ME 370B Energy Systems II: Modeling and Advanced Concepts

Chris Edwards Winter 2023

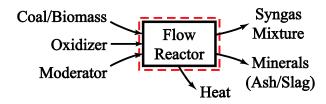
More than you ever wanted to know about... Thermo Calculations with Coal and Biomass

Coal can be a challenging fuel to deal with in thermodynamic calculations. It is a complex mixture of carbon, hydrogen, sulfur, oxygen, nitrogen, and other elements that has no exact chemical formula and varies significantly according to the region where it is formed, its age, depth, handling procedures (e.g. drying), etc.

Biomass presents the exact same difficulties as coal, but its composition is different, and it usually contains significantly more water. The chemical makeup of biomass varies quite widely among the different species from which it is derived, and the requirements for feedstock handling are often more stringent than they are for coal due to its fibrous nature.

As with most things in life, there are relatively simple ways in which the complexities of these fuels can be encapsulated, and if you understand these, working with them does not present much more of a challenge than the other fuels with which you have already dealt. The biggest challenge that coal and biomass present is that the data describing them are often presented in a thermodynamically confusing format. In this document, we will systematically explore complex fuel analysis so that you will be well prepared to deal with any fuel that comes your way.

In this discussion, we will take the approach that we did with simple fuels. To start, we will assume that we know everything we could possibly want to know about the fuel, including its composition and its enthalpy with respect to reference species. As we run through a generalized analysis of combustion and gasification (reforming), we will find that even though we don't have all of that information available, we don't actually need (or want) to know everything, and the data that are measured for these fuels actually does tell us what we *need* (and therefore, want) to know. The remainder of this discussion will mainly use coal as an example, but the analysis is equally applicable to biomass.



The general problem we are interested in is that of a chemical transformation of coal or biomass to some other species or set of species. If the species are combustion products, we refer to the transformation as combustion. If the species are low-molar-mass gases with a significant heating value—carbon monoxide, carbon dioxide, hydrogen, water, methane—we speak of gasification.

If the species are liquid hydrocarbons, we speak of liquefaction. Regardless of the specific objective, we can learn what we need to know by considering a generic gasification problem.

In this process coal or biomass is reacted with an oxidizer (usually air or oxygen) and a moderator (usually water, nitrogen, or carbon dioxide) to separate the mineral matter in the feedstock from the organic components and to transform the organic matter into light, gaseous species. Like autothermal reforming, the energy required to drive the separation is provided by the oxidation of a fraction of the organic matter in the feedstock. Unlike ATR, the complex nature of the feedstocks precludes the use of catalysts. The moderator is used both to control the temperature of the reaction and to tailor the atomic composition as best suited to product-gas requirements.

If we write the energy equation for this reactor using coal as feedstock, it reads

$$\dot{m}_{coal}h_{coal} + \dot{m}_{oxid}h_{oxid} + \dot{m}_{mod}h_{mod} = \dot{m}_{syngas}h_{syngas} + \dot{m}_{ash/slag}h_{ash/slag} + \dot{Q}$$

which simply states that the enthalpy input to the reactor is divided between the product gases, the condensed-phase mineral matter, and heat transfer. Given that we should, in principle, know everything that we put into the reactor (the left side), our task in gasification is to determine the composition, thermal state, and heat transfer (the right side).

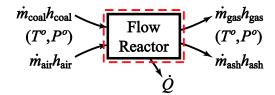
Assuming that the reactor has been designed in such a way that the products come close to achieving equilibrium conditions, this problem can be solved if we have ways to:

- (a) specify the molecular species that are permitted to be formed,
- (b) specify the atoms from which the molecular species are to be assembled,
- (c) specify the pressure or density (or equivalent property) during the assembly (equilibration),
- (d) specify the enthalpy or internal energy (or equivalent property) of the matter, and
- (e) deal with the ash or slag (how much and its enthalpy or internal energy) that is left behind.

If we can address these issues, the problem looks very much like the autothermal reforming problem that we have already treated. In fact the first three items on this list are identical to the ATR problem, they are just a bit more complicated due to the nature of the fuel. Item (d) is also similar, but the solid nature of the fuel makes it a little different and therefore worth discussion. The last item (e) is unique to solid fuels like coal and biomass and essentially different from the fuel processing you have done previously. It is also the source of complications for items (a-d).

Similar to the fuel-processing problem, the approach we take to dealing with item (d) involves the experimental determination of the "heating value" of the coal—a problem with which we are already familiar, but which is a little different here due to the presence of mineral matter. That is where we will begin.

The Heating Value Problem



Determination of the heating value of coal or biomass proceeds along the same lines as for other fuels. Dry coal and air at standard conditions T° , P° are reacted to form gaseous products and ash which are cooled so as to exit at standard conditions. Because of the low exit temperature $(T^{\circ}$ is usually taken as 25°C, P° as 1 bar or 1 atm), the mineral matter exits in the solid phase (ash) as opposed to liquid (slag). The amount of heat transferred is measured, and the results are used to determine the heating value. The energy equation for this process is

$$\dot{m}_{mf}h_{mf} + \dot{m}_{air}h_{air} = \dot{m}_{gas}h_{gas} + \dot{m}_{ash}h_{ash} + \dot{Q}$$

where the subscript mf denotes moisture-free coal. The heating rate in this equation \dot{Q} determines the heating value of mf coal. Both coal and biomass may have significant quantities of moisture associated with them, but if the fuel is reacted in its "wet" state, then you can simply deal with the moisture by assuming it enters the reactor as a separate stream (or enters along with the moderator).

Heating values for coal are usually given on a *moisture-and-ash-free* (*maf*) basis. Moving the term associated with the ash to the left side of the equation and defining $\dot{m}_{maf}h_{maf}\equiv \dot{m}_{mf}h_{mf}-\dot{m}_{ash}h_{ash}$ gives the relationship between the *maf* enthalpy and the measured heat transfer rate as

$$\dot{m}_{maf}h_{maf}+\dot{m}_{air}h_{air}=\dot{m}_{gas}h_{gas}+\dot{Q}$$

Note that since it is possible to measure the amount of ash generated by a unit mass of coal directly, the moisture- and ash-free mass flow rate is known independently, $\dot{m}_{maf} \equiv \dot{m}_{mf} - \dot{m}_{ash}$, and the moisture- and ash-free enthalpy is then determined uniquely by the definition above.

In order to progress further, we must specify how much air is to be supplied and the composition of the gases that are generated in the reactor. Following the same approach as used for conventional fuels, we assume that air is provided in excess of the oxidation requirements and that, accordingly, the gases that are generated correspond to the products of complete combustion (CO_2 for carbon, H_2O for hydrogen, and SO_2 for sulfur). Given the elemental composition of the coal on a per-carbon-atom basis, the reaction balance can be written as

$$\begin{split} CH_{a}S_{b}O_{c}N_{d}Si_{e}Fe_{f}Al_{g}Ca_{h}...+\lambda\bigg(1+\frac{a}{4}+b-\frac{c}{2}+\frac{mor/C}{2}\bigg)\big(O_{2}+3.76N_{2}\big) \to \\ CO_{2}+\frac{a}{2}H_{2}O+bSO_{2}+\big(\lambda-1\big)\bigg(1+\frac{a}{4}+b-\frac{c}{2}+\frac{mor/C}{2}\bigg)O_{2}+\\ \bigg[\frac{d}{2}+\lambda\bigg(1+\frac{a}{4}+b-\frac{c}{2}+morC\bigg)3.76\bigg]N_{2}+min/C \end{split}$$

where $mor/C = 2e + \frac{3f}{2} + \frac{3g}{2} + h + ...$ is the <u>mineral oxygen</u> (atom) <u>requirement per carbon atom</u>

in the coal and $min/C = eSiO_2 + \frac{f}{2}Fe_2O_3 + \frac{g}{2}Al_2O_3 + hCaO + ...$ is the <u>min</u>eral matter generated

per <u>carbon</u> atom in the coal. The importance of keeping track of the mineral matter is that formation of ash requires oxygen. That oxygen must be supplied either by the fuel itself (from coefficient c) or by the air stream. Without correctly accounting for the oxygen requirement of the ash (or slag for high-exit-temperature systems) the atom balances and therefore matter and energy balances will not be correct.

Writing the energy balance with the gaseous product species shown explicitly gives

$$\dot{m}_{maf}h_{maf} + \dot{m}_{air}h_{air} = \dot{m}_{CO_2}h_{CO_2} + \dot{m}_{H_2O}h_{H_2O} + \dot{m}_{SO_2}h_{SO_2} + \dot{m}_{O_2}h_{O_2} + \dot{m}_{N_2}h_{N_2} + \dot{Q}$$

Dividing through by the rate of moisture- and ash-free coal gives

$$h_{maf} + \frac{\dot{m}_{air}}{\dot{m}_{maf}} h_{air} = \frac{\dot{m}_{CO_2}}{\dot{m}_{maf}} h_{CO_2} + \frac{\dot{m}_{H_2O}}{\dot{m}_{maf}} h_{H_2O} + \frac{\dot{m}_{SO_2}}{\dot{m}_{maf}} h_{SO_2} + \frac{\dot{m}_{O_2}}{\dot{m}_{maf}} h_{O_2} + \frac{\dot{m}_{N_2}}{\dot{m}_{maf}} h_{N_2} + \frac{\dot{Q}}{\dot{m}_{maf}} h_{M_2} + \frac{\dot{Q}}{\dot{M}$$

The last term is the heating value of the coal, defined on a moisture- and ash-free basis.

$$q_{maf} = \frac{Q}{\dot{m}_{maf}} = \frac{Q}{\dot{m}_{mf} - \dot{m}_{ash}}$$

Substituting for \dot{Q} in the energy equation and noting that at standard reference conditions the enthalpy of both components of air (oxygen and nitrogen) are zero, yields an expression for the enthalpy of coal (on a *maf* basis) at the standard state as

$$h^o_{maf} = rac{\dot{m}_{CO_2}}{\dot{m}_{maf}} h^o_{CO_2} + rac{\dot{m}_{H_2O}}{\dot{m}_{maf}} h^o_{H_2O} + rac{\dot{m}_{SO_2}}{\dot{m}_{maf}} h^o_{SO_2} + q^o_{maf}$$

This is an important result! Knowledge of h_{maf}^o and the specific heat capacity of the mf coal allows us to satisfy condition (d) on our list above—specification of the enthalpy input.

Since the reaction balance is constructed on a molar basis, it is useful to convert the gas terms on the right side of the expression to a molar basis as well

$$h_{maf}^{o} = \frac{\dot{N}_{CO_{2}}}{\dot{N}_{C}M_{maf/C}} \overline{h}_{CO_{2}}^{o} + \frac{\dot{N}_{H_{2}O}}{\dot{N}_{C}M_{maf/C}} \overline{h}_{H_{2}O}^{o} + \frac{\dot{N}_{SO_{2}}}{\dot{N}_{C}M_{maf/C}} \overline{h}_{SO_{2}}^{o} + q_{maf}^{o}$$

where we have used the fact that we can express the mass rate of *maf* coal on a carbon-rate basis by use of the molar mass per Carbon atom

$$\dot{m}_{maf} = \dot{N}_C M_{maf/C}$$

The molar mass per carbon atom on a *maf* basis may be found by applying the definitions of molar mass and the mass rate of *maf* coal

$$\begin{split} \boldsymbol{M}_{maf/C} &= \frac{\text{mass of maf coal}}{\text{mole of carbon}} = \frac{\text{mass of } mf \text{ coal}}{\text{mole of carbon}} - \frac{\text{mass of ash}}{\text{mole of carbon}} \\ &= \boldsymbol{M}_C + a\boldsymbol{M}_H + b\boldsymbol{M}_S + c\boldsymbol{M}_O + d\boldsymbol{M}_N + e\boldsymbol{M}_{Si} + f\boldsymbol{M}_{Fe} + g\boldsymbol{M}_{Al} + h\boldsymbol{M}_{Ca} + \dots \\ &- e\boldsymbol{M}_{SiO_2} - \frac{f}{2}\boldsymbol{M}_{Fe_2O_3} - \frac{g}{2}\boldsymbol{M}_{Al_2O_3} - h\boldsymbol{M}_{CaO} - \dots \end{split}$$

Grouping common mineral-generating elements together yields

$$\begin{split} M_{\textit{maf/C}} &= M_{\textit{C}} + a M_{\textit{H}} + b M_{\textit{S}} + c M_{\textit{O}} + d M_{\textit{N}} + e \Big(M_{\textit{Si}} - M_{\textit{SiO}_2} \Big) + f \left(M_{\textit{Fe}} - \frac{1}{2} M_{\textit{Fe}_2O_3} \right) \\ &+ g \bigg(M_{\textit{Al}} - \frac{1}{2} M_{\textit{Al}_2O_3} \bigg) + h \Big(M_{\textit{Ca}} - M_{\textit{CaO}} \Big) + \dots \end{split}$$

which upon elimination of the common-element molar masses in each term leads to

$$M_{maf/C} = M_C + aM_H + bM_S + cM_O + dM_N - eM_{O_2} - \frac{f}{2}M_{O_3} - \frac{g}{2}M_{O_3} - hM_O + \dots$$

Finally, all of the mineral-related terms can be cast in terms of the molar mass of monatomic oxygen giving the not too surprising result

$$M_{maf/C} = M_C + aM_H + bM_S + (c - mor/C)M_O + dM_N$$

Note that the <u>net</u> maf oxygen/carbon ratio, (c-mor/C), is the oxygen content determined by *ultimate analysis* of coal on a maf basis and is part of the information that is directly measured for coal or biomass fuels (so you don't need to figure this out!). The same holds true for any other elements that may end up in the ash or slag (unreacted C, trace S, N, ...). Analysis on a maf basis correctly provides the element ratios needed to obtain the molar mass (per unit carbon).

Returning to the expression for the standard-state maf enthalpy, it is apparent that the atom ratios for CO_2 , H_2O , and SO_2 per carbon atom can be taken directly from the reaction balance, yielding

$$h_{maf}^{o} = \frac{\overline{h}_{CO_2}^{o}}{M_{maf/C}} + \frac{a}{2} \frac{\overline{h}_{H_2O}^{o}}{M_{maf/C}} + b \frac{\overline{h}_{SO_2}^{o}}{M_{maf/C}} + q_{maf}^{o}$$

The importance of this expression is that it provides a way to move from the (directly available) *maf* heating value of the coal to knowledge of the standard-state enthalpy of *maf* coal on a mass basis. All that we need now to complete our understanding is to close the loop on how this piece of information enables us to address the original gasification (or combustion, or liquefaction) problem posed above.

Gasification Revisited

Recall that the energy balance for our generic gasification problem was

$$\dot{m}_{mf}h_{mf} + \dot{m}_{oxid}h_{oxid} + \dot{m}_{mod}h_{mod} = \dot{m}_{syneas}h_{syneas} + \dot{m}_{ash/slag}h_{ash/slag} + \dot{Q}$$

(Note: The \dot{Q} in this expression is a general heat transfer rate, not the heating value.)

Expressing the coal and ash/slag enthalpies in terms of their standard-state values and differences from those values, and applying the same strategy as above wherein we combined the coal and mineral matter gives

$$\dot{m}_{mf}\left(h_{mf}^{o} + \Delta h_{mf}^{o}\right) - \dot{m}_{ash/slag}\left(h_{ash}^{o} + \Delta h_{ash/slag}^{o}\right) + \dot{m}_{oxid}h_{oxid} + \dot{m}_{mod}h_{mod} = \dot{m}_{syngas}h_{syngas} + \dot{Q}$$

Replacing terms on the left with the standard-state *maf* enthalpy, and moving the sensible ash/slag enthalpy term back to the right gives

$$\dot{m}_{maf}h_{maf}^{o} + \dot{m}_{mf}\Delta h_{mf}^{o} + \dot{m}_{oxid}h_{oxid} + \dot{m}_{mod}h_{mod} = \dot{m}_{syngas}h_{syngas} + \dot{m}_{ash/slag}\Delta h_{ash/slag}^{o} + \dot{Q}$$

This expression shows that the enthalpy balance can be constructed using the *maf* standard-state value to represent the chemical energy of the coal, the sensible enthalpy of the coal (usually specified via its specific heat capacity, measured on a moisture-free basis) to represent differences from the standard state, and the enthalpy difference of the ash/slag from the standard-state value (ash, as determined in the heating value problem). Note that the ash/slag enthalpy difference may include contributions due to phase transformations as well as sensible-enthalpy. Also note that while the sensible enthalpy term for the coal depends on the inlet temperature, which is typically known, the enthalpy difference term for the ash/slag depends on the outlet temperature which is not known and will require an implicit or iterative approach for solution. Since determination of the heat loss is also likely to require an iterative approach, this poses no new complication.

Consider the specific case of an air-blown (so that we can include nitrogen), slagging gasifier using water as the moderator. The energy equation for this case is given by

$$\begin{split} \dot{m}_{maf}h^o_{maf} + \dot{m}_{mf}\Delta h^o_{mf} + \dot{m}_{O_2,feed}h_{O_2,feed} + \dot{m}_{N_2,feed}h_{N_2,feed} + \dot{m}_{H_2O,feed}h_{H_2O,feed} = \\ \dot{m}_{syngas}h_{syngas} + \dot{m}_{slag}\Delta h^o_{slag} + \dot{Q} \end{split}$$

To solve for the equilibrium composition we need to be able to specify the specific enthalpy of the gas mixture being equilibrated. This can be found by rearranging the energy balance

$$h_{syngas} = \frac{\dot{m}_{maf}}{\dot{m}_{syn}} h_{maf}^{o} + \frac{\dot{m}_{mf}}{\dot{m}_{syn}} \Delta h_{mf}^{o} + \frac{\dot{m}_{O_{2},feed}}{\dot{m}_{syngas}} h_{O_{2}}^{o} + \frac{\dot{m}_{N_{2},feed}}{\dot{m}_{syngas}} h_{N_{2}}^{o} + \frac{\dot{m}_{H_{2}O,feed}}{\dot{m}_{syngas}} h_{H_{2}O}^{o} - \frac{\dot{m}_{slag}}{\dot{m}_{syn}} \Delta h_{slag}^{o} - \frac{\dot{Q}}{\dot{m}_{syn}} h_{syngas}^{o} + \frac{\dot{M}_{N_{2},feed}}{\dot{m}_{syngas}} h_{N_{2}}^{o} + \frac{\dot{m}_{N_{2},feed}}{\dot{m}_{syngas}} h_{N_{2}O,feed}^{o} + \frac{\dot{m}_{N_{2},feed}}{\dot{m}_{N_{2}O,feed}^{o}} h_{N_{2}O,feed}^{o} + \frac{\dot{m}_{N_{2}O,feed}}{\dot{m}_{N_{2}O,feed}^{o}} h_{N_{2}O,feed}^{o} + \frac{\dot{m}_{N_{2}O,feed}}{\dot{m}_{N_{2}O,feed}^{o}} h_{N_{2}O,feed}^{o} + \frac{\dot{m}_$$

Factoring out the *maf*-to-*syngas* ratio this becomes

$$h_{syngas} = \frac{\dot{m}_{maf}}{\dot{m}_{syngas}} \left[h_{maf}^{o} + \frac{\dot{m}_{mf}}{\dot{m}_{maf}} \Delta h_{mf}^{o} + \frac{\dot{m}_{O_{2},feed}}{\dot{m}_{maf}} h_{O_{2}\atop feed}} + \frac{\dot{m}_{N_{2},feed}}{\dot{m}_{maf}} h_{N_{2}\atop feed}} + \frac{\dot{m}_{H_{2}O,feed}}{\dot{m}_{maf}} h_{H_{2}O} - \frac{\dot{m}_{slag}}{\dot{m}_{maf}} \Delta h_{slag}^{o} - \frac{\dot{Q}}{\dot{m}_{maf}} \right]$$

The reaction balance for the species in moisture-free coal of "known" composition can be used to find the flow rate relationships needed. Writing the general reaction balance

$$\begin{split} CH_{a}S_{b}O_{c}N_{d}Si_{e}Fe_{f}Al_{g}Ca_{h}...+&\left(O_{2}/C\right)_{feed}O_{2}+\left(N_{2}/C\right)_{feed}N_{2}+\left(H_{2}O/C\right)_{feed}H_{2}O\\ &\rightarrow\sum_{\substack{i\\svngas}}\left(N_{i}/C\right)Species_{i}+min/C \end{split}$$

emphasizes that in addition to the inlet states, the key parameters for the gasification process are the oxygen/carbon, nitrogen/carbon, and water/carbon ratios of the feed stream(s).

Using these parameters, the mass ratios in the expression for the specific enthalpy of the gas mixture can be found from the appropriate species balances and expressed as

$$\begin{split} \frac{\dot{m}_{maf}}{\dot{m}_{syngas}} &= \left[1 + \left(O_2/C\right)_{feed} \frac{M_{O_2}}{M_{maf/C}} + \left(N_2/O_2\right)_{feed} \left(O_2/C\right)_{feed} \frac{M_{N_2}}{M_{maf/C}} + \left(H_2O/C\right)_{feed} \frac{M_{H_2O}}{M_{maf/C}}\right]^{-1} \\ \frac{\dot{m}_{mf}}{\dot{m}_{maf}} &= \frac{\dot{m}_{maf} + \dot{m}_{slag}}{\dot{m}_{maf}} = \left(1 + ash/maf\right) \\ \frac{\dot{m}_{O_2, feed}}{\dot{m}_{maf}} &= \left(O_2/C\right)_{feed} \frac{M_{O_2}}{M_{maf/C}} \\ \frac{\dot{m}_{N_2, feed}}{\dot{m}_{maf}} &= \left(N_2/O_2\right)_{feed} \left(O_2/C\right)_{feed} \frac{M_{N_2}}{M_{maf/C}} \\ \frac{\dot{m}_{H_2O, feed}}{\dot{m}_{maf}} &= \left(H_2O/C\right)_{feed} \frac{M_{H_2O}}{M_{maf/C}} \\ \frac{\dot{m}_{slag}}{\dot{m}_{maf}} &= \left(ash/maf\right) \end{split}$$

where we have expressed the nitrogen/carbon ratio in terms of the oxygen/carbon ratio of the feed and the nitrogen/oxygen ratio of the oxidizer (air or other, including pure oxygen). The expressions also show the last of the key parameters, the *ash/maf* mass ratio of the feed stream. This can be determined from the proximate analysis of the coal.

With these substitutions the expression for the specific enthalpy of the gas mixture becomes

$$h_{syngas} = \frac{\dot{m}_{maf}}{\dot{m}_{syngas}} \left[h_{maf}^{o} + \left(1 + \frac{ash}{maf} \right) \Delta h_{mf}^{o} + \left(\frac{O_{2}}{C} \right)_{feed} \frac{\overline{h}_{O_{2},feed}}{M_{maf/C}} + \left(\frac{N_{2}}{O_{2}} \right)_{feed} \left(\frac{O_{2}}{C} \right)_{feed} \frac{\overline{h}_{N_{2},feed}}{M_{maf/C}} + \left(\frac{H_{2}O}{C} \right)_{feed} \frac{\overline{h}_{N_{2},feed}}{M_{maf/C}} - \left(\frac{ash}{maf} \right) \Delta h_{slag}^{o} - q_{maf} \right]$$

where $q_{maf} \equiv \dot{Q}/\dot{m}_{maf}$ is the specific heat loss per unit of moisture- and ash-free coal. As mentioned above, because Δh_{slag}^o depends on the equilibrium temperature, the solution procedure

for the syngas composition and state is usually performed iteratively. Note too that specification of Δh_{slag}^o will require knowledge of the specific heat of the ash and slag as well as the latent heat of fusion that accompanies the ash-slag phase change. And Δh_{mf}^o requires knowledge of the specific heat of the mf coal (not maf, but the complete coal without moisture).

These sensible enthalpies are fairly easy to compute, and give us the remaining piece we need for item (d) in our list. Items (a-c) and (e) have also been addressed along the way: We know how to specify what is in the box, how much energy it has, what its thermo-mechanical constraints are (e.g., pressure), and how to handle the stuff that comes out of the box. All that remains is to actually do this with some practical fuels. That can be done with the data on the next couple of pages drawn from Higman and van der Burgt's book *Gasification* (Elsevier, 2003).

Coal and Biomass Data

Proximate Analysis describes the coal <u>as received</u> (ar), that is, with native moisture and ash in place (no drying or reaction having taken place). The only two numbers that you need for thermodynamic calculations are the water and ash content. (The information on volatiles and fixed carbon is important for burner/furnace design.) The water content describes the fraction of the total mass of coal that is lost after the coal is dried, but not burned. The ash content describes the fraction of the total mass of coal that is left as solid matter after the coal has been burned completely. The volatile and fixed-carbon specifications correspond to stages intermediate between drying and full reaction and jointly constitute the maf coal.

Ultimate Analysis is provided on a *maf* basis. This is the atom-by-atom breakdown of all of the elements in coal that will end up in the gas phase upon reaction. It supplies the *a, b, c-mor/C, d* coefficients needed to describe the composition of *maf* coal directly.

Heating Value is defined the same way as for any other fuel (with higher and lower values defined by the exit water state), but it is given on a maf basis—as we saw that we needed it to be in our analysis. It represents the total amount of sensible energy that is liberated as all of the matter accounted for in the ultimate analysis is reacted to form product species.

Ash Analysis gives the breakdown by mass percentage of what is left as a solid after the coal or biomass is fully oxidized. Some of the oxides are present in the raw feedstock, but some of the oxygen in the ash comes from the combustion process (as described in connection with *morC* during the analysis). For thermodynamic purposes, these data are mainly used to define the heat capacity and latent heat of fusion of the ash or slag that emerges from the gasifier.

Table 4-4 Analyses of Various Coals												
	Proximate Analysis, % Mass ar				Ultimate Analysis, % Mass on maf Coal				LHV			
Country	Region	Class	Fixed carbon	Vol. Mater	Water	Ash	С	Н	0	N	s	maf coal MJ/kg
Germany	Rhein	Browncoal	17.3	20	60	2.7	67.5	5.0	26.5	0.5	0.5	26.2
U.S.A.	North Dakota	Lignite	27.8	24.9	36.9	10.4	71.0	4.3	23.2	1.1	0.4	26.7
U.S.A.	Montana	Sub-bituminous	43.6	34.7	10.5	11.2	76.4	5.6	14.9	1.7	1.4	31.8
U.S.A.	Illinois	Bituminous	39.3	37.0	13.0	10.7	78.4	5.4	9.9	1.4	4.9	33.7
Poland	Typical	Bituminous	54.9	35.6	. 5.3	4.2	82.8	5.1	10.1	1.4	0.6	36.1
South Africa	Typical	Bituminous	51.3	32.7	2.2	13.8	83.8	4.8	8.4	2.0	1.0	34.0
China	Datung	Bituminous	50.9	28.1	11.9	9.1	84.4	4.4	9.5	0.9	0.8	33.4
India	Typical	Bituminous	30	23	7	40	75.5	6.4	15.2	1.5	1.4	32.1
Australia	Typical	Bituminous	44.9	41.1	4.5	9.5	81.3	5.8	10.0	2.0	0.9	33.8
Germany	Ruhr	Anthracite	81.8	7.7	4.5	6.0	91.8	3.6	2.5	1.4	0.7	36.2

Table 4-6 Ash Fusion Temperatures and Analysis												
Coal Ash-Melting Point Analysis of Ash a					Ash as	as Oxides (wt%)						
	reducing °C	oxidizing °C	SiO ₂	Al ₂ O ₃	TiO ₂	Fe ₂ O ₃	CaO	MgO	Na ₂ C	K ₂ O	SO ₃	P ₂ O ₅
Pocahontas No. 3 West												
Virginia Bituminous	IDT>1600	IDT>1600	60.0	30.0	1.6	4.0	0.6	0.6	0.5	1.5	1.1	0.1
Ohio No. 9 Bituminous	1440	1470	47.3	23.0	1.0	22.8	1.3	0.9	0.3	2.0	1.2	0.2
Illinois No. 6 Bituminous	1270	1430	47.5	17.9	0.8	20.1	5.8	1.0	0.4	1.8	4.6	0.1
Pittsburgh, WV Bituminous	1300	1390	37.6	20.1	0.8	29.3	4.3	1.3	0.8	1.6	4.0	0.2
Utah Bituminous	1280	1320	61.1	21.6	1.1	4.6	4.6	1.0	1.0	1.2	2.9	0.4
Antelope Wyoming												
Sub-bituminous	1270	1260	28.6	11.7	0.9	6.9	27.4	4.5	2.7	0.5	14.2	2.3
Texas Lignite	1230	1250	41.8	13.6	1.5	6.6	17.6	2.5	0.6	0.1	14.6	0.1
Source: Stultz and Kitto 1992												

Table 4-14 * Ash Components in Various Biomasses as Wt% of Total Ash							
	Straw	Miscanthus	Wood				
CaO	6.5	7.5	37.3				
MgO	3.0	2.5	8.5				
Na ₂ O	1.3	0.2	3.0				
K ₂ O	23.7	12.8	8.6				

Table 4-12 Properties of Various Biomasses								
Biomass	HHV MJ/kg	Moisture wt%	Ash wt%	Sulfur wt% dry	Chlorine wt% dry			
Charcoal	25–32	1–10	0.5–6					
Wood	10-20	10-60	0.25 - 1.7	0.01	0.01			
Coconut shell	18-19	8-10	1–4					
Straw	14–16	10	4–5	0.07	0.49			
Ground nut shells	17	2-3	10					
Coffee husks	16	10	0.6					
Cotton residues								
(stalks)	16	10-20	0.1					
Cocoa husks	13-16	7–9	7–14					
Palm oil residues								
(shells)	15	15						
Rice husk	13-14	9-15	15-20					
Soya straw	15-16	8–9	5-6					
Cotton residue								
(gin trash)	14	9	12					
Maize (stalk)	13-15	10-20	2 (3-7)	0.05	1.48			
Palm oil residues								
(fibers)	11	40						
Sawdust	11.3	35	2					
Bagasse	8-10	40-60	1–4					
Palm oil residues								
(fruit stems)	5	63	5					

Table 4-13 Analysis of Typical Bio	mass
Proximate Analysis	
Volatile matter, wt% maf	>70
Ash, wt% ar	1.5
Moisture, wt% ar	20
Fixed carbon, wt% ar	<15
Ultimate analysis	
C, wt%	54.7
H, wt%	6.0
O, wt%	38.9
N, wt%	0.3
S, v	0.1