ME 370B
Energy Systems II:
Modeling and Advanced Concepts

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Project #5: Coal and Biomass Gasification

Group assignment, due as a PDF file via Canvas, Thursday, February 16, 11 PM

Time to gasify coal and biomass. This week you will build on the code you finished with last week—the one that treats the indirect problem with arbitrary H/C and O/C ratios—and extend it to where it can treat coal and biomass. In the process you will have constructed a code that can treat almost any fuel (natural gas is "coal" with a high H/C ratio, little nitrogen and sulfur, and no ash). This will allow you to tackle most gasification, partial oxidation, autothermal reforming, etc., problems short of municipal waste (where toxic byproducts like dioxin are a key issue).

The key to wrapping your brain around this assignment is the *More than you ever wanted to know about… Coal and Biomass* handout that accompanies this (separate file). It guides you through what coal is, what you need to know about it (data), and therefore how to transition from where you are now to where you need to be. It is not too tough actually—just a little vectoring is required.

Because this is the middle of the quarter, the assignment is a little lighter this week. To that end, while there are still four parts to the assignment, the third is *not* to do cold catalytic conversion of carbonyl sulfide to hydrogen sulfide, and the fourth is *not* to integrate this into a combined-cycle IGCC plant. Instead we would like you to get a little extra sleep the night this is due, or any other night that you may need it. For that effort—*not* doing the analyses mentioned above—you will receive 25 points on each of Parts 3 and 4. (Good luck with your midterms!)

The Objectives

(1) to further understanding and experience with chemical transformations in general, and gasification in particular,

(2) to gain experience in dealing with mineral matter residues (ash/slag) in thermo calculations,

(3) to understand the origin and types of minor-species that result from this type of exergy transformation, and

(4) to develop understanding of how gasification permits a fuel like coal to be used in a combined-cycle power plant in lieu of natural gas (IGCC as an extension of NGCC).

The Assignment

There is not much more we have to say here. Most of what you need to know is in the Coal and Biomass handout. So let's hit the ground running…

(1) 30 Points Extend your model from Part 4 of last week to be able to treat coal and biomass. This will require that additional atoms be added to the mix and that the fuel be treated on a *maf* basis with a known *ash/maf* ratio. Include a heat loss that corresponds to 2% of the fuel's lower heating value and include enthalpy loss due to ash or slag exiting the gasifier (even though it is small). For this purpose it will be sufficient to use average specific heats for the ash and slag (as well as for the feedstock warm up to reactor temperature).

Encapsulate your code in a function that can treat an arbitrary feedstock with specified parameters. Use the function to compare natural gas to bituminous coal and agricultural residue (vegetative) biomass as feedstocks. Use air as the oxidant (commonly used in, low-temperature non-slagging gasification—particularly for biomass).

For the natural gas, use the same composition as you used for the NGCC assignment, but now make it more realistic by adding a little sulfur (50 ppm as H_2S) to the gas. Adjust the methane mole fraction to balance out the sum of the mole fractions to unity. (This is actually a little high—10 ppm would be more realistic—but we would have to nurse Cantera through some equilibration issues if we went that low.) Use a lower heating value of 46.1 MJ/kg and an average specific heat for the fuel gas of 2 kJ/kg-K.

For the coal, use a typical, high-ash, bituminous coal from India as listed in Table 4-4 from van der Burgt (in the coal/biomass handout). Use the proximate analysis to set your *ash/maf* ratio, and the ultimate analysis to set your atom ratios. Assume an ash melting temperature of 1350°C. Take the latent heat of fusion to be 240 kJ/kg and the average specific heat of both the ash and slag to be 1 kJ/kg-K. Assume that the average specific heat of the *mf* coal is 0.7 kJ/kg-K.

For the vegetative biomass use the typical proximate and ultimate analysis data listed in Table 4-13, and use a LHV of 12 MJ/kg *maf*. These correspond to a typical ag-waste product (*e.g.*, husks, straw). Assume an ash melting temperature of 800°C, and that the latent heat and heat capacities of the ash and slag are the same as for the coal listed above. Use 1.3 kJ/kg-K as the specific heat of the *mf* biomass feedstock.[1]

Following along from where you left off last week, fix the water/carbon mole ratio at unity and vary the oxygen/carbon mole feed ratio from near zero to unity. Again assume that the mixture is preheated to 450°C and that the reactor pressure is 10 bar.

[1] Biomass gasification often occurs at relatively low temperatures such that the assumption of chemical equilibrium must be questioned. In fact, for counter-flow gasifiers of the type discussed in class, equilibrium is usually not achieved and significant amounts of non-equilibrium products (e.g., volatile HCs and tar) are produced. However, if the gasification is done in a co-flow configuration, where the presence of ash acts as a catalyst to aid completion of reaction, these systems *can* achieve close to chemical equilibrium output composition, albeit at the expense of a slightly reduced cold gas efficiency. That is the case envisioned here. (Ask me about this if still not clear. CFE)

Make temperature and major species (above 0.1% by mole) plots that compare the three fuels as a function of oxygen/carbon molar feed ratio. Show the major species mole fractions in a linear fashion on this cross-comparison plot. Include horizontal, dashed lines showing the ash melting temperatures for the coal and biomass on the temperature plot, and vertical, dashed lines showing the oxygen/carbon ratios that correspond to these temperatures on the species plots. Since our intent is to design a non-slagging gasifier, we must choose operating conditions that correspond to temperatures that are comfortably below the ash-melting conditions of each fuel. (No such restriction applies to the natural gas so its operating temperature is chosen solely on the basis of performance.)

Because of adverse effects associated with the minor species present in these fuels (particularly those incorporating sulfur and nitrogen) additional conversion or removal of minor species is often required. In order to see what is present in our syngas, make additional semi-log plots of the species with mole fractions above 1 ppm for each of the fuels (use separate plots) vs. oxygen/carbon molar feed ratio. Again show vertical lines corresponding to the ash-melting limitations.

Plot the cold-gas efficiency and syngas yield (moles of $CO + H_2$ per mole of *carbon* introduced into the gasifier) vs. oxygen/carbon molar feed ratio for each feedstock on a series of cross-comparison plots. Plot the three fuels together using a separate plot for each performance metric. (There are no exergy-related plots since we cannot determine the entropy of these complex fuels.)

Note: It is not always possible to equilibrate mixtures with low oxygen feed ratios since we have not included the species required to treat pyrolysis in our property set. For that reason, it is always best to start at the high end of the oxygen feed range and work your way down. At the point where the oxygen becomes too low (which will happen for some fuels but not others) Cantera will balk. This is not numerical gibberish but a reflection of the fact that you are asking for a transformation that cannot be accomplished. If you run into this condition, stop the sweep at the lowest achievable oxygen feed. You will have already swept out the interesting part of the gasification region. (And trust me, you really don't want to tackle pyrolysis!) Also be careful when your exit temperature approaches the ash melting temperature. The latent heat at phase change can wreak havoc with clever numerical methods as they cross this boundary.

(2) <u>20 Points</u> Use your code from above (modified as necessary) to generate footprint plots for neat-oxygen, slagging gasification of Illinois #6 coal in oxygen/carbon and water/carbon feed space (cover the feed range from 0.1–0.5 O_2/C, 0–1.5 H_2O/C, by mole). Use a reactor pressure of 55 bar, and preheat the reactants to 150°C before injection into the gasifier. (These inlet conditions correspond to what is proposed for use with a Conoco/Phillips E-Gas gasifier in the NETL study for IGCC plants.)

Unlike the previous analysis, neglect heat loss through the walls of the gasifier and the enthalpy loss due to slag. This will allow you to start on this a little earlier if you wish (in parallel with the last bits of Part 1), and it will help you to avoid some Cantera gymnastics in equilibrating the mixture over a wide range of conditions. (These can all be handled, but they won't lead you anywhere new, so we will skip them this week.)

Show contour plots for the temperature and major species and for the two performance metrics (CGE, syngas yield). Include a contour on your plots that shows the locus of operating conditions corresponding to the ash-melting temperature of this coal (Table 4-6), recalling that since we are slagging this time, we must maintain the reactor comfortably *above* this temperature.

In addition to the plots above, show contour plots for the minor species hydrogen sulfide H_2S, carbonyl sulfide COS, and ammonia NH_3. This type of oxygen-blown, entrained-flow gasifier is the heart of the IGCC process. Conversion and removal of these species plays a central role in determining the efficiency and capital cost of IGCC as a competitor with pulverized coal, supercritical-Rankine-cycle power plants for base-load electric power generation.

Note: The contour plotting routine requires a full matrix of data values to operate. When gasifying coal, you will run into conditions where there is not enough oxygen to gasify the feedstock without forming solid carbon. Since there is no way to represent solid carbon as an ideal gas, we cannot simply include it in the property set and so we must treat this condition separately. In practice it turns out not to be difficult. All you have to do is to be on the lookout for negative mole numbers for any of the species you use to feed atoms into the gasifier. If you calculate these correctly, then the onset of negative numbers means that there isn't enough oxygen to go around. Given that the contour function wants data at all matrix locations, but you can't calculate data in places where the problem is non-physical, you need to fake out the contour function. This is easy enough to do: When the mole numbers go negative, simply write a zero into the matrix for the rest of the oxygen/carbon sweep. This will cause the contour plotting routine to form a wall of sorts at the boundary where the problem becomes unphysical. Since the plateau formed by the constant value (zero) will have no contours on it (it is a plateau), the plot will appear very much as it should—it will have a well defined demarcation between the real solutions and the (automatically identified) boundary of physical solutions.

(3) 25 Points Get some extra sleep. Do not dream of Cantera, Matlab, gasification, or exergy. (Dreams of a secure, environmentally compatible energy future are, of course, permitted.)

(4) 25 Points Get some more sleep.

The Write-Up

Only the plots are required. As always, please provide a brief statement of how much time was spent on each part of the analysis and what you thought were the most and least useful aspects.

The Deliverables

(1) Plot of Temperature vs. O_2/C ratio for Natural Gas, Coal and Biomass (one plot)
    Include horizontal lines indicating ash melting temperature
  Plot of Major species vs. O_2/C ratio for Natural Gas, Coal and Biomass (one plot, linear)
    Include vertical lines indicating O_2/C ratio corresponding to ash melting temperature
  Plot of Minor species vs. O_2/C ratio for Natural Gas, Coal and Biomass (three plots, semilog)
    Include vertical lines indicating O_2/C ratio corresponding to ash melting temperature
  Plot of CGE vs. O_2/C ratio for Natural Gas, Coal and Biomass (one plot)
    Include vertical lines indicating O_2/C ratio corresponding to ash melting temperature
  Plot of Syngas Yield vs. O_2/C ratio Natural Gas, Coal and Biomass (one plot)
    Include vertical lines indicating O_2/C ratio corresponding to ash melting temperature

(2) Footprint diagrams for coal gasification (0.1-0.5 O_2/C ratio, 0-1.5 H_2O/C ratio)
    Temperature
    All Major Species
        Include locus of ash melting temperature
    Minor Species: COS, H_2S, NH_3
        Include locus of ash melting temperature
    CGE
        Include locus of ash melting temperature
    Syngas Yield
        Include locus of ash melting temperature

(3) Zzzzzzz...

(4) An enthusiastic "Good Morning!" for The Village on Friday.