DEVELOPMENT OF AN ASPEN MODEL OF A DIRECT COAL LIQUEFACTION FACILITY

Howard G. McIlvried
John J. Marano
Burns and Roe Services Corporation

John H. Boyd
Science Applications International Corporation

Development of direct coal liquefaction has seen rapid progress over the past decade and has reached the point where new concepts must be evaluated at the pilot scale. Such experimentation is expensive; and, in order to conserve limited funds, only the most promising developments can be tested in pilot runs. The primary criterion for judging the worth of a new concept is its impact on process economics. It is, therefore, important to be able to perform rapid and accurate (at least relative to the differences between cases) process economics to assist the R&D activity. With that objective in mind, we have developed a new direct coal liquefaction computer model based on the ASPEN simulator.

Although Bechtel, under DOE funding, had previously developed an ASPEN direct coal liquefaction model, the Bechtel model was developed for a different purpose and does not suit our current needs. The Bechtel model basically models the baseline design developed by Bechtel; but, as currently configured, the model does not have the capability to evaluate the effects of process variables, such as pressure, space velocity, gas circulation rate, etc., on process economics. The Bechtel model consists largely of a set of user supplied FORTRAN blocks, one for each plant (coal preparation, hydrogen manufacture, coal liquefaction, gas treating, etc.) in the overall complex, and to evaluate a new case, it is frequently necessary to rewrite one or more of these FORTRAN blocks.

We have chosen a different approach. Our model consists mainly of ASPEN operations blocks together with in-line FORTRAN code and design specifications, as needed. We have included essentially the same plants in our model as are in the Bechtel model, but the level of detail of modeling varies greatly from one plant to another. Those plants which are affected by process variables, such as the coal liquefaction plant, are modelled in more detail than plants, such as sulfur recovery, which are based on well developed technology and which are not affected by process variables, other than individual plant throughputs. Some of the plants of this type are modeled by a single ASPEN separator block.

A major problem faced by anyone planning to model a direct coal liquefaction plant is the complexity of the system with many individual units and a large number of recycle streams. Figure 1 shows a block flow diagram of the Bechtel Base Case. A significant convergence problem would arise were this facility to be modelled exactly as show in this figure. To avoid convergence problems that would arise if all the recycle streams were modeled as they actually exist, some units are modeled in pieces, and then the pieces are summed, after all the rest of the plant is converged, to give total plant feed and product stream rates.

An example of this is the hydrogen cleanup unit, which receives impure hydrogen from direct liquefaction, naphtha hydrotreating, and gasoil hydrotreating and recycles pure hydrogen. This unit is initially modeled as three separate parts, and then the parts are added to give an overall size for use in the costing algorithms. Another example is the gasification unit. This unit gasifies both coal and ROSE Unit bottoms and produces medium Btu fuel gas, in addition to hydrogen. This unit was alsomodelled in three parts.

The Bechtel baseline design consists of 12 major units, as shown in Table 1. Each of these units is included in our model. The only significant differences between our model and the baseline design are that we do not generate electric power and we do not send any phenols to the gasifier.

As mentioned above, the detail with which various units are modelled varies significantly. The most detailed modelling occurs in the coal liquefaction unit, where essentially every major piece of equipment is represented by an ASPEN block. Figure 2 is a schematic of the ASPEN model of the coal liquefaction plant. We did not, however, model the fractionators in detail. These are modeled by separation blocks, and not by plate-to-plate distillations. It was felt that detailed distillation calculations were not necessary and would not add to the accuracy of the model, but they would greatly add to the time required to run the model. In out model, we are only interested in the quantities of the various products, not their exact compositions.

Another approach used to speed up convergence was to converge the material balance first, and then converge the energy balance later in the simulation.

Many units are modelled with one, or at most, a few blocks. These units include the oxygen plant, the sulfur plant, ammonia recovery, and phenol recovery. Figure 3 shows the very simple model of the sulfur plant. Other plants are modelled with slightly more complexity. For example, in hydrogen purification, there are separate blocks for acid gas removal, the membrane unit, the PSA unit, and the compressors. Figure 4 is a schematic of the model for the gasification (hydrogen production) plant. The naphtha and gasoil hydrotreaters were modelled fairly completely.

Another principle we used in developing our model was to configure it so various cases could be run without modifying the model itself, that is by only changing the input data, not the ASPEN blocks themselves. Therefore, most of the required data, such as pressures, temperatures, feed slurry composition, process yields, etc., are entered as parameters in the input file and can be changed by simple editing of the input file. For example, Tables 2 and 3 show the data required for the coal preparation and coal liquefaction plants.

Nevertheless, the model has been carefully written in a modular fashion, so that when it is desired to evaluate a different processing configuration, such as using an in-line hydrotreater in place of the naphtha and gasoil hydrotreaters, it will be relatively easy to modify the model.

As indicated previously, the initial configuration of the liquefaction plant was chosen to duplicate the Bechtel baseline design. One reason for doing this was to have a basis for assessing the validity of the model. To be valid, the model must be able to match the baseline design within a small margin of difference. This version of the model has been successfully completed, and the agreement with the baseline design is quite good. In most cases, for those streams for which data are presented in the Bechtel report, there is at most a few percent difference between the Bechtel design and our model.

In the Bechtel model, each unit has a characteristic flow rate which is used to estimate investment by means of a power law costing algorithm. Using the costing algorithms from the Bechtel model but the corresponding sizing stream rates from our model, the capital investment predicted by our model is off by less than a percent from that given by the Bechtel model, as shown in Table 4.

In addition to capital investments, the other two important pieces of information to obtain from the model are product rates and utility requirements. Again, agreement with the Bechtel Baseline Design is acceptable, as shown in Tables 4 and 5. The reason for the higher phenol yield is, as mentioned above, because we do not send any phenols to the gasifier. We produce slightly more LPG, probably because we use separator blocks rather than distillations. For the same reason, there are minor differecnces in the various distllate cuts, but the overall distillate yield agrees quite closely.

In general, utilities are estimated using the same factors as the Bechtel model. However, duties for all the furnaces are calculated individually. The amount of fuel required is estimated, and enough coal is fed to the gasifier to produce the amount of medium Btu gas needed to just balance the fuel requirement. This includes the heat necessary to raise any net steam requirement. Thus, the only utilities required are purchased electric power and makeup water for the boilers and cooling towers.

As indicated earlier, the gasifier is modelled in three parts. The first part handles gasification of the ROSE unit bottoms. All the ROSE unit bottoms are disposed of in this way. Next, after the model has converged the coal liquefaction plant and the two hydrotreaters, the net hydrogen requirement for the facility is calculated. The second part of the gasifier is then sized to provide the required hydrogen. Finally, the third part is sized to provide the necessary net fuel gas requirement. The three parts are then summed to get total coal and oxygen requirements. These quantities are then used to size the coal processing and oxygen plants. Since this can all be done after other parts of the facility are converged, no recalculation of any other plants is required.

The model prints out a short summary report providing capital investments, utility requirements, and product yields. Tables 4 and 5 show some of the information in this report.

In order to handle calculating the impact of changing operating conditions on Plant 2 (Coal Liquefaction) investment, a FORTRAN subroutine has been written which costs all the equipment items in Plant 2. This subroutine was developed by adding costing algorithms to a subroutine from the Bechtel model which provides sizing of all the Plant 2 equipment. This subroutine provides a platform for adjusting investment as process variables, such as pressure, space velocity, solvent to coal ratio, etc., change.

One other complication deserves to be mentioned and that is the issue of narrow boiling distillate cuts versus wide boiling cuts. Pilot plant data are normally presented as wide boiling cuts, but in some units narrow boiling cuts are necessary for realistic phase equilibrium calculations. Our approach is to enter the data as wide boiling cuts and use ASPEN's ASSAY command to convert the wide boiling cuts to narrow boiling cuts. When narrow boiling cuts are no longer needed, we use dummy RYIELD blocks to convert them back to wide boiling cuts.

In summary, we have prepared a direct coal liquefaction model, based on the ASPEN process simulator. This model runs fairly rapidly, on the order of 5 minutes, and successfully duplicates the Bechtel baseline design. It has been run on both bituminous and subbituminous coals without convergence problems. The next step will be to refine the costing algorithms so that investments in the coal liquefaction plant closely reflect changes in process operating conditions.

PLANTS IN THE BECHTEL BASELINE DESIGN

Plant 1 - Coal Processing

Plant 2 - Coal Liquefaction

Plant 3 - Gas Plant

Plant 4 - Naphtha Hydrotreater

Plant 5 - Gasoil Hydrotreater

Plant 6 - Hydrogen Purification

Plant 8 - ROSE Unit

Plant 9 - Hydrogen Production

Plant 10 - Oxygen Plant

Plant 11 - Sulfur Recovery

Plant 38 - Ammonia Recovery

Plant 39 - Phenol Recovery

PLANT 1 PARAMETERS

PARAMETER 101 ;Water Content of ROM Feed Coal,wt%

PARAMETER 102 ;Ash Content of ROM Feed Coal,wt% MF coal

PARAMETER 103 ;Water Content of Plant 2 Feed Coal,wt%

PARAMETER 104 ;Ash Content of Plant 2 Feed Coal,wt% MF coal

PARAMETER 105 ;Ash Content of Plant 1 Refuse,wt% MF coal

PARAMETER 106 ;Carbon Content of ROM Feed Coal,wt% MF coal

PARAMETER 107 ;Hydrogen Content of ROM Feed Coal,wt% MF coal

PARAMETER 108 ;Sulfur Content of ROM Feed Coal,wt% MF coal

PARAMETER 109 ;Nitrogen Content of ROM Feed Coal,wt% MF coal

PARAMETER 110 ;Chlorine Content of ROM Feed Coal,wt% MF coal

PARAMETER 111 ;Oxygen Content of ROM Feed Coal,wt% MF coal

PARAMETER 112 ;Sulfur Content of Cleaned Coal,wt% MF coal

PlLANT 2 PARAMETERS

PARAMETER 201 ;Solvent to MAF Coal Ratio, lb/lb

PARAMETER 202 ;Resid in Solvent, wt%

PARAMETER 203 ;Ash + IOM in Solvent, wt%

PARAMETER 204 ;Total Hydrogen to MAF Coal Ratio, lb/lb

PARAMETER 205 ;Hydrogen Consumption (MAF Basis), wt%

PARAMETER 206 ;Hydrogen Bleed Rate, lb/lb MAF Coal

PARAMETER 207 ;Reactor Exit Temperature, F

PARAMETER 208 ;Reactor Inlet Pressure, psi

PARAMETER 209 ;Soluable Organics in Lt. Dist., wt%

PARAMETER 210 ;Plant 2 Wash Water Rate, lb/lb MAF Coal

PARAMETER 211 ;Steam to Atm. Tower, lb/lb AT Feed

PARAMETER 212 ;Steam to Vaccuum Tower, lb/lb VT Feed

PARAMETER 213 ;Space Vel. in 1st Rx, lb slurry/hr/ft3

INPUT DATA FOR LIQUEFACTION YIELDS

BLOCK 2R01 RYIELD

MASS-YIELD MIXED H2O 9.51 / H2S 2.86 / NH3 1.39 / CO 0.06 /

CO2 0.14 / C1 1.84 / C2 1.43 / C3 1.52 /

NC4 0.4 / IC4 0.39 / NC5 0.5 / IC5 0.5 /

NAPH 15.12 / LDIST 7.51 / HDIST 25.11 /

LVGO 21.36 / HVGO 0.66 / RESID 8.39 / PHENOLS 0.3

MASS-YIELD NC IOM 7.21

INVESTMENTS

	Our Model		Bechtel Model	
	No. Trains	ISBL, $MM	No. Trains	ISBL, $MM
Plant 1	5	88.8	5	91.0
Plant 1.4	10	87.5	10	87.5
Plant 2	5	932.4	5	932.2
Plant 3	1	26.0	1	25.3
Plant 4	1	14.9	1	15.6
Plant 5	1	73.8	1	74.0
Plant 6	1	159.4	1	152.6
Plant 8	1	43.0	1	42.2
Plant 9	5	264.0	5	263.7
Plant 10	5	177.9	5	191.0
Plant 11	4	45.4	4	46.7
Plant 38	1	40.5	1	40.2
Plant 39	1	18.5	1	13.3
TOTAL		1972.1		1975.3

PRODUCT RATES, LB/HR

	Our Model	Bechtel Design
Propane	31,530	32,422
Butanes	33,855	29,450
Naphtha	225,231	224,290
Light Distillate	104,532	99,876
Heavy Distillate	307,383	300,288
Gasoil	179,917	193,648
Sulfur	59,524	61,722
Ammonia	20,479	20,312
Phenols	3,621	2,707
Ash	213,731	234,340

UTILITIES REQUIREMENTS

	Fuel Gas MMBtu/hr	Power kW	Steam lb/hr	CW gpm
Plant 1	0.	7986.	0.	0.
Plant 1.4	485.	12118.	0.	242.
Plant 2	1318.	59021.	-186756.	7983.
Plant 3	-1525.	824.	416410.	21950.
Plant 4	62.	1095.	26672.	2588.
Plant 5	161.	2174.	30771.	8027.
Plant 6	0.	42083.	62430.	6806.
Plant 8	211.	4559.	25329.	0.
Plant 9	-870.	64653.	-1253920.	50984.
Plant 10	0.	143813.	0.	0.
Plant 11	67.	2965.	-69593.	7733.
Plant 38	0.	1571.	905099.	76585.
Plant 39	0.	1086.	84731.	4490.
Offsites	91.	35783.	28512.	93.
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Total	0.	379731.	69685.	187480.
Bechtel	0.	396295.	74376.	189862.

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