THE USE OF ASPEN PLUS PROCESS

SIMULATOR

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Introduction and Overview

ASPEN PLUS is a process simulator used by engineers to model any type of process for which there is a continuous flow of materials and energy from one processing unit to the next. It is quite versatile as it has been used to model processes in the chemical and petrochemical industries, petroleum refining, oil and gas processing, synthetic fuels, power generation, metals and minerals, pulp and paper, food, pharmaceuticals, and biotechnology.

Flowsheet models are employed throughout. Input to the simulator consists of information normally contained in the process flowsheet such as flow rates, temperatures, pressures, number and compositions of individual streams and the unit operation desired. Output is a complete representation of the performance of the plant, including the composition, flow rates, and properties of all intermediate and product streams and the performance of the various process units.

ASPEN PLUS can be utilized both in the process development and process design phases. During process development, ASPEN PLUS can be utilized as soon as there is a conceptual flowsheet of the process. It can be updated as more information concerning the process is available. It can be used to aid in interpreting pilot plant data and to allow engineers to study many process alternatives.

The ASPEN PLUS models may be used to study trade offs, and to investigate the flexiblity of the plant to handle a wide range of feedstocks. These simulation studies during process design can help avoid costly mistakes before committing to plant hardware.

In addition to providing guidance in process development and plant design, ASPEN PLUS can be utilized as a tool for plant engineers to improve plant operations, to improve yield and throughput, and to reduce energy use in existing plants.

Before proceeding further it is appropriate to provide a brief description of the goal of any process simulator (ASPEN PLUS USER MANUAL, 1981):

> "To obtain the required information about a particular process through the minimum expenditure of engineering and computer resources."

The ASPEN PLUS user manual recommends that the following generalized procedure be followed to help the beginning user develop a methodology for simulation.

1. Determine the scope and level of detail of the information which is desired about the process.

2. Select physical property models from those available in the system or create ones of your own to be used in the calculations. Locate or estimate the parameters and property values required by these models for every component present in the flowsheet.

3. Establish a simulation flowsheet containing unit operation blocks and streams which have been selected in such a way to yield the required information about the process flowsheet, while requiring the minimum amount of computer resources.

4. Select or create an appropriate unit operation model for each block of the simulation flowsheet and specify the parameters required for each block.

5. When necessary, design a control and convergence scheme to achieve the required design specifications and operating conditions in the simulation flowsheet while minimizing computer time.

6. Identify the streams for which additional physical property data are desired, and decide on appropriate table types and accompanying specifications to generate this information.

7. Decide which portions of the process are to participate in economic calculations and establish an economic strategy. This consists of the delineation of cost blocks and sections, the selection of appropriate cost models and utilities, and the selection of a profitability calculation model.

8. Establish the reports that are desired, specify the level of detail of calculation history to be generated, determine the constraints to be imposed on the computer resources, create an input file and perform the simulation.

9. Determine the validity and adequacy of the simulation. Perform additional runs if necessary.

A conceptual understanding of the syntax of the ASPEN input language is required to realize effective and efficient use of the simulator.

ASPEN Input Language

A basic assumption made in selecting the ASPEN input language is that the typical user will be a process engineer who is familiar with process flowsheet calculations. Knowledge of computer programming is not required. The material presented here presents the recommended forms of input for a limited number of applications. The interested reader is referred to the ASPEN PLUS USER MANUAL for considerably more details concerning specific applications.

The ASPEN input language consists of paragraphs, sentences and individual data entries. There are three levels of key words that correspond to this hierarchy: primary, secondary, and tertiary. Key words are system defined words identifying the paragraph, sentence, or individual data value.

Some very specific steps must be followed in developing a flowsheet model to use with the ASPEN PLUS simulator. These steps include:

a. The process flowsheet to be modeled is defined and the purpose of the model is specified.

b. The units of measurement for the input data and output report(s) are selected.

c. The chemical components present in each stream of the process flowsheet are specified.

d. The methods and models to be used to calculate the physical properties are selected.

e. The flowsheet is broken into unit operation blocks and an appropriate model for each block is selected.

f. The feed streams to the process are specified.

g. The performance of each unit operation block is specified.

h. Any additional design specifications are set.

Details of the meaning of each of these steps are provided in ASPEN PLUS An Introductory Manual for the flowsheet representing the hydrogenation of benzene to cyclohexane. An example of the input data file necessary to completely define the process flowsheet is provided along with stream reports and block reports for the reactor, distillation column, and high pressure separator. The stream reports include flow rates in various units, temperatures, pressures, enthalpy, entropy, density, and molecular weight values for the various process streams. The block reports include additional information including convergence tolerance, tower specifications, concentration profiles,

results of flash calculations, and a summary of the flowsheet connectivity by the various streams. The ASPEN PLUS output report for this problem consists of 15 pages. The Introductory manual illustrates 8 pages of this output. These pages include the information of greatest interest to a process engineer using the simulator.

The following example provides an illustration of ASPEN PLUS to simulate a chemical reactor. In particular, the RSTOIC model will be utilized to simulate the reactor used in the synthesis of methanol from hydrogen and carbon monoxide.

Use of the RSTOIC Model for the Methanol Synthesis Reactor

There are six models available in ASPEN PLUS that may be used in chemical reactor simulations. The various models are selected by specifying one of the following acronyms: RSTOIC, RYIELD, REQUIL, RGIBBS, RCSTR, and RPLUG. Each of the six models requires a different input file and produces a different output report. An application of RSTOIC has been selected for this report as it illustrates the principal features of these reactor models. The following table illustrates the input data file for this simulation.

TABLE I-D-1

Input Data File for Methanol Synthesis

```
$ TY INPUT 1.INP
NEW
TITLE 'METHANOL SYNTHESIS'
DESCRIPTION "EXAMPLE OF ICI METHANOL SYNTHESIS"
;
IN-UNITS     ENG
OUT-UNITS    ENG
HISTORY MSG-LEVEL PROPERTIES = 2
COMPONENTS H2 H2/CO CO/CO2 CO2/CH3OH CH4O/H2O H2O
PROPERTIES SYSOP 1 GLOBAL
FLOWSHEET
        BLOCK REACTR     IN=FEED     OUT=PRODS
;
STREAM FEED TEMP = 482     PRES = 450
        MOLE-FLOW = 60
    MOLE-FRAC H2 0.67/CO    0.16/CO2    0.17
;
BLOCK REACTR RSTOIC
        PARAM PRES = 0     DUTY = 0
        STOICH 1 MIXED CO-1/H2 - 1/CH3OH   1
        STOICH 2 MIXED CO2-1/H2 - 3/CH3OH   1/H2O   1
        EXTENT   1   3
        EXTENT   2   0.5
;
STREAM-REPORT
        STANDARD OPTIONS=MOLE-FRAC
$
```

Before presenting the output report that was generated by ASPEN
PLUS from this input file, some specific points will be noted concerning
certain items in the input file.   The ENG following the key words IN-
UNITS and OUT-UNITS indicates that the user has selected the English
engineering set of units for both the input and output variables.   Other
sets including the SI set are available.   The ENG set is the default
set.

The component designations following the key word COMPONENTS
represent the component ID (which the user specifies) followed by the
alias which the ASPEN PLUS simulator utilizes for that particular

component. In this particular example, the component ID and the alias are identical except for methanol.

The specification of SYSOP 1 GLOBAL following the key word PROPERTIES indicates that the user has selected the SYSOP 1 option set to calculate the properties for all streams on the process flowsheet. There are 16 option sets available in ASPEN PLUS. The particular choice of option set depends upon the various properties desired, and the type of mixture selected. SYSOP 1 utilizes the Chao-Seader model to determine the phase equilibrium constants. The ASPEN PLUS Introductory Manual provides guidelines that may be used to select the various option sets along with the specific equaitons used to calculate the various properties once an option set has been selected.

The zeroes following the key words PARAM PRES and DUTY indicate that the reactor is to operate adiabatically with zero pressure drop. The values of 3 and 0.5 which follow the key words EXTENT 1 and EXTENT 2 represent the extent of reactions 1 and 2, respectively.

The following table presents the output report that was generated by the input file just described.

TABLE I-D-2

Output Report

METHANOL SYNTHESIS
DESCRIPTION

EXAMPLE OF ICI METHANOL SYNTHESIS
RUN CONTROL INFORMATION

TYPE OF RUN : NEW
INPUT FILE NAME : INPUT 1
INPUT PROBLEM DATA FILE NAME : RUN 1   UPDATE NO. 0
MAIN CALLING PROGRAM NAME : RUN 1
SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

METHANOL SYNTHESIS
TABLE OF CONTENTS

METHANOL SYNTHESIS
FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
PRODS	REACTR	----	FEED	----	REACTR

FLOWSHEET CONECTIVITY BY BLOCKS

	BLOCK	INLETS	OUTLETS
	REACTR	FEED	PRODS

COMPUTATIONAL SEQUENCE
SEQUENCE USED WAS:
            REACTR
OVERALL FLOWSHEET BALANCE

MASS AND ENERGY BALANCE

CONVENTIONAL COMPONENTS (LBMOL/HR)	IN	OUT	REALTIVE DIFF.
H_2	40.2000	32.7000	0.186567
CO	9.60000	6.0000	0.312500
CO_2	10.2000	9.70000	0.490196E-01
CH_3OH	0.00000E+00	3.50000	-1.00000
H_2O	0.00000E+00	0.50000	-1.00000.

TOTAL BALANCE

	IN	OUT	
MOLE (LBMOL/HR)	60.0000	53.0000	0.116667
MASS (LB/HR)	798.841	798.841	0.629507E-06
ENTHALPY (BTU/HR)	-0.200247E+07	-0.200246E-07	-0.624358E-06

INPUT DATA

STOICHIOMETRY MATRIX:
    REACTION #1:
        SUBSTREAM MIXED:
            -2.00 H_2 -1.00 CO_2 1.00 CH_3OH 1.00 H_2O

REACTION CONVERSION SPECS: NUMBER = 0

REACTION EXTENT SPECS: NUMBER = 2

    REACTION #1 : EXTENT = 3.000 LBMOL/HR
    REACTION #2 : EXTENT = 0.5000 LBMOL/HR

TWO PHASE PQ FLASH

PRESSURE DROP PSI		0.00000E+00
SPECIFIED HEAT DUTY	BTU/HR	0.00000E+00
MAXIMUM ITERATION NO.		30
CONVERGENCE TOLERANCE		0.10000E-03

METHANOL SYNTHESIS
U-O-S BLOCK SECTION

```
REACT - STOICH (RSTOIC) : REACTR (CONTINUED)
                        RESULTS
OUTPUT TEMPERATURE F                        793.23
OUTPUT PRESSURE PSI                         450.00
HEAT DUTY BTU/HR                              0.00000E+00
VAPOR FRACTION                              1.0000
```

While most of the items that appear in this report should be self explanatory, some specific comments concerning its content are now included.

1. Page 3 is not included in the Table of Contents. Page 3 merely includes the acronyms used by ASPEN PLUS in the physical properties section for the various SYSOP option set(s) selected. As SYSOP 0 is the default option set it is always included.

2. Additional information concerning the output stream was provided by ASPEN PLUS. A flash calculation was performed on the output stream and the phase compositions and equilibrium constants for the various species were part of the output report. They were not shown here as the simulator determined that the vapor fraction was 1.0 as shown on page 5 of the output report.

Use of Aspen Plus to Determine Activity Coefficients and Viscosities for Water-Methanol Mixtures

This application illustrates the use of ASPEN Plus to calculate certain thermodynamic and transport properties for specified mixtures. The table below is the input file for this simulation.

TABLE I-D-3

```
        NEW TGS
COMPONENTS H₂O WATER/CH₄O METHANOL
PROPERTIES SYSOP8 GLOBAL
REPORT TABLES
OUT-UNITS SI
DATA
PROP-LIST    GMWSNA 1/GMW SNB 1
BPVAL CH₄O H₂O - 0.8127118/-122.7592
BPVAL H₂O CH₄O 0.8127118/-218.97112
PPTABLES TABLE 1 PROPS
IN-UNITS SI
DESCRIPTION 'SINGLE-PHASE PROPERTIES'
SYSTEM 1 H₂O 1/CH₄O 1
STATE 1    PRES = 101325    TEMP = 298.15
INDEP-VAR 1  TEMP
RANGE 1   SVAL = 273.15    FVAL = 373.15    NINC = 10
DEP-VAR 1   PL   HL   DHVL   VL   COMP = CH₄O  H₂O
INDEP-VAR 2 MOLEFRAC COMP = H₂O
RANGE 2    SVAL = 0    FVAL = 1    INCR = 0.1
DEP-VAR 2 GAMMA COMP = CH₄O  H₂O
TABLE 1 'PURE COMPONENT PROPERTIES' &
        DEP-VAR 3 MULMX
TABLE 1 'PURE COMPONENT PROPERTIES' &
        SYST = 1    STATE = 1    INDEP-VAR = 1 &
        RANGE = 1   DEP-VAR = 1
TABLE 2 'BINARY MIXTURE ACTIVITY COEFFICIENTS' &
        SYST = 1    STATE = 1    INDEP-VAR = 2 &
        RANGE = 2   DEP-VAR = 2
TABLE 3 'MIXTURE VISCOSITY' &
        SYST = 1    STATE = 1    INDEP-VAR = 2 &
        RANGE = 2   DEP-VAR = 3
```

Several comments concerning this input are in order.

1. The values which follow the key word BPVAL represent the
    parameters used in the Wilson equation to determine the
    liquid phase activity coefficients.

2. The pressure and temperture for the input stream are
    specified in SI units.

3. The output reports are requested in SI units.

The important portions of the output report from this input data

file are shown in the following table.

TABLE I-D-4

TYPE OF RUN: NEW
INPUT FILE NAME: INPUT 2
INPUT PROBLEM DATA FILE NAME; RUN 1
UPDATE NO. 0
MAIN CALLING PROGRAM NAME: RUN 1
TGS ONLY RUN

TABLE OF CONTENTS

PHYSICAL PROPERTY TABLES SECTION

(CONTINUED)

PPTABLES (PROPERTIES); TABLE 1
SINGLE-PHASE PROPERTIES
      PURE COMPONENT PROPERTIES

TEMP	DHVL H_2O	VL CH_4O	VL H_2O
K	K/KMOL	CUM/KMOL	CUM/KMOL
2.73150+02	4.48120+07	3.93822-02	1.77177-02
2.83150+02	4.44364+07	3.99376-02	1.78836-02
2.93150+02	4.40537+07	4.05187-02	1.80544-02
3.03150+02	4.36635+07	4.11280-02	1.82304-02
3.13150+02	4.32653+07	4.17681-02	1.84119-02
3.23150+02	4.28589+07	4.24421-02	1.85991-02
3.33150+02	4.24437+07	4.31535-02	1.87925-02
3.43150+02	4.20193+07	4.39064-02	1.89924-02
3.53150+02	4.15852+07	4.47058-02	1.91992-02
3.63150+02	4.11408+07	4.55575-02	1.94135-02
3.73150+02	4.06854+07	4.64683-02	1.96357-02

PHYSICAL PROPERTY TABLE SECTION

PPTABLES (PROPERTIES): TABLE 1 (CONTINUED)
BINARY MIXTURE ACTIVITY COEFFICIENTS

MOLE FRAC H_2O MOL-FR	GAMMA CH_4O		GAMMA H_2O
0.0	1.00000	00	1.87349
1.00000-01	1.00410	00	1.73582
2.00000-01	1.01779	00	1.60854
3.00000-01	1.04391	00	1.49139
4.00000-01	1.08688	00	1.38427
5.00000-01	1.15381	00	1.28724
6.00000-01	1.25687	00	1.20068
7.00000-01	1.41849	00	1.12548
8.00000-01	1.68404	00	1.06351
9.00000-01	2.15848	00	1.01870
1.00000 00	3.13624	00	1.00000

PHYSICAL PROPERTY TABLES SECTION

PPTABLES (PROPERTIES): TABLE 1 (CONTINUED)
MIXTURE VISCOSITY

| MOLE FRAC H_2O MOL-FR	M	MULMX N-SEC/SQ
0.0		3.91909-04
1.00000-01		4.14886-04
2.00000-01		4.37599-04
3.00000-01		4.60087-04
4.00000-01		4.82412-04
5.00000-01		5.04659-04
6.00000-01		5.26948-04
7.00000-01		5.49441-04
8.00000-01		5.72358-04
9.00000-01		5.96002-04
1.00000 00		6.20797-04

INCORPORATING USER MODELS IN ASPEN

ASPEN has two ways of incorporating models for unit operations
not provided by ASPEN. The first way is to use the USER interface
(Chapter 5, ASPEN User Manual Vol. I) that is a standard part of ASPEN.
This interfaces a "personal" model to ASPEN; however, the model does not
become available on a system wide basis. The second way, which is
considerably more complicated, is for the ASPEN System Administrator at
a particular site to build a new model into the ASPEN system so that it
is available to everyone at that site.

We will be illustrating the first way, in which user models will
be incorporated into ASPEN using the USER interface. From the viewpoint
of ASPEN, the USER model is treated the same as any other unit operation
block; i.e., it has an ID, a model type (USER), and its connectivity is
described in a FLOWSHEET paragraph. The USER block obtains values from
inlet stream arrays and block arrays, solves the model equations and
places the computed results into outlet stream arrays and block arrays.
The model allows for from one to four inlet and/or outlet material streams
and for one inlet and/or outlet information stream. Each stream is
passed to the user subroutine through the argument list as a single
array. All stream data are in SI units. In addition, the model allows
the user to pass integer and real variable arrays to the user
subroutine. There may be any number of USER models in a given process
simulation. User model subroutines can call other USER supplied models
as well as ASPEN subroutines (physical property monitors and flash
routines). Figure I-D-1 shows the typical configuration of a USER block

model. Figure I-D-2 presents the connectivity of the flowsheet for the reactor/preheater.

The following example shows how the direct coal liquefaction preheater and reactor models were incorporated into ASPEN. The ASPEN input file, the main subroutine and the ASPEN generated output are presented in Appendix D.
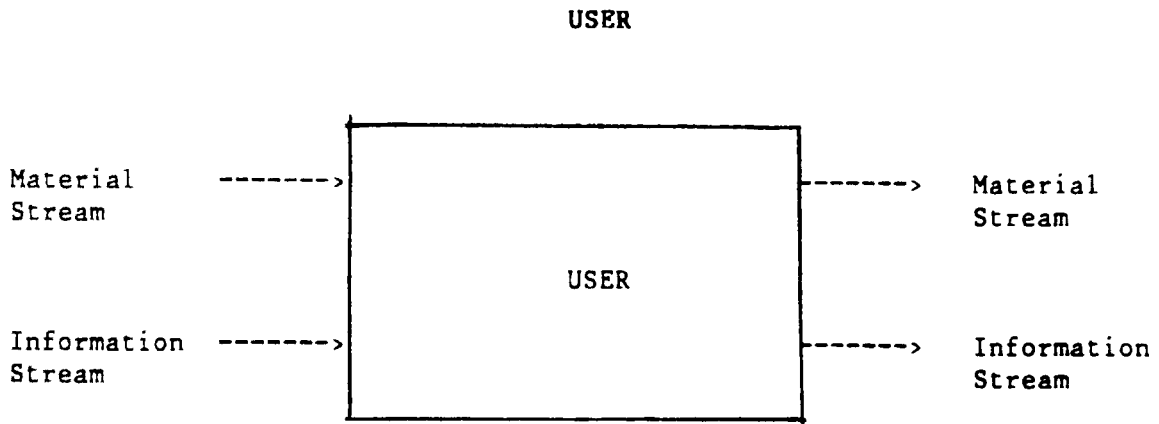
USER

Flowsheet

Inlet: One to four material streams; one information stream
Oulet: One to four material streams; one information stream

Input Specifications

The only required input is a user-supplied subroutine which calculates the flowrate and composition of all exit streams.

For a two-phase flash or three-phase flash, two of the following variables msut be specified: temperature, pressure, vapor fraction, or heat duty. If no specifications are made, the outlet streams wil be flashed at the temperture and pressure specified in the stream vector by the user subroutine.

Input Language

```
       BLOCK    blkid    USER
          SUBROUTINE    model    report
          PARAM    kwd = value
               where kwd's are:
               (NINT)   (NREAL)    (NIW)    (NW)    (NSIZ)
          FLASH-SPECS sid kode kwd = value / . . .
               where kwd;s are:
               (TEMP)   (PRES)    (V)
               (NPK)    (KPH)     (TEST)
               (PEST)   (MAXIT)   (TOL)
```

FIGURE I-D-1.   ASPEN PLUS Input for USER Model

```
                    INT intl . . . .
                    REAL reall . . .
```

where: blkid is the block ID as entered in a FLOWSHEET paragraph.

SUBROUTINE is used to specify the name of the user supplied model
subroutine (model) and, optionally, of the user supplied report
subroutine (report).

PARAM is used to enter array sizes needed by the model.
    NINT is the length of the integer array.
    NREAL is the length of the real array.
    NIW is the length of the integer work array.
    NSIZ is the length of the size array.
       All array sizes default to 1.

FLASH-SPECS is used to specify flash options for any outlet streams that
are to be flashed by the system.
    sid is the stream ID.
    kode is the flash option code.
       0   - Don't flash this tream (Default)
       1   - PH flash
       2   - TP flash
       3   - PV flash
       4   - TH flash
       5   - TV flash
    TEMP is the outlet temperature.
       Default = value stored in stream by user subroutine.
    PRES is the outlet pressure.
       Default = value stored in stream by user subroutine.
    V   is the vapor fraction of the outlet.
       Default = value stored in stream by user subroutine.
    NPK is the number of phases in the outlet stream.
    KPH is the phase kode and is used if NPK = 1.
       1   - vapor (Default)
       2   - liquid
       3   - solid
    TEST is an estimate for the temperature of the outlet stream.
    PEST is an estimate for the pressure of the outlet stream.
    MAXIT is the maximum number of iterations allowed for convergence
       of flash calculations.
       Default = 25
    TOL is the convergence tolerance for flash calculations.
       Default = 0.0001

INT is used to load the integer array with input values.

REAL is used to load the real array with input values.
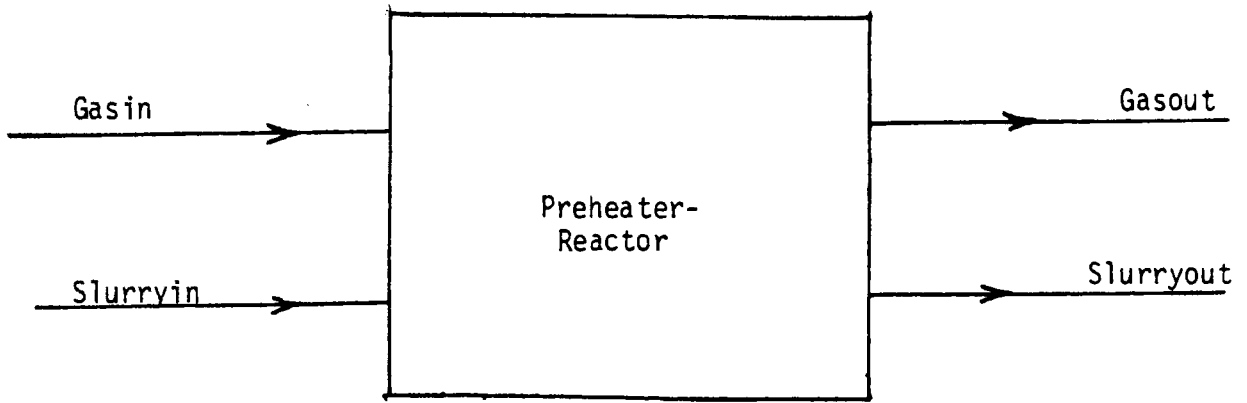

FIGURE I-D-1 (Continued)

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Gasin

Slurryin

Preheater-
Reactor

Gasout

Slurryout

Figure I-D-2: Flowsheet