oxide material additives for the slag chemistry that will control its flow in the gasification chamber. The slag model is based on the assumption that similar slag chemistries will have similar slag viscosities. The basic architecture of the slag model used to predict slag behavior is shown below.



APPROACH

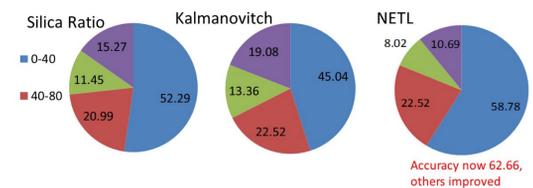
The slag model is being evaluated commercially as part of a technology commercialization program at Eastman Chemical Corp. The slag model data base was expanded in a targeted area of the slag composition using select viscosity models, thermodynamic predictions, viscosity measurements of specific coal ash chemistries, proprietary slag chemistry/viscosity data of Eastman, and special viscosity measurements of actual and synthetic slags with/without additives. Viscosity, temperature, and chemistry data was modeled to predict viscosity behavior.

Coal Slag Viscosity Models Considered

Type	Equation	Model
Empirical	Arrhenius	Watt-Fereday
		Silicate ratio
	Weymann-Frenkel	Urban
		Kalmanovitch
		Browning
Quasichemical		Riboud
		Factsage

Accuracy of Literature Models

Accuracy (°C)	Browning	Urban	Kalmanovitch	Silica Ratio	Riboud	Watt Fereday	Factsage
0-40	35.88	6.87	45.04	52.29	3.05	12.98	26.56
40-80	21.76	24.43	22.52	20.99	10.69	31.68	18.36
80-120	18.70	32.44	13.36	11.45	32.44	24.05	20.31
>120	23.66	36.26	19.08	15.27	53.82	31.30	34.77



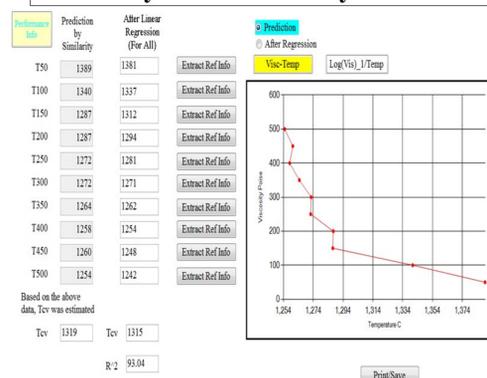
$$\text{Arrhenius: } \eta = A_A \exp\left(\frac{E_A}{RT}\right)$$

$$\text{Weymann-Frenkel: } \eta = AT \exp\left(\frac{10^3}{T}\right)$$

RESULTS

Viscosity predictions using the slag management model developed by NETL has been shown (1) to be of greater accuracy than thermodynamic predictions or predictive models available commercially or in the literature. Testing and validation of the model is still underway. Customization and validation of the model to a specific user's coal ash chemistry is the goal of the current model.

Similarity Model Viscosity Prediction



Data Input

Please Input Slag Chemistry by Weight or Weight Percentage

Weight	Oxide	Weight	Wt. %	Wt. % Without P2O5 & SO3	Mole Fraction	Mole Fraction without P2O5 & SO3	Element Mole Fraction
SiO2 = 36.7	SiO2	36.70	37.54	37.54	0.46	0.46	Si: 0.18
Al2O3 = 29.3	Al2O3	29.30	30.21	30.21	0.22	0.22	Al: 0.14
FeO = 28.28	FeO	28.28	29.16	29.16	0.30	0.30	Fe: 0.60
MgO = 0.9	MgO	0.90	0.93	0.93	0.00	0.00	Mg: 0.00
CaO = 0.9	CaO	0.90	0.93	0.93	0.01	0.01	Ca: 0.00
MgO = 0.3	MgO	0.30	0.31	0.31	0.01	0.01	Mg: 0.00
SiO2 = 0.7	SiO2	0.70	0.72	0.72	0.01	0.01	Si: 0.00
P2O5 = 0	P2O5	0.00	0.00	0.00	0.00	0.00	P: 0.00
SO3 = 0	SO3	0.00	0.00	0.00	0.00	0.00	S: 0.00
							O: 0.84

Sample Name: _____ R = 2.112 X = 0.264 Y = 3.756
 The number of oxygen ions per network-forming ions
 Normalizing oxygen per polyhedron
 Bridging oxygen per polyhedron

BENEFITS AND FUTURE WORK

The gasification of coal to produce syngas generates slag from mineral impurities in the coal that must flow from the gasification chamber. High gasification temperatures create a highly fluid slag that flows easily, but increases refractory liner wear of the gasification chamber (shorting the on-line availability of the gasifier) and that increases downstream fouling and agglomeration. Gasification temperatures that are too low cause slag buildup in the gasification chamber that that can must be removed by its shutdown.

A slag management model developed by NETL allows gasifier users to predict viscosity of molten coal ash (slag) before gasification and to make needed additive adjustments to change slag chemistry, or to blend different coals to achieve desired flow characteristics, permitting improved on-line performance of the gasification process. This model has been shown to improve the accuracy of viscosity predictions over existing commercial models. The model can also be customized with other data or by using proprietary user data to improve its accuracy.

Enlargement of the slag management model to petcoke based carbon feedstock ash viscosity is also possible using recent phase diagram data (2) related to vanadium compounds. The current slag model database was developed using coal as a carbon feedstock. It is possible the existing model would accurately predict petcoke containing slag behavior if vanadium oxide content is below about 4 wt pct., a value where as crystallization of vanadium compounds is not predicted.

ACKNOWLEDGEMENTS

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REFERENCES

- Kwong, K.S., and Bennett, J., "Development of a Slag Management System for Gasification," MOLTEN 2016: 10th International Conference on Molten Slags, Fluxes and Salts, Seattle, Washington, US, May 22-25, 2016.
- Nakano, J., Duchesne, M., Bennett, J., Nakano, A., Hughes, R., and Jung, I.-H., "Chemical and Thermal Influences on the Thermodynamic Stability of the Vanadium-Rich Oxide System," CALPHAD XLV: 45th International Conference on Computer Coupling of Phase Diagrams and Thermochemistry, Awaji Island, Hyogo, Japan, May 29- June 3, 2016.



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