Essential Readings in Light Metals: Alumina and Bauxite.
Edited by Don Donaldson and Benny E. Raahauge.

ASPEN MODELING OF THE BAYER PROCESS

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Summary

The ASPEN simulator was used to model Alcoa's Pt. Comfort Bayer refinery. All areas of the refinery including the lakes and powerhouse were modeled. Each area model was designed to be run stand alone or integrated with others for a full plant model.

The refining plant models were designed to be user friendly, flexible and accurate. User friendly models were made through FORTRAN interfaces that allow easy use by persons with no ASPEN or computer programming knowledge. Flexibility was achieved by building flowsheet options in the model that are available in the plant. Accuracy was accomplished through improved physical property correlations and model verification with plant data. Details on these features and examples of model applications are discussed.

Introduction

Successful chemical process design and operation requires the ability to accurately predict process conditions. Through heat and mass balance calculations, engineers have a tool for determining such changes and raw material and energy consumption. With adequate knowledge of these process parameters, process engineers have opportunities to increase process efficiency, and reduce the cost of operation.

For many years, heat and material balances had to be done by tedious hand calculation. Although hand balances helped engineers make significant process improvements, there were many shortcomings. Simplifying assumptions had to be made so that calculations could be done in a reasonable amount of time. Iterative calculations around recycle processes could be done only a few times and could not obtain tight tolerances.

With the availability of computers, many of the shortcomings of hand calculations were overcome. Tedious calculations could be done quickly; complex process equations could be considered in greater detail. Because many chemical processes used the same unit operations, computer simulation packages were developed to assist engineers in process modeling. The simulation packages model processes with a flowsheet oriented building block approach. This allows engineers/programmers greater flexibility for evaluating flowsheet options and makes the process easier to model conceptually.

ASPEN represents the latest generation of production scale chemical process simulation programs. Because it considers solid components and allows the user to write specific unit operation and physical property models, it is applicable to Bayer process modeling. Alcoa was interested in using ASPEN for Bayer process modeling early on and contributed to its development at MIT. The goal was to develop a general computer model for the Bayer process which could be used for flow sheet evaluations and process improvements. The model was also envisioned as a troubleshooting tool for operations people and as a means for measuring current plant performance against ideal performance.

The modeling effort centered around the Pt. Comfort refinery. Development was a joint effort between the plant and research. Engineers from both locations were involved in assembling the model flowsheets, model coding, the design of the user interface input and output, and model verification.

This paper describes the stand-alone models developed for each area of the refinery and the procedure for full plant integration of these models. The user interface features and the physical property system are discussed, as are plant applications of these models. Several developed models were verified with plant operating data in carefully controlled tests to establish confidence in the modeling approach. Comparisons of model predictions with actual plant operation are shown.

Modeling Pt. Comfort

Model Development

ASPEN models were developed for each major process area. These models can be run stand-alone or combined with other area models for full plant simulation. Because users preferred to work with common process terminology rather than that of the ASPEN program, each model was made to appear as a unique custom program for that area.

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Early in the development, evaluation of flowsheet and operating strategy changes were found to be the major application of models. Initially, evaluation of a flowsheet change required programming changes in the ASPEN input files. This arrangement was hardly ideal from a user's point of view. A programming philosophy was developed to incorporate as many flowsheet flexibilities as possible in the customized models. This allowed many flowsheet changes to be evaluated quickly and easily without any reprogramming.

To ensure that sufficient flexibility was built into each model, the modeling team conducted extensive interviews with the process engineers most likely to use the models. Process flowsheets and modeling assumptions were discussed so that process personnel could get a feel for the model and how it worked. Imminent process changes and future plans were discussed and, when possible, were added to the model. This made the models larger and more complex, but greatly enhanced the process engineer's ability to use the models for flowsheet revision without help from a programmer. Increased flexibility also allowed several similar process units to be covered by one model, thus decreasing model maintenance tasks.

Sometimes process engineers wanted to evaluate a flowsheet change that was beyond the built-in flexibilities of the model. In that case a new ASPEN model had to be developed. For example, if the design of a new heat interchange unit from idle plant equipment was being considered, the process engineers would propose a variety of flowsheet options and discuss them with the modeling team. A model would be developed to evaluate the flowsheet options and to assist in the design of the new unit.

In the course of the process engineer interviews, a model specification document was written. It outlined the user's needs and wants to the programmer, and served as a user's manual for each model. Included in it were process and ASPEN block diagrams, description of inputs and outputs, modeling assumptions, and a user's trouble shooting guide.

All ASPEN process models were written so that users did not have to know how to program with ASPEN. In the customized models, an interactive user interface was set up, making the ASPEN input and syntax transparent to the user. The user's contact with the model consists of a data file containing typical process operating parameters, process configuration options, and material inlet stream composition. The user need only log on to a computer terminal, enter a command specifying the process unit model to be run, and enter process data through an input base file in a line by line prompt mode. The job is submitted automatically when all required inputs are specified. The simulation program is run and results from the job are displayed at the screen and a printed hard copy can be made. Default values for input data are provided in the base file, and the user can also have his own set of defaults. Full screen editing of data files is available to users who find the line by line prompting too slow.

Figures 1A and 1B show a typical input base file and output file for an interactive digestion model. A FORTRAN block, executed first in the ASPEN input file sequence, reads from the input base file, converts the input into ASPEN usable form and passes it to the ASPEN unit operation blocks that make up the model. The simulation portion of the ASPEN input file is executed until the process calculations converge. Then, another FORTRAN block is executed which converts the ASPEN output into terms with which the user is more familiar.

The ASPEN input files with these user interface FORTRAN blocks undergo partial processing before becoming interactive modules for the user. The input translation, FORTRAN compile and link steps are done as the last stage of model development and a load module is stored. This limits the user's wait at the terminal to the simulation execution time.

Physical Properties

Three phases are present in the Bayer process. Solid material is processed in a liquid stream. The liquid is flashed to produce vapor, which is used to heat cold liquor streams. Physical property data is needed for all three phases in order to accurately model the process.

Heat capacity, heats of reaction, boiling point elevation and density are properties commonly used in Bayer process calculations. These properties must be known in order to do accurate material and energy balances. The ASPEN physical property system carries these properties as enthalpy, heats of formation, liquid and vapor fugacity coefficients, and molar volume.

Vapor Properties

For the Bayer process models, water is assumed to be the only component in the vapor phase. Since none of the other components in Bayer liquor are significantly volatile, this assumption seems quite valid. Vapor enthalpy, molar volume, and fugacity coefficient are determined from the 1967 ASME steam table correlations built into the ASPEN physical property system.

Liquid Properties

The model's liquid phase properties are determined for a mixture of water and the following components:

Na_2O	- Caustic not associated with dissolved Al_2O_3
Na_2AlO_4	- Dissolved Sodium Aluminate
Na_2CO_3	- Dissolved Sodium Carbonate (TA-TC)
Na_2SO_4	- Sodium Sulfate
NaCl	- Sodium Chloride
Organics	- Dissolved Organic Compounds

Because Alcoa's version of ASPEN does not have an electrolyte property system, physical properties for Bayer liquor were represented as a mixture of water and pseudo liquid components. A pseudo liquid component represents each of the ionic

```
TITLE FOR THIS SIMULATION:
  SAMPLE BASE FILE FOR DEMO  ..........................85SEP25
L130-001  BEGIN BUILDING 30 INPUT.  40 PSIG STEAM TEMP & PRES (F,PSIA)
           300.0      54.7
L130-002  110 PSIG STEAM TEMP & PRES (F,PSIA)
           400.0     124.7
L130-003  SLURRY ENTRY POSITION CODE.  IF=1 T-1,IF=2 T-2....IF=6 DIG.
           3
L130-004  BLOW-OFF A/TC RATIO
          0.665
L130-005  INTERMEDIATE RATIOS (T1-T5).  THESE ARE IGNORED IF N/A
         .450   .500   .540   .600   .665
L130-006  HEAT TRANSFER COEFICIENTS (T1-T5) (BTU/HR*F*FT**2)
         200    200    250    250    250
L130-007  HEAT TRANSFER AREAS (T1-T5) (FT**2)
         4000.0  4000.0  4000.0  4000.0  4000.0
L130-008  TEMP SET-POINTS:  LAST DIGESTOR AND LIQUOR TO GRINDING (F)
           290.0      212.0
L130-009  LIQUOR TO R-36 (GPM) MAY BE OVERRIDDEN BY 25 MODEL (MIN VAL=1)
           100
L130-010  PRESSURE DROP IN STEAM LINES FOR HEATER STAGES T-1 THRU T-5
           0   0   0   0   0
L130-011  BLOW-OFF TANK PRESSURE RANGE LOWER AND UPPER LIMIT (PSIA)
          14.7     15.0
L130-012  11 & 22 PSIG STEAM WITHDRAWAL (FRACTION FLASH STEAM)
           0.0      0.0
L130-013  FRACTION CONVERSION DATA:  TOTAL BUILDING AL2O3 CONVERSION
          0.98
L130-014  DIGESTER DESILICATION: FRACTION CONVERSION - DSP W/ NACL
           0.0
L130-015  DIGESTER DESILICATION: FRACTION CONVERSION - DSP W/ NA2CO3
           0.5
L130-016  DIGESTER DESILICATION: FRACTION CONVERSION - DSP W/ NA2SO4
           0.0
L130-017  DIRECTION OF LIVE STEAM CONDENSATE IF=1 CRD,IF=0 POWERHOUSE
           0
L130-018  FRACTION OF VAPOR LOST THRU EACH TUBULAR HEATER TO VENT SYSTEM
           .03
L130-019  BUILDING 30 PACKING WATER FLOW (GPM) AND TEMPERATURE
          500      150D0
L125-001  BEGIN BLDG 25A INPUTS.  25A RATIO CODE (=1,ABSOLUTE;=2,CHANGE)
           1
L125-002  25A A/TC RATIO (CODE=1,ABSOLUTE RATIO. CODE=2,RATIO CHANGE)
           .385
L125-003  R-36 CALC CODE(IF=1,NORMAL;=2,VERIFY;=3,25A %SOL;=4,R36 FLOW)
           1
L125-004  25A % SOLIDS (IF GE 0, 25A % SOLIDS),(IF LT 0, 25 % SOLIDS)
           0.5
L125-005  R-2C LIQUOR 'SPILL' (GPM)
           0.0
L125-006  TEMPERATURE SET-POINT FOR 25C CONTACT HEATER (F)
           205.0
L125-007  SPECIFY GRINDING, 25A EXIT TEMPS (OR TEMP DROP IF NEGATIVE)
           165.0   195.0
L125-008  LIME ENTRY CODE(IF=1, 25;=2, 25A INLET;=3, 25A OUTLET;=4, DIG)
           2
```

Figure 1A

Partial Input Base File for
Pt. Comfort Digestion Model

```
 TITLE : PWDIG022 ....TEST RUN.............................85SEP25
 PROPERY SYSTEM LAST UPDATED ON : 84/ 2/16
*               RUN DATE:  9/25/85              *
 SAMPLE BASE FILE FOR DEMO  ..........................85SEP25
****************************************
****************************************
**                                    **
**       PT. COMFORT OPERATIONS       **
**         INDIRECT SLURRY HEATING    **
**                                    **
****************************************
****************************************
    THIS SIMULATION CONVERGED CORRECTLY
     YOU MAY USE THE FOLLOWING OUTPUT DATA

    CHECK THESE RESULTS VS. YOUR SETPOINTS ]
    ----- ----- ------- --- ---- --------- -

    DIGESTER TEMP.                    290.0
    25 CONTACT TEMP.                  205.0
    25A INLET FRACTION SOLIDS        0.5151
    25A OUTLET FRACTION SOLIDS       0.5000
    LIME SLURRY FRACTION SOLIDS      0.1900
    CARBONATION RATE                    0.0

  ALUMINA/CAUSTIC RATIOS
    T-1 EXIT                         0.4500
    T-2 EXIT                         0.5000
    T-3 EXIT                         0.5400
    T-4 EXIT                         0.6000
    T-5 EXIT                         0.6650
    BLOWOFF                          0.6650
    RATIO RISE IN 25A                -.0355
****************************************
*                                      *
*               RESULTS                *
*                                      *
****************************************

****************************************
*                                      *
*   TUBULAR HEATER TEMPERATURES (F)    *
*                                      *
****************************************

        T-1      209.6
        T-2      223.8
        T-3      242.7
        T-4      276.1
        T-5      292.2

****************************************
*                                      *
*FLASH TANK TEMPS (F) & PRESSURES (PSIA)*
*                                      *
****************************************

    B-0      225.9    15.0
    F-7      247.3    22.4
    F-6      268.6    32.7
```

Figure 1B

Partial Output File for
Pt. Comfort Digestion Model

species in Bayer liquor. Properties of the pseudo liquid are set up so that each exerts no vapor pressure and therefore never appears in the vapor phase.

Vapor liquid equilibrium is determined from:

$$x_i \phi^L P_i = y_i \phi^V P$$

where x_i is the liquid mole fraction of component i
ϕ^L is the liquid activity coefficient for i
P_i is the vapor pressure of i
y_i is the vapor mole fraction of i
ϕ^V is the vapor activity coefficient for i
and P is the total system pressure.

For the pseudo liquids, ϕ^L, ϕ^V, and P_i are always zero. Therefore, y_i is always zero. For this reason, water is the only component that impacts vapor liquid equilibrium. P_i and ϕ^V for water are calculated from ASPEN's ASME steam tables. Water ϕ^L is determined from a regression of boiling point data from Dewey (1) and from experiment. The concentration of all liquid phase components and temperature impact water ϕ^L.

Liquid phase enthalpy is calculated from the sum of two parts. The first part is mole weighted sum of heats of formation of all liquid phase components. Standard heat of formation data from the National Bureau of Standards (3) is used. Pseudo liquids are assigned the same NBS heat of formation as its represented ionic species. The organic component's heat of formation is arbitrarily set so that the heat effect of organic reactions is negligible. The second part of the liquid enthalpy equation involves liquor heat capacity. An empirical correlation for heat capacity as a function of temperature and component concentration was derived from experimental measurement. The effect of impurities is included. The heat capacity correlation is integrated with temperature for enthalpy. The form of the ASPEN liquor enthalpy equation is:

$$H = \Sigma\ x_i\ H_{fi} + x_W\ H_W(T) + \Sigma\ x_i \int Cp_i(T)\ dT$$

where H is the liquid phase enthalpy
H_{fi} is the NBS heat of formation at 25°C of component i
H_W is the ASPEN steam table water enthalpy
and Cp_i is the heat capacity of component i in solution (i ≠ water)

At zero ion concentration, H is the ASPEN steam table enthalpy for water.

Similar to enthalpy, liquor molar volume is determined from experimental data. This correlation, also, extrapolates to pure water molar volume at zero concentration.

$$V = x_W\ V_W(T) + \Sigma\ x_i\ V_i(T)$$

where V is the liquid phase molar volume
V_W is the pure water molar volume
V_i is the molar volume of i in solution (i ≠ water)

Solid Properties

A number of solid components are considered in the property system to account for major and minor reactions and impurity balances. These solids are:

Gibbsite
Boehmite
Reactive Silica - carried as Kaolinite
Tricalcium Aluminate
CaO
$CaCO_3$
$CaO.H_2O$
Non Reactive Silica - carried as Quartz
Iron Oxide
P_2O_5
Titania
Desilication Products - (1-1-2 Formula)
w/Carbonate
w/Chloride
w/Sulfate

Additional solids are considered to account for miscellaneous compounds in bauxite which convert caustic in liquor to carbonate, sulfate, chloride, or organate. These do not represent actual solid components but preserve an overall impurity balance.

Solid enthalpy is calculated from the weighted sum of solid heats of formation and from integration of solid heat capacities. Values of the heat of formation and heat capacity were found in the literature for most of the solids listed. In cases where the ASPEN solid component does not represent a real solid, the heat capacity is estimated from a Perry's Handbook equation (4) for naturally occurring solids and the heat of formation is assigned an arbitrary value to make the heats of reaction small.

Literature values for solid density are used when possible. When density data was unavailable for a particular solid, a value of 3000 g/L was assigned.

Individual Area Models

Digestion

Models were developed for the low temperature and high temperature digestion units at Pt. Comfort. Each model determines the steam and raw material usage based on unit flow sheet, operating strategy, and operating parameters. Input data consists of feed stream composition and flow, equipment parameters (heat exchanger surface area and coefficients), and operating parameters (digestion temperature set point, blow off ratio). Results include steam and raw material demands, temperature and pressure profile of flash tanks, temperature profile of heaters and outlet stream flows, and composition.

Digestion unit models can be run in stand alone or full building mode. In the stand alone case, a digestion unit is assumed to have a dedicated bauxite grinding and slurry storage area. This is a good approximation for individual unit evaluations. In the full building mode, the parallel digestion units share one common grinding and slurry storage facility. This model can be used to evaluate

interactions among the units concerning flashed steam and spent liquor sent to grinding.

Because most digestion simulation studies evaluate energy saving projects, the model's energy balance method is very important. Calculations related to the flash tank/heat exchanger network consume a major portion of the simulation time. Input heat transfer coefficient and surface area for each tubular heater are used in an iterative calculation to determine the flash tank pressure that solves the log mean temperature difference for each heat exchanger. For the blow off stage, flash tank pressure limits are specified so that the amount of vapor lost to atmosphere can be determined.

An iterative calculation is used to hit a user specified blow off alumina to caustic ratio set point, by varying the feed slurry flow rate. Bauxite slurry percent solids is maintained by calculating the amount of spent liquor for grinding. An ASPEN user block was written to implement grinding liquor temperature control. Major alumina, silica and lime reactions, as well as minor impurity reactions like P_2O_5 removal and liquor carbonation, are considered. Reaction extents are user specified and are normally based on historical or empirical data. Two ASPEN user blocks were written for digestion reactors. The first is a general reactor which handles all the major and minor reactions possible in digestion. The second dissolves gibbsite or boehmite to achieve a specific alumina to caustic ratio, or ratio increase.

Miscellaneous dilution from pump packing and instrument purge are considered in the model's heat and material balance.

Because many simulation studies concern flow sheet changes, flexibility was built into each digestion model to consider:

- Multiple bauxite and lime slurry entry points
- Multiple condensate withdraw
- Multiple steam entry points
- Multiple grinding liquor sources

In-line FORTRAN was used to implement this flexibility.

Heat Interchange

Models for four unique heat interchange unit flow sheets were developed. Green liquor and spent liquor inlet flow and composition and heat transfer coefficients and surface area are specified. Process evaporation and green/spent liquor outlet temperature are calculated. Log mean temperature calculations are done for each heat exchanger stage by iterative calculation, as in the digestion models. Consideration was made for liquid/liquid heat transfer in plate heat exchangers.

The models are used in studies to determine the process evaporation and test tank temperature for given green and spent liquor flow rates, temperatures and compositions.

Clarification

A single model was developed for Pt. Comfort clarification. Mud slurry from both the high and low temperature digestion units are considered. Mud slurry from each digestion unit passes through sand traps, where the sand fraction is washed and disposed to the lake. The mud fraction is thickened, the overflow filtered, and sent to heat interchange. The thickener underflow is sent to a washing circuit for soda recovery. Last washer underflow is sent to the lake; first washer overflow to filtration.

Several user blocks were developed for clarification modeling. The sand trap block splits the inlet slurry into a sand underflow and mud overflow. This split is determined by a user input sand/mud ratio and percent solids underflow. The thickener model splits the inlet slurry based on a desired underflow percent solids and g/L solids overflow. Both the sand trap and thickener models use ASPEN flash routines to allow user specified heat losses and temperature drops. A counter current decantation (CCD) model was written. This model allows any number of stages, sidestreams, or withdraws. The CCD material balance is determined by user specified underflow percent solids and a stage mixing efficiency as described by Scandrett (2). The user can specify the temperature profile for the CCD cascade, or specify stage heat loss, and have the temperature profile determined by iterative energy balance (7).

Several process reactions are considered in the clarification model. Reactors after the thickeners and sand traps account for autoprecipitation of hydrate through a user specified ratio drop. A reactor block is used to model lime reactions in the causticizer. The amount of lime and steam required for the outside causticization reaction is calculated. The user specifies the fraction of reactive lime that forms calcium carbonate and tricalcium aluminate.

In the stand-alone mode, this model has been used extensively to evaluate operation of the CCD washing circuit. The effect of varying washer dilution and underflow percent solids on caustic recovery has been evaluated. Runs have been made varying the position of washer overflow withdraw to the causticizer to determine the best lime efficiency.

Lake System

The ASPEN lake system model consists of four lakes at Pt. Comfort, the storm lake, clear lake, raw water lake, and mud lake. The purpose of the model is to meet process lake water demand and calculate the plant site water balance.

The major water demands met by each lake are:

Storm Lake:	Supplies accumulated rain water to balance the other lakes
Clear Lake:	Supplies water for precipitation interstage cooling water, precipitation barometric condenser, seed wash, and lime slaking
Raw Water Lake:	Supplies cooling water to rod mills and kilns

Mud Lake: Supplies water for mud washing and heat interchange barometric condensers

Rain and evaporation are considered in each lake balance, determined from user specified run-off and pan evaporation factors, rain and evaporation area.

Hydrate autoprecipitation and atmospheric carbonation are considered for each lake. The user specifies the lake A/TC and TC/TA ratios.

Using inlet flows, lake water demands, and lake bottom percent solids, the model predicts the equilibrium lake concentration, and soda and alumina losses to lake bottom. The rate of mud buildup on the lake bottom is predicted. Also, based on process demands, the model predicts the rate that the mud lake water level rises or falls. Other lake levels are held constant by water transfers between the lakes or by the addition of makeup water from outside the plant. The transfer rates and make-up flow are calculated.

Because it is a steady state model, only long-term steady state predictions are made. It can not predict short-term changes in lake conditions. Although this is not as useful as a dynamic model, it does allow the user to determine the long-term effects of a process change on lake conditions.

Precipitation

Models were developed for batch and continuous precipitation at Pt. Comfort. These models consider all aspects of precipitation from 45A flash to classification and 45E spent liquor tanks.

The 45A area of the models flashes liquor down to a user specified precipitation fill temperature. The amount of cooling water required for the barometric condenser is calculated.

Two user blocks were written to model the actual crystallization process. The first block models a stage or cascade of continuous precipitation. The user specifies the number of stages in the cascade, the cascade temperature profile, tank volume, seed area and green liquor and seed slurry flow. Liquor short circuiting is considered. Yield, solid concentration, and exit liquor composition are calculated. The cascade model uses alumina solubility and growth rate kinetic data developed at Alcoa Laboratories to rigorously calculate hydrate yield (6). This model does not consider particle size distribution. The second user block models a batch precipitator. The same operating parameters and kinetic and solubility data used for the cascade model do the yield calculations for batch. The batch reactor is assumed to be approximated by a long cascade of small volume CSTR reactors.

In both the continuous and batch models, the classification system supplies the user specified seed charge to the precipitation tanks. The user specifies the amount of each type of seed (primary, secondary or tray) to each of the first three tanks in the continuous cascade, or to each unit of tanks in batch. Ratio drops across classification are considered. Because the model is steady state, it is assumed that a seed balance is maintained. The user specified seed charges are always provided. Production is calculated as the amount of solid remaining after the seed charges and the user specified 45E spent liquor solids are supplied.

Liquor for seed slurry injection and water for hydrate and seed washing are calculated. Flows through classification are reported to tell the user if the specified seed charge is achievable.

The models are most often used to calculate production under a given set of temperatures, flows, and seed conditions.

Powerhouse

The powerhouse model for Pt. Comfort determines the fuel required to supply the plant steam and power demands. The user specifies the plant demand for steam from all powerhouse steam headers, compressed air demand, process plant power required, flow and temperature of returned condensate, turbine generator extraction and exhaust flow limits and boiler loading limits.

Gross and net power generated, boiler heat loads, and purchased power requirements are calculated.

The basic strategy used at Pt. Comfort for loading boiler and turbines was built into the powerhouse model; the user can specify loading limits through input to the user interface.

User blocks were written for turbine, turbine generator, and desuperheater/deaerator unit operations. The user is allowed to specify isentropic and mechanical efficiency for the turbines and turbine generators or to have these efficiencies determined as a function of steam flow from a user specified table. Efficiency versus flow data is available from plant or manufacturer's data, and therefore is not frequently changed once set up.

The ASPEN pump block was also modified to allow pump power requirement to be calculated based on manufacturer's pump curves.

This model has been used to evaluate the effect of boiler feed pump pressure on power requirement and to evaluate the impact on power of using lower pressure process steam.

Condensate System

The model for the condensate system provides condensate for the powerhouse, hydrate wash, pump packing, and instrument purge. These demands are met by live and process condensate produced in digestion, heat interchange, the causticization heater, and from the addition of potable water.

Within the model, a hierarchy was developed to supply the hottest condensate first to the powerhouse, then to hydrate wash and finally for packing and purge needs. If there is insufficient condensate, potable water is added to meet the demands. Potable water is first used to meet packing and

purge requirements, and if necessary hydrate wash demand. The amount of potable water needed, if any, to meet these demands is calculated. The model includes provisions for splitting contaminated condensate from the system to waste reclaim.

The condensate model includes a calcination cooler which cools calcined alumina by preheating condensate to the powerhouse. The calcination cooler heat transfer rate is calculated based on inlet alumina and condensate temperature and flow and heat transfer area.

Full Plant Models

Full plant models are assembled from models of the individual process areas. Figure 2 shows a typical full plant flow sheet for Pt. Comfort. Individual area models were coded so that they could be easily combined. To accomplish this, close attention was paid to input file structure, nomenclature and block sequencing.

Each individual model input file is partitioned into easily identifiable sections. The first section isolates information that will be deleted or modified when models are combined. Run control statements, component and property specifications, and other code that is needed only once per input file is found in this section. The overall model sequence appears in this section as well, since the order of execution of a process model in stand alone mode may be different than when it is run in conjunction with other process models.

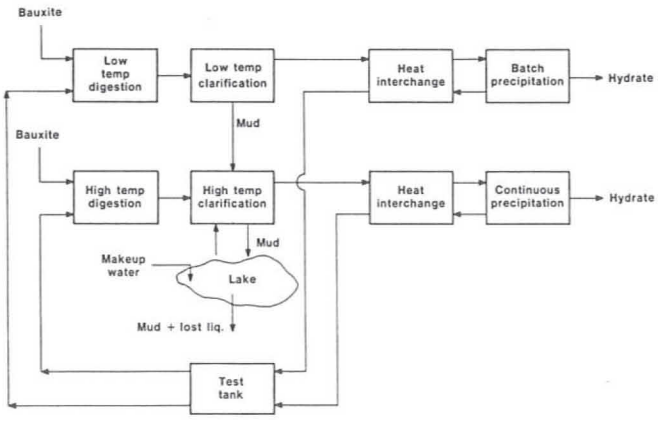
A second section contains the ASPEN input that actually models the process unit. Flow sheet connectivity, unit operation blocks, operating parameters and process control strategy are described in this section. Code in this section can be considered as a self-contained insert for the modeled process unit.

By combining inserts for each area of a Bayer refinery and adding one section of supervisory code and overall sequence, a complete Bayer plant model is created. With this two part structure, it is easy to superimpose overall plant control strategies around the individual area models. For example, dilution in CCD washing can be varied to hit a specified flow rate of spent liquor to digestion.

Within the individual area models, strict rules for names of streams, blocks, FORTRAN variables and statement labels were observed to prevent accidental duplication in the full plant input file. The general naming rule was to end every block, stream and FORTRAN variable name with the unit number and building number of the process being modeled. In this way name conflicts were resolved at the area model level and were avoided in the full plant model.

Much consideration was given to the overall block execution sequence of the full plant model. A sequencing system was devised to ensure that the complex full plant model would work when assembled. Also, overall execution time was reduced by finding a sequence where all recycle streams can be converged simultaneously. In the individual area models, blocks were arranged into specific subsequences. Each subsequence was labeled to indicate where it would be executed in the overall full plant model. Five separate kinds of subsequences were used. One subsequence identified blocks executed only once at the beginning of a simulation, a second for blocks executed only once at the end of a simulation, the third and fourth type of subsequences contained blocks executed once per recycle stream iteration and the fifth contained blocks executed many times per tear iteration. By packaging blocks into subsequences, the procedure for sequencing a newly built full plant model is greatly simplified.

Because of the way individual area input files are structured, named, and sequenced, it is possible to build large full plant input files from the smaller individual area models. Full plant input files can be assembled with relative ease and without ASPEN input translation errors. Although a user needs to be familiar with ASPEN and the structure of the Bayer process model to build a full plant model, this approach allows considerable flexibility.



Full Plant Model Flow Sheet
Figure 2

Training

Models are a great help in doing extensive calculations, but they cannot think. Some input information, such as extents of process reactions, is left up to the user's judgment. Proper choice of this input requires a user's knowledge of engineering and the process. It is imperative that the user understand the assumptions and calculations made in each model. Engineers with the best understanding of the models and the process are best able to apply the models with confidence.

Two courses were given to plant engineers to ensure an understanding of the models. One course was for users, the second for programmers. The user's course was a week long review of completed custom models. Emphasis was placed on hands-on use of the models for solving practical problems. The course was attended by technical and production personnel including superintendents. All received a flavor of the model capabilities and left with the ability to use the models. The programmers' course concentrated on understanding ASPEN and FORTRAN code used in the models and how to modify existing models. This course was attended by plant representatives of the development team and other plant process engineers. Although few of the attendees actively applied programming techniques outside of the course, each had a better understanding of the ASPEN program and its method of calculation.

Verification

The ASPEN models of the Bayer process replace various other mathematical models and material and energy balance calculations done in the past. These calculations were performed by a variety of disciplines and at many levels in the corporation. One of the goals of the modeling project is to put all calculations of this type on an equal basis. Therefore, to establish confidence in their accuracy, the unit models had to be verified against some suitable standards.

Verification was accomplished in a number of ways, including: comparison of results to those of another existing model, testing of the new model at varying conditions for comparison with known trends, and direct comparison of unit models to a steady-state operating unit in the plant.

When possible, comparison to a running plant unit is the preferred verification method. Such comparisons test all the assumptions, convergence methods, and flow sheet details contained in the model at realistic operating conditions. These tests can determine the accuracy of the model and can pinpoint any problem areas for model improvement.

Direct plant-to-model comparisons can be technically difficult. True steady state conditions throughout an operating unit are rare. Often the level of instrumentation needed to operate a process is less comprehensive than needed to define its energy and material balance. Calibration accuracy of the plant instrumentation and chemical analysis accuracy were checked thoroughly for these comparisons.

As an example, for the rigorous verification of the Point Comfort digestion area models, preparations for the plant test involved: inspection and calibration of all flow meters, testing of temperature sensors, installation of some new instrumentation and thermowells, and shutoff of unmetered sidestreams. The plant tests were performed on digestion units that had recently been out of service for overhaul and descaling so that instrumentation errors and operational difficulties caused by scale formation were reduced.

For each digestion verification test, data were gathered at two operating conditions. The only major unmeasured variable was the amount of vapor blown off in the atmospheric flash tanks. Operating conditions were chosen to reduce or eliminate this loss. Each test lasted three to four hours, holding the unit at constant conditions. Other plant areas had to be held as steady as possible in support of the tests.

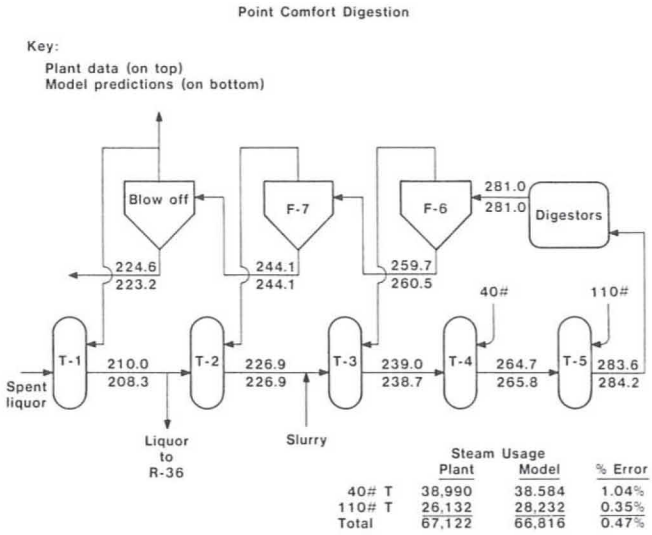
Most of the data collection was performed through the digestion area process computers, which are directly interfaced to about 45 instruments per unit through a multiplexor bank. Data taken from instruments unique to the test were gathered manually every half hour. Spent liquor, bauxite slurry and exit slurry were sampled each hour.

Data manipulation included calculation of temperature compensation factors for all flow meters, averaging of intermediate temperatures and laboratory assay of the samples. Elements as minor as pump packing water flows were considered. The progress of hydrate dissolution through the tubular heaters was found to be important, particularly in the high temperature digestion units, and was closely monitored.

ASPEN input data included spent liquor feed conditions, exit alumina/caustic ratio, and heat exchanger performance variables. The model was used to predict unit temperature profiles, slurry feed flow requirements, steam requirements, flash vapor and condensate flows, and exit slurry compositions.

In early tests, the comparison revealed some important deficiencies in the model, particularly the physical properties used for Bayer liquor. The heat of dissolution of gibbsite was investigated in detail (5) as a result of difficulties in the verification of low temperature digestion. Improved vapor pressure and heat capacity correlations were developed at high temperature digestion conditions to resolve discrepancies between the plant and the model. Additional improvements were made by accounting for liquor impurities and side reactions.

The most recent verification results of digestion have been extremely good. Figure 3 shows the results for a low temperature digestion unit. Steam demand predictions are within one percent of measured values. Average absolute error for temperature predictions is less than 1°F, with the maximum discrepancy being 2°F. Predicted and measured chemical concentrations were within one half percent in most cases. The digestion area models are now believed to be accurate within the limitations of plant measurements.



Low Temperature Digestion Verification Results
Figure 3

The digestion area verification tests were the most rigorous attempted. It is believed that these models sufficiently test the physical property systems and simulation techniques so that many of the other area models can be verified by less stringent means. Everyday users of the models can be confident that the results are the best available.

Applications

The ASPEN simulator has been used in various process engineering analyses at Point Comfort since 1982. In general, the models have been used to predict energy and raw material requirements for various plant equipment configurations. The applications fall under five main categories: production scheduling, optimization of operating targets, process design calculations, capital project justification, and process control and diagnostics.

The production scheduling applications involve using models of the existing plant units to predict steam requirements and other parameters for a given production rate. Different combinations of available equipment will result in different steam usages. These predicted steam values were used to determine energy cost. The energy cost information is combined with other operating cost data to reveal the optimum configuration of the units available. In particular, this method was used to select the number and type of low temperature digestion units to operate at reduced production rates. Also, this method is regularly used to predict energy and raw material costs for budgetary purposes.

For optimization of operating targets, a parametric study of a unit or plant circuit is performed. This can be used to determine the combination of variables for minimum operating cost. For instance, the digestion, evaporation, and powerhouse area models were used to determine the best available steam extraction and exit pressures for the turbine generators. The steam flow rates required for digestion and evaporation at each combination of steam pressure, production rate, and yield were determined. These data were used in the powerhouse model to predict electrical energy production and natural gas demand for each case. The best operating target has the minimum total cost of gas and purchased power.

Process design and capital project justification applications are handled in a similar fashion. An ASPEN model is developed which allows comparison of alternative designs for new equipment in the existing plant. Studies with these models reveal which design is the most favorable in terms of operating cost and assist in the economic analysis of the proposal. The positive or negative impact of a project on other plant areas can be assessed. This can be extremely important, since cost savings in one area are sometimes negated by decreased efficiency in another.

ASPEN models have been used for several such design calculations at Point Comfort. For example, several options were considered for preheating bauxite slurries in tubular heat exchangers. The analysis of options was simplified by development of a single digestion unit model allowing selective utilization of these options. In another case, a ten-stage regenerative evaporator was to be converted into a heat interchange unit. An ASPEN model was used to determine the number of regenerative stages needed for this unit. Such calculations were done exclusively by hand in previous years, in some cases delaying the justification of a project.

The use of ASPEN models in process control is still in the development phase. One possible use for the models is the calculation of steady state operating targets throughout the plant for use by the process control computers. Periodic execution

of a unit or plant model would provide information helpful in deciding if a particular section of the plant is not in balance. If these data can be interfaced directly with process computers, automatic selection of flow controller set points could be made, bringing the plant back in balance. Unit models are already used in a diagnostic mode, where temperature profile expectations in the heat interchange units are compared to on-line data. The comparisons give timely indication of heat exchanger scaling or waterlogging problems.

The main limitation of on-line process control applications is the relatively long processing time and size of machine needed to run the ASPEN models. Currently, the turnaround time for the models is too long for effective real-time processing of results. Also, economic justification for a machine capable of running large simulations is difficult for a single plant. Solutions to these problems will involve simplification of models for the real-time environment, material balance only simulations, general improvements to the software architecture and improvements in hardware execution speed and cost.

Conclusions

The ASPEN simulator can be applied to the Bayer process to model individual operating units and full plants. User supplied FORTRAN helps to make the ASPEN models easy to use by people with limited programming experience. Detailed process simulations can be done quickly, easily and accurately.

The modeling effort for the Point Comfort refinery was successful because of close interaction between plant and research engineers. Close attention was paid by the modeling team to the end users' needs for flexibility and accuracy. User training was an important part of model development.

The models have been used by plant engineers for various flow sheet evaluations. Most often, flow sheet changes or operating strategies were evaluated to reduce energy and raw material consumption.

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