

# Process Simulation with ASPEN PLUS

---

## CHE654 Course Notes

### Section 2: Output Files and Miscellaneous Topics

These course materials are applicable to Version 8.4 of ASPEN PLUS

ASPEN PLUS™ is a trademark of Aspen Technology, Inc., Burlington, MA, U.S.A.

# ASPEN PLUS Output Files

---

- User Interface contains all the simulation results
- But it may be desirable to get a hard copy of the results or a complete report
- ASPEN PLUS Report File
  - \*.REP file : contains simulation results
  - Select Export in File pulldown menu to generate it
- ASPEN PLUS History File
  - Select History in Summary Group under Simulation Home in the ribbon to look at it
  - Can then save the file or print it
  - Contains detailed calculation history and diagnostic messages

# File Management in ASPEN PLUS

---

- An ASPEN PLUS run generates many files, many of them just temporary.
- The important files you should be aware of:

<u>File Type</u>	<u>Extension</u>	<u>Format</u>	<u>Description</u>
Compound	*.apwz	Binary	File containing all input specifications, simulation results, and intermediate convergence information, in addition to other (normally) external files which the simulation needs. This can include user subroutines, DLOPT files, EDR input files for rigorous HeatX models, embedded Excel spreadsheets, and other files.

# File Management (Cont'd)

---

<u>File Type</u>	<u>Extension</u>	<u>Format</u>	<u>Description</u>
Document	*.apw	Binary	Quick restart file containing simulation input and results and intermediate convergence information
Backup	*.bkp	ASCII	Archive file containing simulation input and results
Input	*.inp	Text	Simulation input
Run Message	*.cpm	Text	Calculation history shown in the Control Panel
History	*.his	Text	Detailed calculation history and diagnostic messages
Summary	*.sum	ASCII	Simulation results
Report	*.rep	Text	Simulation report

# Export in File Pulldown Menu

The screenshot shows the Aspen Plus V8.4 interface with the 'Export' dialog box open. The dialog is titled 'Export' and is currently showing the 'Save as type' dropdown menu. The file name is 'Air Compression Example'. The file type list includes:

- Backup Files (\*.bkg)
- Backup Files (\*.bkp)
- Report Files (\*.rep)
- History File (\*.his)
- Summary Files (\*.sum)
- Input Files (\*.inp)
- Input Files with Graphics (\*.inp;\*.apmbd)
- Run Messages (\*.cpm)
- XML Results File (\*.xml)
- Problem Definition File (\*.appdf)
- EO Solver Report File (\*.atslv)
- DMO Solver Active Bounds Report File (\*.atact)

A red box highlights the 'Export' dialog, and a red arrow points to the file type list. A red text box on the right says 'Different types of files you can generate'.

In the background, a table titled 'Air Compression Example' is visible. The table has the following data:

Stream ID		AIR-FEED	COMP-AIR	COOL-AIR
Temperature	F	60.0	870.4	600.0
Pressure	psia	14.70	220.00	220.00
Molar Frac		1.000	1.000	1.000
Molar Flow	lbmol/hr	100.000	100.000	100.000
Mass Flow	lb/hr	2885.040	2885.040	2885.040
Volume Flow	cuft/hr	37928.442	6527.137	5203.502
Enthalpy	MMBtu/hr	-0.012	0.572	0.371
Molar Flow	lbmol/hr			
2		79.000	79.000	79.000
2		21.000	21.000	21.000

# Frequently Used ASPEN PLUS Files

---

- **Compound File** (\*.apwz) and **Document File** (\*.apw)
  - ASPEN PLUS main file, created under Save or Save As.
  - Contains simulation input and results including graphics.
  - Usually very large (0.5 MB - 10 MB)
  - Binary file; therefore, version-dependent
- **Backup File** (\*.bkp)
  - ASPEN PLUS archive file, created under Save As or Export
  - Contains the same information as \*.apw but opens slower
  - Usually small (50 KB - 0.5 MB)
  - ASCII file; therefore, version-independent

## Frequently Used ASPEN PLUS Files (Cont'd)

---

### □ **Input File** (\*.inp)

- ASPEN PLUS input file, created under Export.
- Contains only input in keywords format; very small file
- Convenient for debugging and viewing the entire flowsheet input
- Text file; therefore, version-independent

□ Note: All Document, Backup, and Input files can be opened by ASPEN PLUS but the Input files will not retain the original drawing of the flowsheet.

# ASPEN PLUS Stream Specifications

---

- The Material Streams Sheet is used to:
  1. Define the flow rates, compositions, and thermodynamic states of all process feeds.
  2. Provide initial guesses for tear streams.



# Sign Convention for Heat and Work in A+

---

□ Energy equation:

$$H_{\text{out}} + Q_{\text{out}} + W_{\text{out}} = H_{\text{in}} + Q_{\text{in}} + W_{\text{in}}$$

□ Heat supplied to a block (e.g. reboiler, heater) is (+)

□ Power supplied to a block (e.g. pump) is (+)

# Miscellaneous Topics in User Interface

---

## □ Exporting Stream Results

- To a printer
- To Microsoft Excel

## □ Creating a new (user-defined) units set for input data and output results

## □ Creating a PFD (Process Flow Diagram) of a flowsheet

# Exporting Stream Results

Press these buttons to copy individual streams to the clipboard

Click File to get a hard copy

Press this Select-All button to copy stream data to the clipboard

	AIR-FEED	COMP-AIR	COOL-AIR
Substream: MIXED			
Mole Flow lbmol/hr			
N2	79	79	79
O2	21	21	21
Total Flow lbmol/hr	100	100	100
Total Flow lb/hr	2885.04	2885.04	2885.04
Total Flow cuft/hr	37928.4	6527.14	5203.5
Temperature F	60	870.427	600
Pressure psia	14.7	220	220
Vapor Frac	1	1	1
Liquid Frac	0	0	0
Solid Frac	0	0	0
Enthalpy Btu/lbmol	-121.539	5717.35	3709.96
Enthalpy Btu/lb	-4.21275	198.172	128.593

Press these buttons to copy data of a row

# Microsoft Excel after Pasting from the Clipboard

	AIR-FEED	COMP-AIR	COOL-AIR
Substream: MIXED			
Mole Flow lbmol/hr			
N2	79	79	79
O2	21	21	21
Total Flow lbmol/hr	100	100	100
Total Flow lb/hr	2885.04	2885.04	2885.04
Total Flow cuft/hr	37928.44	6527.137	5203.502
Temperature F	60	870.4268	600
Pressure psia	14.7	220	220
Vapor Frac	1	1	1
Liquid Frac	0	0	0
Solid Frac	0	0	0
Enthalpy Btu/lbmol	-121.5394	5717.349	3709.957
Enthalpy Btu/lb	-4.212745	198.1723	128.5929
Enthalpy MMBtu/hr	-0.0121539	0.5717349	0.3709957
Entropy Btu/lbmol-R	0.7903291	2.13319	0.4469793
Entropy Btu/lb-R	0.027394	0.0739397	0.015493
Density lbmol/cuft	0.00263654	0.0153206	0.0192178
Density lb/cuft	0.0760653	0.4420069	0.5544419
Average MW	28.8504	28.8504	28.8504
Liq Vol 60F cuft/hr	85.79137	85.79137	85.79137

# Creating a New Units Set

---

- There are already many A+ built-in units sets for input data and output results.
  - 3 main sets: **ENG, MET, SI**
  - Variations of main sets: **METCBAR, METCKGCM, SI-CBAR**
  - e.g. METCKGCM is the metric set in which T is in °F and P is in kg/cm<sup>2</sup>
  
- User may wish to create his own units set or customize an existing set.
  
- The easiest way to create a new units set is to copy from an existing one.

# Creating a New Units Set (Cont'd)

---

## □ To create a new units set:

1. Select Units Sets under Home in the ribbon.
2. Click the New button in the Object Manager.
3. Specify an ID for the new units set.
4. Specify whether you want to make this new units set global. If you specify “global”, this new units set will apply to the entire simulation.
5. Select an existing units set from which you want to copy. SI is the default.
6. Now, customize any keyword to the desired unit (e.g. specify Volume Flow in “gal/min”).

# Creating a New Units Set (Cont'd)

The screenshot shows the Aspen Plus V8.4 interface with the 'Unit Sets' configuration window open. The window title is 'Air Compression Example.apw - Aspen Plus V8.4 - aspenONE'. The 'Unit Sets' window contains a table with the following data:

Name	Status
ENG	Input Complete
MET	Input Complete
METC	Input Complete
SI	Input Complete
SI-CBAR	Input Complete
US-1	Input Complete

Below the table are buttons for 'New', 'Edit', 'Delete', 'Copy', 'Rename', 'Hide', 'Reveal', and 'Paste'. The 'New' button is highlighted with a red arrow pointing to the text 'Press this button to create a new units set'. A red bracket groups the first six rows of the table, with the text 'The 6 built-in units sets' next to it. A red arrow points from the 'Unit Sets' folder in the left-hand 'All Items' tree to the text 'Select Units Sets under Setup in the Menu Tree'. The bottom of the interface shows the 'Model Palette' with 'Mixers/Splitters' selected, and the Windows taskbar at the bottom right shows the date and time as 10:20 AM 5/6/2014.

# Creating a New Units Set (Cont'd)

Simulation Main Flowsheet Unit Sets - US-1

Copy from: SI

Flow related

Mass flow: kg/sec

Mole flow: kmol/sec

Volume flow: gal/min

Flow: kg/sec

Flux: cum/sqm-sec

Mass flux: kg/sqm-s

Temperature related

Temperature: K

Delta T: K

Inverse temperature: 1/K

Pressure related

Pressure: N/sqm

Delta P: N/sqm

Delta P / Height: N/cum

I lead: J/kg

Inverse pressure: sqm/N

Volume Flow changed to the unit of "gal/min"

Six categories of unit keywords

1. Standard
2. Heat
3. Transport
4. Concentration
5. Size
6. Miscellaneous