

# Using Models To Select Operating Conditions for Gasifiers

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The gasifier is probably the most important component in an IGCC cycle because it provides a means for converting solid fossil or opportunity fuels into clean gaseous fuels, liquid fuels or chemical feedstocks. In a recent DOE Industry survey, improved performance of entrained-flow gasifiers and the use of computer simulation to address problems hindering their operation have been identified to be critical for the success of Integrated Gasification Combined Cycle (IGCC) power plants [Clayton et al, 2002].

Through funding from a DOE Vision 21 project, Reaction Engineering International (REI) has developed comprehensive Computational Fluid Dynamics (CFD) models and mechanistic-based process models for entrained flow gasifiers, and incorporated them into a flexible system model or workbench for a Vision 21 plant. Our efforts on gasifiers are focused on the dominant, commercially available gasifier configurations: single-stage and two-stage, pressurized, oxygen-blown systems [Holt, 2001]. In this paper we present an overview of our Vision 21 program and focus on the application of the gasifier Process Model developed for rapid assessment of effects of operating conditions on gasifier performance.

For the single-stage gasifier, emphasis is on down-fired systems that contain a single injector along the gasifier centerline. However, configurations with multiple injectors or an up-fired orientation have also been studied. For the two-stage gasifier we have selected for study an up-flow design with multiple feed inlets that can be opposed or tangentially fired. The two-stage gasifier consists of two sections connected by a diffuser. Each section can have two or four feed injectors. The first stage is assumed to be a slagging combustor used to remove a high fraction of the ash as slag and to provide hot gases to the second stage. Ash particles are deposited on the wall as slag for both classes of gasifiers. Proper slagging behavior is important for protecting the refractory-lined walls of the gasifier from the harsh environment within the gasifier. Examples of commercial sized single-stage, down-fired gasifiers are those used at the Polk Power Station, Eastman Chemical plant, and the gasifier test facility at the Freiberg R&D center in Germany. Examples of commercial-sized, two-stage gasifiers are the opposed-fired gasifier used at the Wabash River power plant and the air-blown, tangentially-fired systems being developed in Japan. Although our focus is on oxygen-blown, slurry-fed, pressurized systems, the same modeling tools can be used to model air-blown, dry-feed or atmospheric systems. Our gasifier model development efforts are strengthened through collaborations with Neville Holt of the

Electric Power Research Institute (EPRI), Prof. Terry Wall and his colleagues at the Collaborative Research Center for Coal and Sustainable Development (CCSD) in Australia, and Prof. Klaus Hein from the Institute for Process Engineering and Power Plant Technology (IVD) at the University of Stuttgart, Germany.

## **IGCC VISION 21 PROCESS WORKBENCH**

The gasifier models are embedded within an IGCC process workbench simulation tool that REI has developed within a DOE Vision 21 project [Bockelie, 2003]. The process workbench can be used to analyze the performance and emissions from Vision 21 energy plant systems as well as other Advanced Power Generation systems that are focused on near zero emissions of pollutants and green house gases. The workbench has been developed as a tightly-integrated problem-solving environment, with plug and play functionality, which contains an array of tools and models that communicate in a seamless manner. A hierarchy of models is provided in the workbench, ranging in complexity from simple reactor models to sophisticated CFD-based models. The available component models include:

- Gasifiers – entrained flow; transport reactor;
- Heat Exchangers – syngas cooler, heat recovery steam generator (HRSG), recuperator;
- Air Separation Unit (ASU);
- Gas Clean Up (warm, hot) – cyclone, chlorine guard, bulk desulfurizer, sulfur polisher;
- Gas Turbine Equipment (turbine, compressors, expanders, combustors);
- Solid Oxide Fuel Cells (SOFC) and SOFC Exhaust Gas Combustors (dump, catalytic);
- Membrane Based Gas Separation Units – water gas shift membrane reactor.

The models can be computed locally or on geographically dispersed computers. The workbench provides support for using “virtual sensors” to indicate equipment (or model) operation problems (e.g., refractory temperatures out of range). The workbench provides the capability to interrogate a simulation at multiple levels of detail. Data visualization is performed using software from the Iowa State University Virtual Reality Applications Center, that allows displaying simulation results on systems ranging from inexpensive desktop PCs to large-scale immersive virtual reality environments. The process workbench can be used to perform simulations and visualize results for individual components, “sub-systems” within the plant, or overall plant performance. Compared to currently available tools, our IGCC process workbench provides a substantial increase in flexibility, ease of use, model selection, solution interrogation, and simulation sophistication.

Using the feedback loop capability of the process workbench allows including the effects of nearby down-stream processes on the gasifier calculations. Hence, the effects of char recycle and flue gas recycle can be included in the gasifier calculations. This also provides the capability to study the impact of water-gas shift reactions downstream of the gasifier, prior to the take-off for cooled syngas recycled to the gasifier. Last, because data available in the open literature is typically reported for “clean” syngas at a point downstream of the gasifier, using the process workbench allows accounting for these additional processes and thereby facilitates model benchmarking.

## **GASIFIER OPERATING CONDITIONS**

The focus in this paper is on the selection of the operating conditions for single-stage and two-stage “generic” cylindrical gasifiers. The pressure in a gasifier is normally determined by the end application. For the current generation of IGCC plants, the gas turbine governs the selection of the gasifier pressure, which is typically in the range of 20 to 30 atmospheres. For chemical plants, pressures are dictated by the pressure in the units to which the syngas from the gasifier is sent, and are typically in the range of 60 to 80 atmospheres. The operating changes that need to be modeled, in addition to pressure, are:

- fuel switching: coal type – petcoke, wastes;
- feed system: wet (slurry) versus dry ( $N_2$ ,  $CO_2$ );
- fuel-oxidant ratio;
- coal ash composition and its impact on slagging properties; and
- char recycle and flue gas recycle.

The CFD model calculates the following output parameters:

- carbon conversion, cold gas efficiency;
- syngas properties:
  - flow rate, temperature, heating value;
  - species composition (typically up to 20 species are tracked);
    - major:  $CO$ ,  $CO_2$ ,  $H_2$ ,  $H_2O$ ,  $N_2$ ,  $O_2$ ,
    - minor:  $H_2S$ ,  $COS$ ,  $CH_4$ ,  $NH_3$ ,  $HCN$ , ...
- fly ash properties (carbon content, particles size distribution);
- slag efficiency (fraction of total ash removed as slag, unburned carbon content).

In addition, the following distributions within the gasifier are calculated:

- temperature and composition within the gas;
- ash deposition rates and properties of ash layer on gasifier walls (composition, temperature, viscosity, thickness, carbon content);
- heat flux to the walls and the rate of heat extraction for different thermal boundary conditions, e.g. refractory or cooled walls.

The criteria for selecting the operating conditions are that the carbon conversion efficiency should be high, the cold gas efficiency (the fraction of the heat of combustion of the fuel that is available in the cooled syngas) should be a maximum, and the temperature for a single-stage or the first stage of a two-stage gasifier should be high enough to enable the slag to flow freely. These requirements can be used to define the oxygen/carbon ratio,  $H_2O$ /carbon ratio, and gasifier volume. Since CFD-based gasifier models can require significant computational time to arrive at a steady-state solution, we have developed a simple model that can be used for rapid calculations either within an energyplex workbench or as a preprocessor to narrow the range of operating conditions for a CFD model. The model, its validation, and selected application are described below.

## **PROCESS FLOW SHEET GASIFIER MODEL (STEADY-STATE)**

The process flow sheet gasifier model consists of three submodels: a zonal, equilibrium submodel with heat transfer; a carbon burnout submodel; and a model of the quench zone

downstream of the gasifier. The zonal submodel calculates the equilibrium exit gas concentration and temperature given a prescribed backside temperature and wall resistance. Heat loss through the walls and heat absorbed by the ash in the solid fuel (e.g., coal) are accounted for in the model. An ash viscosity submodel developed for the CFD gasifier flowing slag model is used to calculate a representative ash viscosity and critical viscosity temperature. The fuel burnout and char recycle are required inputs to the zonal submodel obtained from the burnout submodel, while the gas and radiation temperatures are the required inputs into the burnout submodel obtained from the zonal submodel.

A schematic of the one stage and two stage process flow sheet gasifier models are illustrated in Figures 1a and 1b, respectively. For particle burnout we use kinetic parameters that include the intrinsic kinetics of the reactions of the various carbons with oxygen, carbon dioxide, and water vapor, models for the pore diffusion, and the evolution of physical properties (porosity, surface area, particle diameter) developed by the CCSD in Australia. The detailed kinetic models are used to obtain power law kinetics that are easily incorporated into the process and CFD models. There is a paucity of data at high pressures, but the CCSD has embarked in a systematic program to fill in the gaps and provides the results to REI as they become available as part of our collaboration.

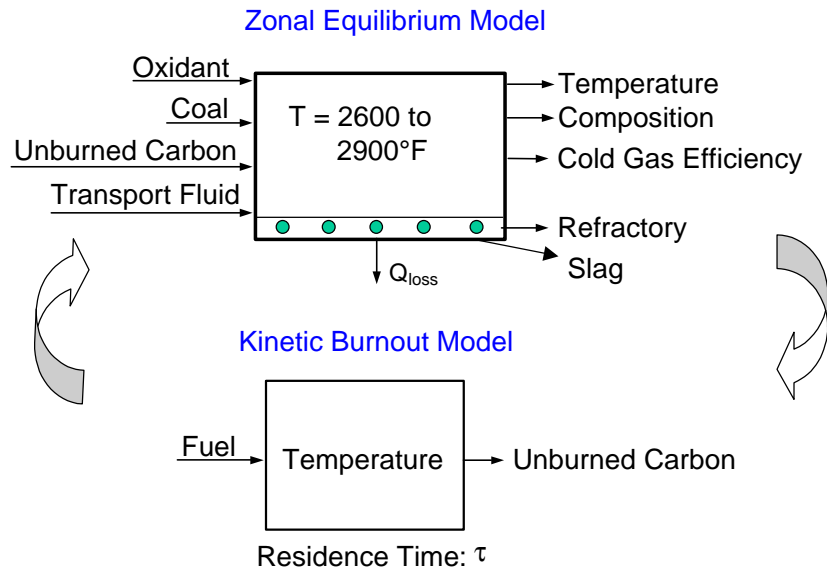


Figure 1a. Schematic for the one stage, process flow sheet gasifier model.

In general, two-stage gasifiers are operated with the first stage serving as a combustion stage, which provides the heat needed to drive endothermic gasification reactions in the reducing second stage. The first stage is operated close to stoichiometry, while the remaining feed-stock fuel is introduced in the second stage with very little or no oxidant. In the two-stage model, staged fuel injection is easily handled. Iterations proceed in the first stage between the particle burnout, equilibrium, and heat transfer models until the exit temperature is converged (see Figure 1b). The same iterations for the second stage then follow, except that any unburned particles from the first stage are also integrated in the second stage.

The process inputs for the model include: the fuel properties; flow rate, composition and temperature of the slurry (or transport gas for dry feed), oxidant, recycled char and recycled syngas. The inputs to describe the reactor include the gross geometry (height, diameter) and the wall properties.

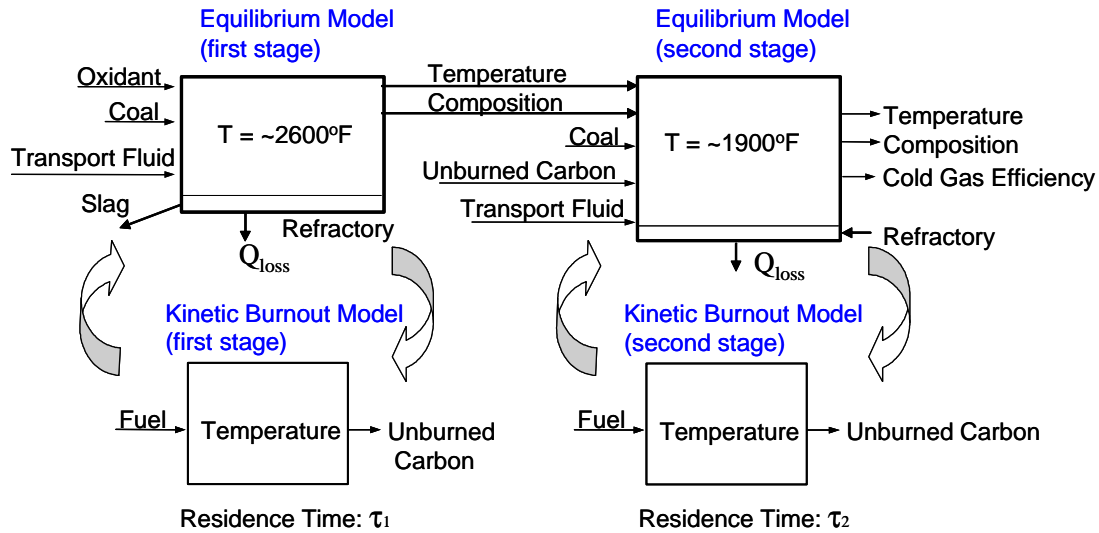


Figure 1b. Schematic for the two-stage, process flow sheet gasifier model.

## QUENCHING OF GASIFIER OUTPUT

The gases leaving the gasifier may be cooled at different rates depending upon the design of the process. Mechanisms of cooling, listed in order of decreasing cooling rate, include injection of recycled cooled syngas, firetube heat exchangers, heat-exchange platens, and radiant coolers. The temperature at the exit plane of a single stage gasifier is high enough that reactions will continue until it is quenched. The result of this cooling on the gas composition is to increase the concentrations of  $\text{CO}_2$  and  $\text{H}_2$  at the expense of those of  $\text{CO}$  and  $\text{H}_2\text{O}$ . As a consequence, the temperature at which the water-gas shift equilibrium reaction ( $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$ ) is equilibrated in the product syngas decreases. This is evident in Fig. 2, in which the water-gas shift equilibrium constant of the quenched product gases is shown as a function of cooling rate for gasifier outlet temperatures of 1900, 2241, and 2577°F. No reactions occur downstream of the reactor for an exit temperature of 1900°F (representative of the exit temperature of a two-stage gasifier), as evidenced by the constancy of the equilibrium constant. As the exit temperature is increased, however, significant reactions occur at the lower cooling rates, as seen for exit temperatures of 2241 and 2577°F (representative of the range of exit temperatures of single-stage gasifiers). The lower cooling rates of 200°F/s may represent values in radiant coolers. The values on the order of 1000°F/s are representative of the use of cooling in firetubes. Higher values on the order of 50000°F/s can be obtained by rapid mixing with recycled cooled syngas.

The frozen water-gas shift equilibrium constant in Fig. 2 can be translated into a temperature at which the reactions are effectively frozen. The results of doing so are shown in Fig. 3, where the equilibration temperature is shown as a function of the cooling rate of the gasifier product gases, for gasifier exit temperatures of 1900, 2241, and 2577°F. It can be seen that as the cooling rate is increased to levels in excess of 50000 °F/s the gas composition is quenched at levels close to that at the gasifier outlet. As the cooling rate is decreased, the temperature drop before the syngas composition freezes increases. A rule of thumb for the differential between the exit and frozen temperatures that is used in the industry (Holt, 2001) is 150°F, but it can be seen that this drop is a function of both the gasifier exit gas temperature and the quench system design.

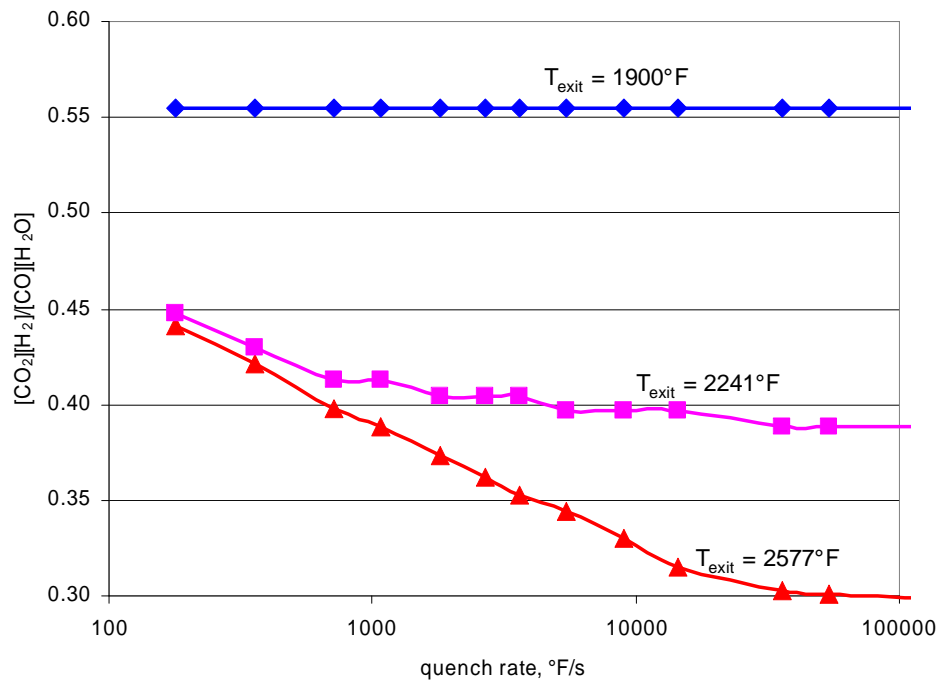


Figure 2. Effect of quench rate on water-gas shift equilibrium constant for syngas produced in gasifiers with exit temperatures of 1900°F, 2241°F and 2577°F.

It should be pointed out that the impact on gas composition and cold gas efficiency due to the temperature differentials is small. Results for the gas composition for different cooling of 180°F/s, 5400°F/s and 180000°F/s are shown in Table I. The simulations were carried out for conditions corresponding to a dry-fed, oxygen-blown, Shell gasifier processing 2560 tons per day of Illinois #5 coal. The coal is pulverized and pre-dried to less than 2 percent moisture, and then transported to the gasifier by high-pressure nitrogen. Oxygen of 95 percent purity is supplied by the Air Separation Unit. Over the wide range of quench rates studied, measurable differences in the gas concentrations of H<sub>2</sub>O and CO<sub>2</sub> are seen, but the absolute changes are small enough not to have a significant impact on the syngas heating value or cold gas efficiency.

The effect of syngas quench rate on the water-gas shift equilibrium can therefore be considered to have a second order effect.

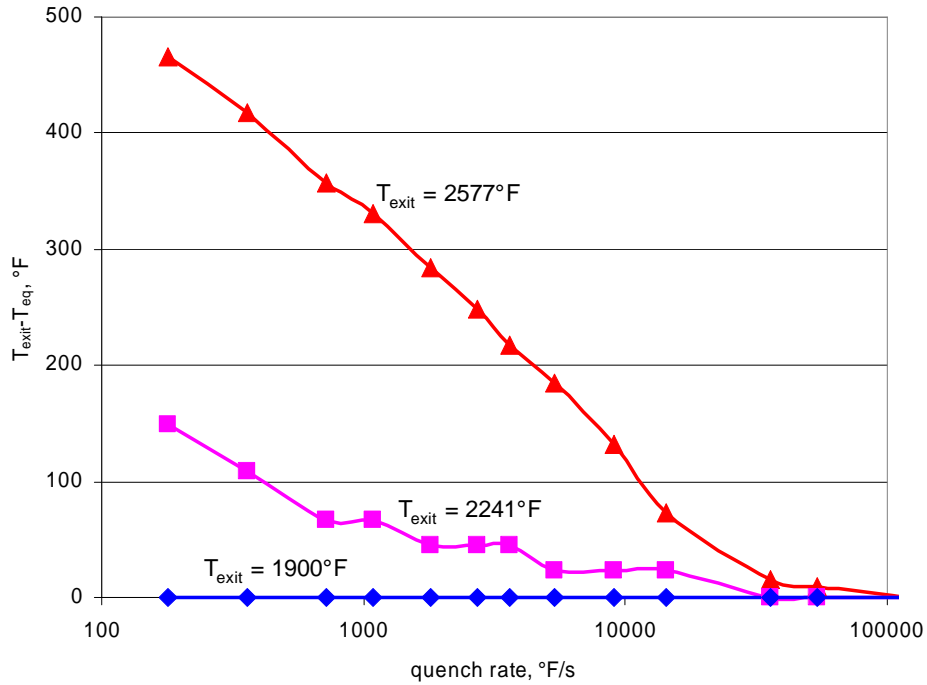


Figure 3. Difference between gasifier exit temperature,  $T_{exit}$ , and the water-gas shift equilibrium temperature,  $T_{eq}$ , for gasifier exit temperatures of 1900°F, 2241°F and 2577°F.

Table I. Impact of quench rate on gas composition and heating value.

	<b>B&amp;V</b>	<b>Model</b>	<b>180°F/s</b>	<b>5400°F/s</b>	<b>180000°F/s</b>
Exit Temperature, °F	-	2615	441	441	441
Carbon Conversion, %	-	99.1	99.1	99.1	99.1
Mole Fraction: CO	0.6284	0.6173	0.6100	0.6160	0.6170
H <sub>2</sub>	0.2837	0.2264	0.2340	0.2280	0.2270
H <sub>2</sub> O	0.0122	0.0492	0.0418	0.0476	0.0491
CO <sub>2</sub>	0.0104	0.0391	0.0465	0.0407	0.0392
CH <sub>4</sub>	0.00030	0.00004	0.00003	0.00004	0.00004
H <sub>2</sub> S	0.0106	0.0121	0.0121	0.0121	0.0119
COS	0.0008	0.0011	0.0011	0.0011	0.0010
Ar	0.0093	0.0105	0.0105	0.0105	0.0105
N <sub>2</sub>	0.0440	0.0439	0.0439	0.0439	0.0439
LHV of Syngas, Btu/lb	5207.5	4522.7	4517.5	4521.3	4524.3
HHV of Syngas, Btu/lb	5486.2	4765.0	4760.0	4763.6	4767.1
HHV of Syngas, Btu/SCF	297.0	277.9	277.7	277.9	277.8
Cold-Gas Efficiency (LHV), %	79.5	79.5	79.4	79.5	79.5

## VALIDATION OF THE PROCESS MODEL

The gasifier vendors and user community are very protective with information on process design and operation so that validation of models is not easy, and needs to be based on whatever information has been made public. Among the data available in the public domain are those on two single-staged gasifiers, one with a slurry feed and one with a dry feed. These have been used to test the validity of the Process Model.

The Cool Water (1990) coal demonstration unit used a Texaco oxygen-blown gasifier designed to process up to 1000 tons of coal per day fed as a water slurry, at an operating pressure of approximately 42 atmospheres, and with an exit temperature between 2100°F and 2500°F. The operating conditions and the coal compositions for six cases selected for validating the Process Model are shown in Table II. The Cool Water gasifier has refractory walls; therefore, in the simulations, the gasifier was assumed to be nearly adiabatic (wall heat transfer resistance was fixed at 1 m<sup>2</sup>·K/W). The four coals used in the trials were: Illinois #6, Pittsburgh #8, SUFCo, and Lemington. The composition and higher heating values (HHV) calculated from the Process Model are compared with those from the Cool Water plant in Table III. Excellent agreement, within two percent, is obtained between the calculated and measured syngas heating values. The agreement with the data on gas composition is also very commendable, particularly for cases 3, 4, and 5. Note that in all the cases, the predicted hydrogen sulfide (H<sub>2</sub>S) and carbonyl sulfide (COS) concentrations are higher than reported; this is because the reported syngas composition is that after cleaning, while the simulated results are essentially the dry syngas, all formed H<sub>2</sub>S and COS during gasification remain in the gas. The methane concentrations are underpredicted by the model. The methane in the gasifier effluent is believed to be a residual of the pyrolysis products and therefore will be underestimated by the equilibrium model. It should be noted, however, that since information on the char reactivities was not available these were adjusted to fit the char burnout, so the char burnout model was not critically tested here.

The second system used for validation is a Shell Gasifier, which differs from the Texaco design in being up-flow, having a membrane wall, and using dry gas transport. Eurlings and Ploeg (1999) report the performance of three Shell coal gasification processes at Harburg (Germany), Houston and Demkolec (the Netherlands). Results are given for a number of international coals and coal blends. The comparisons here are with the data for two coals, an Illinois #5 coal and a Drayton coal, for which coal analyses were available. Pre-dried coals (about 2 % moisture) are transported to the gasifier by high-pressure nitrogen. The operating conditions for these processes are given in Table IV. Note that coal properties are those after coal milling and drying. Carrier nitrogen flow rates were not reported in Eurlings and Ploeg (1999); in the calculations, these flow rates were adjusted so that the nitrogen concentration in the syngas was the same as that reported in the paper. The syngas compositions, lower and higher heating values, and cold gas efficiencies calculated with the Process Model are compared with the Shell data in Table V. The agreement between model and measured results are satisfactory. Since the heat transfer to the membrane wall was not available it was selected to be in the range of 46 to 250 kW/m<sup>2</sup>. It will be shown later that the results are not sensitive to the rate of heat removal within this range.

The only data available to the authors for a two-stage gasifier was the incomplete documentation in the DOE project reports on the Wabash River plant. The Wabash River gasifier is an E-Gas

oxygen-blown, up-flow, two-stage gasifier operating at a pressure of 400 psia (27 atmospheres). It has processed two different coals (Hawthorn coal and Miller Creek coal), a blend of the two, and petroleum coke. Two of the fuels were modeled here: a sub-bituminous coal and a petroleum coke. Properties of these fuels can be found in Wabash River Project Report (2002). The model predictions are compared with the plant data in Table VI. Since the oxidant flow rate was not reported it was adjusted in the Process Model so that the predicted gasifier exit temperature was close to 1900°F as reported for the two-stage gasifier. It is clear from the table that the syngas compositions predicted by the Process Model are similar to the plant data, though there are some discrepancies, due primarily to the unknown oxidant flow rate and the fuel concentration in the slurry for the case of the petroleum coke. The predicted syngas thermal flows for both cases are in good agreement with the reported data.

Table II. Operating conditions and fuel properties for the Cool Water gasifier.

Case	1	2	3	4	5	6
Coal Type	Illinois #6	Pitt.#8	SUFCo	SUFCo	SUFCo	Lemington
Dry coal feed rate, tons/day	1000	934	1000	1100	1000	1000
Dry, wt%, C	72.21	77.74	71.85	71.45	72.20	69.82
H	4.94	5.32	4.94	4.88	5.04	4.49
S	3.08	2.66	0.43	0.47	0.36	0.42
N	1.57	1.45	1.22	1.21	1.13	1.55
O	6.92	5.46	12.74	11.94	12.59	8.32
Ash	11.28	7.37	8.82	10.05	8.68	15.40
HHV, Btu/lb	12820	14100	12360	12443	12530	12232
as-recd, HHV, Btu/lb	11552	13438	11125	11321	11276	11114
Slurry Conc., wt%	63.4	59.3	60.6	61.7	59.7	62.9
Oxygen flow rate, kscfh	915	933	888	978	907	912
Oxygen purity, %	99.5	99.5	99.5	99.5	99.5	99.5

Table IV. Operating conditions for the Shell gasifiers.

Case	1	2	3	4
Coal type	Illinois #5	Illinois #5	Drayton	Drayton
Pre-dried, moisture, wt%	2.2	2.1	1.5	2.0
ash, wt%	14.2	10.6	12.3	12.2
LHV, Btu/lb	11351	11781	11953	11910
Coal flow rate, kg/s	1.033	1.814	1.588	19.832
Oxidant flow rate, kg/s	0.868	1.524	1.477	17.453
Steam flow rate, kg/s	0.000	0.000	0.000	1.396
Carrier N <sub>2</sub> , kg/s	0.168	0.178	0.159	1.983
Gasifier pressure, barg	20	24	24	27

Table III. Comparison of Process Model results with data from Cool Water Gasifier

Case	1		2		3		4		5		6	
	<b>CW</b>	<b>Model</b>	<b>CW</b>	<b>Model</b>	<b>CW</b>	<b>Model</b>	<b>CW</b>	<b>Model</b>	<b>CW</b>	<b>Model</b>	<b>CW</b>	<b>Model</b>
Exit Temperature, °F	-	2464	-	2656	-	1983	-	2075	-	2142	-	1724
Carbon Conversion, %	96.5	96.5	96.4	96.4	98.5	98.5	98.1	98.1	96.2	96.2	98.0	98.0
Mole Fraction: CO	0.4488	0.4697	0.4427	0.4954	0.4297	0.4162	0.4366	0.4359	0.4277	0.4238	0.4420	0.3938
H <sub>2</sub>	0.3846	0.3427	0.3942	0.3347	0.3813	0.3721	0.3814	0.3672	0.3790	0.3624	0.3686	0.3536
CO <sub>2</sub>	0.1548	0.1697	0.1547	0.1546	0.1807	0.2025	0.1733	0.1884	0.1889	0.2063	0.1795	0.2211
CH <sub>4</sub>	0.00160	0.00005	0.00160	0.00002	0.00210	0.00177	0.00220	0.00089	0.00040	0.00039	0.00070	0.02241
Ar+N <sub>2</sub>	0.0102	0.0076	0.0065	0.0069	0.0062	0.0060	0.0063	0.0061	0.0040	0.0059	0.0093	0.0076
H <sub>2</sub> S+CO <sub>S</sub>	0.0003	0.0102	0.0003	0.0083	0.0000	0.0014	0.0000	0.0015	0.0000	0.0012	0.0000	0.0014
HHV of Syngas, Btu/SCF	266.0	264.1	267.3	263.2	259.4	252.8	261.7	256.6	256.4	250.6	257.9	259.4

Table V. Comparison of Process Model predictions with data obtained in Shell gasifiers

Case	1		2		3		4	
	<b>Shell</b>	<b>Model</b>	<b>Shell</b>	<b>Model</b>	<b>Shell</b>	<b>Model</b>	<b>Shell</b>	<b>Model</b>
Exit Temperature, °F	-	2302	-	2514	-	2386	-	2624
Carbon Conversion, %	> 99	99.0	>98.5	98.7	-	99.3	>98	98.1
Mole Fraction (dry): CO	0.6270	0.6308	0.6410	0.6499	0.6530	0.6537	0.6340	0.6261
H <sub>2</sub>	0.2550	0.2577	0.2660	0.2667	0.2620	0.2659	0.2840	0.2899
CO <sub>2</sub>	0.0220	0.0078	0.0160	0.0054	0.0160	0.0123	0.0150	0.0188
N <sub>2</sub>	0.0880	0.0888	0.0650	0.0633	0.0650	0.0637	0.0620	0.0616
others	0.0080	0.0150	0.0120	0.0146	0.0040	0.0044	0.0050	0.0035
LHV of Syngas (dry), Btu/lb	4732.8	4832.5	4950.9	5050.1	4975.6	5036.2	5114.6	5121.3
HHV of Syngas (dry), Btu/lb	4954.9	5060.1	5186.8	5288.8	5206.8	5272.6	5372.3	5385.6
Cold-Gas Efficiency (LHV), %	75.5	79.5	77.2	77.3	78.0	78.7	78.6	79.4

Table VI. Comparison of Process Model results with data reported for the Wabash River Gasifier

	Typical coal		Petroleum coke	
	Wabash	Model	Wabash	Model
Pressure, psia	400	400	400	400
Fuel, ton/day	2450	2450	2000	2000
Oxidant, ton/day	-	1982	-	1747
Coal, %	60	60	-	54.5
Slurry water, ton/day	1633	1633	-	1670
Mole fraction: N <sub>2</sub>	0.019	0.021	0.019	0.016
Ar	0.006	-	0.006	-
CO <sub>2</sub>	0.158	0.209	0.154	0.143
CO	0.453	0.375	0.486	0.475
H <sub>2</sub>	0.344	0.385	0.332	0.356
CH <sub>4</sub>	0.019	0.001	-0.005	0.002
HHV, Btu/scf	272		268	
Syngas, MBtu/hr	1690	1694	1690	1911
Exit temperature, °F	1900	1933	1900	1978

The comparison between the results of the Process Model are satisfactory considering the difficulty of obtaining complete documentation on field data for gasifiers. This is not surprising, since Ruprecht et al. (1988) presented a model with components, energy balance, carbon oxidation correlation, and water-gas shift equilibrium that parallel those in the Process Model. They report “very satisfactory” agreement between the model results and experiments as part of the development of an oxo synthesis plant of Ruhrchemie. Unfortunately, critical parameters such as the water-gas shift equilibrium temperature, gas composition, and cold gas efficiency were blanked out of the publication so that a quantitative comparison between the present model and the model presented is not possible. The trends in the paper (figures with ordinates not labeled), however, provide reassurance that the approach we are using is valid and the agreement with the incomplete data reported above provides further reassurance.

## PARAMETRIC STUDIES

The Process Model can now be used to study the effects of a wide range of parameters, such as coal or other solid fuel composition, reactor volume, pressure, oxygen/carbon ratio, steam/carbon ratio, pressure, wall heat extraction, dry versus slurry feed, feed preheat. Selected parametric studies will be conducted to show the importance of different parameters. A base case of a gasifier operated at 30 atmospheres, with an Illinois #6 coal, a coal slurry feed with 65% slurry concentration, a slurry temperature of 77°F, a coal flow rate of 25.8 kg/s, an oxidant (95%O<sub>2</sub>, 5%N<sub>2</sub>) flow rate of 13.9 kg/s and a temperature of 77°F, and a heat extraction rate of 100 kW/m<sup>2</sup>. In running the parametric analysis one choice is to vary the parameters keeping the gasifier volume fixed, which is what is expected for changing the process variables for an existing gasifier. However, for the present case the parameter variation was so large that it was decided to vary the volume to keep the carbon conversion efficiency constant, since so many of the observed changes were a consequence of the effect of the parameters on carbon conversion efficiency.

The effect of the heat extraction on gasifier performance for the case of fixed carbon conversion efficiency is seen in Table VII. The range of heat extraction rates were varied from adiabatic (0) to a value of 200 kW/m<sup>2</sup> on the high end of a membrane wall heat transfer rate. It can be seen

that the extraction rates are a small fraction of the total heat input so that the changes in gas composition, gas heating value, and cold gas efficiency are correspondingly small. The change in gas temperature of 60K (108°F) is large enough to affect the kinetics of gasification so that the impact on carbon conversion efficiency could be significant, as will be shown later.

Table VII. Effect of heat extraction on gas composition, exit temperature, and cold gas efficiency (carbon conversion maintained constant).

Heat Extraction, kW/m <sup>2</sup>	0	50	100	150	200
Exit Temperature, °F	2538	2543	2516	2489	2462
Thermal Input, MW	700.6	700.6	700.6	700.6	700.6
Thermal Output, MW	526.7	526.6	526.4	526.3	526.2
Carbon Conversion, %	97.9	97.9	97.9	97.9	97.9
Mole Fraction: CO	0.3529	0.3519	0.3509	0.3499	0.3489
H <sub>2</sub>	0.2487	0.2497	0.2506	0.2516	0.2526
H <sub>2</sub> O	0.2626	0.2616	0.2606	0.2596	0.2586
CO <sub>2</sub>	0.1118	0.1127	0.1137	0.1147	0.1157
CH <sub>4</sub>	0.00001	0.00001	0.00002	0.00002	0.00002
H <sub>2</sub> S	0.00653	0.00654	0.00654	0.00654	0.00655
COS	0.00032	0.00032	0.00031	0.00031	0.00031
N <sub>2</sub>	0.0165	0.0165	0.0165	0.0165	0.0165
Syngas Flow Rate, kg/s	59.92	59.92	59.92	59.92	59.92
LHV of Syngas, Btu/lb	3315.3	3314.5	3313.7	3312.8	3311.9
HHV of Syngas, Btu/lb	3781.6	3780.7	3779.9	3779.0	3778.1
CGE (HHV), %	75.2	75.2	75.1	75.1	75.1

A similar result is seen on the impact of pressure in Table VIII. The volume of the reactor was decreased as the pressure was increased to maintain a constant carbon conversion efficiency. This results in a fraction of the energy input being lost to the wall, but since the heat loss does not significantly influence the gasifier performance this is not significant. Furthermore, the major equilibrium reactions such as the water-gas shift do not involve a volume change on reaction so that the effect of pressure on the gas phase composition is negligibly small.

The effect of slurry concentration in Table IX is dramatic. The impact of the water mass on the temperature in the gasifier is enormous. The variations provided here are unrealistic but make the point on the decrease in gasifier temperature on exit and the increase in cold gas efficiency with increases in water content.

The last parametric variation was that of carbon conversion efficiency, varied here by changing the gasifier length, as shown in Table X. Again, the range of parameters is not realistic but makes the point of how sensitive the performance of the gasifier is to changing carbon conversion.

From these parametric studies it can be seen that the parameters of greatest importance are the pressure because of the effect of gasifier volume, the slurry concentration because of the impact of moisture on temperature and the gasifier performance, and any parameter (furnace length, oxygen concentration, furnace temperature) that affects the carbon conversion efficiency. Because of the interdependence of the parameters it is difficult to draw conclusions from varying

one parameter at a time. The next section provides a parametric study that shows the impact of multiple parameters on performance and illustrates how this can be used to home in on preferred operating conditions.

Table VIII. Effect of pressure on gasifier performance for a fixed carbon conversion.

Pressure, atm	20	30	55	75	100
Exit Temperature, °F	2516	2516	2516	2518	2518
Thermal Input, MW	700.6	700.6	700.6	700.6	700.6
Thermal Output, MW	526.4	526.4	526.4	526.4	526.3
Carbon Conversion, %	97.9	97.9	97.9	97.9	97.9
Mole Fraction: CO	0.3509	0.3509	0.3509	0.3509	0.3508
H <sub>2</sub>	0.2507	0.2506	0.2505	0.2504	0.2502
H <sub>2</sub> O	0.2606	0.2606	0.2607	0.2607	0.2608
CO <sub>2</sub>	0.1137	0.1137	0.1137	0.1137	0.1138
CH <sub>4</sub>	0.00001	0.00002	0.00005	0.00010	0.00018
H <sub>2</sub> S	0.00654	0.00654	0.00654	0.00654	0.00654
COS	0.00031	0.00031	0.00031	0.00032	0.00032
N <sub>2</sub>	0.0165	0.0165	0.0165	0.0165	0.0165
Syngas Flow Rate, kg/s	59.92	59.92	59.92	59.92	59.92
LHV of Syngas, Btu/lb	3313.7	3313.7	3313.4	3313.2	3312.8
HHV of Syngas, Btu/lb	3780.0	3779.9	3779.7	3779.4	3779.1
CGE (HHV), %	75.1	75.1	75.1	75.1	75.1

Table IX. Effect of slurry concentration on gasifier performance for a fixed carbon conversion.

Slurry Concentration, %	48	65	83
H <sub>2</sub> O Flow Rate, kg/s	27.97	<b>13.90</b>	5.29
Exit Temperature, °F	1740	2516	3308
Thermal Input, MW	700.6	700.6	700.6
Thermal Output, MW	546.5	526.4	511.9
Carbon Conversion, %	97.9	97.9	97.9
Mole Fraction: CO	0.1946	0.3509	0.4832
H <sub>2</sub>	0.2700	0.2506	0.2379
H <sub>2</sub> O	0.3430	0.2606	0.1764
CO <sub>2</sub>	0.1705	0.1137	0.0734
CH <sub>4</sub>	0.00289	0.00002	0.00000
H <sub>2</sub> S	0.00531	0.00654	0.00758
COS	0.00012	0.00031	0.00057
N <sub>2</sub>	0.0130	0.0165	0.0198
Syngas Flow Rate, kg/s	73.98	59.92	51.30
LHV of Syngas, Btu/lb	2600.7	3313.7	3924.3
HHV of Syngas, Btu/lb	3178.0	3779.9	4292.6
CGE (HHV), %	78.0	75.1	73.1

Table X. Effect of carbon conversion on gasifier performance.

Gasifier Length, m	0.029	0.1	1.1	5.5	9.9
Exit Temperature, °F	4296	3837	2892	2516	2413
Thermal Input, MW	700.6	700.6	700.6	700.6	700.6
Thermal Output, MW	68.3	247.5	447.9	526.4	541.1
Carbon Conversion, %	36.3	64.0	88.7	97.9	99.6
Mole Fraction: CO	0.0185	0.2146	0.3254	0.3509	0.3536
H <sub>2</sub>	0.0064	0.0989	0.2079	0.2506	0.2599
H <sub>2</sub> O	0.6168	0.4797	0.3186	0.2606	0.2486
CO <sub>2</sub>	0.2730	0.1792	0.1235	0.1137	0.1138
CH <sub>4</sub>	0.00000	0.00000	0.00000	0.00002	0.00003
H <sub>2</sub> S	0.00000	0.00102	0.00623	0.00654	0.00659
COS	0.00000	0.00009	0.00035	0.00031	0.00031
N <sub>2</sub>	0.0213	0.0195	0.0172	0.0165	0.0164
Syngas Flow Rate, kg/s	47.33	52.98	58.03	59.92	60.27
LHV of Syngas, Btu/lb	163.7	1546.3	2855.6	3313.7	3396.0
HHV of Syngas, Btu/lb	620.6	2009.9	3320.4	3779.9	3862.5
CGE (HHV), %	9.8	35.3	69.9	75.1	77.2

## SELECTION OF OPERATING CONDITIONS

For the baseline case of the Illinois #6 coal water slurry considered above, the H<sub>2</sub>O/coal(dry-ash-free) and O<sub>2</sub>/coal(daf) were varied systematically. Increasing O<sub>2</sub>/coal(daf) at a fixed H<sub>2</sub>O/coal results in a systematic increase in temperature and in carbon conversion efficiency. However, there is a value beyond which increases in H<sub>2</sub>O/coal(daf) result in increases in the decrease in the syngas heating value as CO is converted to CO<sub>2</sub> and H<sub>2</sub> is converted to H<sub>2</sub>O. This results in a peaking in the cold gas efficiency (see Fig. 4). We would wish to select values of O<sub>2</sub>/coal(daf) and H<sub>2</sub>O/coal(daf) that lie on the locus of maximum cold gas efficiency that can be seen in Fig. 4. Another constraint is imposed by the need for the slag to flow freely out of the gasifier. The criterion used is that the temperature should be selected to yield a viscosity below a critical value of say 25 Pa·s. For the Illinois #6 the critical temperature is about 1627K (2469°F). The locus for this temperature is shown on Fig. 4. The slagging region is to the right of this line. The conditions close to the knee of the slagging curve provide the desired high cold gas efficiency, high temperature and as is shown on Fig. 5 a carbon conversion efficiency of about 98%. If the carbon conversion efficiency is inadequate then the gasifier length can be changed but this will require repeating the calculations, when significant changes in conversion are expected. For the present, the optimum conditions therefore correspond to an O<sub>2</sub>/coal(daf) of about 0.85 and an H<sub>2</sub>O/coal(daf) of about 0.05. Reducing the H<sub>2</sub>O/coal(daf) would not present a penalty and would probably reduce operating complexity so that may be preferred. Fig. 4 provides an illustration of how the Process Model can be used to select the operating conditions to use in gasifiers. Figures 5 through 10 provide the plots for carbon conversion efficiency, temperature, CO, H<sub>2</sub>, CO<sub>2</sub>, and H<sub>2</sub>O mole fractions. The use of these plots to select operating conditions for gasifiers can be used to evaluate different design configurations and also provides input conditions for the more detailed process design optimization using CFD.

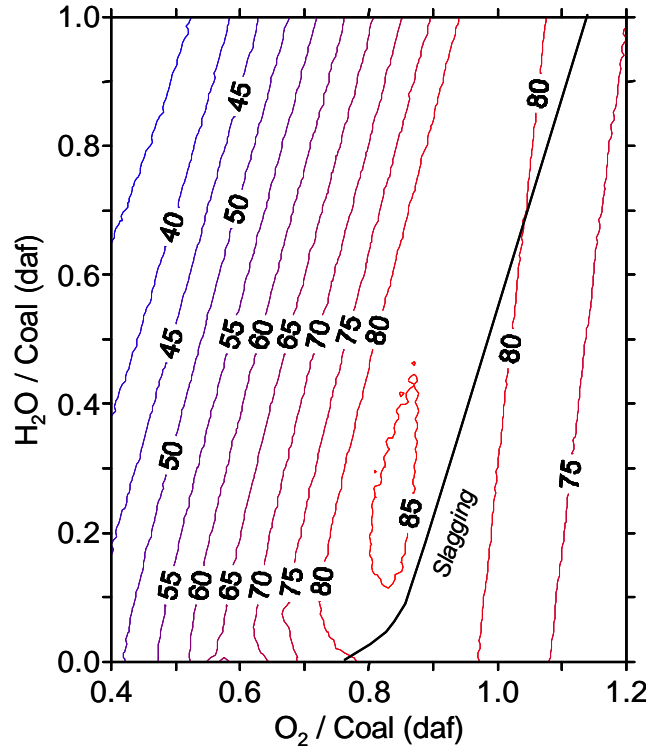


Figure 4. Effect of  $\text{H}_2\text{O}/\text{coal}$  (daf) and  $\text{O}_2/\text{coal}$  (daf) on cold gas efficiency (HHV) (single-stage gasifier, 30 atm, Illinois #6 coal), solid line is locus for slagging conditions.

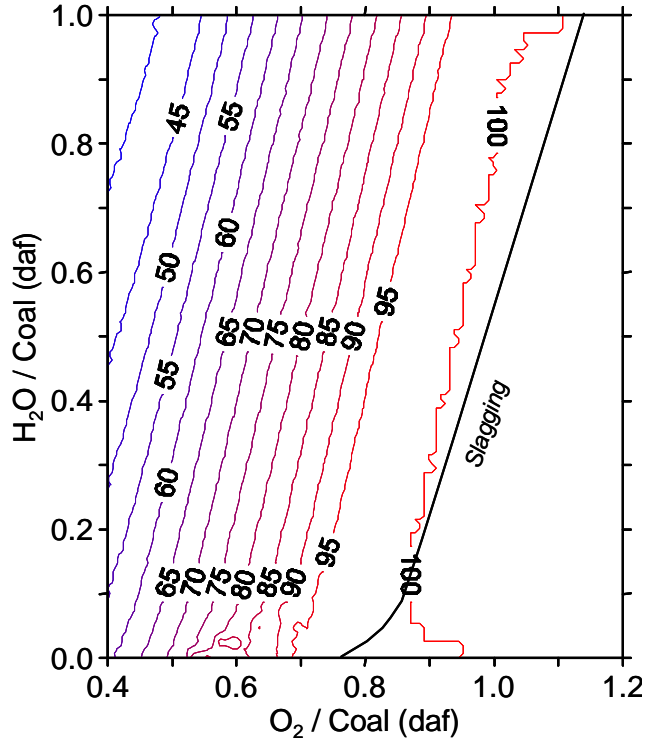


Figure 5. Effect of  $\text{H}_2\text{O}/\text{coal}$  (daf) and  $\text{O}_2/\text{coal}$  (daf) on carbon conversion (single-stage gasifier, 30 atm, Illinois #6 coal).

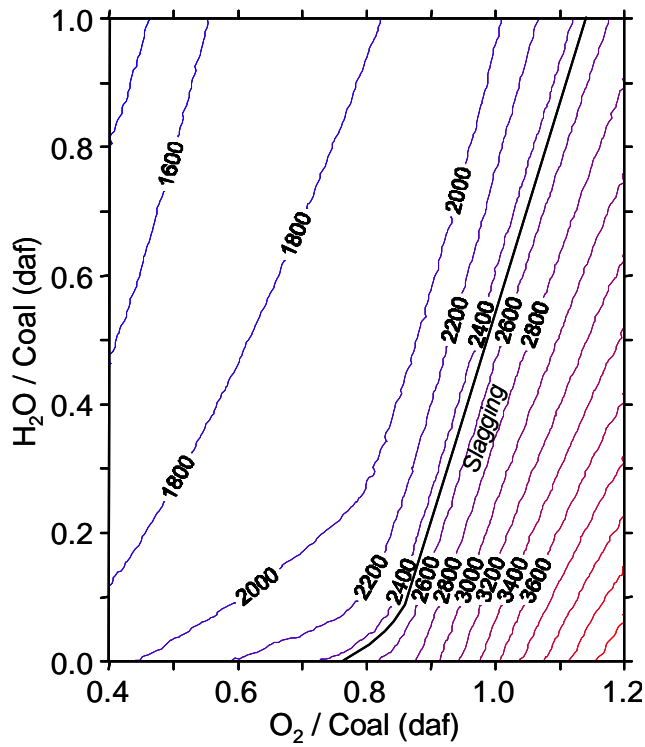


Figure 6. Effect of H<sub>2</sub>O/coal (daf) and O<sub>2</sub>/coal (daf) on gasifier exit temperature (°F) (single-stage gasifier, 30 atm, Illinois #6 coal).

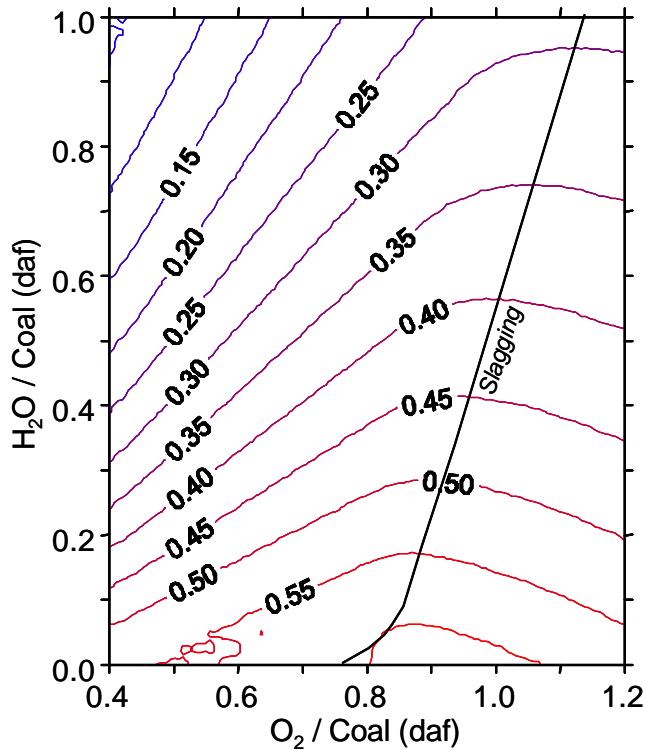


Figure 7. Effect of H<sub>2</sub>O/coal (daf) and O<sub>2</sub>/coal (daf) on CO mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal).

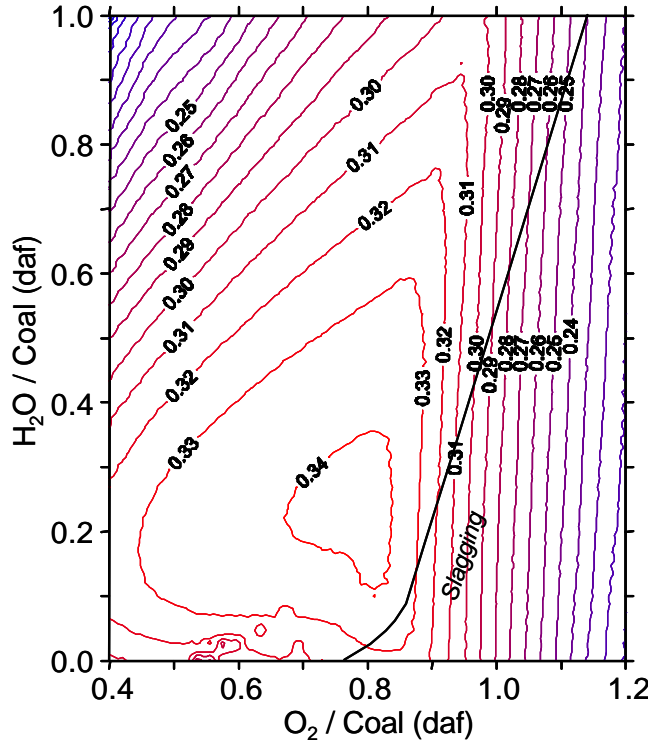


Figure 8. Effect of H<sub>2</sub>O/coal (daf) and O<sub>2</sub>/coal (daf) on H<sub>2</sub> mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal).

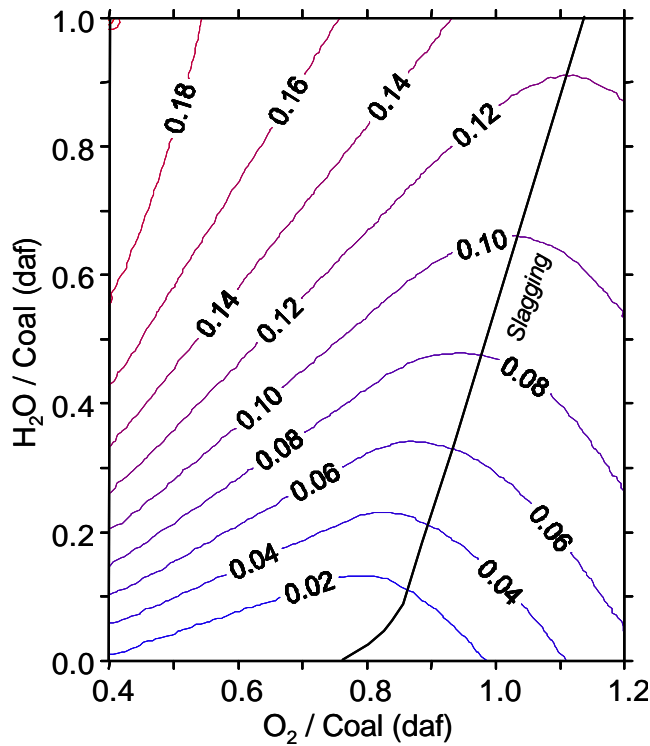


Figure 9. Effect of H<sub>2</sub>O/coal (daf) and O<sub>2</sub>/coal (daf) on CO<sub>2</sub> mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal).

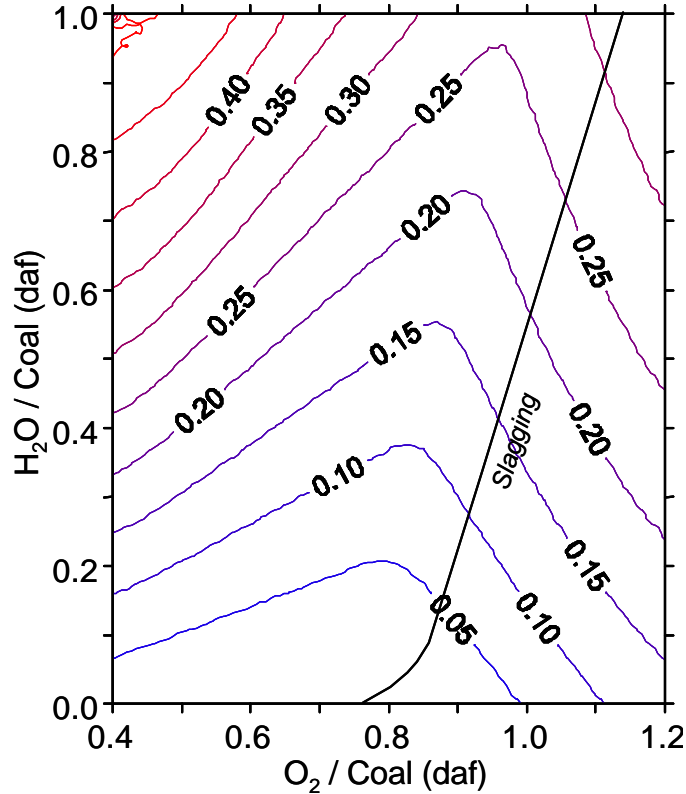


Figure 10. Effect of  $\text{H}_2\text{O}/\text{coal}$  (daf) and  $\text{O}_2/\text{coal}$  (daf) on  $\text{H}_2\text{O}$  mole fraction (single-stage gasifier, 30 atm, Illinois #6 coal).

## CFD GASIFIER MODELS

The Process Model provides a good first approximation for process conditions that can be used as inputs for a CFD model. There are a number of issues, however, that cannot be addressed by the simple model. These include consideration of flame stability that have been shown to impose upper limits on the  $\text{H}_2\text{O}/\text{coal}$  at a given  $\text{O}_2/\text{coal}$  [Smoot et al., 1984], the formation of soot and tars that imposes a lower limit on the  $\text{O}_2/\text{coal}$ , the amount of ash rejected as ash that determines the length to diameter ratio of the gasifier, the overheating of the injector nozzle or refractory that requires the maximum acceptable heat flux at the injector. Such question can be addressed by the use of CFD codes, such as *GLACIER*, REI's proprietary comprehensive two-phase, reacting flow CFD code that can be used to model a broad range of steady, turbulent reacting flows ([http://www.reaction-eng.com/modeling\\_tools/glacier.html](http://www.reaction-eng.com/modeling_tools/glacier.html)). For modeling entrained flow gasifiers, we have incorporated sub-models to account for flowing slag along the gasifier walls and gasification reaction kinetics [Bockelie, 2002a, b]. The flowing slag model is sufficiently general to account for backside cooling (e.g., a water jacket) to create a frozen slag layer on the refractory surface. Other considerations involve the startup and shutdown of the gasifier, and issues such as the build up of an insulating slag layer on the refractories before exposing them to the peak heat fluxes. These require the use of transient CFD models such as *AIOLOS* ([http://www.ivd.uni-stuttgart.de/english/aiolos\\_e\\_fh.html](http://www.ivd.uni-stuttgart.de/english/aiolos_e_fh.html)). This code was originally developed for coal combustion but has been adapted to entrained flow gasifiers by the incorporation of sub-models for gasification reactions. The Process Model described in this paper provides a good

complement to these models and enhances their capabilities by providing a rapid means of developing the approximate operating parameters and reactor configuration before using the time-consuming CFD codes to address the detailed questions.

## **SUMMARY**

In this paper we have described a Process Model for gasifiers that consists of a module that allows for equilibrium gas phase reactions and enthalpy balances for the gasifier, a submodel that calculates the carbon combustion efficiency for chars of different reactivity, and a quench model that can allow for the reactions between the exit of the gasifier and the temperature at which the reactions are quenched. The difference between the gasifier exit temperature and the water-gas shift equilibrium temperature has been found as a function of exit temperature and quench rate. Although the temperature differential can be as high as 460°F at low quench rates (radiant coolers) and high gasifier temperatures (2580°F), the impact on gasifier performance of making this correction is second order. The model has been found to give gas compositions and cold gas efficiencies in good agreement with the limited data in the literature. Parametric studies about a baseline condition were carried out to show that heat loss and pressure had little impact on cold gas efficiency but that small variations in slurry concentration and reactor length (impact on carbon conversion) had a major impact. A procedure was proposed for calculating oxygen/fuel, steam/fuel ratio, and reactor length for use in rapid evaluations of gasifier performance or as inputs to CFD calculations to address a number of issues that cannot be addressed by the Process Model.

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