

Modeling Absorption Chillers in ASPEN

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Abstract

The oil and gas industry is an immense energy consumer. However, absorption chillers can utilize sources of waste heat in the plant to provide useful cooling or refrigeration, which is especially valuable in the oil and gas industry. To this end, we have modeled several absorption chiller designs in ASPEN in order to integrate them directly into plant models. This paper details the modeling procedure as well as the results for a single and double effect water/lithium bromide chiller. In order to evaluate the accuracy of the ASPEN absorption cycle models they were compared to published data from other models. Results of comparison for the single effect water/lithium bromide design indicate both models agree within 3% deviation for all cycle parameters. These absorption cycle models will allow investigation into the benefits of using absorption chillers for waste heat utilization in the oil and gas industry.

1. Introduction

1.1 Absorption Chillers

An absorption chiller is a closed loop cycle that uses waste heat to provide cooling or refrigeration. Absorption chillers' use has been limited by their relatively poor efficiency at delivering cooling compared to vapor compressions cycles. For comparison, an absorption chiller typically has a coefficient of performance (COP) between 0.5 and 1.5, while modern vapor compression cycles have COPs in excess of 3.0. However, absorption chillers continue to be practical because they are able to utilize low temperature (<100°C) heat to provide cooling. In this sense, a COP for an absorption chiller cannot be compared to the COP of other cooling cycles because the input energy for an absorption chiller can be essentially free, as it would have otherwise unused in most processes. Thus, in processes where low temperature waste heat is available and cooling is desired, it often makes sense to implement an absorption chiller to increase the overall energy efficiency of the process. Absorption chillers use a refrigerant-absorbent pair as a working fluid. By far, the two most common combinations used are water/lithium bromide and ammonia/water. This paper focuses on water/lithium bromide designs. Furthermore, cycles can be half, single, double, or even triple effect. Multi-effect cycles require more components and higher temperature waste heat, but have higher COPs. This paper focuses on modeling of single and double effect absorption chillers.

1.2 ASPEN

ASPEN is a process modeling software suite. One of these programs is ASPEN Plus, which allows for steady-state process modeling [1]. The user interface is predicated on a library of ready-made, user editable component models based in Fortran. By connecting these components by material, heat and work streams, and providing sufficient inputs, the user is able to model complex processes. ASPEN is particularly a favorite software in the petroleum industry.

1.3 Modeling History and Impetus for an ASPEN Model

Absorption chillers have been modeled in the past in a variety of ad hoc programs, including a program by Lazzarin et al. [2]. Modern modeling is usually done by one of two programs: ABSIM, developed by Oak Ridge National Laboratory [3, 4], and Engineering Equation Solver (EES), developed at the University of Wisconsin [5, 6, 7]. EES modeling allows the user to compute thermophysical properties of working fluids, providing results with very good accuracy when compared to experimental results [8]. However, there are a number of limitations to EES. Equations must be written out manually, making modeling of complex processes tedious and susceptible to user errors. There is a lack of modeling analysis tools, such as sensitivity analysis and optimization. Unfamiliar users may be confused by the user interface, which is text-based. Finally, it is difficult to integrate a model into a larger process model. A model in ASPEN Plus would improve upon or solve all of these issues.

1.4 Objective

The goal of this study was to create working models for a single and double effect water/lithium bromide absorption cycles in ASPEN Plus. The model should upon completion be ready to work stand-alone or able to be integrated into a larger process model. Additionally, the model should only require realistic inputs from the user. This includes various temperatures (waste heat, cooling temperature, etc), heat exchanger and pump performance values, and quantity of heat available or desired cooling. It should provide all useful results, either directly, or readily available with simple calculations. Such results include pressures, heat duties, cycle COP, mass flow rates, etc. Finally, the model should be verifiable when compared to results of another modeling software, such as EES.

2. Modeling Approach

2.1 State Points and Assumptions

To start, it would be useful to discuss some basic operating principles of the absorption cycle as illustrated in Figure 1. Heat is added at the generator (also known as a desorber), separating gaseous refrigerant and liquid solution. The gaseous refrigerant is sent to the condenser, where it rejects heat to a medium temperature sink, usually ambient. It is expanded, and then evaporated using heat input from low temperature, which results in useful cooling. The solution is also expanded, and then recombines in the absorber. Normally, a solution heat exchanger is also included for increased performance. It is placed between the generator and the two pressure changing devices.

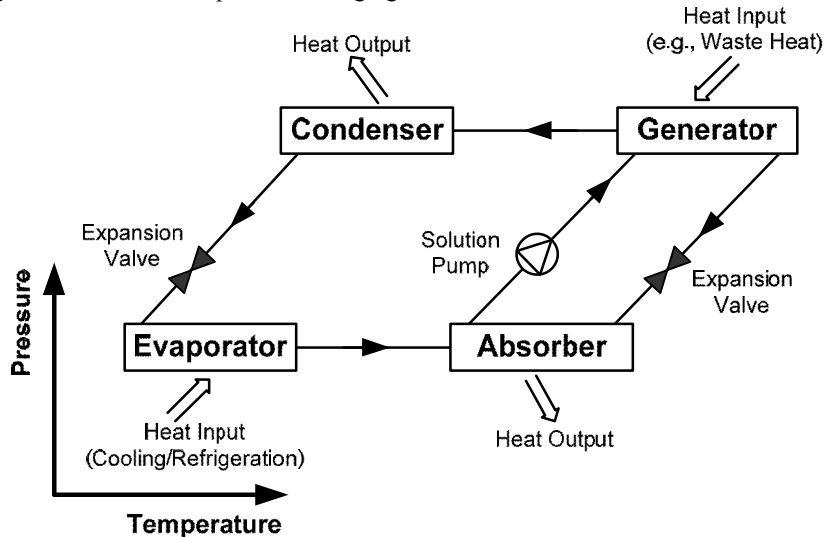


Figure 1. Absorption cycle operating principle [9].

A double effect absorption cycle operates under the same principle, except that a higher pressure level is added. Some of the solution leaving the desorber is pumped to a higher pressure desorber. The resultant refrigerant is condensed in the higher pressure condenser and fed to the lower pressure condenser. The solution exiting the higher pressure condenser is sent back to the lower pressure desorber. Finally, in a double effect cycle, the external heat is added to the higher pressure desorber, while the higher pressure condenser rejects heat to the lower temperature desorber.

For expediency, the following convention will be used for state points and will be adhered to throughout the paper. For the single effect cycle, the absorber exit is state one, the pump exit is state two, the solution heat exchanger exit leading to the desorber is state three, the liquid exit of the absorber is state four, the solution heat exchanger exit leading to the solution valve is state five, the solution valve exit is state six, the gas exit of the desorber is state seven, the condenser exit is state eight, the refrigerant valve exit is state nine, and the evaporator exit is state ten. For the double effect cycle, states 1-10 describe the lower half of the cycle and are identical to the states of the single effect cycle. States 11-19 describe the upper half of the cycle using the same numbering system (i.e. state 11 is equivalent to state 1). The following basic assumptions in Table 1 were made for the single effect cycle. Further assumptions or modeling decisions will be explained in greater detail in following sections. A similar set of assumptions were made for the double effect cycle, as enumerated in Table 2.

Table 1. State point assumptions for the single effect cycle.

State(s)	Assumption
1	Vapor quality of 0
2	Determined by the solution pump model
3	Determined by the SHX model
4 & 7	Saturated liquid and saturated vapor respectively; the mass flow rate ratio between states 4 and 7 is determined by the temperature of the waste heat available
5	Determined by the SHX model
6	Determined by the solution valve model
8	Vapor quality of 0
9	Determined by the refrigerant pump model
10	Vapor quality of 1

Table 2. State point assumptions for the double effect cycle.

State(s)	Assumption
1	Vapor quality of 0
2	Determined by the lower solution pump model
3	Determined by the SHX model
4 & 7	Saturated liquid and saturated vapor respectively; the mass split between states 4 and 7 is determined by the temperature of the heat coming from the upper condenser
5	Determined by the SHX model
6	Determined by the solution valve model
8	Vapor quality of 0
9	Determined by the refrigerant pump model
10	Vapor quality of 1
11	Vapor quality of 0
12	Determined by the upper solution pump model
13	Determined by the SHX model
14 & 17	Saturated liquid and saturated vapor respectively; the mass low rate ratio between states 14 and 17 is determined by the temperature of the waste heat available
15	Determined by the SHX model
16	Determined by the solution valve model
18	Vapor quality of 0
19	Determined by the refrigerant pump model

Both sets of assumptions were chosen because they are commonly used assumptions for absorption chiller modeling [10]. Adhering to the same assumptions as other models commonly do will allow for an “apples to apples” comparison of the ASPEN model to other models.

2.2 Property Method Selection

The first and most crucial step in the modeling process was finding a suitable property method for the water/lithium bromide mixture. At this point it should be pointed out that except for very common fluids, ASPEN does not use look-up tables for property data. Instead, the user must select a property method based on operating conditions, fluid characteristics, etc. As a result, there is an error inherent to any model created in ASPEN. This should not be taken as a deterrent, as even look-up tables will have some errors due to interpolation. Rather, it is a warning to the potential user to select the property method wisely when modeling in ASPEN. The ASPEN developers suggested the ELECNRTL property method was chosen for the water/lithium bromide solution based on the operating conditions and fluids being modeled. As the name suggests, it is a method designed for electrolytes. To use it properly, the user must select the relevant components (in this case, water and lithium bromide) and use the electrolyte wizard, which will generate a series of reactions. In this case, the only relevant reaction was the dissociation of lithium bromide. For the states that are pure water (7-10), the steamNBS tables [11] were used. Since look-up tables are available for pure steam, the property data induced error will be much smaller.

2.3 Component Breakdown and Modeling

As alluded to in the introduction, modeling ASPEN plus is based in taking a process and breaking it down into more simple components, also known as “blocks”. For example, a gas turbine could be

decomposed into a compressor block, a combustion chamber block, and a turbine block. While this allows the user to model complex processes more easily, there is a certain level of subjectivity involved. Thus, some of the decisions made in the following section could have been done in a different way. However, every effort will be made to point out these instances.

The following section is an in-depth description of the component breakdown used to produce the models. It is intended to act a guide for anyone who would like to recreate or modify the described models. Many simple components (pumps, valves, etc) could be modeled simply by selecting the equivalent block in ASPEN, while others did not have an exact analogue. Naturally, much more time will be spent on the latter instance, as these components may have required further assumptions or multiple blocks to model. Finally, it should be noted that in this section, the goal was only to produce a running model, not one with realistic inputs. The adaptation to realistic inputs is described in section 2.4.

2.3.1 State Point 1

Because ASPEN uses a sequential solver, it is necessary to model a “break” in closed cycles to give inputs to the model. For both the single and double effect cycles, this break was inserted at state point 1. In other words, the exit of the absorber (stream 1A) and the inlet of the pump (stream 1) are not connected (see the overall process flow diagrams in section 2.5). If these two fluid streams give the same results (which is to be expected; they represent the same state!), this is evidence of a well formulated problem. This was verified throughout the modeling process and found to be consistently satisfied. The break in state 1 allows for inputs to be given for the pump inlet. For now, these inputs were the low side pressure, a vapor quality of zero, the mass flow rate, and the concentration of water and lithium bromide.

2.3.2 Pumps

Pumps are used in the following instances, between states 1 and 2 in both models and between states 11 and 12 in the double effect model. Pumps require only one input, the exit pressure. One could also include pump efficiency, but the default value of 100% was used because of the negligible effect on the overall cycle of picking a different efficiency (the pump work is several orders of magnitude smaller than the heat duties of other components).

2.3.3 Valves

The other pressure change devices needed to model the cycle are valves. For the single effect cycle there is one refrigerant and one solution valve, for the double effect cycle there are two of each. The valve model is self-explanatory; one only needs to give the exit pressure or some equivalent (i.e. pressure ratio).

2.3.4 Solution Heat Exchangers

A solution heat exchanger (SHX) is used once in the single effect cycle. Heat is transferred from state 4 (the hot side inlet) to state 2 (the cold side inlet), resulting in states 5 (the hot side exit) and 3 (the cold side exit). It is used in the same spot in the double effect cycle, as well as to transfer heat from state 14 (the hot side inlet) to state 12 (the cold side inlet), resulting in states 15 (the hot side exit) and 13 (the cold side exit). This was modeled using two heater blocks, connected by a heat stream to indicate that the heat rejected on the hot side was to be added to the cold side. A screen shot of this part of the model is shown in Figure 2. Assuming no pressure drop, the only two unknowns are the exit temperatures. One unknown was described by assuming a heat exchanger effectiveness, defined below.

$$\varepsilon = \frac{T_4 - T_5}{T_4 - T_2} \tag{1}$$

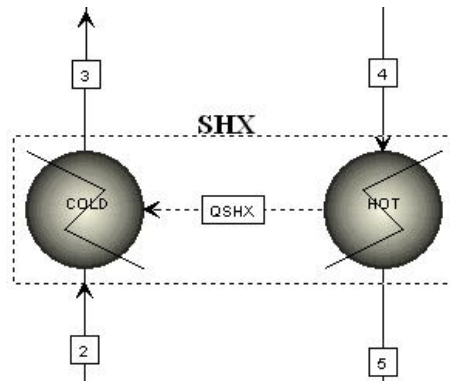


Figure 2. SHX model in ASPEN.

This sets T_3 . The model now knows the amount of heat lost from states 4 to 5, and matches this to the amount of heat gained from states 2 to 3, setting T_3 . To implement the heat exchanger effectiveness equation, a calculator block was used.

2.3.5 Condensers

The condensers were modeled as heater blocks. Assuming no pressure drop, the only input necessary is to specify a vapor quality of 0 at the exit. Since the refrigerant is pure water, the property method for this component, as well as any refrigerant-only components, should be changed to steamNBS for improved results. The condenser model is used three times, once in the single effect cycle and twice in the double effect cycle (at middle and high pressures). The middle pressure condenser has two inputs: the refrigerant coming from high pressure and the refrigerant coming from the middle desorber. Modeling the condensers using the heater block model introduces a new assumption, that heat is being added at constant temperature. Based on previous EES modeling, this has proven to be an essentially inconsequential assumption [10]. However, one could model the condenser as a heat exchanger rather than a heater to eliminate this approximation, if one were so inclined.

2.3.6 Evaporators

Modeling the evaporators was very similar to modeling the condensers. The evaporator was modeled as a heater block using the steamNBS property method. The inputs to the model were zero pressure drop and a vapor quality of 1 at the exit. This model is used one time each in the single and double effect cycles. Note that the caveat about using a heater in the model rather than a heat exchanger applies for the evaporator model as well.

2.3.7 Absorbers

The absorber is modeled as a heater block with two inputs, the exit of the evaporator and the exit of the solution valve. The inputs are zero pressure drop and zero vapor quality. The absorber model is used once in the single and double effect cycles. The caveat about using a heater in the model rather than a heat exchanger applies for the absorber model as well.

2.3.8 Desorbers

To this point, modeling components has been relatively straightforward, as they all involved simple processes like pressure changes, heat addition or rejection, mixing, or some combination. Desorbers, on the other hand, involve separating components, which makes them much more difficult to model. The desorber in the single effect cycle and the high pressure desorber in the double effect cycle have similar inputs and requirements; thus, they have the same design. They are:

- Single inlet (stream 3 in the single effect, 13 in double effect)
- Saturated vapor outlet (stream 7 in the single effect, 17 in double effect), which is pure water
- Saturated liquid outlet (stream 4 in the single effect, 14 in double effect), which is solution

An assumption needs to be made about the vapor outlet stream. In this model, it was assumed to be the saturation temperature of the liquid solution at state 3. This was chosen to correspond to the assumption made in the EES model, but could be easily altered [10]. The mass split between the two outlet streams and the liquid output temperature is dictated by the temperature of the heat input to the cycle. To accomplish these requirements, three heater blocks and a flash block were used. The flash is used to separate vapor and liquid. Its inputs are zero pressure drop and outlet temperature (based on the temperature of the heat input into the cycle). However, this gives the vapor stream the same temperature as the liquid stream, which would not meet the assumption stated in the previous paragraph. Thus, a heater block is added to reduce the temperature of the vapor stream to the saturation temperature of the inlet stream. To keep this heat internal to the desorber, a second heater block is added at the inlet, where the heat can be added. The final heater block raises the inlet stream to liquid saturated temperature, which allows a calculator block to reference the liquid saturation temperature of the inlet stream for the purpose of setting the outlet vapor stream temperature. A screenshot of the model in ASPEN is shown in Figure 3.

The middle pressure desorber in the double effect cycle has different inputs and requirements:

- Two inlets (streams 3 and 16)
- Saturated vapor outlet (pure water, stream 7)
- Two saturated liquid solution outlets (stream 11 to upper cycle, and stream 4 to lower cycle)

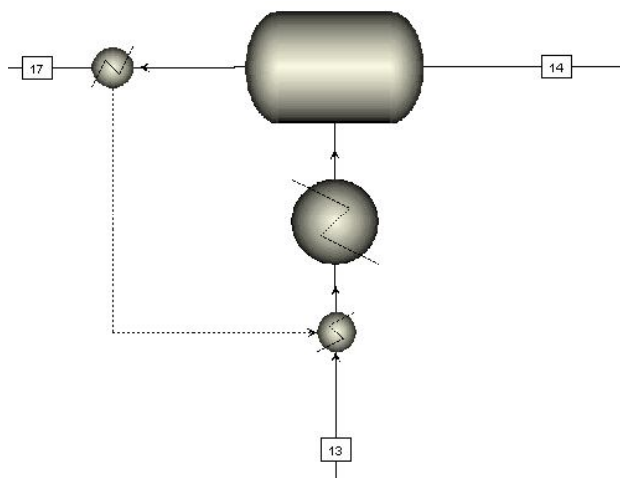


Figure 3. Desorber model for single effect and double effect at high pressure.

As can be seen in the ASPEN screenshot in Figure 4, stream 3 is split based on the requirement that the upper condenser and middle pressure desorber have the same magnitude heat duty. This is accomplished with a splitter block. The solution entering the upper cycle is raised to saturation temperature with a heater block and is sent to the upper half of the cycle as stream 11. The remaining solution mixes with the other inlet stream. The temperature at which this solution is flashed is based on the assumption that the solution concentrations are the same for the upper and lower half of the cycle. It is used to determine the temperature necessary in the upper condenser. Finally, as in the other desorber design, the vapor outlet temperature must be adjusted. Thus, the final heater block sets the outlet temperature equal to the temperature of stream 11 (which is a saturated liquid). The vapor goes to the middle pressure condenser and the liquid goes to the lower half of the cycle. For every component, zero pressure drop was assumed.

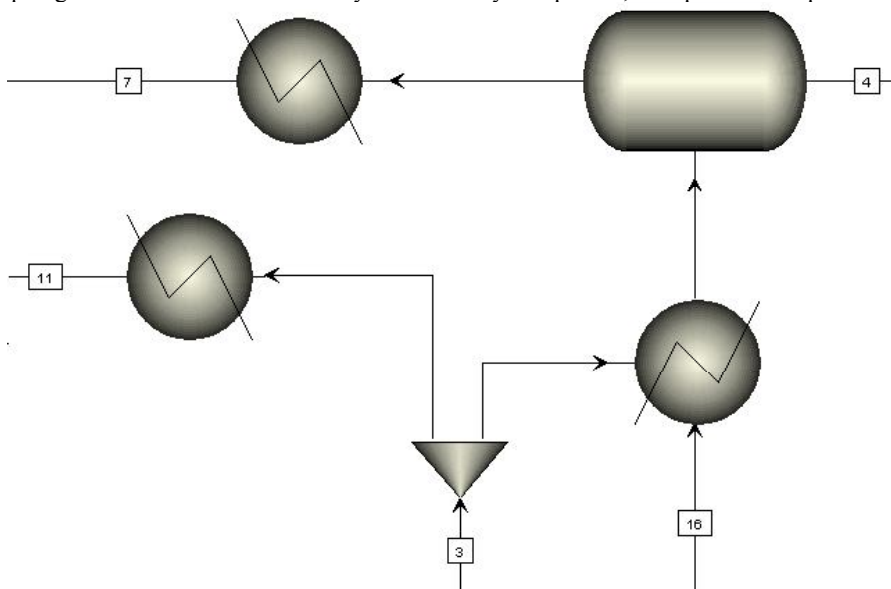


Figure 4. Desorber model for double effect at middle pressure.

For both of these desorber models, the combination of components is intended to represent the physical desorber. Thus, to obtain the heat duty of the desorber, one should add the duties of the individual components.

2.4 Adaptation to Desired Inputs

Now that the two working models have been created, it is time to use realistic inputs to define such as operating pressures and concentrations. Those inputs are:

- Either quantity of waste heat available or desired cooling load
- Evaporator exit temperature (related to desired cooling temperature)*
- Condenser and absorber exit temperatures (related to ambient temperature, or whatever other medium they are rejecting heat to)*
- (Upper) desorber exit temperature (related to temperature of available waste heat)*

**How cycle temperatures relate to cooling, waste heat, or ambient temperature is up to the user. One could make any number of assumptions; for example, they could assume a pinch temperature or UA value.*

Each of those inputs defines a pressure, concentration, or mass flow rate, as enumerated below. For both cycles, either waste heat available or cooling load defines the mass flow rate through the (bottom) pump. For the double effect cycle, the mass split between the upper and lower cycles is given by the specification that the high pressure condenser and middle pressure desorber have the same magnitude heat duty. For both cycles, evaporator exit temperature defines the low pressure. For both cycles, absorber exit temperature defines the solution concentration at the absorber exit. In the single effect cycle, the condenser exit temperature defines the high pressure. In the double effect cycle, the middle pressure condenser exit temperature defines the middle pressure. Both of these are related to ambient temperature. Also in the double effect cycle, the high pressure condenser exit temperature defines the high pressure. This temperature is based on the temperature of the middle pressure desorber (where it rejects heat to), for example by assuming a pinch temperature or an overall heat transfer coefficient (i.e. a UA value). In the single effect cycle, the temperature at the liquid exit of the desorber (related to the temperature of the available heat) defines the concentration at the desorber exit. This can be specified by changing the temperature in the flash block (i.e. a design spec is not necessary). The same is true of the high pressure desorber in the double effect cycle. Finally, the temperature of the middle pressure desorber in the double effect cycle is set by assuming the concentration at the liquid exit of both desorbers is the same. To accomplish this in ASPEN, the user should define a design spec, instructing ASPEN to vary the appropriate variable so that another variable reaches the design spec. For example, to meet the desired cooling load, one would tell ASPEN to vary the total mass flow rate until the desired evaporator duty was met.

2.5 Final Models

The final models in ASPEN are shown in Figures 5 and 6. For the double effect cycle, the desorbers were placed in hierarchy blocks to reduce clutter. For the desorber model designs, see section 2.3.8.

3. Results and Model Verification

3.1 Energy Conservation Verification

As one way of verifying each model, an energy conservation check was performed, shown below. If the magnitude of the energy into the cycle was not equal to the magnitude of the energy out of the cycle, there would be cause for concern. Thus, for each model, a set of results were used to perform this verification.

$$E_{in} + E_{out} = 0 \quad (2)$$

For the single effect cycle:

$$|Q_{Condenser} + Q_{Absorber}| + |Q_{Evaporator} + Q_{Desorber} + W_{pump}| = 0 \quad (3)$$

$$11.434 + 13.924 - 10.772 - 14.585 = 0$$

$$0 = 0$$

For the double effect cycle:

$$|Q_{Condenser} + Q_{Absorber}| + |Q_{Evaporator} + Q_{Desorber} + W_{pumps}| = 0 \quad (4)$$

$$197.70 + 442.15 - 372.49 - 267.36 = 0$$

$$0 = 0$$

3.2 Model Verification

For this model to be of any use its results should be verified. Thus, the ASPEN models were compared with the EES models pre-developed by Herold et al. [10]. As was alluded to in section 2 of this paper, the same assumptions were made in creating the ASPEN models as were used in these EES models to facilitate a fair comparison.

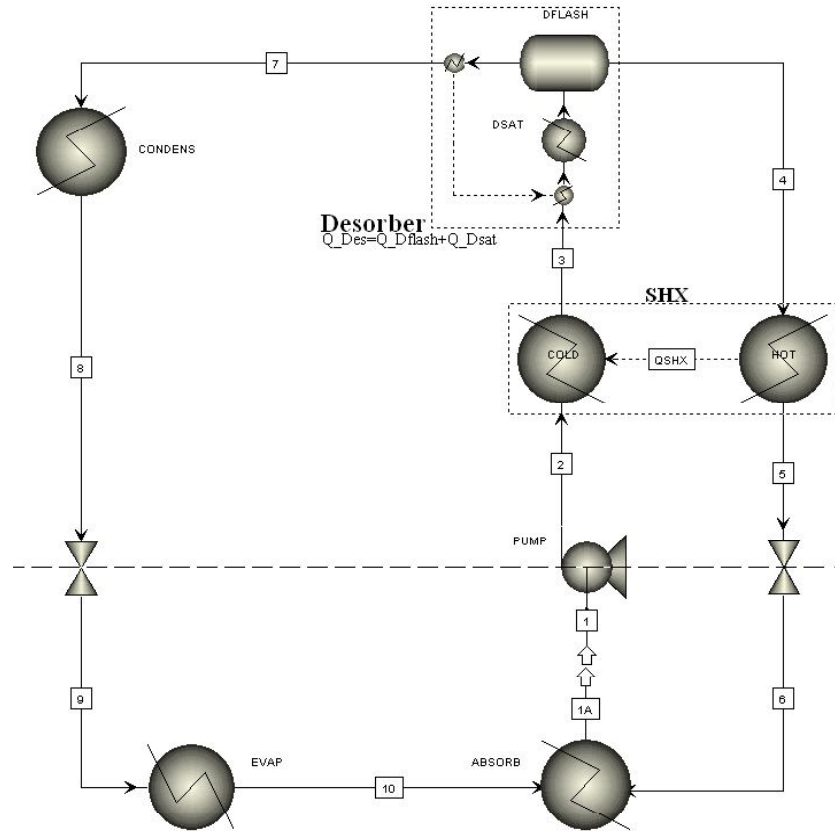


Figure 5. Single effect cycle final model.

3.2.1 Single Effect Cycle

Table 3 details the model verification performed. Note that the evaporator heat duty discrepancy is marked as not applicable because its duty was used as an input to the model. The results are very promising; no parameter has more than a 3% error, with many below or near 1%. Those that have errors between two and three percent are all heat duties, which reflects the imperfect property method used in ASPEN.

3.2.2 Double Effect Model Verification

Table 4 details the model verification performed. Note that the desorber heat duty discrepancy is marked as not applicable because its duty was used as an input to the model. The double effect model's discrepancy is larger but still less than 7%. Again, most of the parameters with larger errors are heat duties due to the property method selection.

Table 3. Single effect cycle verification.

Parameter	Units	EES	ASPEN	Discrepancy
P_{low}	kPa	0.673	0.6715	0.22%
P_{high}	kPa	7.445	7.4606	0.21%
Concentration, LiBr Strong Solution		56.7	57.4	1.23%
Concentration, LiBr Weak Solution		62.5	62.57	0.11%
$Q_{absorber}$	kW	14.297	13.924	2.61%
$Q_{condenser}$	kW	11.427	11.434	0.06%
$Q_{desorber}$	kW	14.952	14.585	2.45%
$Q_{evaporator}$	kW	10.772	10.772	N/A
COP		0.720	0.739	2.52%

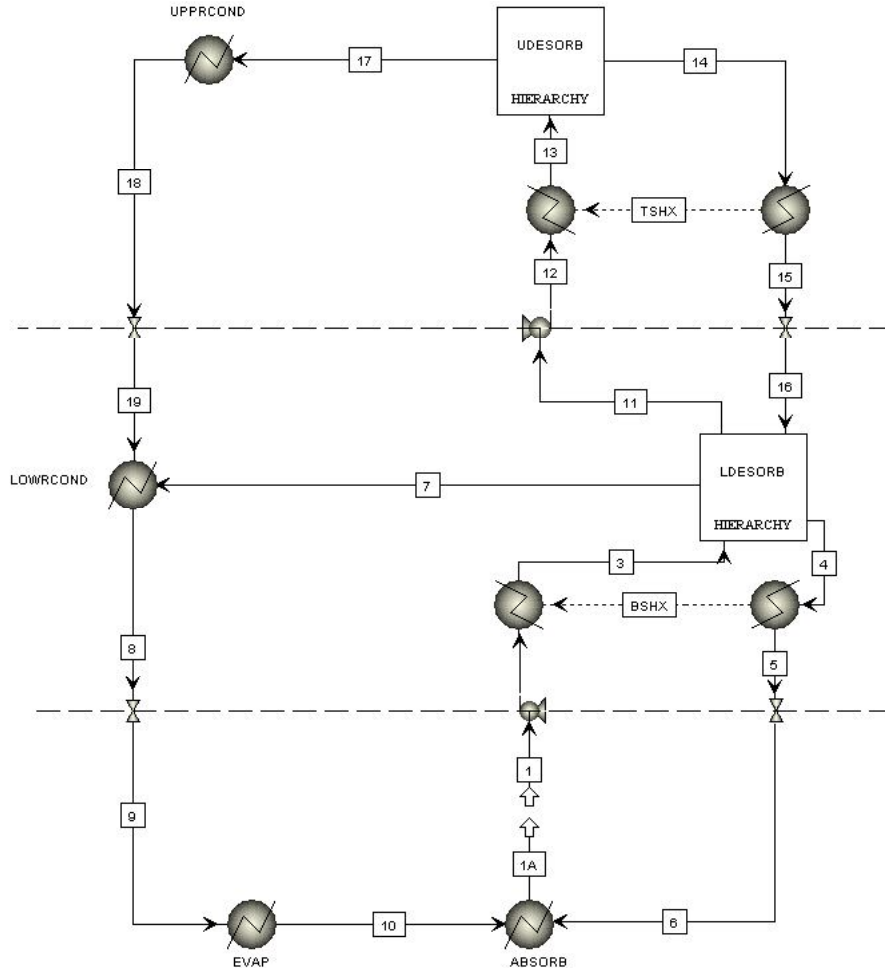


Figure 6. Double effect cycle final model.

Table 4. Double effect cycle verification.

Parameter	Units	EES	ASPEN	Discrepancy
P low	kPa	0.8810	0.8805	0.06%
P middle	kPa	4.1780	4.1776	0.01%
P high	kPa	64.2970	62.3972	2.95%
Concentration, LiBr Strong Solution		52.76	52.72	0.07%
Concentration, LiBr Weak Solution		61.96	61.94	0.03%
Q absorber	kW	435.99	442.15	1.41%
Q cond/des	kW	192.68	199.97	3.78%
Q middle condenser	kW	185.61	197.70	6.51%
Q evaporator	kW	354.19	372.49	5.16%
Q upper desorber	kW	267.39	267.36	N/A
COP		1.325	1.393	5.18%

4. Conclusions

This paper details the process used to create two absorption cycle models in ASPEN: one for a single effect and one for a double effect water/lithium bromide cycle. Both cycles use realistic inputs and provide all outputs of interest. Verification with EES models shows only small discrepancies. This indicates that the models are sufficiently accurate, since the EES models compare well with experimental data. However, the ASPEN models have many advantages over models created in EES. They will be much more user-friendly and visually appealing to a casual user. They can be created quicker, and can be more readily integrated into larger processes. Finally, any assumptions made in model creation can be altered with modest effort as desired by the user.

Nomenclature

$1, 2, 3, \dots$	State points 1, 2, 3...
COP	Coefficient of performance
E	Energy
EES	Engineering Equation Solver
SHX	Solution heat exchanger
P	Pressure
Q	Heat duty
T	Temperature
UA	Overall heat transfer coefficient
W	Work
ε	Heat exchanger effectiveness

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Dr. Reinhard Radermacher, Ph.D., is a Professor in the Department of Mechanical Engineering at the University of Maryland. He holds an M.S. and Ph.D. in Physics from the Munich Institute of Technology. Dr. Radermacher is an internationally recognized expert in heat transfer and working fluids for energy conversion systems, including heat pumps, air-conditioners, and absorption chillers.

Dr. Saleh Al Hashimi, Ph.D., an Assistant Professor in the Department of Chemical Engineering at The Petroleum Institute, United Arab Emirates. He has expertise in mathematical modeling, catalysis and waste heat management. He has been interested in applying novel systems to the petroleum industry to make better use of the waste heat generated. Some of his recent publications in this area focus on crude oil stabilization and polycarbonate plants.

Dr. Peter Rodgers, Ph.D., is Associate Professor of Mechanical Engineering at The Petroleum Institute, U.A.E. He has extensive experience in thermofluid modeling and experimental characterization. His current research activities are focused on waste heat utilization in the oil and gas industry; the development of polymeric heat exchangers for sea water cooling applications; computational fluid dynamics; electronics reliability; and engineering education. He is presently a member of several international conference program committees, and serves as program co-chair for both EuroSimE 2009 and Energy 2030. He has authored or co-authored over 60 journal and conference publications.