

Detailed Modeling of Distillation Technologies for Closed-Loop Water Recovery Systems.

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This paper presents efforts to develop chemical process simulations for three technologies: the Cascade Distillation System (CDS), the Vapor Compression Distillation (VCD) system and the Wiped-Film Rotating Disk (WFRD) using the Aspen Custom Modeler and Aspen Plus process simulation tools. The paper discusses system design, modeling details, and modeling results for each technology and presents some comparisons between the model results and recent test data. Following these initial comparisons, some general conclusions and forward work are discussed.

Detailed Modeling of Distillation Technologies for Closed-Loop Water Recovery Systems.

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Nomenclature

<i>ACM</i>	= Aspen Custom Modeler
<i>AP</i>	= Aspen Plus
<i>CDS</i>	= Cascade Distillation System
<i>DCT</i>	= Distillation Comparison Test
<i>ESM</i>	= Equivalent System Mass
<i>ISS</i>	= International Space Station
<i>PCPA</i>	= Pressure Control and Purge Assembly
<i>TC</i>	= Trim Cooler
<i>THP</i>	= Thermoelectric Heatpump
<i>VCD</i>	= Vapor Compression Distillation
<i>WFRD</i>	= Wiped Film Rotating Disk
<i>WRS</i>	= Water Recovery System

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I. Introduction

The ability to recover and purify water through physico-chemical processes is crucial for realizing long-term human space missions, including both planetary habitation and space travel. Although short-duration missions have relied on storage and transport instead of on-board water recovery, an estimated requirement of 8 to 15 kg of water per crewmember per day will pose a significant launch penalty and significant barrier to longer duration missions¹. Therefore, future water recovery, purification, and processing technologies should possess the ability to accept wastewater streams from various sources (gray water, urine, and condensate from humid air) and recycle them to a high level of chemical purity and potability. These processes also must be able to function in both zero-gravity and low-gravity environments while consuming modest power resources and requiring little maintenance and few consumables. Eventually, such systems may even be expected to operate in a completely closed-loop fashion with the ability to recover most of the water from various waste streams.

Several technologies, including reverse osmosis², catalytic and electrochemical processes³, and distillation³ have been explored as candidates for next generation water recovery systems (WRS). Because of the robust nature of distillation processes, vacuum distillation has been actively pursued as a technology for water recovery¹. Distillation at very low pressures has demonstrated the ability to significantly reduce power requirements over traditional distillation technologies and has therefore been developed for space applications. This report discusses the development of dynamic process simulations for the CDS, VCD and WFRD technologies.

Detailed chemical process simulations are useful tools for designing and optimizing complex systems and architectures for human life support. Dynamic and steady-state models of these systems help contrast the interactions of various operating parameters and hardware designs, which become extremely useful in trade-study analyses. Aspen Custom Modeler (ACM) is a chemical process modeling package that has the ability to perform both steady-state and dynamic simulations and has been used frequently for developing detailed models for various engineering analyses^{4,5}. Dynamic modeling is particularly useful because it allows the ability to study a process technology in great detail, identifying process limits as well as process dynamics. Because life support processes are often highly sensitive to disturbances and seldom reach true steady-state conditions, dynamic modeling and data are crucial to developing robust descriptions of the process dynamics.

By relating operating and hardware-related variables to process efficiency, it is possible to optimize the unit sizing and its operating parameters. Accurate models can even generate data for a wide variety of operating conditions, which can then be used to develop a process control strategy that is based on process-specific operating data instead of a generalized theoretical description. Detailed models can also simulate off-nominal scenarios that are rare, difficult, or even dangerous to reproduce, which can help in sizing for worst-case operating conditions. Ultimately, the goal of modeling is to develop accurate dynamic descriptions of processes that can be used to optimize the complete life support architecture by considering process efficiency, equivalent system mass (ESM), and the general operating limits of the technologies. For water recovery, such comparisons will be made between technologies like the VCD, WFRD and CDS.

This report presents the status of modeling efforts for the CDS, VCD and WFRD water recovery technologies. The report discusses system design, modeling details, and modeling results for each technology and then presents some general conclusions and forward work. Updates to this report will be made available as the three models gain greater fidelity and accuracy. Eventually, the three water processing technologies will be evaluated using ESM metrics, test data and model results in order to optimize the water processing architecture for the life support systems. Modeling will also be used to design and evaluate process control schemes.

II. Technology Descriptions

The systems that have been modeled are the CDS, VCD and the WFRD. Even though all three of these systems rely on distillation technology to reclaim water, they vary in their design and operation. The following presents a brief discussion of the mechanical and operating principles of each processor. Further details are provided elsewhere^{4,5}.

A. Cascade Distillation System (CDS)

The CDS is being developed in conjunction with Honeywell International Inc. and Thermodistillation. The CDS presents a variant on the vacuum rotary distillation concept through a multistage rotating distiller coupled with a thermoelectric heat pump that provides heating and cooling. The vacuum is provided by a mechanical pump that reduces the distiller chamber pressure to 50 mmHg. Heat transfer surfaces between the stages serve to capture the heat of vaporization and transfer it to the adjacent stage. Figure 1 presents a schematic of the CDS.

The multistage vacuum rotary distiller (CD5 in the diagram) consists of chambers (stages) with rotating heat transfer surfaces separating brine and condensate and with stationary pitot-tube pumps providing liquid transfer between stages. Feed waste water is fed into the fifth stage of the CD5 and is partially vaporized using heat from condensation of vapor from the fourth stage. Countercurrent flow of brine and vapor/condensate occur as a result of heating the most concentrated brine in the first stage. This leads to a temperature gradient between stages, increasing in the direction of brine flow and decreasing in the direction of condensate flow. The heat of vaporization is captured by heat transfer surfaces within the stages and used to heat the liquid in the next stage. Once the brine has reached a maximum concentration, it is fed into a separate holding tank. A cooled condenser stage provides final condensate collection.

Heat energy for the process is supplied by a thermoelectric heat pump (THP)^{6,7}. A portion of the liquid from stage one is fed to the heat pump and then recirculated back to the distiller to supply heat for the process. This heat energy is actually drawn from a portion of the recovered water as a recirculating water stream. The THP itself requires less power than a traditional heater, and since it uses thermal energy from the cold side to heat the hot side, it functions as both the condenser and the reboiler stages of a traditional distillation column. Reducing the pressure inside the distiller using the vacuum pump reduces the distillation temperature thus reducing power requirements even further¹. Since the THP generates heat from electrical resistance within the device, a trim cooler (TC) is used to remove additional heat from the colder recirculating stream.

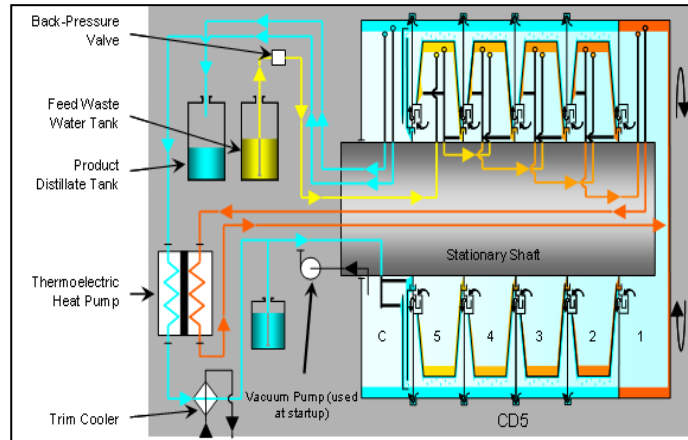


Figure 1. Schematic description of Cascade Distillation System⁸. The blue stream represents distiller water flow while the yellow stream indicates the flow of waste water (urine). The brine is represented by the orange stream.

B. Vapor Compression Distillation

The VCD system is a single-stage distillation process that has been developed at Marshall Space Flight Center for the International Space Station (ISS). The distillation assembly, the primary component of the Vapor Compression Distillation system, appears in Figure 2.

Wastewater is deposited in a thin film along the inner evaporator surface of the rotating drum. As water evaporates, it is pulled into the compressor through the hollow stationary shaft. The compressor raises the saturation temperature and pressure of the water vapor, and the compressed vapor then passes into the condenser, where it condenses on the outer surface of the rotating drum, in thermal contact with the evaporator surface. The resulting heat flux from the condenser to the evaporator, driven by the saturation temperature difference, drives the further evaporation of water inside the evaporator, and the VCD process thus recovers the latent heat of evaporation/condensation.

The evaporator pickup tube (Recycle Out) collects the wastewater not evaporated inside the evaporator. This concentrated wastewater (brine) flows through a recycle loop and is mixed with fresh wastewater for reprocessing. The condensed water vapor is collected from the condenser by the product water pickup tube (Product Out). The condenser is periodically purged (Purge Out) to remove non-condensable gases and to maintain the operating pressure.

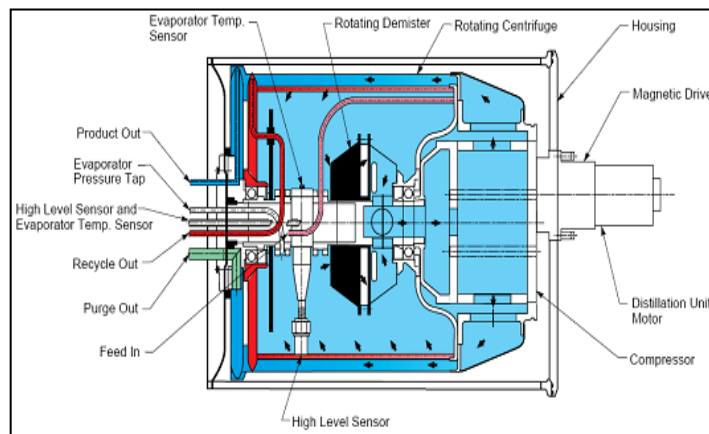


Figure 2. VCD distillation assembly schematic⁹⁻¹².

The VCD evaporator process nominally operates at 3.4 to 5.5 kPa (0.5 to 0.8 psia) and ambient temperature (32 to 43°C, 90 to 110°F). Further details of the VCD process and system, including other components such as fluids pumps, the recycle filter tank, etc., are provided elsewhere^{9,10,11}.

C. Wiped Film Rotating Disk (WFRD)

Thin film distillation offers improved efficiency by enhanced heat transfer. In the WFRD system, a preheated feed is sprayed onto a rotating hollow disk assembly to create a thin film. The film evaporates quickly and the vapor is compressed and fed into the condenser section (the inside of the hollow disk assembly) of the unit. The heat of condensation is transferred back to the evaporating film hence conserving some energy. The overall process consumes less energy than a traditional distillation system. In essence the film evaporates via a combined convection/conduction process. Figure 3 presents a schematic for the WFRD evaporator assembly and Figure 4 presents the process flow diagram for the WFRD system.

The basic operation for distillation within the WFRD can be summarized by Figure 3. The hot feed is sprayed onto the hollow rotating disk within the partially evacuated still. As the fluid evaporates it is pumped out through the “vapor out” port and fed into the inside portion of the hollow rotating disk through the “heating steam” port. The vapor is moved from the outside of the rotating disk to the inside using an external compressor. As the vapor condenses, the heat of condensation is conducted through the wall of the rotating disk assembly and used to evaporate more of the feed. This combination of processes results in efficient evaporation with low power consumption. Feed that is not evaporated becomes enriched with waste byproducts while the vapor consists primarily of water and volatile gases. The enriched brine is disposed through the brine scoops on the outside of the rotating disks while the collected distillate (pure water) is sent to the distillate tank through a product tube. The entirety of the process is discussed using Figure 4 below.

As mentioned earlier, the evaporated feed (vapor) is moved from the outside portion of the hollow rotating disk assembly to the inside of the hollow disk where it is condensed. The external compressor is shown in Figure 4. Figure 4 also shows the flow paths for the brine and distillate collection. It is also worth noting the integration of various streams for heat exchange. For example, feed is heated by the hot brine exiting the evaporator loop and heated again by the hot liquid product exiting the condenser. This heat exchanged between hot and cold streams provides substantial savings in operational power.

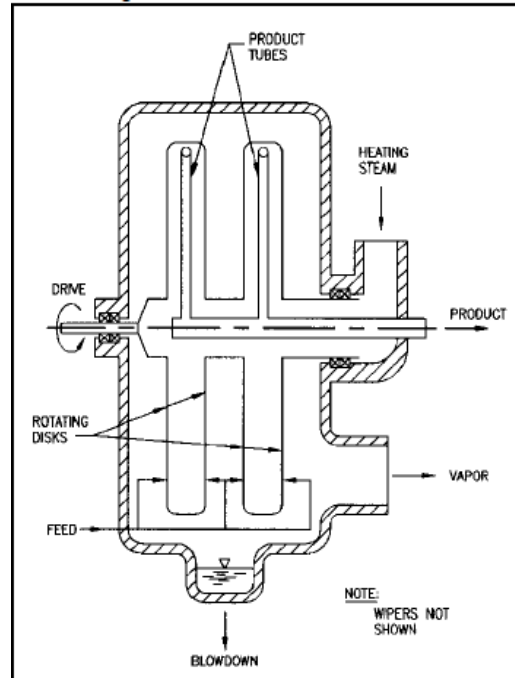


Figure 3. WFRD Evaporator Assembly Schematic¹².

III. Modeling Principles

For water modeling, ACM interfaces with the thermo-chemical properties subroutines and databases in Aspen Plus (AP), which provides electrochemical and thermodynamic relations that describe component solubility and phase behavior in the model system. AP provides an extensive database of intrinsic physical properties for chemical species as well as several methods for determining thermodynamic, physical and state properties.

A salt water system (NaCl-H₂O) was used for the initial modeling of the technologies. Once the initial models appeared to operate successfully, the salt-water system was replaced with an ERSATZ waste water formulation and the models were run with the ERSATZ model containing a host of inorganic and organic components found in typical urine and humidity condensate streams. The current model for the feed was based on the results of the distillation comparison test (DCT). The DCT Feed uses 24 of the most prevalent components found during the DCT and incorporates phenomena such as solids precipitation and production of VOCs and non-condensable gases such as carbon dioxide.

For all three technologies, separation was modeled using flash calculation routines supplied by ACM. For the WFRD and VCD, one flash calculation was used to predict the split between liquid (and solid) and vapor, while five sequential flash calculations were used to model the CDS. Although the flash is the most straight forward and logical choice for predicting the separation between liquid and vapor, it does rely upon assuming thermodynamic

equilibrium with the processors. Although equilibrium flash may be a reasonable assumption, especially for a multi-staged distiller like the CDS, it may not be as robust for a single stage unit like the WFRD or the VCD, particularly when modeling the affects of process upsets.

III. Results and Discussion

At present, preliminary models for the CDS, VCD, and the WFRD have been completed. In addition to the processor models, a model for the DCT Feed formulation has been developed in AP, and the CDS and WFRD have been adapted to the new model.

Figure 5 presents the ACM flowsheet for the CDS. The CDS process simulation includes a number of models for individual components of the system. The multistage rotary vacuum distiller is modeled as a number of stages; five evaporating stages and five condenser stages.

Each evaporator stage passes evaporated water to the adjacent condenser stage and the heat of condensation is passed to that stage's evaporator (except for Stage 1). The split between vapor and liquid phases is calculated by the rigorous flash routines mentioned earlier. The THP and the TC are modeled as heat exchangers. The THP equations are based on the operation of a thermoelectric heater that draws heat from the cold loop and passes it to the hot loop. Since the inefficiencies of the THP (due to electrical resistance) have not been characterized in great detail, the model uses empirical factors to replicate the efficiency. The trim cooler operates as a conventional countercurrent single pass heat exchanger and incorporates heat transfer coefficients based on the manufacturer's data. The recirculation flow rates for the hot and cold loops are fixed and balanced and the target water temperature for the distillate is fixed. The cooling water flow rate is fixed in order to achieve the target distillate temperature. Feed and production rates are allowed to vary and are determined by the model based on the process operating parameters.

The chemistry within the process simulation is based on thermodynamic data generated by AP and all aqueous components are tracked during mass balance calculations as neutral (apparent) species as opposed to ionic species to improve the efficiency of the calculations. Vapor-liquid equilibrium calculations are performed using actual true-component compositions (considering ionic species). The DCT feed also incorporates solid formation in parts of the CDS such as the feed tank and the evaporator sections. Since only water vapor and gases reach the condenser blocks, solids formation was not calculated in these blocks.

Figures 6 – 8 present urea mole fraction (X_{Urea}), stage temperature ($^{\circ}C$) and stage pressure (bar), respectively, within each of the five evaporator stages of the CDS. As expected, the highest urea concentration, stage temperature and stage pressure were predicted at Stage 1, the stage closest to the brine recirculation loop, with the lowest values predicted for stage 5. The simulation also models the successive enriching of the brine in Stage 1 by the slow removal of water from the waste input stream. Similar calculations of pressures, temperatures and species concentrations can be generated for the condenser side components. Concentrations of any individual liquid phase species can be tracked using plots similar to Figure 6.

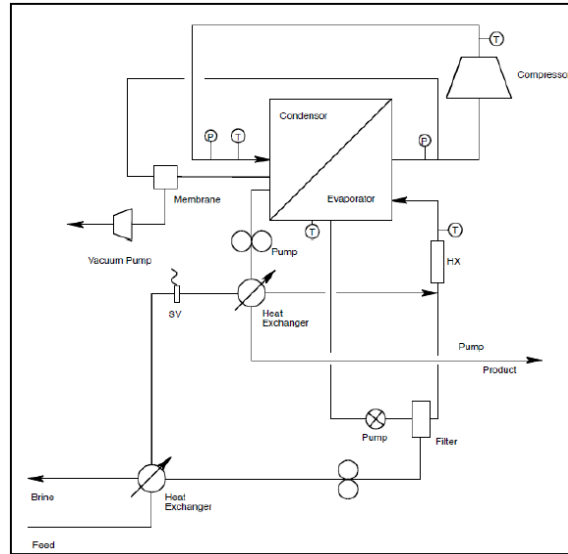


Figure 4. WFRD schematic¹².

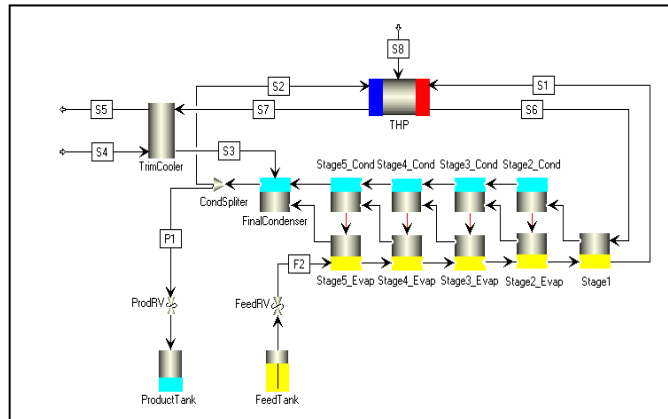


Figure 5. ACM flowsheet model of Cascade Distillation System. The multistage rotary vacuum distiller is represented by five evaporating and compressing stages.

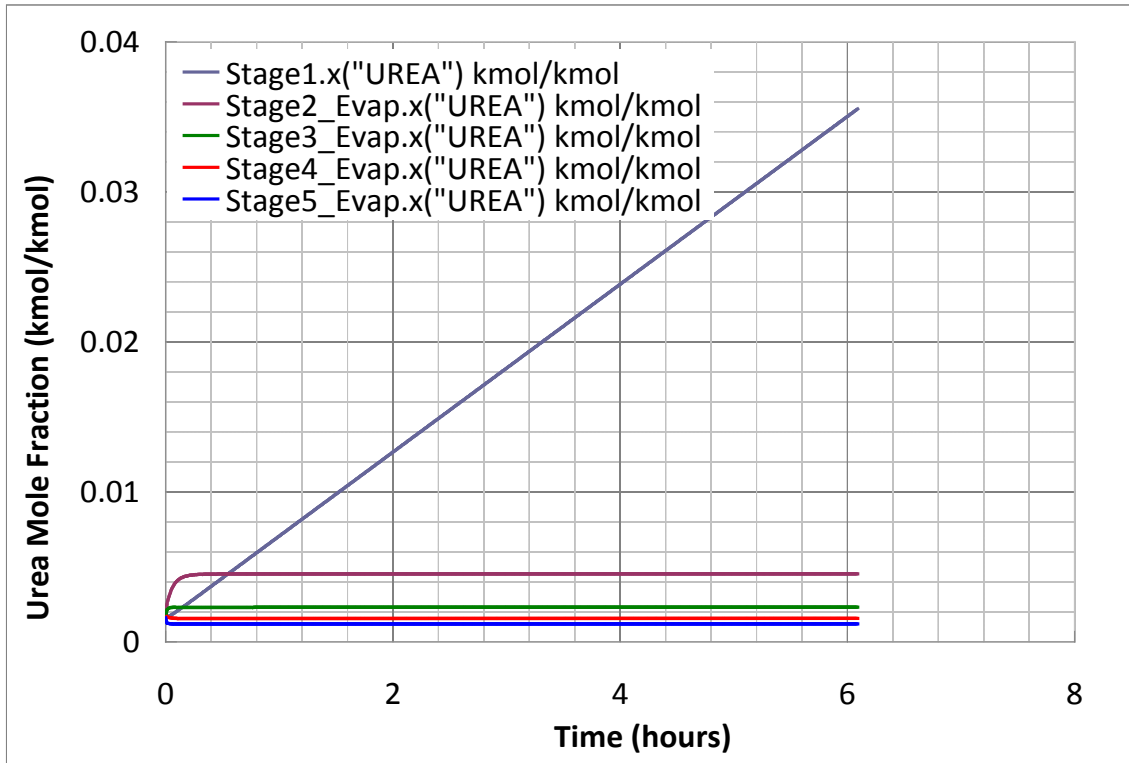


Figure 6. Variation of Urea concentration in evaporator stages of the CDS. Stage 1 is closest to the brine recirculating loop. Stage 5 is closest to the brine final condenser.

Stream chemistry, pH in particular, showed reasonable agreement between the DCT and the modeling results. For the feed stream the pH variation between the model and the test was small (less than 5%). For the brine and distillate streams, the pH variation between model and experiment was within 10% in both cases. Small to marginal deviations in stream chemistry are expected since the model uses only a portion of the components detected during the DCT.

Figures 7 and 8 illustrate the gradient of temperature and pressure (respectively) over the evaporating stages of the CDS. The temperature and pressure varies in correspondence with the enrichment of the brine over the stages of the CDS. Stage 1, the most concentrated stage, exhibits the highest temperature and pressure due to boiling point elevation effects. These predictions are made by Aspen Plus's thermodynamic calculations.

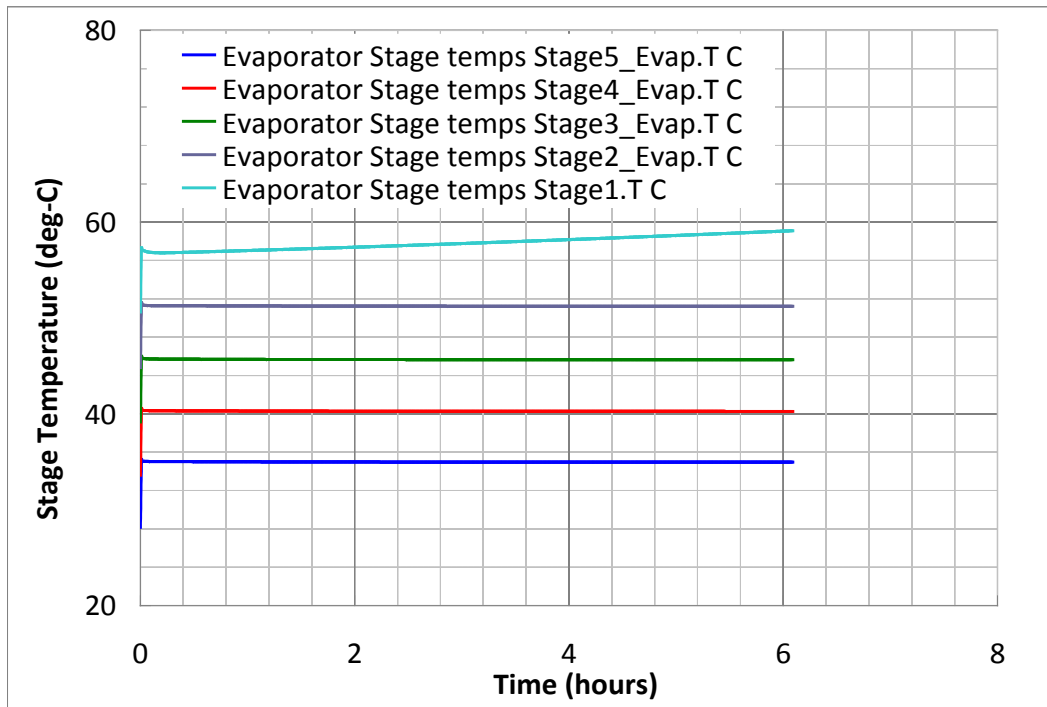


Figure 7. Variation of temperature in evaporator stages of the CDS. Stage 1 is the stage closest to the brine recirculating loop. Stage 5 is the stage closest to the brine final condenser.

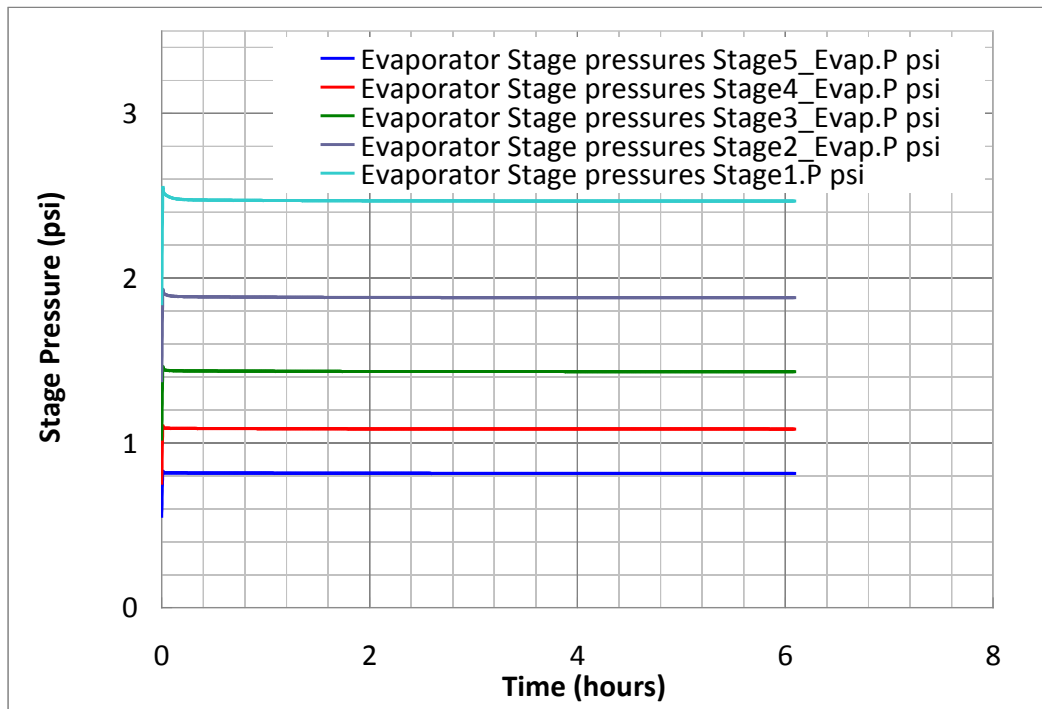


Figure 8. Variation of pressure in evaporator stages of the CDS. Stage 1 is the stage closest to the brine recirculating loop. Stage 5 is the stage closest to the brine final condenser.

The model predicts a distillate flow rate of 4.7 l/hr and predicts an energy consumption rate of 265 W by the THP. Although the distillate production rate appears to be within observed values (~ 4.5 l/hr), the THP power consumption appears lower than documented values (~300 W). At present, the model assumes that all gases from

the feed are removed before distillation. It will be also necessary to use ACM's estimation tools to refine model parameters (such as heat transfer coefficients) based on the test data. In addition, the CDS model does not incorporate energy consumption by the rotating distiller and therefore the total energy consumption of the system is not predicted.

Figure 9 presents an ACM flowsheet of the VCD system. This model has been updated to process the ERSATZ waste water formulation.

The current model lumps the liquid hold-up volume of the evaporator and recycle filter tank together in the DA_Evaporator stage and treats the volume as well mixed. A more detailed model of the recycle loop is currently being developed that will provide a more realistic dynamic description of VCD batch processing and start-up behavior. The compressor model assumes an idealized compressor with a fixed efficiency. The Pressure Control and Pump Assembly (PCPA) is modeled as a total condenser and the additional condensate is collected as part of the distillate.

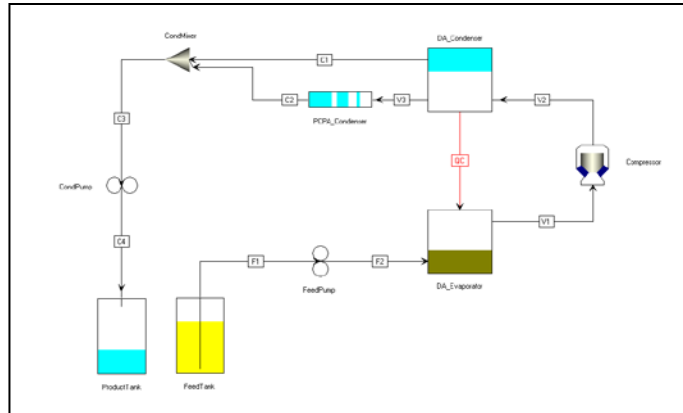


Figure 9. ACM representation of the VCD system. The rotating distiller is modeled as two equilibrium stages.

Estimates of the internal pressures and temperatures of the evaporator and condensers are provided by Figures 10 and 11 respectively. Internal temperatures for the condensers and the evaporator show reasonable agreement with the DCT results.

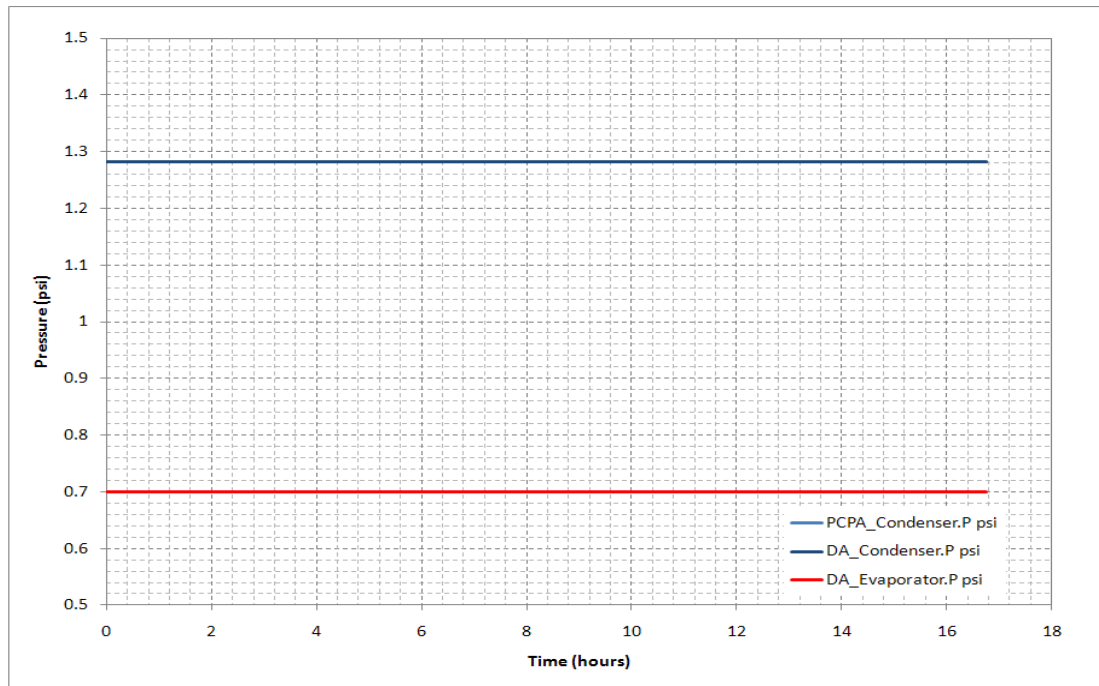


Figure 10. VCD Evaporator and Condenser pressure predictions.

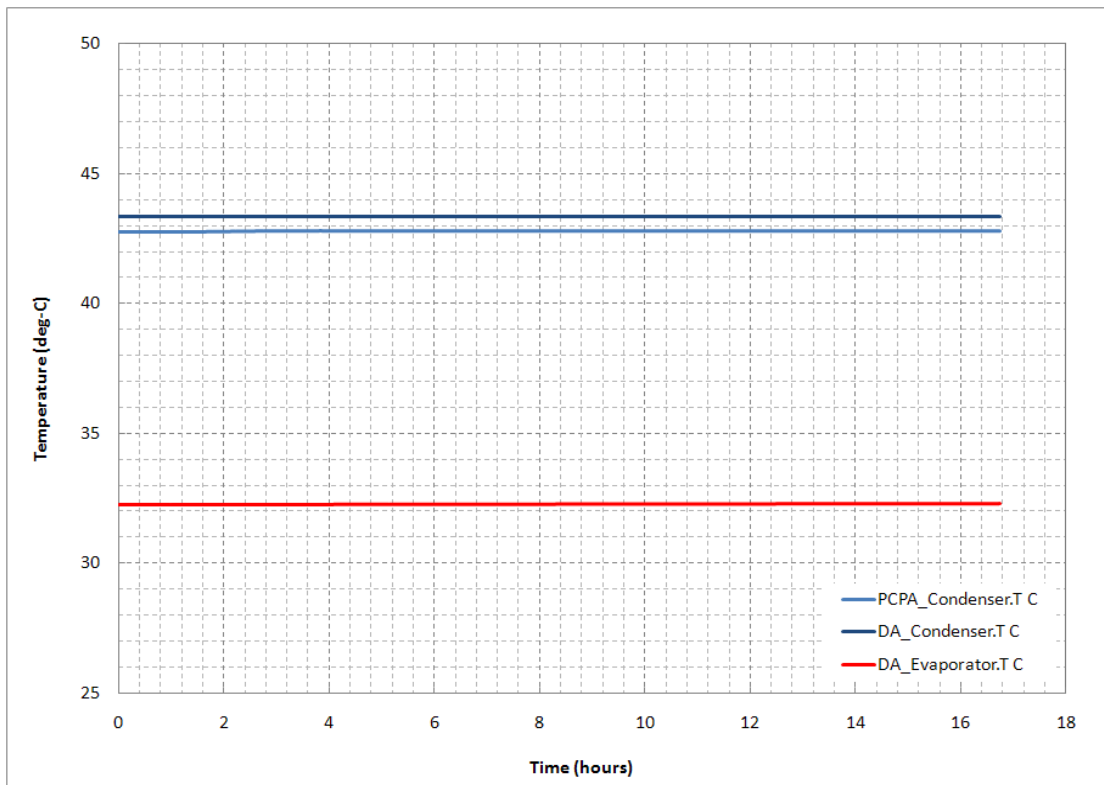


Figure 11. VCD Evaporator and Condenser temperature predictions.

Figure 12 presents an ACM flowsheet of the WFRD system. The single stage Rotating Disk Evaporator is modeled as two blocks; an evaporating side and a condensing side. The compressor is modeled as an adiabatic compressor with a fixed efficiency.

Flash routines are used to determine the vapor/liquid split for the exit streams from the evaporating side and a similar flash routine is used to determine the amount of condensate formed. The film thickness is determined (as a total hold-up) from a combination of the mass and energy balances in each block. The film thickness is calculated by approximating the holdup as a cylinder of fluid. The heat transfer between the two sides as well as the heat transfer coefficient is calculated from the energy balance between the condensing and evaporating sides. The heat transferred out the condensing side block is the exact amount required to produce vapor from the evaporating side. Some of the operating parameters, such as the evaporator pressure and the brine recycle rate were fixed values, similar to those used in the DCT.

Figures 13 - 15 provide estimates of the film thickness and internal pressures and temperatures (evaporating and condensing sides) respectively.

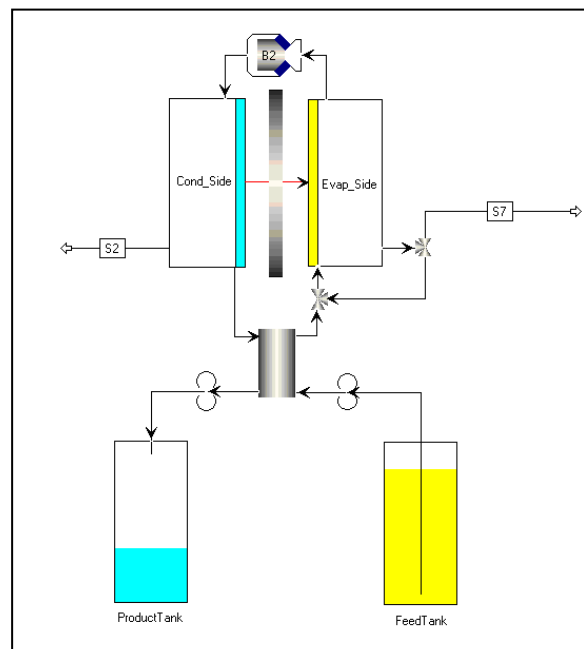


Figure 12. ACM flowsheet model of the Wiped Film Rotating Disk system. The rotating distiller is modeled as two equilibrium stages.

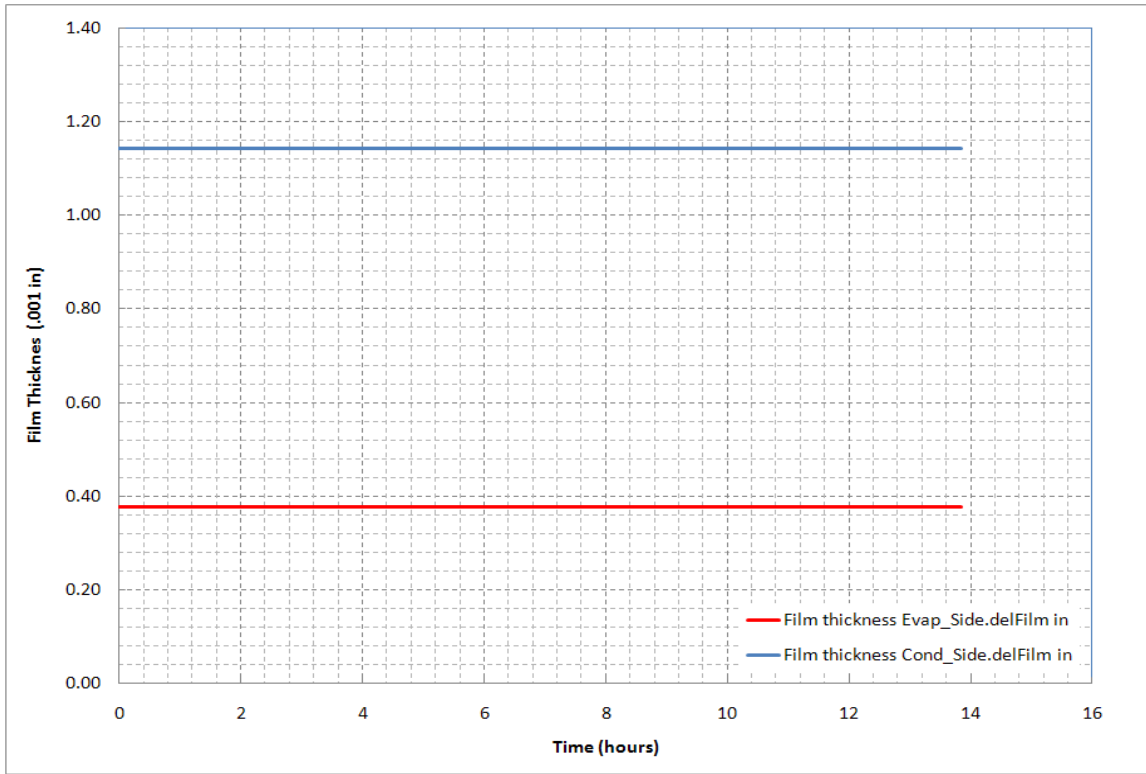


Figure 13. WFRD Evaporator and Condenser side film thickness estimates.

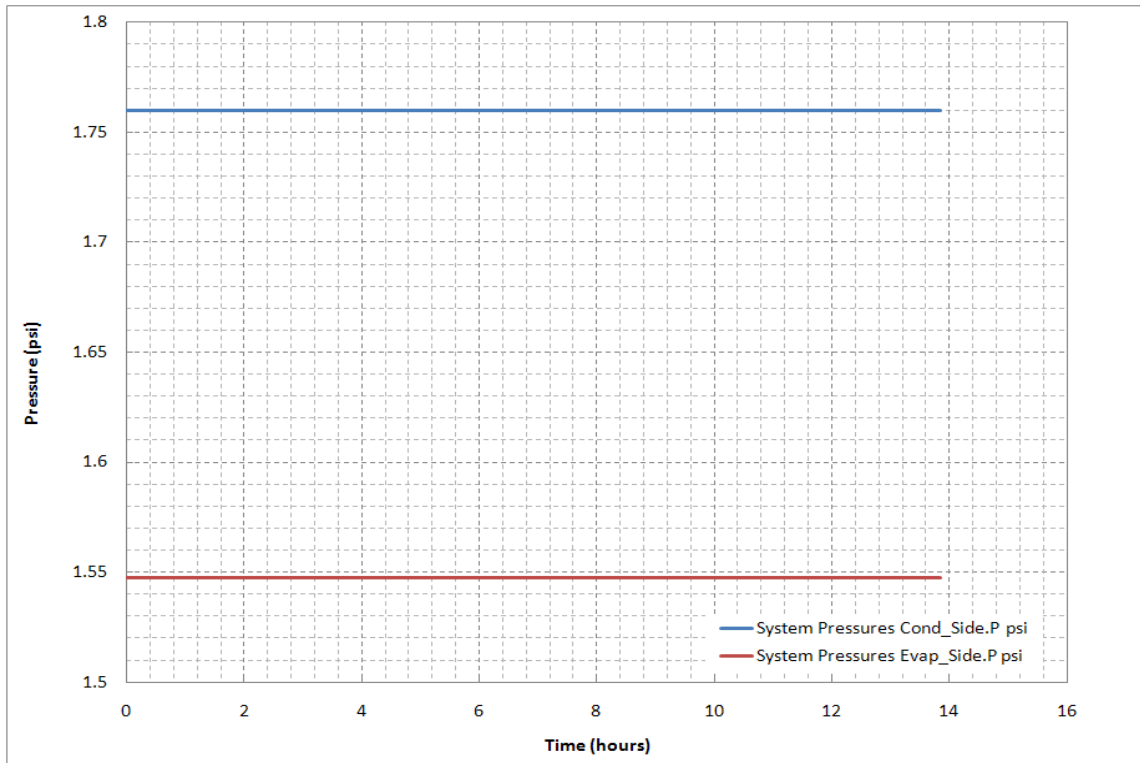


Figure 14. WFRD Evaporator and Condenser side pressure estimates.

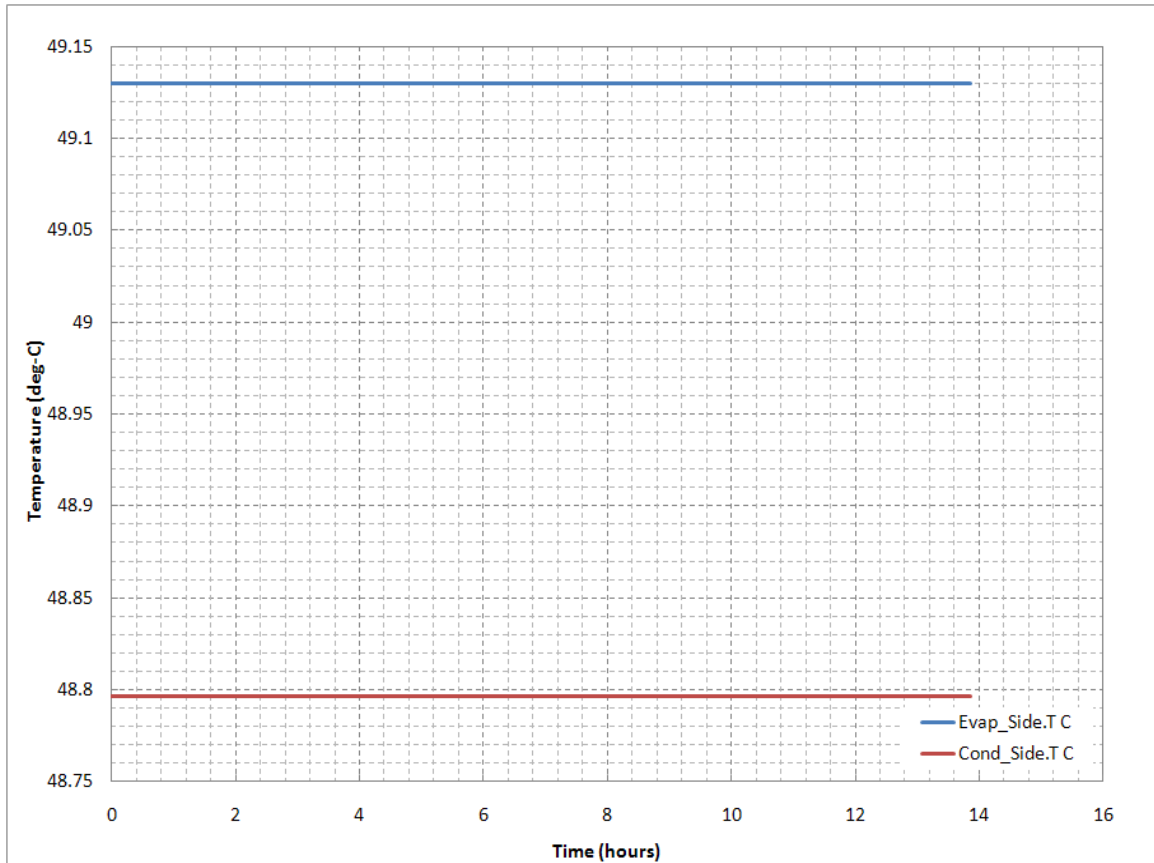


Figure 15. WFRD Evaporator and Condenser side temperature estimates.

Because there is no information on film thickness measurements for the current configuration, the ratio of the film thicknesses between the evaporating and condensing sides was fixed, based on literature values¹³. The film thickness values obtained by the model showed reasonable agreement (within 10%) of values during previous demonstrations of the WFRD¹³. Heat transfer coefficients, based on these film thicknesses have yet to be compared to those for the current configuration.

The internal pressure estimates showed significant deviations from values in the DCT data¹⁴. These deviations were mainly due to convergence issues in model. The compressor exit pressure estimate from the model was significantly lower than the condenser side pressure in the test due to convergence issues.

Temperatures reported by the model are theoretical temperatures (based on thermodynamic equilibrium) within the evaporator and condenser sides and are not necessarily equivalent to the evaporator and condenser temperatures during a test. In particular, the condenser side temperatures reflect the temperature after the vapor has condensed. Therefore the temperatures reported in the model may be more reflective of the actual film temperature vs. the bulk temperature within the unit. Although there was good agreement between theory and experiment for the evaporator side temperature, significant deviation (~25%) was found between model predictions and the DCT results for the condenser side temperature. Although, this deviation can be partially attributed to the convergence issue discussed earlier, it may also highlight the differences that may result from assuming a stable equilibrium with the condenser side. In the actual process, condensation may occur faster than thermal equilibrium can be realized.

Specific energy consumption predicted by the model (for the compressor) was high (50 W-hr/kg) when compared to the test results (~30 W-hr/kg)¹⁴ which may be a result of the differences in pressure between the test and the model. These results are presented in Table I.

Significant deviations between the model and the test results were also seen in the pH values for the feed, brine and the distillate streams. Although the feed pH values showed much lower deviations (less than 10%), the

distillate pH predicted by the model was greater than the test results by 30% and conversely the brine pH predicted by the model was 30% lower than the brine pH during the DCT. These results are presented in Table I.

Table I. Comparison between DCT results and model predictions for the WFRD.

Property	Data ^{13,14}	Model	Deviation
P, Compressor In (torr)	82.0	80.0	-2.44%
P, Compressor Out (torr)	110	91.0	-17.27%
T, Compressor In (C)	52.6	49.1	-6.65%
T, Compressor Out (C)	75.0	65.0	-13.33%
compressor specific energy (W-hr/kg)	25.0	50.0	100.00%
Condenser Film thickness (mils)	0.95	1.11	16.84%
Evaporator film thickness (mils)	0.33	0.38	15.15%
Feed pH	2.25	2.09	-7.11%
Distillate pH	3.5	4.66	33.14%
Brine pH	1.8	1.32	-26.67%

IV. Conclusion

Detailed simulations for three distillation technologies, CDS, VCD, and WFRD were developed using ACM. The CDS and the WFRD models have been updated to simulate distillation of a complex feed stream similar to that used in the DCT. The current VCD model processes the ERSATZ urine formulation and the DCT version is being developed. This report presents some preliminary modeling results along with comparisons of the model predictions with test results from the DCT.

At this point it is necessary to further refine and validate models of the individual components to ensure that they accurately represent the hardware. Convergence issues and stability of the simulations pose significant hurdles to model operation. Some preliminary work to improve stability of the models has been undertaken using AP. One solution may involve reducing the number of components, while retaining key chemical interactions like solids precipitation.

Acknowledgments

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