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Evaporation and NARS

Nitric Acid Mass Balance Summary: 2000–2005

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by

Benjamin D. Kreutzberg, Richard L. Ames, and Kenneth M. Hansel

ABSTRACT

A compilation of the historical nitric acid processing data for the evaporation and nitric acid recycle system (NARS) in TA-55 has provided general acid mass balance trends, as well as the location of missing information in both the evaporation system and NARS data logs. The data were accumulated during the calendar years 2000 to 2005. After making a number of processing assumptions, the empirical system information was used to create an interactive spreadsheet that predicts, with moderate accuracy, some of the various stream variables for the combined evaporation and acid recycle processes. Empirical data and interactive calculations were compared to an Aspen Plus™ simulation of the process.

1.0 INTRODUCTION AND BACKGROUND

The overall objective of this project was to optimize nitric acid process data collection procedures in the plutonium processing facility (TA-55), PF-4, room 401. There are two principal acid processing unit operations located in the room 401 facility: the evaporator and nitric acid reprocessing system (NARS). Results of this effort, detailed below, were a compilation of nitric acid processing data for the evaporator, NARS, and mass balance summary for the production years 2000 through 2005. In addition, an interactive spreadsheet was constructed from the process data, a simulation of the process was completed using Aspen Plus™ process simulation software (which was compared with actual process data), and suggestions were made for future data collection activities given lessons learned from the analysis process.

1.1 Process Overview

The evaporator system serves to separate contaminant materials from process nitric acid waste streams generated by acid unit operations within the facility. The contaminant materials are then cemented for long-term storage. The purified acid distillate, or overhead product, from the evaporator can then be sent to NARS to be concentrated, recycled to purification operations, or discarded as waste to Technical Area 50 (TA-50).

The first step in the task was to compile available acid-processing data. For the evaporator the data for the years 2000 through 2005 were quite complete. However, the

NARS system has seen only limited operation since 2002 and a total of 16 runs were available. Once the data were compiled into an Excel™ spreadsheet, historical averages were compiled and used to design and construct an interactive spreadsheet in order to predict the results of possible future runs, given certain process assumptions.

Next, research into the construction of the interactive spreadsheet available database programs was conducted. The goal was to select a suitable program to use for the future data entry for both systems and to replace or supplement the paper forms currently in use.

Finally, an acid system simulation was conducted using Aspen Plus™ software at Colorado School of Mines. The simulation provided insight into the limitations of some of the assumptions made during the earlier phases of the project, and may suggest ways to improve how data are collected in these systems.

By completing this project we have begun the process of determining which information is needed to make records complete (mass balance), determining the most efficient methods of data collection, and initiated the task of automating data entry, storage and manipulation for both the evaporator and NARS systems. The compilation project has also generated a valuable summary of historical data, identified a useful tool to predict and model the processes, and highlighted data collection areas that need improvement.

1.2 Process Notes

Although the process block flow diagrams in this report accurately show the unit operations, they do not show the detail of each acid treatment process. The larger tanks on the diagrams are, in reality, batteries of tanks; each measures 6 in. in diameter. Measurements of material levels in these tanks are approximations based on the personal experience of the technicians making the measurements. Most of the smaller individual tanks are calibrated for volume.

As for the evaporator unit operation, there are actually two evaporators, both located within a contamination control room (sub-room to 401). Similarly, the entire NARS process is enclosed in another contamination control room along with two support slab tanks and the NARS process sampling system. In preparation for data analysis it was possible to view the processes, which greatly increased the level of understanding of the scale and operation and the logistics of material processing.

2.0 DATA ANALYSIS

The first phase of the project was to compile data from existing hard-copy data run sheets into an Excel™ database. The information compiled was then used for the later stages of the project.

2.1 Evaporator Acid Processing

Nitric acid processing data for the evaporator were available from November 2000 through February 2005, when over 200 runs were conducted and recorded. Figure 2.1 shows the flow diagram for the evaporator, and Appendix I shows the system with all storage tank systems that support the unit operation. Nomenclature for evaporation system variables is located in Appendix II.

The unit operation consists of two parallel thermosiphon evaporators which are based on the principles of liquid-vapor equilibrium for boiling nitric acid. However, only one evaporator is online at any given time. In preparation for a run, fresh feed is introduced into the system and temporarily stored in STK1 and STK2 feed tanks before being processed through the evaporator. The evaporator is charged with approximately 40 liters of feed solution, steam heat is initiated, and prior to reaching the steady state operating temperature, the product is routed to recycle storage tank TS-14. Once the system reaches steady state, the purified nitric acid overheads are sent to TA-50 (waste processing), the NARS process, or recycled to acid unit operations. The bottoms from the evaporator, which contain most of the contaminant material, can be removed from the evaporator for cementation or held until the next run.

For evaporation, processing data were available from two sources including individual run sheets and tank logs. The run sheets indicated how much feed material was processed during a particular run and typically where the feed solution was generated. The sheets then had a note section detailing the timeline for events for each run. For each recorded time, pertinent tank levels were listed, as well as important procedural steps. These data were normally sufficient to determine material flow paths.

Figure 2.1 – Evaporator process flow.

In some cases, the notes on the run sheets were either ambiguous or not sufficiently detailed. In these cases, the tank logs were needed to provide supplemental information. These logs detailed material stored in the various tanks and were also the only way to determine nitrate concentration of the products. To determine acid molarities, a simple weighted average formula was used because the product was typically distributed among several tanks. Many assumptions were necessary to complete the analysis. For example, rinse water was added when removing bottoms from the system, and because the exact amount added was not recorded for each run, operators were consulted and we recommended that approximately 10 liters of added wash solution be used as an assumption.

Once all available data were entered into the spreadsheet, a volume balance was performed and average values were calculated for use in the interactive spreadsheet. Finally, a nitrate mole balance was performed to determine the molarity of the feed, but because this value was unknown, it was not possible to determine an overall error or delta value for the nitrate concentration of the system.

The principal difficulty encountered while compiling the evaporator data was interpreting the run sheets. Specifically, it was often fairly difficult to determine the volume of material being generated as product. The largest source of error was the assumption that conserved volume and tank measurement error. In reality, volume was not a conserved quantity, as was assumed to perform the material balances. Because the streams are almost entirely nitric acid and water, the assumption is not especially inaccurate (as demonstrated in the Aspen Plus™ simulation discussed in section 3.5), but there were some minor volumetric fluctuations inherent in the different concentrations present. Although some of the tanks were volumetrically calibrated, the tank measurements were performed by visual estimation that led to errors in tank levels in the source data.

The compiled historical evaporation processing data have been used as baseline information for overall mass balance, process simulation, lessons learned, and as groundwork for the NARS version of the database.

2.2 Nitric Acid Recycle System (NARS) Acid Processing

Data for the NARS were available from May 2001 to July 2003. During this period, 16 runs were conducted and recorded. Figure 2.2 shows the process flow for the system, and located in Appendix I is a version of this flow diagram that includes tank support system details. In addition, variables that are present in the system are defined in Appendix II.

Figure 2.2 – NARS Process Flow.

The NARS process was designed to produce concentrated nitric acid from dilute evaporator overheads. This acid can be recycled to other processes, resulting in a reduction of the total amount of acid needed and waste produced. The feed is introduced into the distillation column from feed tanks TS-12 and TS-13 and is recirculated until the column reaches steady state. Once separation begins, the distillate, which is almost pure water, is sent to the red and blue tanks. The bottoms, which are typically concentrated acid product, are sent through the slab tanks to storage tanks T-9 and T-10. From there, the nitric acid can be recycled to other unit operations.

The NARS data were retrieved from two sources, the NARS electronic run sheets and room 401 tank logs. Unfortunately, certain information was not available because the wastes from this process were not accountable (since they do not contain radioactive materials). The run sheets showed the feed data quite reliably, but distillate and bottoms data were incomplete, at best. Sometimes, the volumes sent to the red and blue tanks could be determined from the tank logs, although it was not always possible to correlate runs to log entries. The product volume and acid concentration were sometimes in the run sheets, sometimes in the tank logs, but sometimes not present at all. If volume and concentration data for any material that was recycled to the feed tanks could not be located, estimates had to be made.

As with the evaporator, it was assumed that 40 liters of water were added per run for the purpose of rinsing equipment and system startup. Other estimates were based on the observed trends and a general knowledge of the process. Three runs had too little

information to make informed guesses and were not used in spreadsheet calculations. That left 13 runs for data analysis and spreadsheet calculations.

Once assumptions were made in order to fill voids in the process data, a volume balance was again used to determine the amount of material processed. Although the data summary generated by this section of the project may contain significant errors, it allowed for the creation of the interactive spreadsheet, and the data is likely valuable, given the approximate nature of the spreadsheet. The most meaningful piece of information gathered is that more data need to be collected for the acid recycle system (additional runs) and that future data collection must be complete.

3.0 RESULTS AND PROJECTIONS

Once the evaporator and NARS run data were compiled, averages were generated and the information was used to create an average run data spreadsheet and an interactive spreadsheet. Results from the interactive spreadsheet were compared with the results of an acid system Aspen Plus™ simulation. In addition, the experience gained during the data compilation phase served to determine the parameters for recommendations for a new database system.

3.1 Summary of Average Run Data

Table 3.1 shows the average processing data for the evaporation system on a per run basis, as illustrated in Figure 2.1. In summary, approximately 500 liters of product was generated from an estimated 550-liter batch of feed (including recycle acid and makeup water). Data on the exact volume of bottoms produced before dilution were not available, so it was assumed that 15 liters of 10 molar solution were produced, which was then diluted to the bottoms volume using approximately 10 additional liters of water. It was also assumed the nitrate concentration for the product was 6.7 molar (this value was extrapolated from post-2003 historical trends) when the data was not recorded. For the 222 evaporator runs where data were available, the outputs exceeded the inputs by about 3500 liters, or an average of approximately 21 liters per run (3 percent by volume). The most likely cause of this discrepancy was the addition of makeup water added above the 25 liters for each run. It should be noted that, in some cases, inputs exceeded outputs, and the values are simply averages.

Table 3.1 – Average Evaporator Historical Data

Evaporator Stream	Volume (L)	Concentration (M)
V _{ts-14}	52	1.0
V _{wa} (makeup water)	21	0.0
V _{feed}	478	7.7
V _{fts-14}	64	1.0
V _{prod}	516	6.7
V _{bot}	20	5.5
Delta volume	21	–

For the 13 NARS runs evaluated, the average per run data is shown in Table 3.2, as illustrated in Figure 2.2. In summary, approximately 250 liters of 12M acid bottoms was produced for each 700-liter run. It was assumed that 40 liters of water were added per run for the purpose of rinsing equipment and system startup. Inputs exceeded outputs by about 10 liters on average, or about 130 liters for all 13 runs. The nitrate balance showed that outputs exceeded inputs by a total of about 4900 moles of nitrate, for an average of approximately 375 moles per run. It should be noted that approximately 11% of the acid recycle system data was estimated from process knowledge

Table 3.2 – Average NARS Historical Data

NARS Stream	Volume (L)	Concentration (M)
V_{feed}	671	5.4
V_{left}	174	3.5
V_{top}	277	0.0
V_{prod}	250	11.6
V_{wa} (makeup water)	40	0.0
Delta Volume	10	—

3.2 Interactive Spreadsheet

The interactive spreadsheet was intended to allow technicians to model the combined evaporator and NARS processes. It will allow operators to predict some variables after inputting either their desired results or their observed measurements. The spreadsheet includes both the evaporator and NARS processes, although it can be used for either one independently. Figure 3.1 shows a flow diagram of the combined system.

Figure 3.1 – Combined process flow diagram.

Some variables change very little from run to run and can be accurately assumed to be very close to the average. Using this principle, it was possible to create Section A of the spreadsheet to require seven variables and return the other six. There was some restriction as to which variables must be defined. For example, the user must specify either V_{top} or V_{prod} in the NARS segment of the process. Without this information, the spreadsheet would not be able to calculate the splitting ratio. Section A of the interactive spreadsheet includes nine potential combinations of user-defined and calculated parameters. These combinations were intended to cover the more common (and useful) situations that a technician may wish to model.

For section B of the spreadsheet, one additional assumption was made that the ratio of V_{top} to V_{prod} in NARS is a constant 1.1, which was determined by examining the system historical data. The assumption makes Section B less accurate but also allows the spreadsheet to function with one less user input. This allows for an estimation of product produced from a given feed if NARS functions according to the predicted averages. An additional listing of assumptions is included as Appendix III.

In both A and B cases, the intention was that the spreadsheet be used only as a rough guide. There are potentially significant variations in the assumed parameters, which can adversely affect the results. Further, as in the data compilation phases, volume is treated as a conserved quantity. In addition, for Section B, the splitting ratio is the average of only 13 runs. The value would probably be somewhat different if more runs were conducted.

To test the spreadsheet, a test model was entered and the results compared with the actual values. Table 3.3 shows the values calculated by the spreadsheet in comparison to the corresponding actual values using Section A, line 4 and Section B, line 17 of the spreadsheet. This sample is based on the evaporator run on December 3, 2001, which was then sent to NARS the next day.

Table 3.3 – Section Interactive Spreadsheet Comparison

Variable	Actual Value	Calculated Value-A	Calculated Value-B
V_{feed} (evap)	540	549	532
M_{feed} (evap)	7.15	6.27	6.5
V_{prod} (evap)	550	550	533
M_{prod} (evap)	6.7	6.1	6.25
V_{feed} (NARS)	430	Not calculated	413
M_{feed} (NARS)	4.3	6	6.25
V_{top} (NARS)	340	255	238.2

This example demonstrates that, although Section A gives better results, the difference is not significant, given system assumptions. In addition, the example shows that the NARS portion of the spreadsheet is less accurate than that of the evaporator largely because of the lack of NARS data and the stream estimates made.

This spreadsheet may ultimately be the most useful portion of this project. Despite the potential sources of error, it should model the actual process well enough to make general predictions. For example, a technician could enter the desired products and determine a reasonably accurate prediction of the feed volume and concentration. In addition, once additional NARS data are generated, this part of the spreadsheet can be improved.

3.3 Database Software Analysis

Another objective of this task was to conduct a preliminary evaluation of using a computer database to log and compile acid processing data in the future. The new database program would need to allow an individual to print run sheets for the purpose of material accountability. In order to have this sort of functionality, the program should be able to access inputs from input forms. This method of input most likely simplifies the process, and it gives a much tidier appearance than the line-by-line approach needed for an Excel spreadsheet. The new program must also be able to track running statistics as data are entered.

As a result of our preliminary evaluation, the preferred software was Microsoft Access™. Other database packages were briefly evaluated and some appeared to be adequate, but none was more suitable for chemical flow work than Access™.¹ Simply stated, Access™ appeared to meet all the specific requirements and had the additional advantage of being widely available within NMT Division. Screenshots of both the sample entry form and tabular spreadsheet are located in Appendix IV. This sample database is solely intended to demonstrate the basics of how the final database would work. Data are entered on the form and then translated into the spreadsheet-type database.

3.4 Database Design Recommendations

During the early phases of the project, much of the data were taken from run sheets and tank logs. These data sources were sometimes inefficient and difficult to understand. To obtain useful information from run sheets and tank log data, a level of familiarity with both the process and data entry methods is required. When the new database is designed, we recommend that a number of changes be made to the methods used to archive data. The most useful database feature would be direct entry for all inputs and outputs. The easiest method to implement would be to have additional entry fields for the new data, whereby users could enter, e.g., the total fresh feed in one field, the total recycled feed in another, and the various products in other individual boxes. This technique would allow new information to be available while retaining information about the tank levels, which is required for accountability purposes. These fields could also be designed to pinpoint or identify the exact destinations of outputs.

An item that was frequently missing or difficult to find was nitric acid concentration, and when acid concentration was available, it was often in tank logs that were incomplete. It would be more effective to record the acid concentration of every tank and every flow, if the information was available. If this data could be provided, it should be entered in a new entry field located near to the pertinent volume fields, or if it were not available, an estimate could be made. In summary, by improving data entry and compilation

techniques, it will be much easier to retrieve information about either individual runs or totals and averages for multiple runs.

3.5 Aspen Plus Simulation

Aspen Plus™ is a chemical process flow program package that models steady state operations.² Although the processes of concern were not steady state, Aspen Plus™ can still accommodate them. The principal goal of the Aspen Plus™ simulation was to determine the accuracy of the assumptions that were made in the previous phases of the project. Appendix V includes the process flow diagram (PFD) and run sheet generated by Aspen Plus™ as well as empirical vapor-liquid equilibrium (VLE) data.³

Because Aspen Plus™ models only steady state operations, it was necessary to set a basis of 1 hour. For example, if 200 liters total feed was processed, that value was entered as 200 liters per hour. Since all measurements will be in the same form, the hours can be ignored when analyzing the results.

The first goal was to compare the nitric acid/water binary VLE regression curve with the curve obtained experimentally in 2003 by Dr. Steve Yarbrow (Appendix V).³ Table 3.4 and Figure 3.1 show the VLE data generated by Aspen Plus™ for water, along with the equation for the regression curve. The data generated by Aspen Plus™ do not compare well with the empirical values generated by Yarbrow.³ This was the case when Yarbrow compared his empirical data to Aspen™ VLE in 2003, and the likelihood is that there have not been major changes to the Aspen Plus™ VLE data in the last two years. Until Aspen Plus™ is equipped with more accurate nitric acid/water VLE data, all of the Aspen Plus™ results for this system should be viewed with some skepticism.

Table 3.4 – Binary VLE Data Generated by Aspen Plus™

Temp °C	X _a	Y _a	X _w	Y _w	K _a	K _w
100.907	0.010	0.017	0.990	0.983	1.656	0.993
101.691	0.050	0.081	0.950	0.919	1.614	0.968
101.780	0.100	0.157	0.900	0.843	1.566	0.937
102.154	0.150	0.229	0.850	0.771	1.521	0.908
102.985	0.201	0.297	0.799	0.703	1.479	0.880
104.479	0.251	0.361	0.749	0.639	1.440	0.853
106.899	0.301	0.421	0.699	0.579	1.401	0.828
110.659	0.351	0.478	0.649	0.522	1.365	0.803
115.785	0.401	0.533	0.599	0.467	1.329	0.779
118.633	0.451	0.585	0.549	0.415	1.296	0.757

Figure 3.1 – Aspen Plus™ VLE graph with regression, for water.

When comparing the Aspen Plus™ results with the empirical data, a single data run was selected from the database: The first evaporator run with no bottoms sent to cementation (bottoms carryover) was conducted on October 16, 2002, and the consecutive run when bottoms were sent to cementation was conducted on October 28, 2002. The combined products were then sent to NARS and processed on October 30, 2002. These data were selected as the NARS run was complete and none of the data were estimated.

Table 3.5 shows the comparison of the actual stream values and the values computed by Aspen Plus™. As can be seen, the volumes do not balance in either case and are especially inaccurate around NARS. This clearly shows a major flaw in one of the principal assumptions made in the project: that volumes were additive. However, this assumption did not significantly impact the results of the comparison between the Aspen Plus™ simulation and the actual process data, but the previous phases all used the additive volume assumption extensively. Regardless, the flow data compare quite well with the actual values, indicating a fairly good match with the data.

Table 3.5 – Aspen Plus™ Data vs. Collected Data

	V_{feed}	V_{wa}	V_{bot}	V_{prod}	$V_{\text{TA-50}}$	V_{f}	V_{water}	V_{fw}	V_{top}	V_{p}
Actual flow (l)	840.1	25	26	970	130	840	40	not taken	470	340
Aspen Plus™ flow (l/hr)	840.1	25.0	25.6	839.3	0.0	839.3	40.0	879.2	478.8	338.5
Actual Conc. (M)	7.64	0	5.77	6.4	6.4	6.4	0	not taken	0	12
Aspen Plus™ Conc. (M)	7.64	0.00	5.85	7.47	0.00	7.47	0.00	7.13	4.88	11.61

The Aspen Plus™ value for V_{prod} was much more reasonable than the actual value, which does not seem in line with corresponding feed volumes. This discrepancy requires the zeroing of $V_{\text{TA-50}}$ (acid volumes sent to TA-50 as waste) in order to get V_{f} near to the empirical value. The most likely explanation for the discrepancy is that either the volumetric value for V_{prod} was incorrectly measured or the data sheet was misinterpreted and that the value is actually near the Aspen Plus™ value. This phenomenon probably also caused errors in the calculated nitrate concentrations by changing the total amount of nitrate and influencing the calculated nitrate concentration of the feed, which was then used for the Aspen Plus™ simulation. Aspen Plus™ then had a higher nitrate concentration than shown by actual process data leading to error in the nitrate concentrations of V_{prod} and all of the flows in NARS. Because of the imprecise correlation of the tank data and evaporator run data, the misinterpretation of run sheet data seems the more likely scenario. Despite this major source of error, the nitrate concentrations were similar when comparing Aspen Plus™ results with actual process data.

In summary, the Aspen Plus™ simulation compared well with the actual process data in terms of the volumetric balance, though not as well in terms of nitrate material balance. Perhaps more important, the Aspen Plus™ simulation confirmed that volume was not a conserved quantity. This confirmation suggests that some of the inaccuracies, detailed in the previous sections, were a result of calculations based on treating volume as a conserved quantity. The Aspen Plus™ simulation also demonstrated why improved data recording would be very helpful.

4.0 CONCLUSIONS

In conclusion, the major results of this task provided a better understanding of both the evaporator and NARS processes and the identification of areas where the system data collection needs additional organization. More specifically, the compilation of the historical data has provided general mass balance trends, as well as having shown locations of missing information in both the evaporation system and NARS. Having made a number of processing assumptions, we used the empirical system information to create the interactive spreadsheet that predicts, with moderate accuracy, some of the various stream variables for the combined evaporation and acid recycle processes. Also, database investigations indicated that Microsoft Access™ would meet the data collection needs of the process. Finally, the Aspen Plus™ simulation produced data that compared well with empirical process data and helped to show the limited accuracy of some of the assumptions made, specifically the assumption that volume was a conserved quantity.

Results from this task will eventually lead to a streamlined system for data entry and analysis in room 401. It has also produced the interactive spreadsheet that may prove to be a useful tool for everyday operations. In addition, those involved have a better knowledge base and clearer understanding of the needed direction for the evaporation and NARS data compilation system.

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APPENDICES

Appendix I Flow Diagrams with Tanks

Figure I-1 – Evaporator with tanks.

Appendix I (continued)
Flow Diagrams with Tanks

Figure I-2 – NARS with tanks.

Appendix II Nomenclature

Evaporator System Nomenclature

Inputs

V_{feed} – the volume of fresh material initially fed into one of the STK tanks. (It is often necessary to subtract the hot distillate.) The nitrate molarity is calculated through a nitrate balance.

$V_{\text{fts-14}}$ – The volume of hot distillate fed from TS-14. The nitrate concentration is assumed to be ~1M.

V_{wa} – The total volume of water added. No nitrates are present. Assumed to be 25-L when a bottoms dump occurs and 0-L when there is no bottoms dump.

Outputs

V_{prod} – The volume of material sent to tanks LA16, LA17, and LA19 for disposal by TA50 or reprocessing through NARS. The nitrate molarity is a weighted average of the partial flows (V_1 , V_2 , V_3).

V_{bot} – The volume of material sent to cement. The composition is assumed to be 15-L of 10M solution, diluted to the correct volume with additional water.

$V_{\text{ts-14}}$ – The volume of hot distillate leaving the evaporator and sent to TS-14. The nitrate concentration is assumed to be ~1M.

Tank Levels

V_{left} – The volume (if any) of hot distillate which remains in TS-14. The nitrate concentration is assumed to be ~1M.

$V_{\text{inventory}}$ – The volume of material initially present in TS-14. The nitrate concentration is assumed to be ~1M.

Additional flows

V_1 , V_2 , V_3 – the partial flows that make up V_{prod} . Molarities are logged in the LA-19 tank information.

Appendix II (continued)

Nomenclature

NARS Nomenclature

Inputs

V_{feed} – The volume of fresh material initially fed from TS-12 and TS-13. The nitrate molarity is recorded on the run sheets.

V_{wa} – The total volume of water added. No nitrates are present. Assumed to be 40-L based on knowledge of the process.

Outputs

V_{top} – The volume of nearly pure water sent to the red and blue tanks. No nitrates are assumed to be present.

V_{prod} – The volume of material sent to tanks T-9 and T-10 for reuse. The nitrate molarity is recorded on either the run sheets or tank logs.

V_{left} – The volume of partially-enriched product that is returned to the feed tanks. No information about its nitrate concentration was available, so assumptions were based on knowledge of the process.

Aspen Plus TM Nomenclature

X_a – Mole fraction nitric acid in the liquid.

Y_a – Mole fraction nitric acid in the vapor.

X_w – Mole fraction water in the liquid.

Y_w – Mole fraction water in the vapor.

K_a – Distribution coefficient for nitric acid: Y_a/X_a .

Y_w – Distribution coefficient for water: Y_w/X_w .

Appendix III

Interactive Spreadsheet Assumptions

Overall Spreadsheet Assumptions and Notes

1. No recycle stream calculations are included. The assumption is that everything is completely processed.
2. It is assumed that the evaporator is dumped for only the products of the current run; there is no residue from previous runs, nor will the evaporator bottoms be combined with a future run.
3. The following values are based on historical trends: V_{wa} , V_{bot} , M_{bot} for the evaporator and V_{wa} and M_{top} for NARS.

Section B Additional Assumptions and Notes

1. The objective of Part B is to make “quick and dirty” calculations without requiring much input. The main assumption is that the ratio of product to tops in the NARS system is constant at approximately 1.1:1.
2. This assumption is normally acceptable, although the NARS product composition depends mainly on how the process is run.

Appendix IV Sample Access Plus™ Database Screenshots

Form

Sample Access Database : Database (Access 2000 file format)

Open Design New X

Objects

- Tables
- Queries
- Forms
- Reports
- Pages
- Macros
- Modules

Groups

- Favorites

Create form in Design view

Create form by using wizard

Main Table

Main Table

#Name?

Date
6/27/2005

ID
1

Volume from TS-14
20

Feed Volume
250

Volume to bottoms
25

Volume to TS-14
20

Volume of product
225

NARS?
☐

Recycle?
☒

Record: 1 of 4

Figure IV-1 – Sample Access™ database entry form.

Microsoft Access

Type

File Edit View Insert Format Records Tools Window Help

Main Table: Table

ID	Date	Feed Volume	Volume from TS	Volume to bottol	Volume to TS-1	Volume of produ	Recycle?	NARS?	Calculated Mole
1	6/27/2005	250	20	25	20	225	☒	☐	
2	3/26/2002	300	300	25	0	575	☒	☒	
3	2/5/1999	520	0	25	30	465	☐	☒	
4	2/7/2005	6	5	0	0	0	☐	☒	0
*(AutoNumber)		0	0	0	0	0	☐	☐	0

Record: 1 of 4

Table IV-2 – Sample Access database run entries.

Appendix V Aspen Plus™ Flow

Figure V-1 – Aspen Plus™ flow diagram.

Appendix V (continued)
Aspen Plus™ Flow

Table A-1 – Aspen Plus™ Run Sheet

	V _{FEED}	V _{WA}	V _{BOT}	V _{PROD}	V _{TA-50}	V _F	V _{WATER}	V _{FW}	V _{TOP}	V _P
Substream: MIXED										
Mole Flow mol/hr										
HNO ₃	6418.4	0.0	150.0	6268.4	0.0	6268.4	0.0	6268.4	2337.3	3931.1
WATER	26219.1	1344.8	921.4	26642.5	0.0	26642.5	2151.7	28794.2	20102.8	8691.4
Total Flow mol/hr	32637.5	1344.8	1071.4	32910.8	0.0	32910.8	2151.7	35062.5	22440.0	12622.5
Total Flow kg/hr	876.8	24.2	26.1	875.0	0.0	875.0	38.8	913.7	509.4	404.3
Total Flow l/hr	840.1	25.0	25.6	839.3	0.0	839.3	40.0	879.2	478.8	338.5
Temperature C	93.0	50.0	91.7	91.7		91.7	50.0	89.8	36.1	31.6
Enthalpy J/kmol	-2.6E+08	-2.8E+08	-2.6E+08	-2.6E+08		-2.6E+08	-2.8E+08	-2.6E+08	-2.7E+08	-2.5E+08
Enthalpy J/kg	-9.6E+06	-1.6E+07	-1.1E+07	-9.7E+06		-9.7E+06	-1.6E+07	-1.0E+07	-1.2E+07	-7.8E+06
Enthalpy Watt	-2.3E+06	-1.1E+05	-7.9E+04	-2.4E+06		-2.4E+06	-1.7E+05	-2.5E+06	-1.7E+06	-8.8E+05
Entropy J/kmol-K	-1.7E+05	-1.6E+05	-1.6E+05	-1.7E+05		-1.7E+05	-1.6E+05	-1.7E+05	-1.7E+05	-2.0E+05
Entropy J/kg-K	-6.3E+03	-8.7E+03	-6.7E+03	-6.3E+03		-6.3E+03	-8.7E+03	-6.4E+03	-7.6E+03	-6.3E+03
Density kmol/cum	38.850	53.792	41.784	39.210		39.210	53.792	39.881	46.867	37.286
Density kg/cum	1043.666	969.074	1015.985	1042.437		1042.437	969.074	1039.283	1063.969	1194.253
Average MW	26.864	18.015	24.315	26.586		26.586	18.015	26.060	22.702	32.029
Liq Vol 60F l/hr	741.119	24.274	22.892	742.500	0.000	742.500	38.838	781.338	460.398	320.940
Molarity mol/l	7.64	0.00	5.85	7.47	0.00	7.47	0.00	7.13	4.88	11.61

Table A-2 – Binary VLE Data Generated by Yarbro³

Temp °C	X _a	Y _a	X _w	Y _w	K _a	K _w
100	0.000	0.000	1.000	1.000	0.000	1.000
104	0.067	0.003	0.933	0.997	0.045	1.069
104.5	0.072	0.006	0.928	0.994	0.079	1.071
106.5	0.102	0.010	0.898	0.990	0.098	1.102
107	0.110	0.012	0.890	0.988	0.109	1.110
108.5	0.135	0.020	0.865	0.980	0.148	1.133
109.5	0.141	0.023	0.859	0.977	0.163	1.137
110.5	0.162	0.035	0.838	0.965	0.216	1.152
111.5	0.181	0.042	0.819	0.958	0.232	1.170
114.5	0.217	0.082	0.783	0.918	0.378	1.172
115.5	0.233	0.096	0.767	0.904	0.412	1.179
117.5	0.282	0.165	0.718	0.835	0.585	1.163
119.2	0.348	0.297	0.652	0.703	0.853	1.078