# AUTOMATED INFORMATION RETRIEVAL FOR EFFICIENT AND CONSISTENT GRADING OF FLOWSHEETS DEVELOPED IN ASPEN® PLUS PROCESS SIMULATOR

# SCOTT C. JACKSON, DOROTHY SKAF Villanova University • Villanova PA 19085

odeling with ASPEN<sup>®</sup> can generate large stream reports that can be difficult to understand at a high level. Being able to quickly understand the overall process implications from large flowsheets generated by ASPEN<sup>®[1,2]</sup> is an important requirement when developing new processes. For example, a new adiponitrile process<sup>[3-5]</sup> developed by DuPont from 1995 – 2005 (subsequently sold and implemented by Koch Industries, Inc.) was at the time the largest flowsheet model ever developed by DuPont. Techniques to electronically scan through stream and unit operations reports allowed for a quick optimization of the process where understanding effects of multiple recycles and impurity buildup were critical to the success of the process development.

Unlike the massive flowsheets developed at DuPont, the challenge in the senior design class is not the size of the process flowsheets but the large number of flowsheets submitted. There is a need to consistently access data packed into the stream reports for grading of the many flowsheets while providing timely feedback to the students. In the course, all design groups typically work on variants of the same chemical process, so there are common unit operations between the various designs, although the process specifications and process details can be quite different between groups. Even for a relatively simple process, a long list of process parameters must be monitored to determine the suitability of the process Dorothy Skaf is an associate professor of chemical engineering and past department chair at Villanova University. She joined the Villanova faculty in 1988 where she has taught continuously with the exception of a one-year Fulbright appointment at Qatar University. Dorothy has published in the areas of material treatments for improved hardness and electrical conductivity, graphite fiber production and nanofiber applications in catalysis and waste treatment, and value recovery from biodiesel processing wastes. She has several publications related to heterogeneous photocatalysis for waste treatment and/or value recovery and



is currently working on a project for treatment of food processing waste. She has taught numerous undergraduate and graduate courses. Dorothy earned her B.S in chemical engineering from Princeton University and her M.S. and Ph.D. in chemical engineering from the University of Pennsylvania.



Scott Jackson is a visiting professor of chemical engineering at Villanova University. Prior to joining Villanova, he worked for the DuPont Company as a senior research fellow in diverse roles in a number of businesses. Areas of expertise include separations and reaction kinetics for nylon intermediates, for fluorocarbons/fluoropolymers, new technologies for enhanced oil recovery, and electronic material processing. Scott has taught or co-taught courses in senior design, engineering economics, unit operations lab, heat transfer, and petroleum engineering. He received his B.S. in chemical engineering form

Cornell University and his M.S. and Ph.D. from the University of Delaware.

© Copyright ChE Division of ASEE 2019

design and grade the assignment. In addition, ASPEN® can allow some physically unrealistic conditions to occur, for example, negative pressure drops across some unit operations, including heat exchangers. Monitoring

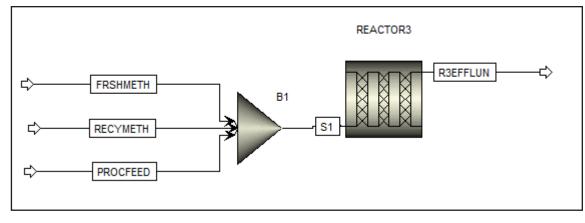


Figure 1. Simple flowsheet example.

these unrealistic conditions can be readily done using this algorithm.

The burden of accurately accessing key parameters in the flowsheet is increased by the range of different stream and unit operation names in the flowsheet. These names are ASPEN<sup>®</sup> defaults or are generated by the students as the flowsheet is developed. This makes it difficult to find key data, since streams and unit operations containing these parameters have different names across different flowsheets. Despite these obstacles, the techniques developed at DuPont were successfully applied to a grading algorithm at Villanova University.

This article documents the use of an EXCEL spreadsheet specially developed at Villanova University to retrieve information from ASPEN® custom stream reports to consistently and automatically grade flowsheets developed in ASPEN® Plus v8.8 as part of the senior design course. The techniques described here are applicable to ASPEN® Plus v9.0 with only minor revisions. The EXCEL functions are used to identify block and stream information. Stream names arbitrarily assigned by ASPEN® or by the students can be handled using EXCEL's lookup and reference functions<sup>[6-10]</sup> on an ASPEN® custom stream report copied into an EXCEL file. Block names associated with those unit operations can be found in the ASPEN® block summary report that can also be copied into the same EXCEL file as the ASPEN® custom stream report. Once stream names entering or exiting a unit operation are known, then EXCEL functions can glean information from the ASPEN® custom stream report, enabling automatic calculation of key parameters for use in a grading rubric.

# THE "STREAM SUMMARY" VS. "CUSTOM STREAM SUMMARY"

One of the keys to automating flowsheet grading is the ability to pull information from a stream summary report. The stream summary and the custom stream summary can be readily copied and pasted into an EXCEL spreadsheet. This can be done by first clicking on the upper left block of the stream or custom stream summary table. The lefthand column of the stream summary will become a light yellow color. Typing "control A" (select all) and then "control C" (copy) will copy all of the data in the stream summary table. Open an EXCEL spreadsheet. Click on a cell location in the EXCEL spreadsheet (this cell location will define the upper lefthand corner location of the data to be pasted). Type "control V" (paste) to paste the entire stream summary into the EXCEL sheet.

The stream information in EXCEL can be readily used to calculate various process characteristics. However, there is no connectivity information in the stream summary report. The inlet and outlet streams to the unit operations are not identified. Despite this, for flowsheets where there are no changes in the stream names—that is, the purpose of the stream is consistent across all the flowsheets to be graded—then relatively simple lookup and reference functions such as HLOOKUP<sup>[6]</sup> can be used to access the required stream information. This function will be discussed below.

When stream names are changing between flowsheets, then an ASPEN<sup>®</sup> custom stream summary report is used to find a stream name entering or leaving a given unit operation. The custom stream summary table contains the stream connectivity information that is used to automatically identify the inlet and outlet streams for each block.

# FINDING NAMES OF INLET AND OUTLET STREAMS FOR EACH BLOCK

Figure 1 and Figure 2 illustrate a simple flowsheet and the corresponding custom stream report that will be used to describe details of a method to extract arbitrarily named streams entering or leaving a block in a flowsheet. Copies of the EX-CEL file used in these examples are provided as additional information by contacting the author at scott.c.jackson@ villanova.edu. In Figure 1, three streams are combined, sent to a mixer, MIXER1, and subsequently fed to reactor, REAC-TOR3. In the reactor, methyl methacrylate (component name is MMA in Figure 2) is produced by the reaction of methanol

1	L	M	N	0	Р	Q	R	
1								
2								
3		Units	FRSHMETH	PROCFEED	R3EFFLUN	RECYMETH	S1	
4	From				REACTOR3		MIXER1	
5	То		MIXER1	MIXER1		MIXER1	REACTOR3	
6	Substream: MIXED							
7	Phase:		Liquid	Liquid	Liquid	Liquid	Liquid	
8	Component Mole	Flow						
9	TBUTANOL	KMOL/HR	0	0.000558476	0.000558476	0	0.000558476	
10	NITROGEN	KMOL/HR	0	0	0	0	(	
11	MMA	KMOL/HR	0	1.15	32.10558	0.5	1.65	
12	02	KMOL/HR	0	0	0	0	(	
13	MEOH	KMOL/HR	42	1	30.54442	18	61	
14	MAA	KMOL/HR	0	42	11.54442	0	42	
15	MLEIN	KMOL/HR	0	0	0	0	(	
16	WATER	KMOL/HR	0	84	116.4556	2	86	
17	Component Mole	Fraction						
18	TBUTANOL		0	4.36E-06	2.93E-06	0	2.93E-06	
19	NITROGEN		0	0	0	0	(	
20	MMA		0	0.00897382	0.1684001	0.0243902	0.00865458	
21	02		0	0	0	0	(	
22	MEOH		1	0.00780332	0.1602116	0.8780488	0.3199571	
23	MAA		0	0.3277395	0.0605527	0	0.2202983	
24	MLEIN		0	0	0	0	(	
25	WATER		0	0.655479	0.6108326	0.0975609	0.4510871	
26	Mole Flow	KMOL/HR	42	128.1506	190.6506	20.5	190.6506	
27	Mass Flow	KG/HR	1345.771	5276.3	7284.919	662.8481	7284.919	
28	Volume Flow	CUM/HR	1.88432	5.689316	8.291648	0.904355	8.492257	
29	Temperature	C	87	87	80	87	93.50282	
30	Pressure	BAR	3.3	3.3	2.886315	3.3	3.3	
31	Vapor Fraction		0		-	0	(	
32	Liquid Fraction		1		-	1		
33	Solid Fraction		0	0	0	0	0	

Figure 2. Custom stream report for flowsheet shown in Figure 1.

(component name MEOH) with methacrylic acid (component name MAA). The three streams that are mixed to form the reactor feed (stream S1) are fresh methanol (FRSHMETH), recycled methanol (RECYMETH), and methacrylic acid (stream PROCFEED). In the case being considered here, none of the stream names are known beforehand. To evaluate this simple flowsheet, possible grading criteria might include:

- 1. A reasonable pressure match for streams entering the mixer
- 2. Reasonable / realistic pressure drops across the mixer and reactor
- 3. Reasonable yield and conversion for the limiting reagent
- 4. Limits on side product formation
- 5. Operation within temperature limitations dictated by the catalyst and the cooling system

For example, to determine the MAA conversion across RE-ACTOR3, the molar flow rates of MAA into and out of REAC-TOR3 are needed. Both can be found using the HLOOKUP<sup>[6]</sup> function as follows if the stream names are known:

HLOOKUP(Lookup\_value, Table\_array,row\_index\_ number,[range\_lookup]) returns the value of a cell in a given matrix defined by the "Table\_array" at the intersection of a column defined by "Lookup\_value" and a row defined by "row\_index\_number." The optional argument "Range\_lookup" should be set to "FALSE" to assure an exact match for the "Lookup\_value." This eliminates issues with the way ASPEN<sup>®</sup> has sorted the stream names vs. how EXCEL expects the values to be sorted.

The information for the molar flow rate of MAA into REACTOR3 is contained in stream S1. HLOOKUP("S1", \$N\$3:\$R\$40, 12,FALSE) will search the custom stream report, Figure 2, and return a value of 42 (KMOLE/HR) for the MAA flow rate. HLOOKUP will go across the top row of the designated matrix (\$N\$3:\$R\$40) until the column with "S1" at the top is found (column R in Figure 2). The function then looks down that column for the value in the 12th row. The value of 12 is the row number within the matrix (row 14 - row 3 + 1) that contains the molar flow rate of MAA for each stream. Absolute references are used to define the matrix since this will make it easier to copy and paste this function elsewhere in the spreadsheet. The matrix to be searched needs to encompass all the streams in the custom stream report. The first column of the matrix should be at the first stream (Ieft-most stream) of the report and should not include the component and

unit columns (columns L and M in Figure 2). In the same fashion, the function HLOOKUP("R3EFFLUN",\$N\$3:\$R \$40,12,FALSE) returns a value of 11.54442 (KMOLE/HR), which is the molar flow rate in the outlet of the reactor. With these two values, the conversion in REACTOR3 can be readily calculated. To apply this HLOOKUP function to multiple designs four things should be followed:

- 1. The starting point (upper left cell) of the matrix must be in exactly the same location in every EXCEL sheet that contains a flowsheet.
- 2. The value of the appropriate row number can be assigned to a global variable name (go to Formulas... Define Name). For example, the name "MAA\_M\_flow" has a value of 12 in the EXCEL sheet used in this example.
- 3. The stream names into and out of REACTOR3 must be fixed and known ahead of time in order to use the HLOOKUP function in this fashion.
- 4. The array to be searched can be much wider than the actual number of streams in the custom stream report. That is, the HLOOKUP function will work if there are blank columns that are searched to the right of the columns that have data. This allows the algorithm to search the custom stream reports despite the changing number of streams that each group may elect to have.

Flowsheets that do not have consistent stream names are challenging. In this case, the correct stream name must be supplied in some automatic manner as the first argument in the HLOOKUP function. Manually searching for the correct stream name is exhausting, time consuming, and prone to errors. As will be shown below, stream names can be automatically determined even on flowsheets where the stream names change from flowsheet to flowsheet. Information needed to calculate each of the performance goals in a grading scheme can still be gathered from the custom stream table using these stream names that are then used as arguments in the HLOOKUP function. The needed stream names across a given unit operation can be identified using the MATCH<sup>[7]</sup> and INDEX<sup>[8]</sup> functions. The combination of these functions is a powerful tool that ultimately allows the identification of multiple randomly named streams entering or leaving a single unit operation.

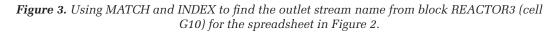
MATCH(lookup\_value, lookup\_array, [match\_type])

 returns the location of a cell in an array (lookup\_array) containing a specified text string (lookup\_value).

 The match\_type should be specified as "0" in order to give an exact match. That is, the MATCH
 function returns an integer corresponding to a
 relative column value in a row segment. For example
 =MATCH("REACTOR3",\$N\$4:\$R\$4,0)

as applied to the custom stream report, Figure 2, for the simple flowsheet, Figure 1, would search row 4 (this row lists the unit operations that the stream is coming "From") through columns N to R for an exact match for

fx =INDEX(\$N\$3:\$R\$5,1,(MATCH(G10,\$N\$4:\$R\$4,0))) H10 ¥ ( D Ε F G H E 7 streams in unit op stream out unit op stream out 8 9 FRSHMETH **REACTOR3** 10 PROCFEED MIXER1 **R3FFFIUN** 11 RECYMETH =INDEX(\$N\$3:\$R\$5,1,(MATCH(G10,\$N\$4:\$R\$4,0))) Row 4 for "from" the unit op 12 #N/A 13 INDEX(\$N\$3:\$R\$5,1,(MATCH(G10,\$N\$5:\$R\$5,0))) Row 5 for "to" the unit op OR =INDEX(\$N\$3:\$R\$5,1,(MATCH(E10,\$N\$4:\$R\$4,0))) 14



"REACTOR3." That match occurs in the third column of this array (column P). In this example, the MATCH function would return a value of 3. The array to be searched can be much wider than the actual number of streams in the custom stream report. That is, the MATCH function will work if there are blank columns that are searched to the right of the columns that have data. This allows the algorithm to search the custom stream report despite the changing number of streams that each group may elect to have. In the example above, MATCH("REACTOR3",\$N\$3:\$Z\$5,0) would have worked as well as long as columns S through Z were blank.

 INDEX(array, row\_number, [column\_number])-- returns the contents of a cell at a specified relative location (row\_number and column\_number) in a given array. For example =INDEX(\$N\$3:\$R\$5,1,3) would return the value or text string at row 1, column 3 of the array defined by absolute cells N to R to R to a that position (Figure 2) is "R3EFFLUN." As in the case for the MATCH function, the array to be searched can be much wider that the actual number of streams in the custom stream report as long as the extra columns are blank.

3. The INDEX is combined with the MATCH function to provide a single command to find a stream entering or leaving a known unit operation. For example, =INDEX (\$N\$3:\$R\$5,1,(MATCH("REACTOR3",\$N\$4:\$R\$4,0))) is asking for the stream coming from "REACTOR3" in the simple flow sheet, Figure 1. In this case it is "R3EF-FLUN."

Information in Figure 2 will be used to demonstrate application of these functions to identify the names of single streams entering or leaving a unit operation. All stream names are listed in row 3 of Figure 2. The unit operation where each stream originates is listed in row 4. This is designated by ASPEN<sup>®</sup> as the "From" unit operation in Figure 2. The unit operation where each stream goes is listed in row 5. This is designated by ASPEN<sup>®</sup> as the "To" unit operation in Figure 2. By inspection of Figure 2, it is apparent that the stream coming "From" "REAC-TOR3" is "R3EFFLUN" (the text string in cell P3). To identify

this stream name automatically, the block name "REACTOR3" must be known. To start the search for the streams associated with this unit operation, this block name has been typed into cell G10 of the spreadsheet, Figure 3. If the unit operation names are not fixed, then the block name can be found by setting cell G10 equal to the block name found elsewhere in the EXCEL spreadsheet. For example, the ASPEN<sup>®</sup> block summary report can be pasted into the spreadsheet to provide the block name.

Figure 3 shows how the names of the streams originating "From" and flowing "To" "REACTOR3" are determined from the information in Figure 2. The block name, "REACTOR3," is typed into a cell (G10). Cells in adjacent columns (F10 and H10) will be used to hold the identified names of streams entering and leaving "REACTOR3," respectively. This logic can be readily expanded to other unit operations by using absolute references for the vector to search in the MATCH function

and the array to search in the INDEX function. Consequently, these cells can be copied and pasted next to the name of any unit operation to identify the outlet and inlet streams coming from and going to that unit operation. The only difference between functions used to find the inlet and outlet stream is the second argument in the MATCH function. For the inlet streams, the MATCH function used the fifth row for the search (\$N\$5:\$R\$5). For the outlet streams, the MATCH function used the fifth row for the streams the fourth row (\$N4:\$R\$4). For both the inlet and outlet streams the first argument of the MATCH function used the unit operation name in cell R31.

## FINDING MULTIPLE INLET AND OUTLET STREAMS FOR BLOCKS

The search procedure is complicated if blocks have multiple inlet and outlet streams. The MATCH function only provides the first instance of a stream name in a vector of "To" or "From" names. Therefore, the functions COLUMN,<sup>[9]</sup> ADDRESS,<sup>[10]</sup> and INDIRECT,<sup>[11]</sup> are combined with MATCH and INDEX to automate the search for multiple inlet or outlet streams.

- The COLUMN<sup>[9]</sup> function is used to calculate the absolute starting position for the subsequent search. That is, COLUMN(\$N\$3) returns a value of 14 since column N is the fourteenth column.
- 2. The ADDRESS(row\_number, column\_number) is used to obtain the address of a cell in a work sheet. For example, ADDRESS(3,14) would return the absolute cell location of \$N\$3. This function is used to convert the relative position of a cell within the search matrix to the address of the cell within the spreadsheet. There are optional parameters available for this function that are not used here.
- 3. INDIRECT(ref\_text) converts a string, ref\_text, into a cell reference within a formula without changing the formula itself.

С D 3 4 5 6 INDEX(\$N\$3:\$R\$5.1.B9) match1 match2 for last for next input input stream out (from left) unit op stream stream stream in (to right) stream out 8 9 =MATCH(E10,\$N\$5:\$R\$5,0) FRSHMETH 10 =MATCH(D9,\$N\$3:\$R\$3,0) PROCFEED MIXER1 **REACTOR3** 11 =MATCH(D10,\$N\$3:\$R\$3,0) RECY 12 =MATCH(D11,\$N\$3:\$R\$3,0) =INDEX(\$N\$3:\$R\$5,1,(MATCH(G10,\$N\$4:\$R\$4,0))) "Row 4 for "from" the unit op" 13 INDEX(\$N\$3;\$R\$5.1.(MATCH(G10.\$N\$5;\$R\$5.0))) "Row 5 for "to" the unit op =INDEX(\$N\$3:\$R\$5,1,(MATCH(E10,\$N\$4:\$R\$4,0))) 14 OR 15 =(MATCH(\$E\$10,INDIRECT(ADDB (COLUMN(\$N\$3)+B10))):\$R\$5,0 SS(5,(COLUMN(\$N\$3)+B11))):\$R\$5,0 16 =(MATCH(\$E\$10,INDIRECT(ADD =(MATCH(\$E\$10,INDIRECT(ADDRESS(5,(COLUMN(\$N\$3)+B12))):\$R\$5,0) 17 18 =INDEX(INDIRECT(A DRESS(3.(COLUMN(\$N\$3)+B10)));\$R\$5.1.C10) =INDEX(INDIRECT(ADDRESS(3,(COLUMN(\$N\$3)+B11))):\$R\$5,1,C11) 19 =INDEX(INDIRECT(ADDRESS(3,(COLUMN(\$N\$3)+B12))):\$R\$5,1,C12) 20

To identify multiple streams going "To" or coming "From" a

block, a series of searches must be done—one search for each stream going into or out of a block. That is, if there are three streams going into a mixing block, three searches must be done to find all three streams. In practice a fourth search that returns an error will confirm that there are only three streams. Each new search must start at the column immediately after the location of the stream found by the previous search. The search for multiple inlet or outlet streams requires careful use of both locked cells, relative cells, and nested functions. The logic of this automatic recursive search will be illustrated using "MIXER1" block and the information in Figure 2 and Figure 4 as described below.

- 1. Cell B9 of Figure 4: MATCH is used to search N5 to R5 (the row of "To" streams) for the first occurrence of streams entering "MIXER1."
- 2. Cell D9 of Figure 4: INDEX uses the result in cell B9 to identify the name of the first stream entering "MIX-ER1."

A second search for streams entering "MIXER1" is done involving formulas in cells B10, C10, and D10.

- 3. Cell B10: MATCH searches N3 to R3 for the name of the last found stream (in cell D9) to identify the location of this first entering stream.
- 4. Cell C10: MATCH searches a reduced matrix for the next stream entering "MIXER1." The search area is redefined using COLUMN and the results in B10. The INDIRECT function is used with ADDRESS and COLUMN functions to define the starting point of this reduced matrix.
- 5. Cell D10: INDEX uses the reduced matrix and the result in cell C10 to find the name of the next stream entering "MIXER1." As above, the INDIRECT function is used with ADDRESS and COLUMN functions to define the starting point of the reduced matrix.
- 6. Cells B10, C10, and D10 can be copied down until EXCEL responds #N/A for the next input stream (for

Figure 4. Finding the first of multiple streams into a mixer, MIXER1, using INDEX, MATCH, and INDIRECT functions.

example, cell D12 in Figure 4) indicating that all input streams have been identified.

7. This sequence can be copied for each unit operation simply by changing the search string representing the block name.

Below is a more detailed explanation of each of these steps using the formulas in Figure 4 and the information in Figure 2. In cell B9 of Figure 4 the MATCH function is used to search for the first instance of a stream entering the block "MIXER1" (this unit operation name is the address \$E\$10 of the MATCH function). The first instance is found in column 1 of the \$N\$5:\$R\$5 vector. The column number is used in the INDEX function (located in cell D9 of the spreadsheet) to find the name of the "To" stream, *i.e.*, "FRSHMETH."

A recursive search is created to glean any additional streams that enter "MIXER1." The complete set of functions used to search for the next stream going "To" the mixer "MIXER1" is shown in Figure 4. The column number of the first "To" stream is determined in cell B10. This value, 1, is used in the INDEX function to begin a search starting in column number 2 within the N3:R3 block(one column past the column where the first "To" was found). In cell C10, ADDRESS(5,(COLUMN(\$N\$3)+B10)) calculates the value of the starting cell to start the next search. That address is O5. The INDIRECT function in cell C10 tells EXCEL the cell reference from ADDRESS is in text string format and is to be converted to a location in the address with ":\$R\$5" as the boundaries of an array. In this case the array is O5:\$R\$5 in cell C10. The INDIRECT function is the key to letting EXCEL know to use this calculated cell address as the first part of an array address. With the array (or vector) defined, the MATCH function is used to look through that array for the next occurrence of the unit operation called "MIXER1" (value in cell E10). The contents of cells B10, C10, and D10 can readily be copied down to additional cells to find all the "To" streams to unit operation "MIXER1" as shown in Figure 4. It is necessary to use the appropriate absolute and relative references in the formulas in cells B10, C10, and D10 to copy the formulas correctly. When these formulas are copied down, a value of "#N/A" is returned for the unsuccessful search for a fourth inlet stream to "MIXER1." For example, if the block of cells from B9 to H12 were copied anywhere in the EXCEL spreadsheet and renamed the unit operations in cells E10 and G10, these copied functions would find the streams entering and leaving those new unit operations.

It is possible to nest the commands in B10 and C10 into the command in D10. However, these nested commands are difficult to debug. It is recommended to apply a stepwise approach, as shown here, to find multiple stream names in or out of a unit operation. Very powerful debugging facilities in EXCEL were used in developing the information retrieval algorithms described above. For example, "Trace dependents" and "Trace precedents" functions under "Formulas" menu allows a visual interpretation of the parameters going into a given set of functions. Arrows pointing to affected cells or arrays are highlighted with ease, as is shown in Figures 3 and 4.

#### **GRADING ALGORITHM**

The specific grading algorithm to be used will depend on the purpose of the assignments and the sophistication of the process development being attempted in a class. What is described here is just a piece of one grading algorithm used at Villanova. The intent of using lookup and indexing functions described in this article is to provide the needed data in a consistent manner for whatever grading algorithm is used.

For each assignment, student teams submit an EXCEL file containing the custom stream report. They are instructed to make certain to paste the custom stream report into a specific cell. For example, in Figure 2, that cell was L3. In addition, tables of key unit operations are also provided in the same EXCEL spreadsheet submitted by the students. In this way, changing names of unit operations can be used in the search algorithms describe above. The EXCEL files for each group are compiled into an EXCEL workbook with each sheet in the workbook being named for each student group. The search functions and grading rubric are also copied into each tab in the free space next to where the custom stream report was pasted. The search functions will immediately be populated by the correct stream names and values for the key parameters used in the grading rubric. A score will automatically be calculated for each item in the grading rubric. Some adjustment may be needed for a unit operation with multiple streams entering or leaving it. For example, the overhead of a distillation column will not always be the first stream found coming out of the column.

An example of a rubric is shown in Figure 5 for a large custom stream report. In this example, the rubric occupies columns B through M in the EXCEL tab. The custom stream report starts in column X of the EXCEL tab. A list of scoring criteria is in column C with target values for each criterion in column E. Grading elements are automatically calculated or determined based on the characteristics of the pertinent identified streams. The values of the grading element are shown in column D. For example, the molar yield of MMA from methanol is calculated in Figure 5, cell D6, (arrowed). This calculation uses the HLOOKUP function to find the MMA molar flow ("MMA\_row") in the MMA product stream (MMAPROD - shown in cell J6) in the custom stream table. The HLOOKUP function finds the methanol molar flow ("MEOH\_row") in the fresh methanol stream (FRSHMETHshown in cell H6) in the custom stream table. The ratio gives the molar yield – in this case 0.9920. Other grading elements are calculated and compared to desired values. Tolerances shown in columns L and M are used to determine whether the calculated grading element merits 0, 1, or 2 points (out of 2 points) for each performance criteria.

1	B C	D	E	F	G	н	1	J	K	L	М
								_			
					Score	out of					
					76	80				tolerances	
		value	desired value	figure of merit		1st stream	2nd stream	3rd stream	4th stream	for +2	for +1
1	1 Overall Yield of MMA from isobutanol?	0.9873	1	-1.3E-02	2	BUTANOL		MMAPRO	D	-0.02	-0.04
L	2 Yield of MMA form methanol?	0.9920	1	-8.0E-03	2	FRSHMET	н	MMAPRO	D	-0.02	-0.04
	3 Is the MAA production of 42 kmole/hr (+2%) met?	42.34384	42	0.0281867	2	<b>B-BOTS</b>				0.04	0.08
	4 Is the MAA stream purity met?	0.9999936	>0.98	0.9999936	2	<b>B-BOTS</b>				0.98	0.97
	5 Product MMA Pressure (atm) 4atm <p<6 atm<="" td=""><td>3</td><td>5</td><td>2</td><td>0</td><td>MMAPRO</td><td>D</td><td></td><td></td><td>1</td><td>1.99</td></p<6>	3	5	2	0	MMAPRO	D			1	1.99
k.	6 Product MMA Temperture (C ) 35C <t<45c< td=""><td>138.0506</td><td>30</td><td>108.0506</td><td>0</td><td>MMAPRO</td><td>D</td><td></td><td></td><td>5</td><td>10</td></t<45c<>	138.0506	30	108.0506	0	MMAPRO	D			5	10
8	7										
-	8									1	
8	9									1	
ł.	10										
5	Is the fresh feed butanol flow rate just a little above 42 11 kmole/hr?	42.4	42	0.0095238	2	BUTANOL				0.05	0.1
	Is the Mlein recycle stream close to the azeotrope 12 composition?	0.6528644	0.6586	0.0087087	2	S12				0.1	0.15
	Is methacrolein recycle stream reconditioned before 13 reactor 2? [vapor fraction]	1	1	0	2	HIPADIST				0.1	0.15

Figure 5. Grading rubric and metrics used to evaluate the designs.

Each tab in this EXCEL file is a complete grading record for a submitted flowsheet. The individual student's name or team's name can be used to label the tab. A summary sheet, Figure 6, is used to pull the final scores from each worksheet tab. The INDIRECT and AD-DRESS function are used to



Figure 6. Collecting the scores into a summary sheet.

find the name of the tab (in column H of Figure 6) and pull in the value of the score that is in a fixed location of G3 in each of the tabs (3,7 in the ADDRESS function – Figure 6). That is, at cell G3 in each respective tab is the final grade for each flowsheet. The combination of the ADDRESS and INDIRECT functions extracts that value of the final grade from each tab and places it into this summary tab.

### SUMMARY

Despite the complexity of changing stream names and changing unit operation names in ASPEN<sup>®</sup> flowsheets developed by students in the Villanova senior design class, it is possible to consistently provide the needed data that is packed in an ASPEN<sup>®</sup> custom stream report for a scoring algorithm. In this way the automated scoring of many flowsheets in EXCEL is possible. The key steps are:

1. Copy the custom stream summary into EXCEL and use the lookup and reference functions in EXCEL. Pasting the information to a consistent location in a blank EX-CEL worksheet assures that the search algorithms and rubric formulas will always be looking at the flowsheet information in the same location in the spreadsheet.

- 2. Copy any needed ASPEN® block summary reports (unit operations tables) in the same manner into the EXCEL file. As in the custom summary report, paste the information in a consistent location.
- 3. Identify which unit operations need to be examined in order to gather the required information for the grading rubric.
- 4. Using the lookup and reference functions in EXCEL as described above, find all the stream names going into or out of those unit operations.
- 5. For multiple streams entering or leaving a unit operation, make certain you know which one carries the needed information—the overhead from a distillation column vs. the bottom product, for example. This is the only instance where it may be required to look at the flowsheet to get the correct stream names. The other option is to instruct students to start the name of any distillate product streams with a "D" and any bottoms streams with a "B." Consequently, the first stream found leaving a distillation column would always be the bottoms product while the second stream found would always be the distillate product.

- 6. Decide what key pieces of information are needed from each stream. Define the rows for those key pieces of information as global variable names.
- 7. Use the stream names and the global names of the rows in an HLOOKUP function to find specific pieces of information to be used in a grading item.
- 8. Once an algorithm for pulling information out of an ASPEN<sup>®</sup> simulation is complete for a single spreadsheet, that tab can be copied and renamed in the EXCEL book. A new matrix of stream and unit operations can be copied over the previous data in the copied tab and the calculations will automatically be done.

The effort to develop and test the EXCEL grading file was rewarded by the ability to quickly, accurately, and consistently evaluate many ASPEN<sup>®</sup> flowsheets. The plan is to include this type of grading algorithm as a standard practice in future senior design courses at Villanova University.

#### ACKNOWLEDGMENTS

We would like to thank Axalta Coating Systems for supporting this senior design problem and for the technical expertise shared with the class. Their comments to the students were much appreciated by all.

#### REFERENCES

1. Haydary J (2018) Chemical process design and simulation: Aspen Plus

and Aspen Hysys applications (John Wiley & Sons, Inc., New York) ISBN: 978-1-119-08911-7.

- Aspen Plus background information created by Aspentech and retrieved from <<a href="https://www.aspentech.com/en/products/engineering/aspenplus">https://www.aspentech.com/en/products/engineering/aspenplus</a> on Sept 5, 2018.
- Jackson SC & McKinney RJ (2005) Process for catalyst recovery from hydrocyanation product mixtures. US Patent 6,936,171, issued Aug. 30, 2005.
- Jackson SC & McKinney RJ (2005) Process for the preparation of nickel/phosphorous ligand catalyst for olefin hydrocyanation. US Patent 6,897,329, issued May 24, 2005.
- Jackson SC & McKinney RJ (2005) Process for the preparation of a nickel/phosphorous ligand catalyst. US Patent 6,844,289, issued Jan. 18, 2005.
- Microsoft EXCEL HLOOKUP function explained. Retrieved from <a href="https://support.office.com/en-us/article/hlookup-functiona3034eec-b719-4ba3-bb65-e1ad662ed95f">https://support.office.com/en-us/article/hlookup-functiona3034eec-b719-4ba3-bb65-e1ad662ed95f</a>> on Sept 5, 2018.
- Microsoft EXCEL MATCH function explained. Retrieved from <<a href="https://support.office.com/en-us/article/match-function-e8dffd45c762-47d6-bf89-533f4a37673a">https://support.office.com/en-us/article/match-function-e8dffd45c762-47d6-bf89-533f4a37673a</a>> on Sept 5, 2018.
- Microsoft EXCEL INDEX function explained. Retrieved from <https://support.office.com/en-us/article/INDEX-function-A5D-CF0DD-996D-40A4-A822-B56B061328BD> on Sept 5, 2018.
- Microsoft EXCEL COLUMN function explained. Retrieved from <https://support.office.com/en-us/article/COLUMN-function-44E8C754-711C-4DF3-9DA4-47A55042554B> on Sept 5, 2018.
- Microsoft EXCEL ADDRESS function explained. Retrieved from <https://support.office.com/en-us/article/ADDRESS-function-D0C26C0D-3991-446B-8DE4-AB46431D4F89> on Sept 5, 2018.
- Microsoft EXCEL INDIRECT function explained. Retrieved from <https://support.office.com/en-us/article/INDIRECT-function-474B3A3A-8A26-4F44-B491-92B6306FA261> on Sept 5, 2018. □