University of Strathclyde Engineering

Department of Mechanical Engineering

Modelling, Implementation and Simulation of a Single-Effect Absorption Chiller in MERIT

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Signed: **RONALD MUHUMUZA** Date: **10.09.2010**

To my Late Mother

Abstract

Absorption chillers can play a significant role in electrical energy conservation since they can be powered on heat energy. However, their deployment needs to be carefully assessed and evaluated to ensure successful installation and this can be done by using some available energy systems simulation and appraisal computer packages. The main goal of this study is to research thermophysical models and simulation techniques for vapour absorption chillers to assist in their development and implementation into MERIT, an energy systems evaluation simulation computer package that supports the analysis of new and renewable energy schemes. To extend the list of energy technologies existing in MERIT, suitable vapour absorption chiller mathematical models were required to allow simulations that include thermal air conditioning systems. Thus, to pioneer the simulation of vapour absorption chillers in MERIT, the H_2O-LiBr single-effect absorption chiller was considered.

Existing literature relating to modelling single-effect H_2O-LiBr absorption chillers was reviewed and a decision taken on the most suitable model development approach. The steady state modelling approach was adopted which entailed formulating and solving a system of mass balance, energy balance and heat transfer equations. The complete steady state problem constituted 100 equations which were solved using Engineering Equation Solver (EES). By solving the system of equations at various operating temperatures, data representing an operating map were generated. From this operating map, appropriate explicit curve fit expressions representing the general characteristics of the system of mass, energy balance and heat transfer formulations of the working pair were derived using MATLAB. Results from derived explicit mathematical models were verified against results from the complete system of thermophysical models solved with EES and good agreement was achieved.

The developed explicit models were then implemented in MERIT using Microsoft Visual C++ as two absorption chiller operation modes: *follow heating* and *follow cooling* which users can select from an input drop down menu in the MERIT user interface. Hypothetical cooling demand and heat supply profiles were assembled and used in the application of the developed models and results are presented and

discussed. Overall conclusions, areas of further study and lessons learnt by the author during the period of this research are presented.

Acknowledgements

I would like to dedicate this work to everyone who helped me directly and indirectly during the course of my project. More importantly I want to thank with utmost gratitude Dr. Paul Strachan and Dr. Jun Hong for spending their time to provide me with all the guidance and support I needed to complete my project on time. Again, I can't thank enough Dr. Jun Hong for providing me his time and potential when my C++ programming skills were challenged until we got it all moving in the right direction. To the two of you, I would like to say that you enabled me to attain the right level of focus and optimism that I needed to take this work right to the end.

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Prof. Joseph Clark provided me with invaluable insight into the understanding of how MERIT works so that I understood what was possible and impossible in the programming of MERIT. This enhanced my understanding of the program flow.

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To my WIFE who endured the challenging year of my fulltime absence from our family while I undertook this MSc deserves more than words. And my parents who sacrificed everything they had to make me what I am, this GOD GUIDED achievement belongs to you.

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Notation and Units

Q	Rate of heat transfer (kW)
T	Absorption chiller internal component temperature (K)
ΔT	Temperature difference (K)
h	Specific enthalpy (kJ/kg)
X	Concentration of aqueous LiBr solution (%)
$\dot{m}$	Mass flow rate (kg/s)
λ	Circulation ratio (-)
W	Work (kW)
v	Specific volume (m^3/kg)
P	Pressure (kPa)
ε	Effectiveness (%)
C	Specific heat capacity (kJ/kg.K)
U	Overall heat transfer coefficient (kW/m^2.K)
A	Total available heat exchange surface area (m^2)
K	Constant (-)
B	Dühring coefficient (-)
t	Temperature of streams external to chiller components (^{o}C)
$\Delta\Delta t$	Characteristic temperature function (^{o}C)
$\Delta\Delta t'$	Adjusted characteristic temperature function (^{o}C)
COP	Coefficient of performance
COP_{max}	Maximum coefficient of performance
COP_{actual}	Actual coefficient of performance
η	Efficiency
IPLV	Integrated part load value
EES	Engineering Equation Solver
ABSIM	ABsorption SIMulation program
ABSML	ABsorption System Modelling Library
TRNSYS	TRaNsient SYstem Simulation program

Suscripts

g	Generator
a	Absorber
c	Condenser
e	Evaporator
r	Refrigerant
s	Aqueous LiBr Solution rich in refrigerant (strong solution)
w	Aqueous LiBr solution poor in refrigerant (weak solution)
n	Index (1,2,…)
sol	aqueous LiBr solution
sat	Saturated condition/saturated state
lmtd	Logarithmic temperature difference
chill	Chilled stream
cool	Cooling stream
hot	Hot stream
p	Pump
HX	Heat exchanger
SHX	Solution heat exchanger

Chapter 1

Introduction

1.1 Introduction

Today, the world is experiencing increasing population with an almost proportional increase in the use and destabilisation of natural resources caused by increased production and industrial activity. This has brought about environmental damage which is argued to be shifting the earth's stability and ecological carrying capacity to constantly renew itself[1]. This state of events termed "*Growthmania*" by Dally[1], threatens the earth and its inhabitants. Current terms such as global warming, ozone layer depletion, pollution, green house gasses and green house effect can be directly linked to growthmania which is substantially dominated by one of the most lucrative engineering activity i.e. energy production and energy use. To this effect, we need to become more and more concerned about energy efficiency and energy conservation.

In the European Union, electricity consumption for cooling increased from 22,879 GWh per year in 1990 to 51,636 GWh per year in 2000 and further increases up to 109,631 GWh per year in 2015 and 114,579 GWh in 2020 are predicted[2]. Basing on the Defra[3] CO_2 emission factor of 0.537kg/kWh which accounts for grid losses, these figures imply emissions of 589MtCO_2 and 615MtCO_2 in 2015 and 2020 respectively. The world demand for cooling is constituted by residential and commercial buildings, with the highest consumption being in the USA[4]; making them key contributors to global energy-related CO_2 and SO_2 emissions. In a number of cities, this can be largely attributed to the use of electric vapour compression air conditioning and refrigeration systems which use refrigerants that are environmentally undesirable.

Although many have questioned the existence and the validity of linking greenhouse gasses to global warming we must as a matter of precaution reduce energy related SO_2 and CO_2 emissions from fossil fuelled electrical power utilities. This can be done through reducing the electrical demand on such plants. Other proposals including retiring them and constructing renewable generating facilities, using scrubbers in coal power plants, using low sulphur coal, co-firing and converting the coal power generating technology to use cleaner fuels have been suggested. However, the latter options unlike the former can have a significant impact on the cost of electricity.

Because it can be economical, energy conservation through the reduction of electric demand on electrical networks and through reduction of transmission losses by the use of low grade thermal driven refrigeration and air conditioning systems in Combined Heat and Power (CHP) and Combined, Cooling, Heating and Power (CCHP) systems has gained a lot of attention. This is implemented by using vapour absorption systems that can use the heat generated as a by product of any prime movers to provide cooling. Absorption chillers can also be direct fired by cheap fuels that can make them more economical than vapour compression systems.

In many countries, electrical peak demand coincides with the period in which solar intensity is very high due to the increased need for air conditioning in such periods. In such cases, the available solar radiation can be trapped using solar collectors or solar concentrators to provide hot water or steam for driving absorption chillers and this can prove invaluable both in reducing peak demand and improving reliability and stability of electrical grids. All these opportunities have in the recent years stimulated the development and production of vapour absorption chillers. Moreover, numerous research studies have been done on performance improvement of various absorption chiller configurations.

A number of absorption systems exist or are in prototype stages and they include half-effect, single-effect, double-effect, triple-effect, resorption and Generator-Absorber Heat Exchanger (GAX). The common working fluid pairs in these systems are H_2O-LiBr in which H_2O is the refrigerant and LiBr is the absorbent; and H_2O-NH_3 in which NH_3 is the refrigerant and H_2O the absorbent. Systems using the H_2O-LiBr working pair provide cooling above 0°C and are prevalent in air conditioning applications while systems using the H_2O-NH_3 working pair can achieve subzero temperatures which are suitable for refrigeration. In addition, H_2O-LiBr systems are typically manufactured for large commercial cooling applications whereas H_2O-NH_3 systems are typically for residential and light commercial refrigeration applications.

It is also worth noting that although H_2O-NH_3 systems can achieve subzero temperatures, they are less efficient (low COP) than H_2O-LiBr and NH_3 is discouraged in air conditioning applications due to its toxicity. New working pairs have also been developed[5, 6, 7, 8] and their performance studied but there seems not to be a choice that supersedes the characteristics of the already mentioned common two.

This thesis contains the work done in the modelling and implementation of a single-effect absorption chiller with the H_2O-LiBr working pair in MERIT. Extensive studies have been done on the modelling and simulation of H_2O-LiBr absorption chillers in the effort to achieve optimum performance. The author studied existing literature to establish the various modelling approaches. In this thesis, effort is made to categorise the various research material and models that were encountered for a single-effect H_2O-LiBr absorption chiller. A modelling approach is then selected and used to support model implementation and simulation in MERIT.

MERIT is a computer program developed by University of Strathclyde to support the development of new and renewable energy schemes. Appropriate energy solutions are obtained by matching between user specified demand profiles and possible inbuilt supply technologies when deployed separately or in any combination. The addition of an absorption chiller model would allow supply/demand matching options for cooling (in addition to the current capabilities of electricity and heating) to be included in the analysis of potential applications.

The selected model was first set up in Microsoft Excel to enable quick verification of outputs with results obtained in various published material. Good agreement of results was achieved and implementation approaches for programming the model into MERIT were devised as will be explained in chapter 4.

1.2 Objectives

A number of technologies have been implemented in MERIT but presently, there is no functional absorption chiller technology. The overall purpose of this thesis is therefore to research absorption chiller models and simulation techniques for a basic absorption chiller to assist in the development and implementation of its model into MERIT.

Specific objectives

More specifically, the purpose of this thesis was to:

- To research the modelling approaches used in performance study simulations of single-effect absorption chillers and choose the appropriate one for implementing in MERIT
- To provide the single-effect absorption chiller simulation functionality in MERIT that would estimate the suitability of the absorption chiller in utilising the heat available at any time to meet cooling demand
- To provide the single-effect absorption chiller simulation functionality in MERIT that would provide an estimated prediction of the heat required to meet cooling demand
- To develop appropriate mathematical models for accomplishing the above specific objectives and implement them into MERIT using Microsoft Visual C++
- To evaluate the accuracy of the developed mathematical models
- To test, present and discuss simulation results obtained using the models implemented in MERIT

1.3 Methodology

The following activities provided the enabling efforts for accomplishing the above mentioned objectives,

- In the initial stages, focus was directed towards gaining an exhaustive understanding of the field of thermal driven air conditioning and refrigeration systems. Particular attention was paid to modelling and simulation of them. Relevant scientific articles from a number of bibliographic databases were obtained and read which provided a foundation for literature review.
- The various mathematical modelling approaches that existed in literature were carefully explored and one selected for preliminary modelling of a single-effect absorption chiller in Microsoft Excel. The equations were implemented successfully and results and various graphs relating the various absorption chiller variables plotted. This was to gain a full understanding and first-hand synthesis of the simulation results for quick comparison with results obtained by other authors.
- Using EES and MATLAB the required mathematical models were constructed and their output tested and validated against the outputs of the physical model selected from existing models presented in literature review.
- Appropriate subroutines or functions for incorporating into the main Microsoft Visual C++ development environment for MERIT were formulated and applied using appropriate hypothetical cooling load and heat supply profiles.

1.4 Report layout

This work has five chapters. Chapter 1 starts off with the general important ideas that motivate research into absorption refrigeration and air conditioning technologies and presents the objectives of this study. In Chapter 2 some theory key to the understanding of vapour absorption chillers; particularly those based on the H_2O-LiBr working pair is reviewed in brief to inform the reader of some key terms and concepts that will be used in other chapters.

Chapter 3 presents a detailed review of literature regarding the absorption cycle models together with the mathematical equations for all the absorption chiller components. Effort is made to discuss utility of the modelling approaches with regard to the objectives of this thesis. Then in Chapter 4 a modelling approach is selected out of those presented in literature review and implemented into Microsoft Visual C++; the Integrated Development Environment (IDE) in which MERIT is developed. Testing and simulations are performed and results presented.

Chapter 5 concludes the work with a brief summary highlighting the main aspects of this thesis and recommendations for further study.

Chapter 2

Background on Absorption Chillers

2.1 Introduction

The development of absorption technology started in the early 1700's through 1860. During this period both the H_2O-LiBr and the H_2O-NH_3 machines had been produced with the former machine introduced for cooling of industrial processes and the latter for ice making and food storage[9]. Since then, the two machines have become commercialised and can be acquired in various cooling capacities.

This chapter provides some fundamental aspects as well as key terms relevant to the H_2O-LiBr vapour absorption machines and serves as a foundation to the remaining chapters.

2.2 Vapour absorption systems terminology

Table 2.1 is a summary of some key terminology that will frequently be used in the description of the H_2O-LiBr absorption chiller. Clear definition of these terms is important for any model formulation. There are other terminology of significance as defined by Kang et al.[10] which have not been included here but are relevant for advanced vapour absorption cycles.

Terminology	Definition
Number of effects	Number of refrigerant generation/re-generation processes
Number of stages	Number of solution circuits for an evaporator/absorber set
Basic cycle	Single-stage cycle
Strong solution	Rich in refrigerant
Weak solution	Poor in refrigerant

Table 2.1: Some terminology in vapour absorption systems[10]

2.3 Desired characteristics of working fluids

The operating characteristics of any absorption cycle depends on the characteristics of the working pair. This working pair must be selected to closely match the key requirements outlined in Table 2.2.

Fluid	Desirable properties	Reason
Refrigerant	High latent heat	Reduces mass flow
	Moderate pressure at condensing temperature	Reduces strength requirement for condenser and generator
	Relative low triple point	Limit on evaporating temperature
	Low vapour specific volume	Ease of vapour transport
Absorbent	Negligible vapour pressure	Negates the vapour separation or rectification requirement
	High affinity for refrigerant	Greater affinity means a likelihood of high refrigeration capacity in the evaporator
Solution	Low specific heat	Reduces solution heat exchanger duty
	Low specific volume	Reduces pump work
General properties	Low viscosity	Increases heat transfer coefficient and reduces pipe work losses
	Low surface tension	Improves absorber operation
	Low toxicity	Safety
	Chemically stable	Improves system life
	Low cost	Economy

Table 2.2: Desirable properties of working fluids[11]

In particular, the H_2O-LiBr working pair exhibits some undesirable characteristics with respect to the above properties i.e. crystallisation and corrosion. To avoid crystallisation, the H_2O-LiBr cycle must operate within strict limits of solution concentration and temperature. Because the concentration of the aqueous solution during chiller operation is closely tied to component operating temperatures, an operating concentration range of

50% to 65% kg LiBr per kg water vapour is commonly specified as one of the control strategies. Moreover, LiI is sometimes added in the H_2O-LiBr solution to overcome the problem of crystallization[12]. Corrosion is avoided or reduced by the use of anti-corrosive agents. These anti-corrosives must be selected such that they do not attack internal piping and component walls which would lead to degraded cycle performance. Anti-corrosives commonly employed in H_2O-LiBr chillers include lithium nitrate and lithium chromate.

2.4 The vapour absorption systems

Vapour absorption systems are in the technology class of heat pumps. Heat pumps are machines used to transfer heat from a low temperature source to a high temperature sink. This direction of heat flow requires significant amount of work input into the heat pump as per the second law of thermodynamics. Whereas this work input is accomplished by the supply of electricity to the compressor in the vapour compression heat pump, it is by contrast accomplished by the supply of heat in vapour absorption heat pumps.

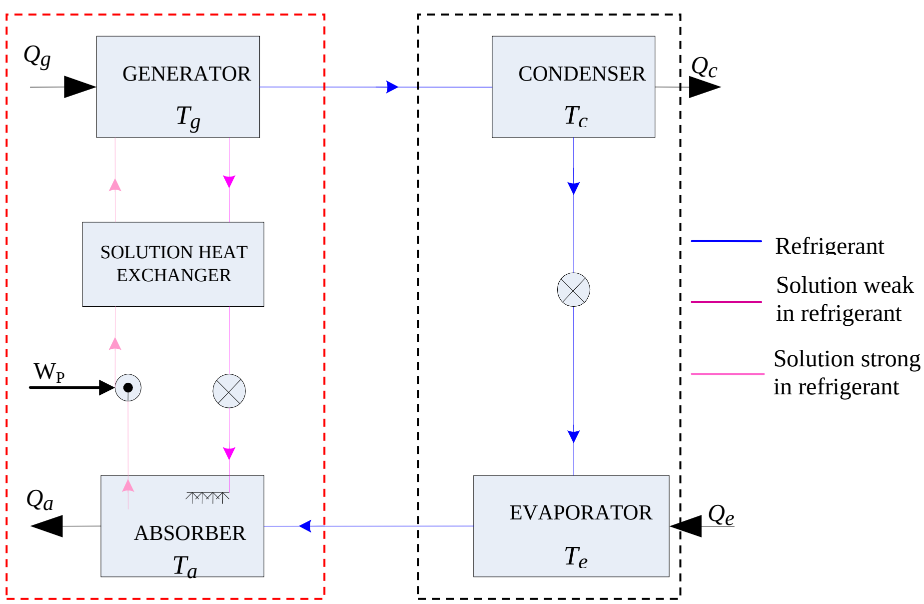


Fig 2.1: Single vapour H2O-LiBr absorption cycle

Fig 2.1 is a basic vapour absorption cycle using H_2O-LiBr as the working pair in which H_2O is the refrigerant and LiBr the absorbent. The cycle is a single-stage or single-effect type. It can be visualised as a combination of two cycles i.e. the work producing cycle (red dotted box) and a refrigeration cycle (black dotted box).

When the cycle is in operation, a large amount of heat Q_g is supplied at a temperature T_g where by $T_g > T_c >= T_a > T_e$. The cycle is then able to cause cooling effect at a temperature T_e by drawing heat Q_e from the medium being cooled. This, in addition to the heat of condensation of refrigerant and the heat of mixing of refrigerant and absorbent i.e. ($Q_c + Q_a$) are rejected to the environment. The work input W_P into the pump is the only electrical supply to the cycle and is very small compared to the heat input.
The cycle in Fig 2.1 can be shown on a *T-s* diagram in which the work producing cycle is combined with a refrigeration cycle as shown in Fig 2.2. It is assumed that the processes in both cycles are reversible.

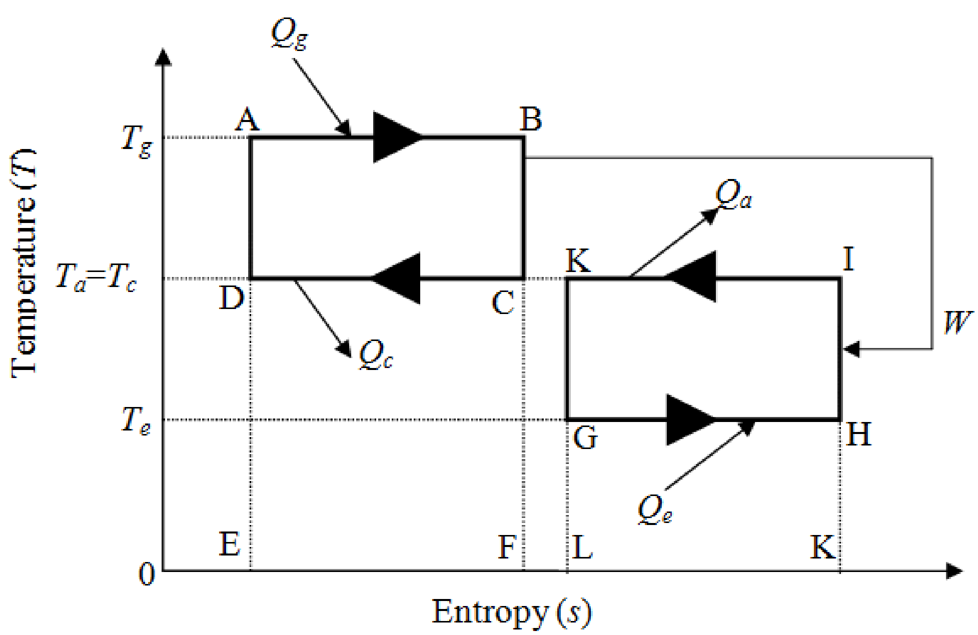


Fig 2.2: Carnot cycle for a basic vapour absorption system[13]

When the first law of thermodynamics is applied to the ideal cycle and the small work input to the pump is neglected equation 2.1 is obtained,

$$Q_g + Q_e = Q_a + Q_c \tag{2.1}$$

Also in a reversible cycle there is no entropy generation, thus

$$\frac{Q_g}{T_g} + \frac{Q_e}{T_e} = \frac{Q_a}{T_a} + \frac{Q_c}{T_c} \tag{2.2}$$

When it is assumed that the condenser and the absorber are operating at a common temperature, and equation 2.1 is substituted into equation 2.2, the coefficient of performance (COP_{max}) of a reversible Carnot thermal driven cycle can be determined by equation 2.3. It is defined as the ratio of the rate of heat removal from the cooled medium to the rate of energy input for a complete plant under designated operating conditions,

$$COP_{\text{max}} = \frac{Q_e}{Q_g} = \frac{T_e}{T_a - T_e} \cdot \frac{T_g - T_a}{T_g} \tag{2.3}$$

COP_{max} is the maximum possible coefficient of performance for a basic vapour absorption system that operates at component temperatures T_e, T_g and T_a=T_c.

2.5 Performance of real cycles

Real cycles however include irreversibilities and continuous changes in operating conditions which affect their overall performance. In defining the performance of real absorption chillers, the terms efficiency, seasonal performance and rated performance are often used. Coefficient of Performance is also used as a measure for expressing the energy performance of absorption systems but the values of Q_e and Q_g used are actual values obtained after all the important irreversibilities have been taken into account. The term efficiency is used to imply the percentage of maximum possible performance that can be obtained from the absorption chiller and is given by equation 2.4.

$$\eta = \frac{COP_{actual}}{COP_{\max}} \tag{2.4}$$

The rated performance is the one often provided by the manufacturer. Seasonal performance is a parameter of significant concern. It is used to gauge the portion of energy that is actually used for the intended purpose in relation to the total energy paid for[14]. The rated efficiency can be dramatically higher than the seasonal efficiency but control systems can be installed along with air conditioning systems to close the gap between seasonal and rated efficiency[14]. These control systems however increase the overall cost of any air conditioning project. As such all these performance parameters need to be evaluated to ensure an optimum system is selected and installed.

2.6 Part load performance

Most systems operate at less than full load for virtually all hours in a year. If the system is oversized, this causes even a greater number of part load operating hours. Performance measurement indices that take chiller part load conditions into account include Integrated Part Load Value (IPLV) and European Seasonal Energy Efficiency Ratio (ESEER)[2]. IPLV is used in North America. They are calculated with a weighted formula that takes variation of Energy Efficiency Ratio (EER) - (in the case of ESEER) and variation of COP (in case of IPLV) with the load rate and the variation of air or water inlet condenser temperature into account as shown in equation 2.5. COP and EER are essentially similar except that for COP, both the cooling energy delivered and the input energy supplied are in the same units e.g. kW while for EER they are expressed in Btu/h and kW respectively. IPLV and ESEER have been evaluated by Eurovent[2] to be more accurate in predicting chiller performance as compared to COP and EER.

$$\mathrm{ESEER} = \mathrm{A} \times \mathrm{EER}(100\%) + \mathrm{B} \times \mathrm{EER}(75\%) + \mathrm{C} \times \mathrm{EER}(50\%) + \mathrm{D} \times \mathrm{EER}(25\%) \tag{2.5a}$$

$$\mathrm{IPLV} = \mathrm{A} \times \mathrm{COP}\,(100\%) + \mathrm{B} \times \mathrm{COP}(75\%) + \mathrm{C} \times \mathrm{COP}(50\%) + \mathrm{D} \times \mathrm{COP}(25\%) \tag{2.5b}$$

In the equations, A, B, C and D are percentages of operating hours also called weighting coefficients at each load condition and their current values for air and water cooled chillers are as shown in Table 2.3 and Table 2.4 respectively.

	ESEER		IPLV	
Part load ratio	Temperature (ºC)	Weighting coefficients	Temperature (ºC)	Weighting coefficients
100%	35	3%	35	1%
75%	30	33%	26.7	42%
50%	25	41%	18.3	45%
25%	19	23%	12.8	12%

Table 2.3: ESEER and IPLV conditions for air cooled chillers[2]

	ESEER		IPLV	
Part load ratio	Temperature (ºC)	Weighting coefficients	Temperature (ºC)	Weighting coefficients
100%	30	3%	29.4	1%
75%	26	33%	23.9	42%
50%	22	41%	18.3	45%
25%	18	23%	18.3	12%

Table 2.4: ESEER and IPLV conditions for water cooled chillers[2]

One of the approaches taken to reduce part load operation is to install multiple small capacity systems such that the total running system at a given time is just enough to meet the required load[14]. The units that are not required can be shut down. The total system can be controlled by an energy management system (EMS) that continually monitors the load thus triggering units to kick in and out depending on the needed capacity.

2.7 Obtaining working fluid properties for cycle analysis

Thermodynamic properties of the working fluids are of key importance when assessing the performance of any absorption cycle. The common properties of interest i.e. enthalpies and concentration of the H_2O-LiBr solution as well as pure water are normally evaluated at internal cycle state point temperatures. The basic setting of equilibrium states points of any complete absorption cycle can be represented on a Dühring chart (Fig 2.3). Superimposed on the chart is a setup of a single-stage absorption chiller such as one in Fig 2.1 with the letters representing the positions of the main components. The blue dots indicate flow of water vapour (GC and EA) and pure liquid water (CE) while the red lines indicates flow of LiBr aqueous solution. Given the operating temperatures of the main absorption chiller components, the cycle can be drawn on as shown in Fig 2.3 and concentrations of the LiBr aqueous solution can be read off directly.

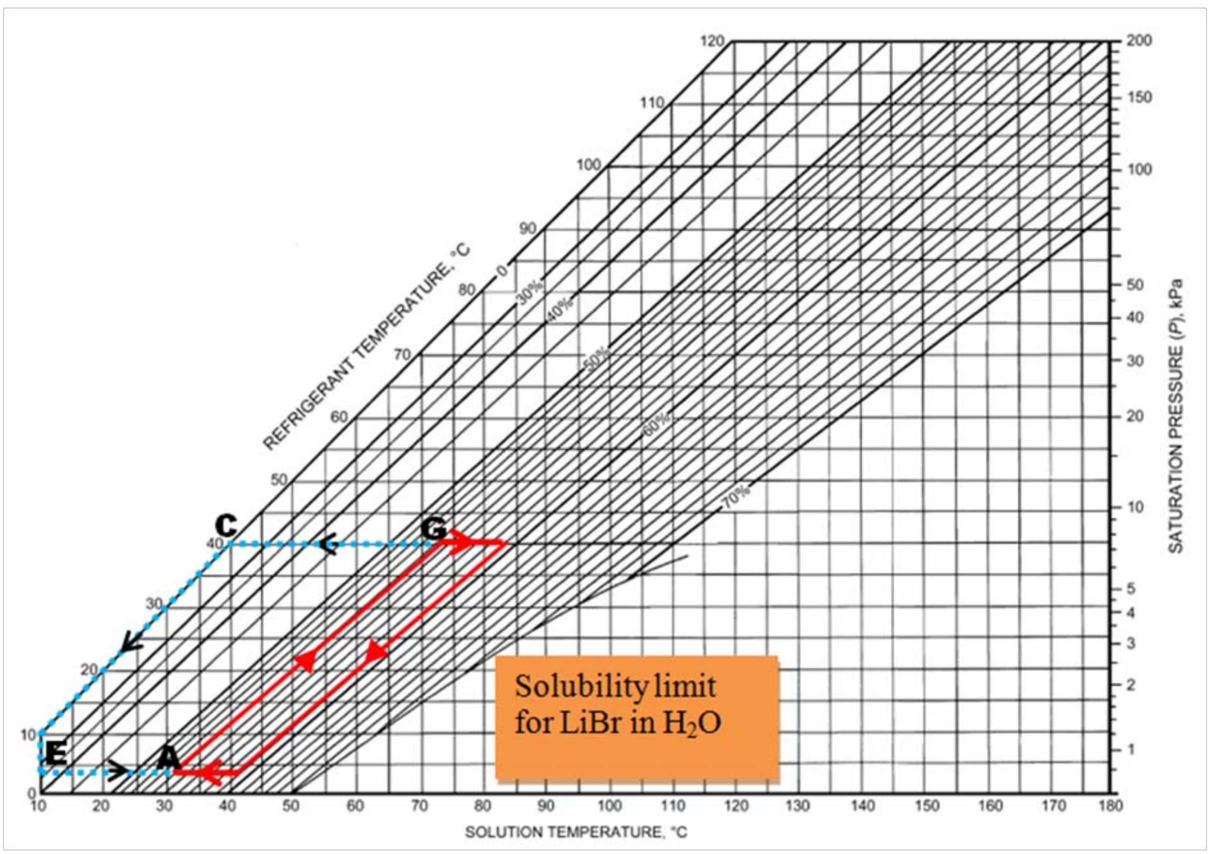


Fig 2.3: Equilibrium chart for aqueous LiBr solutions

Fig 2.4 is another chart where the enthalpies of aqueous LiBr of concentration ranging from 0 to 70% can be obtained. In both charts there are points at different pressures and temperatures where LiBr begins to crystallise from the solution. These points are indicated by the crystallisation line or the solubility limit line visible on the charts.

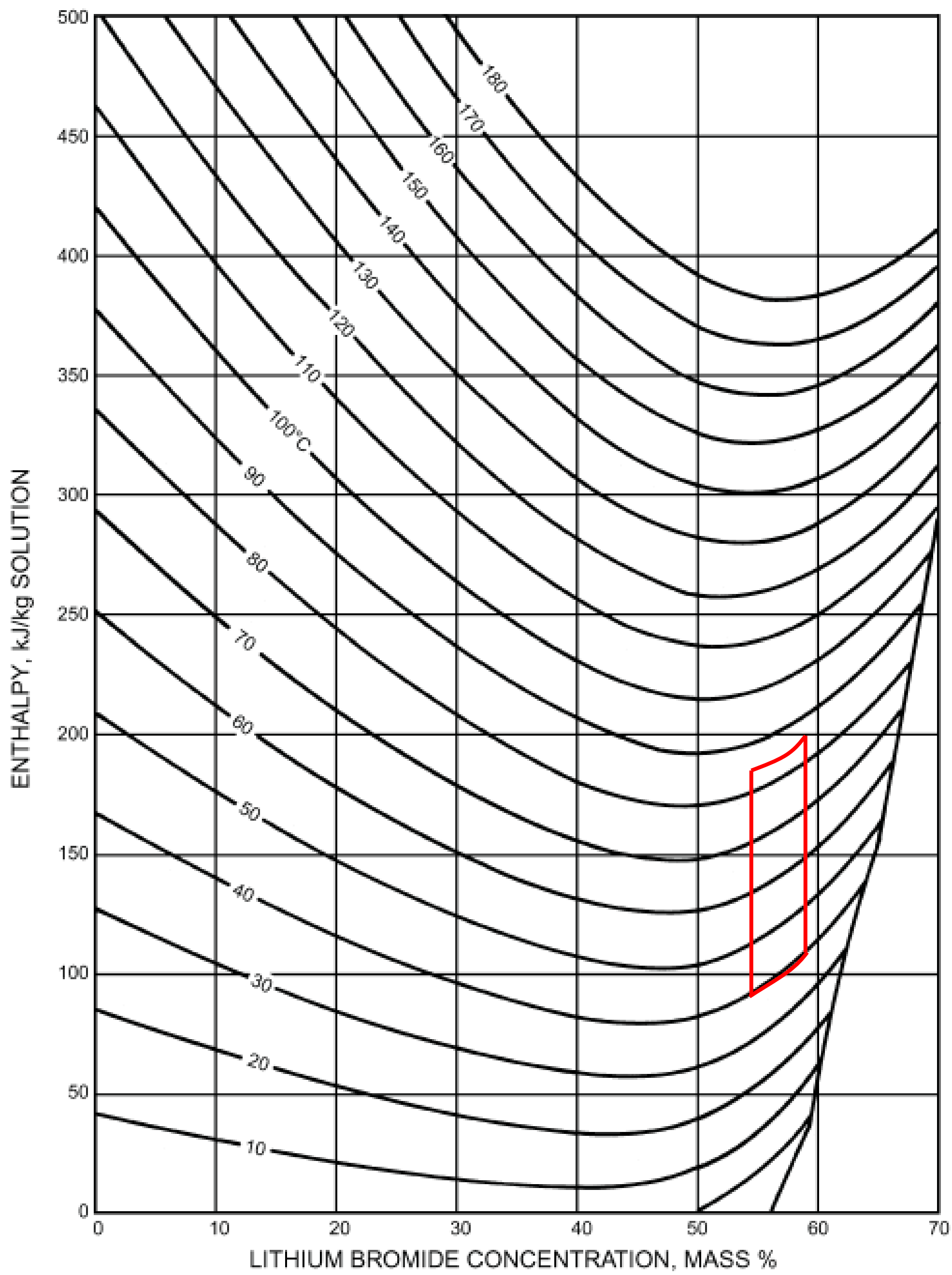


Fig 2.4: Enthalpy-concentration diagram for H_2O-LiBr solutions

However, computer modelling would necessitate alternative and efficient means of obtaining the thermodynamic properties of solutions of the working pair. Polynomial expressions for obtaining thermodynamic properties e.g. enthalpy and temperature of the H_2O-LiBr solutions at equilibrium conditions have been derived[15] to aid in computer simulations. Also expressions or curve fits for determining specific enthalpies of pure refrigerant (H_2O) have been derived. These expressions have been used in the design of H_2O-LiBr absorption machines with good level of accuracy[16].

Equation 2.3 is a relationship between the temperature of the refrigerant (H_2O) T_r, aqueous LiBr solution temperature T_s and its concentration X where A_n and B_n are constants[15]. It assumes that the refrigerant is pure water without LiBr contamination.

Refrigerant temperature (°C) is given by,

$$T_r = \left(T_{sol} - \sum_{n=0}^{n=3} \mathrm{B}_n \mathrm{X}^n \right) \Big/ \sum_{n=0}^{n=3} \mathrm{A}_n \mathrm{X}^n \tag{2.3a}$$

Solution temperature (°C) is given by,

$$T_{sol} = \sum_{n=0}^{n=3} \mathrm{B}_n \mathrm{X}^n + T_r \sum_{n=0}^{n=3} \mathrm{A}_n \mathrm{X}^n \tag{2.3b}$$

The coefficients attached to variables of the above equations are,

$$\begin{array}{ll} \mathrm{A}_0 = -2.00755 & \mathrm{B}_0 = 124.937 \\ \mathrm{A}_1 = -0.16976 & \mathrm{B}_1 = -7.71649 \\ \mathrm{A}_2 = -3.133362 \times 10^{-3} & \mathrm{B}_2 = 0.152286 \\ \mathrm{A}_3 = 1.97668 \times 10^{-5} & \mathrm{B}_3 = -7.95090 \times 10^{-4} \end{array} \tag{2.3c}$$

The enthalpy relation for H_2O-LiBr solutions at equilibrium conditions can also be obtained using the following expression.

$$h = \sum_{n=0}^{n=4} \mathrm{A}_n \mathrm{X}^n + T_s \sum_{n=0}^{n=4} \mathrm{B}_n \mathrm{X}^n + T_s^2 \sum_{n=0}^{n=4} \mathrm{C}_n \mathrm{X}^n \tag{2.4a}$$

Where the coefficients attached to the variables are as follows.

$$
\begin{array}{lll}
A_0 = -2024.33 & B_0 = 18.2829 & C_0 = -3.7008214\times10^{-2} \\
A_1 = 163.309 & B_1 = -1.1691757 & C_1 = 2.8877666\times10^{-3} \\
A_2 = -4.88161 & B_2 = 3.248041\times10^{-2} & C_2 = -8.1313015\times10^{-5} \\
A_3 = 6.302948\times10^{-2} & B_3 = -4.034184\times10^{-4} & C_3 = 9.9116628\times10^{-7} \\
A_4 = -2.913705\times10^{-4} & B_4 = 1.8520569\times10^{-6} & C_4 = -4.4441207\times10^{-9}
\end{array} \quad (2.4b)
$$

2.8 Types of absorption chillers

This section is a summary of the various types of absorption chillers. Single-effect and double-effect machines are the two commercialised types but other efficient absorption cycle types have been studied and are either being developed or at prototype stage.

2.8.1 Single-effect absorption chiller

Fig 2.5 is a typical schematic of a commercially available single-effect, indirect fired absorption machine using H_2O as a refrigerant. The major visible components include generator, evaporator, condenser, absorber, solution and refrigerant pumps and a solution heat exchanger.

As shown, the upper shell of the absorption chiller contains generator and condenser (both at a common higher pressure), while the lower shell contains the evaporator and absorber (both at a common lower pressure). Because the machine operates at near perfect vacuum in both shells it is hermetically sealed to avoid air leakage that would degrade its performance.

The dilute solution of H_2O (refrigerant) and LiBr (absorbent) in the generator is heated by a stream of steam or hot water. As the solution boils, the refrigerant vapour is transferred to the condenser where it is condensed to liquid refrigerant losing its heat of condensation to the cooling water (condensing water). The more concentrated hot solution left in the generator flows to the absorber through a heat exchanger.

The liquid refrigerant then flows by gravity from the condenser through an orifice or liquid trap to the evaporator in which it is evaporated at low pressure by the heat carried by the chilled stream thus resulting into cooling effect. Refrigerant liquid that remains un-evaporated is circulated continuously through the evaporator by means of a refrigerant pump. In the absorber, the more concentrated solution that came from the generator absorbs the water vapour from the evaporator due to its strong absorbing affinity between the two working fluids.

As the vapour is absorbed the solutions becomes dilute and releases heat of condensation and heat of dilution or mixing which is carried away from the absorber by the same cooling water that cools the condenser. The dilute solution is then pumped by the solution pump via the heat exchanger to the generator for re-concentration.

The heat exchanger (also called the solution heat exchanger) is used to cool the hot concentrated solution from the generator and to preheat the diluted solution from the absorber. This helps to keep the temperature of the absorber low and improves the absorption process. Also as the heat carried by the hot concentrated solution from the generator is used to preheat the dilute solution flowing to the generator, the heat requirement in the generator is reduces which improves the coefficient of performance of the machine.

The typical common pressure for the evaporator and the absorber is about 0.7kPa while that for the condenser and the generator is about 6kPa[17].The COP of a single-effect absorption chiller ranges from 0.6 to 0.8 and the driving temperatures are in the range of 90 to 100°C for a water cooled system. The driving temperature for air-cooled systems need to be about 30K higher[18].

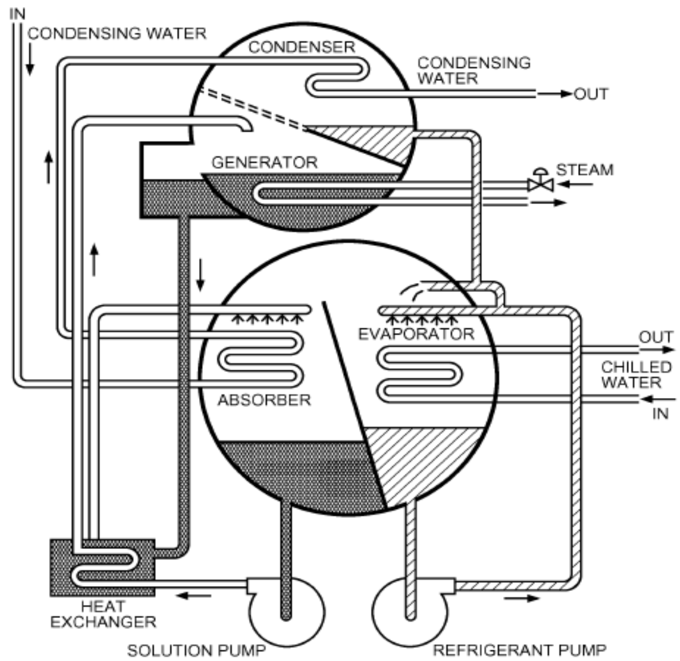


Fig 2.5: Schematic of a commercial single-effect absorption machine [17]

2.8.2 Double-effect absorption chiller

Referring to Fig 2.6, a double-effect chiller is basically a single-effect cycle with an extra generator (high-temperature re-generator, i.e. HTRG) and an additional heat exchanger (HRTX) between the two generators. Because of the high pressure in the HTRG, refrigerant vapour condenses at a temperature, high enough to heat and boil the aqueous solution in the low-pressure generator (LTRG) which increases the refrigerant yield thus increasing the refrigeration capacity and the COP. The particular double-effect machine shown in Fig 2.6 is the parallel flow type because the solution strong in refrigerant is split between the two generators.

The other existing machine is the series type double-effect cycle in which after some refrigerant has been boiled out of the solution from the absorber in the low pressure generator, it is transferred to the high pressure generator for further boiling to evaporate more refrigerant.

Pressures encountered in double-effect machines approach atmospheric pressure. This makes refrigerants with low boiling temperatures like NH_3 impracticable[18]. The COP of a typical water-cooled double-effect H_2O-LiBr chiller ranges between 1.2 to 1.3 and the driving temperature is in the range of 150 to 170°C[18].

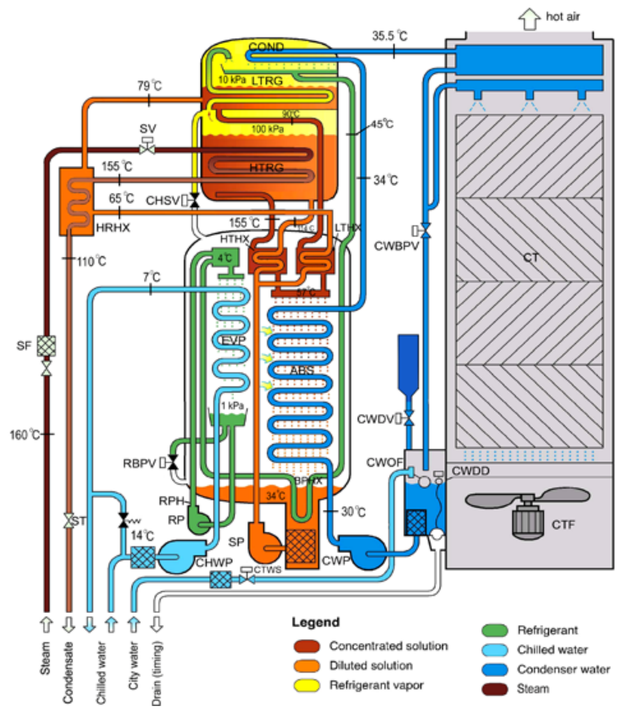


Fig 2.6: Steam fired double-effect absorption machine (parallel flow type) [19]

2.8.3 Other types of absorption chillers

The half-effect, triple-effect, generator-absorber heat exchanger (GAX) and resorption cycles are other types of absorption configurations that have been created and their detailed configuration and operating principles have been presented by Srikhirin et al.[9]. The half-effect cycle can attain COPs in the range of 0.3 to 0.4. For a water cooled half-effect cycle, driving temperatures in the range from 60 to 70°C are required while for an air-cooled cycle driving temperatures of about 30K higher are required[18].

Triple-effect cycles have gained significant interest in the effort to further improve the performance of heat driven cooling systems. They are obtained by adding an additional high pressure generator to the double-effect cycles. Again triple-effect cycles can be made parallel flow or serial flow in the same way as the double-effect cycles. However, outcomes from studies conducted by Grossman[20, 21] suggest that the triple-effect cycle with parallel flow configuration yields the highest COP.

The GAX absorption cycle is based on the fact that a single-effect absorption cycle can perform at COPs as high as typical in double-effect machines by incorporating a generator-absorber heat exchanger (GAX). All these systems and their thermodynamic cycle representations; as well as other configurations not mentioned here have been studied by Srikhirin et al.[9], Kim[18] and Wang & Chua[22].

Chapter 3

Mathematical Models

3.1 Introduction

This chapter reviews thermodynamic cycles and mathematical models that have been used in literature for the assessment and performance study of single-effect H_2O-LiBr absorption chillers.

Modelling can be defined as the application of basic physical laws on a system to derive mathematical expressions that represent its interconnected components and subsystems. In general, vapour absorption system modelling and simulation studies that were encountered in literature were either machine specific or generalised (i.e. modularised for applying to various absorption machine cycle configurations). Models also differed depending on the working fluids that were employed in a particular cycle.

While some models focused on stand alone systems, some modelling and simulation efforts were focused on modelling hybrid systems such as an absorption chiller integrated with solar collectors or other waste heat generating prime movers. In addition other modelling and simulation efforts relating to absorption chillers were focused at designing or sizing absorption chiller components or studying the performance of alternative designs of individual vapour absorption machine components for a particular cooling capacity. Modelling and simulation were also sometimes supported by experiments to verify applicability of theoretical outcomes.

The study of absorption chiller cycles and mathematical models assisted the author in deciding on the kind of model that would be appropriate for implementation in MERIT. The desired accuracy and complexity of the model as well as the time available for completing implementation were the main influencing factors to the choice of the modelling approach.

3.2 Steady state models

Steady state models have been used extensively in the design, optimisation and performance study of engineering systems and components. With respect to single-effect vapour absorption chillers, various research efforts have used steady state models to predict performance, assess the effectiveness of new working fluids, establish relationships between parameters, optimise chiller components and to study hybrid system assemblies for combined cooling, heating and power (CCHP).

At least three kinds of single-effect absorption cycle configurations can be found in literature and they include:

- Basic cycle without external flows
- Basic cycle with external flows
- Basic cycle with refrigerant heat exchanger

3.2.1 Basic cycle without external flows

In this cycle, interactions between the cycle and the external cooling, heating and chilled water flows are neglected and mathematical relations are formulated based on the internal operating temperatures of the generator, evaporator, condenser and absorber. These internal operating temperatures may be determined from actual running measurements or assumed by first reasonable estimate to cycle performance[23]. The other input required in these models is the effectiveness of the solution heat exchanger.

Fig 3.1 is the representation of the basic single-effect absorption cycle commonly used in performance studies and steady state simulations. It is the most basic cycle of a single-effect absorption chiller. In this model, each component is treated as a black box (in other words, the heat transfer processes going on across the components are ignored). The cycle has been drawn with its components oriented as shown to illustrate the concentrations and temperatures in the system as previously depicted on the Dühring diagram shown in Fig 2.4. The coloured side of the cycle carries the refrigerant i.e. water vapour (7,10) and liquid water (8,9). The strong solution (see Table 2.1) goes from the absorber to the generator and is represented by state points 1, 2 and 3. After water vapour has been boiled off, it flows from the generator via state points 4, 5 and 6 back to the absorber as a weak solution where it absorbs the vapour refrigerant coming from the evaporator.

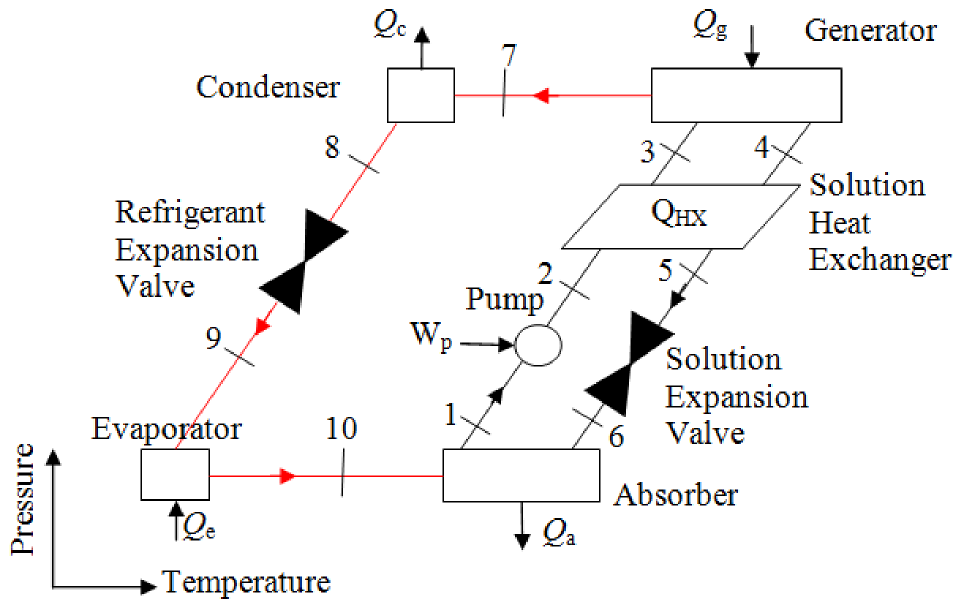


Fig 3.1: Basic single-effect H_2O-LiBr absorption chiller model

In order to analyse the cycle in Fig 3.1, thermodynamic properties of the internal state points need to be determined first. As it can be difficult to evaluate those state points, the following simplifying assumptions are commonly made:

- The pressure drops and heat losses in and across the chiller components are considered negligible.
- The liquid refrigerant leaving the condenser (state point 8) and the vapour leaving the evaporator (state point 10) are assumed to be saturated at their respective saturation temperatures.
- The strong solution leaving the absorber (state point 1) and the weak solution leaving the generator (state point 4) are assumed to be saturated and at equilibrium conditions at their respective temperatures. With this assumption, enthalpies at these state points can easily be obtained from the Dühring chart or by using appropriate polynomials H_2O-LiBr solution properties.
- The refrigerant vapour leaving the generator (state pint 7) is assumed superheated at the generator temperature.

- Flow restrictors (i.e. the refrigerant and solution expansion valves) and the pump are considered adiabatic and isentropic.
- All liquid in the evaporator is evaporated and only vapour goes to the absorber.

With these assumptions, simulation of the single-effect absorption cycle proceeds by writing appropriate steady state mass and energy balance equations for each of the components as follows.

Absorber

Total mass balance:

$$\dot{m} + \dot{m}_w = \dot{m}_s \tag{3.1a}$$

$$\dot{m}_w = \lambda \dot{m} \tag{3.1b}$$

$$\dot{m}_s = (1+\lambda)\dot{m} \tag{3.1c}$$

Where $\dot{m}$ is the mass flow rate of the refrigerant, $\dot{m}_s$ is the mass flow rate of the strong aqueous LiBr solution and $\dot{m}_w$ is the mass flow rate of the weak aqueous LiBr solution.

Lithium-bromide mass balance:

$$\dot{m} + (1 - \mathrm{X}_w)\dot{m}_w = (1 - \mathrm{X}_s)\dot{m}_s \tag{3.1d}$$

$$\lambda = \frac{\mathrm{X}_s}{\mathrm{X}_w - \mathrm{X}_s} \tag{3.1e}$$

Where λ is the circulation ratio and X the concentration of the aqueous LiBr solution with the subscripts, *s* and *w* representing the strong and weak solution respectively as defined in Table 2.1.

Energy balance:

$$Q_a = \dot{m}h_{10} + \lambda \dot{m}h_6 - (1+\lambda)\dot{m}h_1 = \dot{m}[(h_{10} - h_1) + \lambda(h_6 - h_1)] \tag{3.1f}$$

Solution pump

Mass balance:

$$\dot{m}_1 = \dot{m}_2 = \dot{m}_s \tag{3.2a}$$

Energy balance:

$$W_p = \dot{m}_s\left(h_2 - h_1\right) = \dot{m}\left(1+\lambda\right)\left(h_2 - h_1\right) \tag{3.2b}$$

If the strong solution is assumed to be incompressible, then

$$W_p = \dot{m}v_{sol}\left(1+\lambda\right)\left(p_2 - p_1\right) = \dot{m}v_{sol}\left(1+\lambda\right)\left(p_c - p_e\right) \tag{3.2c}$$

Solution heat exchanger

Mass balance:

$$\dot{m}_2 = \dot{m}_3 = \dot{m}_s \tag{3.3a}$$

$$\dot{m}_4 = \dot{m}_5 = \dot{m}_w \tag{3.3b}$$

Energy balance:

$$Q_{HX} = \dot{m}\left(1+\lambda\right)\left(h_3 - h_2\right) = \dot{m}\lambda\left(h_4 - h_5\right) \tag{3.3c}$$

The solution heat exchanger effectiveness ε_{HX} is defined as:

$$\varepsilon_{HX} = \frac{Q_{actual}}{Q_{\max}} = \frac{\dot{m}_w C_{p,w}\Delta T_w}{\dot{m}_w C_{p,w}\Delta T_{\max}} = \frac{T_4 - T_5}{T_4 - T_2} \tag{3.3d}$$

Inlet temperature of strong solution entering into the heat exchanger is approximately equal to the inlet temperature of the strong solution entering the pump i.e. $T_2 = T_1$. So from this T_5 can be calculated using equation 3.3d.

Generator

Mass balance:

$$\dot{m}_3 = \dot{m}_7 + \dot{m}_4 \tag{3.4a}$$

Energy balance:

$$Q_g = \dot{m}h_7 + \dot{m}\lambda h_3 - \dot{m}(1+\lambda)h_4 = \dot{m}[(h_7 - h_4) - \lambda(h_3 - h_4)] \tag{3.4b}$$

Solution expansion valve

$$\dot{m}_5 = \dot{m}_6 = \dot{m}_w \tag{3.5a}$$

$$h_5 = h_6 \tag{3.5b}$$

Condenser

Mass balance:

$$\dot{m}_7 = \dot{m}_8 = \dot{m} \tag{3.6a}$$

Energy balance:

$$Q_c = \dot{m}(h_7 - h_8) \tag{3.6b}$$

Condenser pressure:

$$P_c = P_g = P_{sat}(T_c) \tag{3.6c}$$

Refrigerant expansion valve

$$\dot{m}_9 = \dot{m}_8 = \dot{m} \tag{3.7a}$$

$$h_9 = h_{10} \tag{3.7b}$$

Evaporator

Mass balance:

$$\dot{m}_9 = \dot{m}_{10} = \dot{m} \tag{3.8a}$$

Energy balance:

$$Q_e = \dot{m}(h_{10} - h_9) \tag{3.8b}$$

Evaporator pressure:

$$P_e = P_a = P_{sat}(T_e) \tag{3.8c}$$

Coefficient of performance

$$COP = \frac{Q_e}{Q_g + W_p} \approx \frac{Q_e}{Q_g} \tag{3.9}$$

The second law efficiency or exergetic efficiency is given by:

$$\eta_{II} = \frac{COP}{COP_{\max}} = \frac{Q_e}{Q_g}\left(\frac{T_g}{T_g - T_c}\right)\left(\frac{T_c - T_e}{T_e}\right) \tag{3.10}$$

Equations (3.1 to 3.10) are based on the calculation of internal enthalpies for H_2O-LiBr solution, refrigerant vapour and refrigerant liquid which require knowledge of these properties. Where a computer model is sought, it would be easier to work with polynomial curve fits for calculation of properties of H_2O-LiBr solutions, water vapour and liquid water than to attempt implementing property charts and tables. Moreover, methods for solving the polynomials such as the Newton-Raphson method are well established and can easily be implemented in computer models.

The basic model without external fluids provides a fairly good framework to understanding the performance of the single-effect absorption chiller and has been used by a number of researchers[24, 25, 26]. The main drawback with this model however is that it neglects the heat transfer processes going on between the external fluid and the working pair which causes the analysis to result in higher COP values than actually observed in practice. Also in reality, not all the refrigerant entering the evaporator is evaporated as suggested in the assumptions. Nevertheless, the model itself has been found invaluable because it provides sufficient knowledge in understanding the performance of a single-effect absorption machine.

Also, because this model ignores external streams that would flow through the cycle components, it becomes difficult when the analyst wishes to obtain the actual temperature of chilled water leaving the evaporator for example. This model is therefore just suitable for obtaining a rough picture about cycle performance in relation to changes in average internal temperatures of the cycle components.

3.2.2 Basic model with external flows

In this model, the assumptions made concerning internal state points are the same as in the previous model except that cycle interaction with external flows is now considered. The external flows of interest include the cooling water, heat supply medium (e.g. hot water, steam or hot oil) and chilled water as shown in Fig 3.2. The internal state points characterise the thermodynamic properties of H_2O-LiBr solution (points 1–6), water vapour (7, 10) and liquid water (8, 9). The external state points characterise the thermodynamic properties of the heat supply medium (11, 12), cooling medium (13, 14,15) and the chilled medium (16, 17).

In this case, the evaporator, absorber, condenser and generator components are treated as heat exchangers. They are then modelled by formulating heat and mass balance relations at the four corners in addition to the energy and mass balance expressions already presented under sub-section 3.2.1 for the cycle without external flows. Therefore the implication of considering external heat and mass transfer processes is the increase in the number of equations to be solved. This also contributes dramatically to the nonlinearity of the total system of equations for which a systematic process of equation counting and variable matching must be followed in order to determine the optimum number of inputs required to solve the equations simultaneously.

Mathematical models for the heat exchangers may be based on the UA formulation or the NTU formulation. Both have been used in literature. Based on the UA formulation, the additional equations resulting from external flows are as follows,

For the evaporator

$$Q_e = UA_e \Delta T_{lmtd,e} = \dot{m}_{chill}\left(h_{16} - h_{17}\right) \tag{3.11a}$$

Where

$$\Delta T_{lmtd,e} = \frac{\left(\left(T_{16} - T_{10}\right) - \left(T_{17} - T_{10}\right)\right)}{\ln \dfrac{\left(T_{16} - T_{10}\right)}{\left(T_{17} - T_{10}\right)}} \tag{3.11b}$$

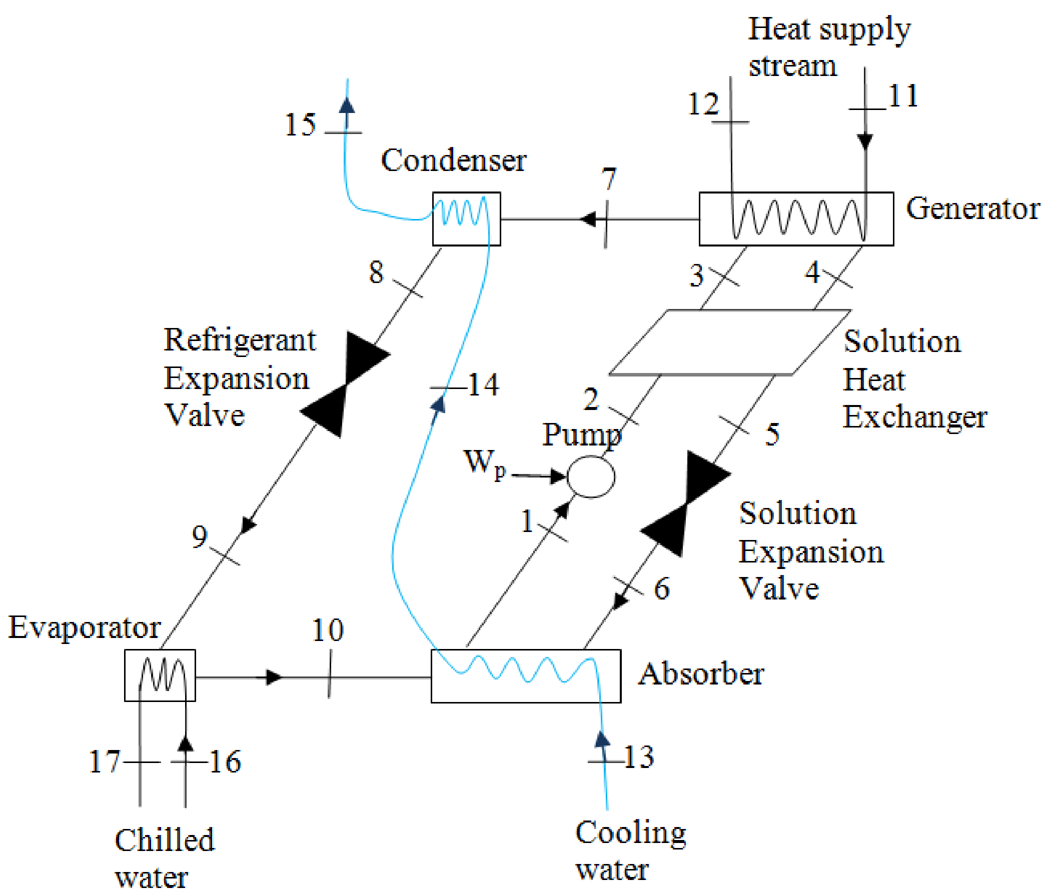


Fig 3.2: Basic single-effect H_2O-LiBr absorption chiller model with external flows

For the condenser

$$Q_c = UA_c \Delta T_{lmtd,c} = \dot{m}_{cool}\left(h_{15} - h_{14}\right) \tag{3.12a}$$

Where

$$\Delta T_{lmtd,c} = \frac{\left(\left(T_8 - T_{14}\right) - \left(T_8 - T_{15}\right)\right)}{\ln\frac{\left(T_8 - T_{14}\right)}{\left(T_8 - T_{15}\right)}} \tag{3.12b}$$

For the absorber

$$Q_a = UA_a \Delta T_{lmtd,a} = \dot{m}_{cool}\left(h_{13} - h_{14}\right) \tag{3.13a}$$

$$= \dot{m}h_{10} + \dot{m}_s h_4 - \dot{m}_w h_1 - Q_{SHX} \tag{3.13b}$$

Where

$$\Delta T_{lmtd,a} = \frac{\left(\left(T_6 - T_{14}\right) - \left(T_1 - T_{13}\right)\right)}{\ln\frac{\left(T_6 - T_{14}\right)}{\left(T_1 - T_{13}\right)}} \tag{3.13c}$$

For the generator

$$Q_g = UA_g \Delta T_{lm,g} = \dot{m}_{hot}\left(h_{11} - h_{12}\right) \tag{3.14a}$$

$$= \dot{m}h_7 + \dot{m}_s h_4 - \dot{m}_w h_1 - Q_{SHX} \tag{3.14b}$$

Where

$$\Delta T_{lmtd,g} = \frac{\left(\left(T_{11} - T_4\right) - \left(T_{12} - T_3\right)\right)}{\ln\frac{\left(T_{11} - T_4\right)}{\left(T_{12} - T_3\right)}} \tag{3.14c}$$

For the solution heat exchanger

$$Q_{SHX} = UA_{SHX} \Delta T_{lm,SHX} \tag{3.15a}$$

Where

$$\Delta T_{lmtd,SHX} = \frac{\left((T_4 - T_3) - (T_5 - T_2)\right)}{\ln \frac{(T_4 - T_3)}{(T_5 - T_2)}} \tag{3.15b}$$

If the modeller is more interested in investigating the impact of specific absorption chiller component characteristics such as diameter of heat exchanger tubes, number of tubes and length of heat exchangers, more detail can be incorporated in the *UA* value. This is done by applying detailed heat transfer models accounting for conduction and convection effects between external streams and internal streams.

Effectively this model uncovers the detail that was ignored by the model presented under sub-section 3.2.1. The less detailed equations 3.1 and 3.3 in the previous model are now replaced by the more detailed equations 3.13 and 3.14. The rest of the internal mass and energy balance equations presented in the previous model apply for this model too. For any given number of inputs, the system of equations is normally solved iteratively by existing solvers such as EES[13], TRNSYS[24] and ABSIM[35].

With regard to the purpose of this thesis, adopting this model would necessitate the development of a comprehensive and robust equation solving algorithm just like the one implemented in EES and ABSIM. It is an algorithm based on the Newton-Raphson variant and concepts of sparse matrices and Gaussian elimination. Because of the nonlinearity of the system of equations more than one solution is possible but only one is correct. Initial guesses are provided and suitable boundaries set for all variables to ensure that the iterative process returns the correct solution.

Clearly this model yields more accurate results and the impact of assumptions to the results obtained is minimised. However, the amount of time accruing to algorithm formulation, coding, testing until deployment can be significant.

3.2.3 Basic model with refrigerant heat exchanger

In other modelling endeavours, a refrigerant heat exchanger (RHX) is incorporated in the single-effect absorption chiller to study its effect on the overall performance of the cycle as shown in Fig 3.3. The mathematical modelling process remains the same as in sub-section 3.2.2 except that appropriate energy balance must be performed at the refrigerant heat exchanger and a choice can be made between the *UA* and the NTU heat transfer modelling approaches.

Such a cycle was studied by Karamangil et al.[27] and Kaynakli[28] but they did not consider heat transfer models for the external streams; rather, they concentrated on determining the internal state point enthalpies and heat rejected or absorbed at the cycle components based on the modelling approach of sub-section 3.2.1. In particular, Kaynakli[28] performed a sensitivity study on effects of changes in internal component temperatures (i.e. generator, absorber, condenser and evaporator temperature) and produced a number of graphs to support findings.

However, the study by Kaynakli[28] yielded an important result that incorporating a refrigerant heat exchanger improves the overall performance of the single-effect absorption chiller by a maximum of only 2.8% as compared to a maximum improvement of 44% attributed to incorporating the solution heat exchanger. Based on this result, the refrigerant heat exchanger is not necessary in the cycle.

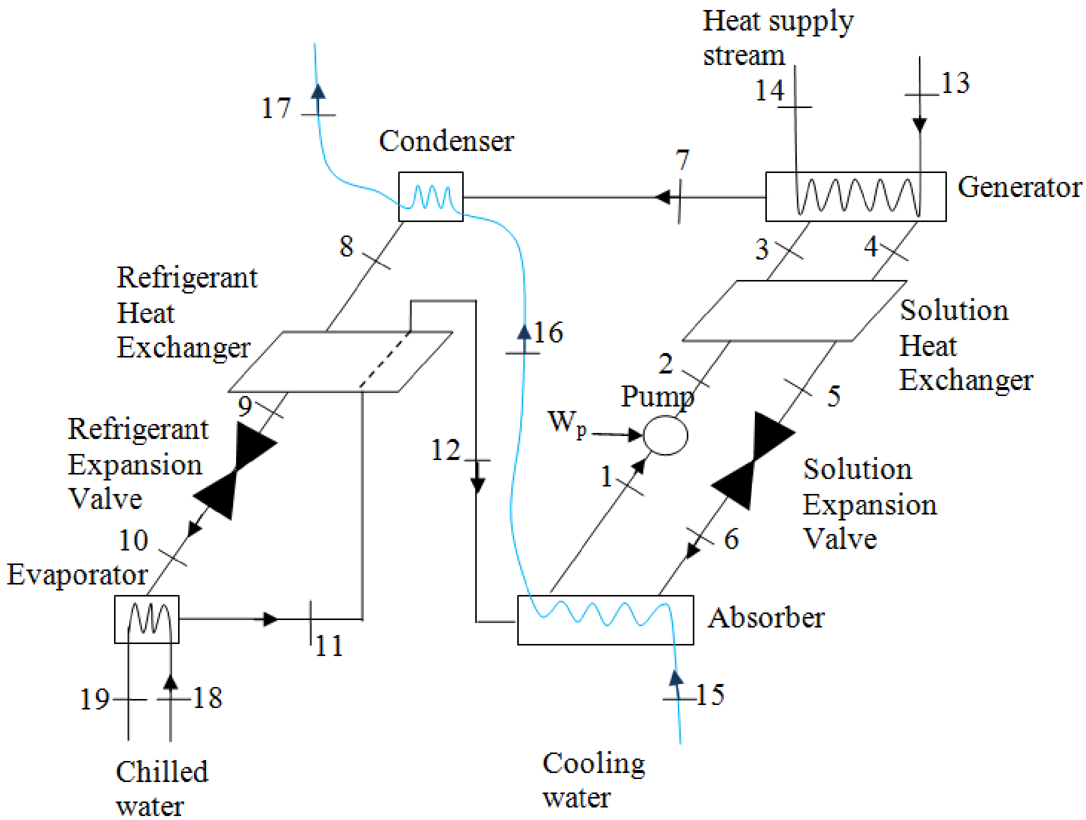


Fig 3.3: Simple model with refrigerant heat exchanger

3.3 Dynamic models

Modelling and simulation of transient behaviour of changing absorption chiller inputs and outputs can be done by using dynamic models[29, 30, 31, 32]. This is important so that thermal powered cooling systems can guarantee economic viability, operability and reliability. Absorption chillers have a high thermal mass consisting of their internal heat exchangers, the absorbing solution and the externally applied heat transfer media[30]. Because of this it takes much longer for an absorption chiller to attain steady state operating conditions when there is a slight change of any input parameter. Engineers therefore need to perform dynamic simulations to better understand and design appropriate absorption chiller controls.

For example, if it is desired to control the output temperature of the outgoing chilled water from the evaporator, it might be very helpful to perform a dynamic study. A possible objective of such a dynamic study could be to determine how much time it takes an absorption chiller to return to its steady state operating condition when there is a change in any available inputs (e.g. hot stream temperature).

Dynamic modelling has been performed by other authors. Kohlenbach & Ziegler[30], used dynamic modelling to study the impact of thermal mass on the transient response of performance for a single-effect absorption chiller when input conditions change and validated results experimentally with very good agreement. A similar dynamic modelling study had been performed earlier by Jeong et al.[29] with similar general conclusions.

Later, Fu et al.[33] designed an object-oriented dynamic modelling library named ABSML detailed mathematical models and an aim of supporting design of chiller control systems. The main components (i.e. absorber and generator, condenser and evaporator) were modelled as shell and tube heat exchangers characterised by lumped systems of equations involving phase change on the shell side. Solution heat exchangers were represented by discretised mathematical models while pumps were represented by simple models.

The author acknowledges that dynamic models are invaluable in providing the much needed insight about the transient behaviour of absorption systems as well as design of control systems for achieving reliable thermal driven cooling systems. In particular they may provide the best way to assess demand and supply matching of combined heat and power systems in MERIT. However the mathematical complexity involved with dynamic models and the time resource for implementing them need careful consideration.

3.4 Modular and custom cycle approach

Here, the individual components in the cycle are modelled separately to enable the user to combine them and compose any cycle configuration (e.g. single, double and triple-effect, with various working fluids). Such an implementation was first done by Grossman and Wilk[34] and later by Grossman and Zaltash[35]. They wrote subroutines for various chiller components which would be called by the main program based on the cycle diagram composed by the user. The mathematical models they implemented were steady state energy and mass balance equations as has already been presented under sub-sections 3.2.1 and 3.2.2 with similar assumptions.

Although this approach provides the users with capabilities of assembling any cycle configuration of their choice, software development for MERIT does not need this level of complexity. In addition since there is currently no absorption chiller model in MERIT, it would be sufficient to succeed in modelling one type of cycle configuration first before attempting the modular and custom cycle approach.

3.5 The characteristic equation

When a cycle is completely modelled using thermodynamic models as has been discussed in sub-sections 3.2.1 and 3.2.2, equations of non-linear structure result which can be difficult to solve, requiring equation solvers. To reduce this complexity, studies have been done in which a characteristic equation that fits absorption chiller catalogue data or experimental data[36, 37] is used.

The characteristic equation was derived by Albers et al.[36] to depict the part load behaviour of single-effect absorption systems. The derivation went through steady state formulation of heat transfer, mass and energy balance equations for the chiller components to arrive at a linear relationship between cooling capacity (Q_e) and the characteristic temperature function ($\Delta\Delta\mathrm{t}$) as in equation 3.16.

$$\Delta\Delta\mathrm{t} = Q_e\left(K_g + K_a + \left(K_c + K_e\right)B\right) + \left(K_{sg} + K_{sa}\right) \qquad (3.16a)$$

Where

$$\Delta\Delta\mathrm{t} = \left(\mathrm{t_g} - \mathrm{t_a}\right) - \left(\mathrm{t_c} - \mathrm{t_e}\right)B \qquad (3.16b)$$

When experimental or catalogue data representing the performance of a particular single-effect absorption chiller is available, constants K_g, K_a, K_c, K_e, K_{sg} and K_{sa} can be determined. B is a parameter that accounts for the different slopes of the boiling lines in the Dühring plot and its value under normal operating conditions is in the range 1.1 to 1.2 and does not change strongly[36].

Albers et al.[36] then used equation 3.16 together with the experimental data shown in Fig 3.4 and Fig 3.5 to obtain a relationship between cooling capacity and external cycle temperatures for a 10kW machine. For the shown data, a simple relation was obtained as shown in equation 3.17.

$$Q_E = 0.42 \cdot \Delta\Delta t' + 0.9 \qquad (3.17a)$$

Where

$$\Delta\Delta t' = t_G - 2.5 \cdot t_{AC} + 1.8 \cdot t_E \qquad (3.17b)$$

and t_G, $t_{A,}$ $t_{C,}$ t_E are arithmetic mean temperature values of inlet and outlet of the external water loops at the generator, absorber, condenser and evaporator, t_{AC} is the arithmetic mean temperature value of t_A and t_C while $\Delta\Delta t'$ is the adjusted characteristic temperature function obtained from equation 3.16b. Using equation 3.17, Fig 3.6 relating the cooling capacity to the derived characteristic function was obtained. More work concerning the use of the characteristic equation for the single-effect and double-effect absorption chillers has been done by Puig-Arnavat et al.[38].

Due to its simplicity, the characteristic equation can be of great help in overcoming the difficulties encountered through using some hard-to-solve nonlinear steady state and dynamic mathematical models. Moreover, it enables the consideration of part load behaviour of absorption chillers since experimental data and data in manufacture’s catalogues is taken into account. However, the characteristic equation can only be established for specific absorption chillers for which experimental performance data is available.

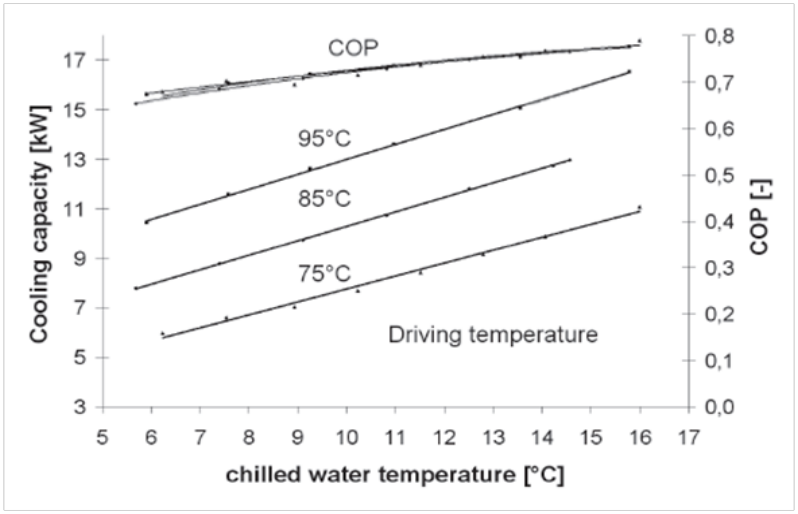


Fig 3.4: Cooling capacity and COP dependence on chilled water and driving heat temperatures[36]

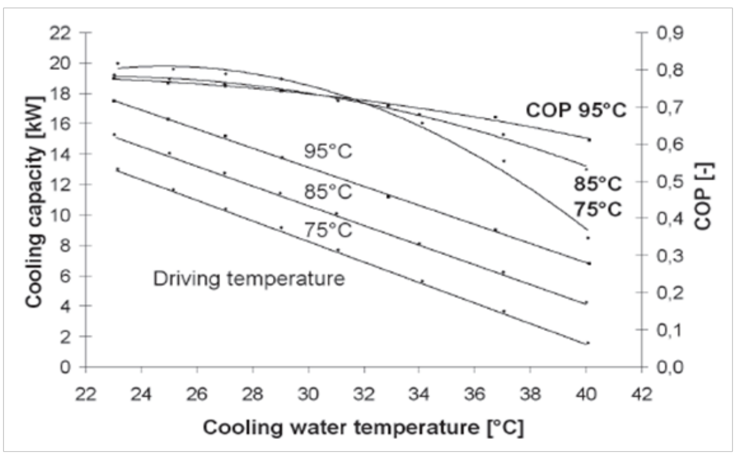


Fig 3.5: Cooling capacity and COP dependence on cooling water and driving heat temperatures[36]

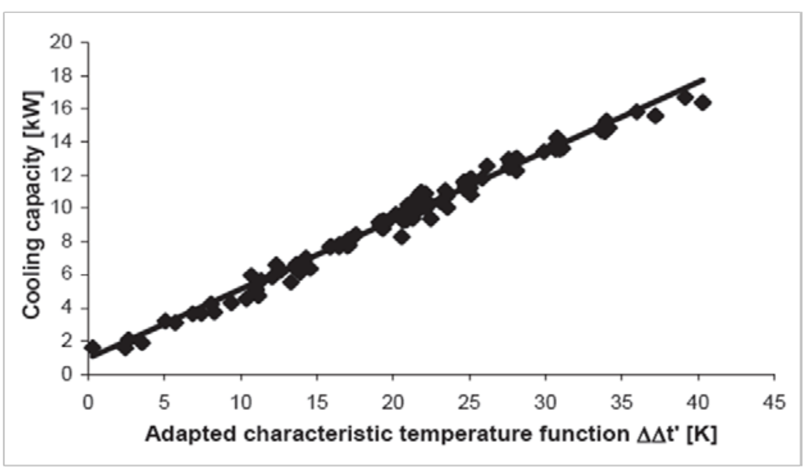


Fig 3.6: Characteristic plot of a 10kW single-effect absorption chiller[36]

3.6 Artificial neural network (ANN) models

More research has proposed that absorption machines can be modelled easily and accurately using artificial neural networks. Manohar et al.[39] presented an artificial neural network model for a double-effect absorption chiller and claimed chiller performance prediction with an error of $\pm$1.2%. The model employed the back propagation learning algorithm and 1000 experimental data sets were used to train the network.

Sencan et al.[40] on the other hand employed the artificial neural network approach to derive very simple expressions for determining the thermodynamic properties of LiBr-water and LiCl-water solutions for a single-effect absorption system. Enthalpy data derived from experiments done by other researchers was applied to train the network using the back propagation algorithm and a correlation coefficient of 0.999 was claimed.

Although ANN provide a simpler way of modelling absorption systems they require myriad experimental training data sets to achieve accuracy within the context of their application. Moreover, although Sencan et al.[40] tried to use enthalpy data obtained from experiments ANNs in general ignore physical modelling fundamentals and their accuracy can only rely on accurately executed experiments. Therefore unless otherwise utilised, ANNs would not elect as the modelling approach of first choice for MERIT.

3.7 Other models

A model capable of describing the behaviour of absorption cycles with a convenient number of characteristic constants for quick simulation of absorption systems was presented by Kim and Ferreira[41]. In their paper, the model was applied to several examples of single-effect absorption chillers using various working fluids but because of its many simplifications, it may not adapt well enough to reproduce the performance of commercial or experimental chillers.

The processes going on in the absorber and the generator are complex. Some studies have attempted to model the absorber and the generator[42, 43, 44] in detail to achieve greater accuracy. For the absorber the weak aqueous LiBr solution from the generator is sprayed over horizontal tubes in which cooling water flows, forming a falling film around the tubes. The water vapour from the evaporator is absorbed into the falling film solution as it flows around tubes. The resulting strong solution collects in the bottom of the absorber from where it is pumped back to the generator. In the generator, water vapour separates from the entering strong solution under the influence of external heat supply.

Detailed modelling of the absorber and the generator seeks to represent these process accurately using numerical methods to solve the resulting partial differential equations across an appropriately discretised mesh of the component. The absorber is commonly modelled as a falling-film heat exchanger[43, 45, 46]. In regard to modelling an absorption chiller in MERIT, this level of detail can be difficult to achieve because of the many nonlinear mass and energy balance equations that need to be solved simultaneously. Getting a correct solution to the nonlinear system of equations would necessitate a robust solver algorithm. Moreover this solver when applied to MERIT would need to be executed for hundreds of iterations at each time step, implying a greater memory requirement.

3.8 Conclusions

In this chapter absorption chiller models and modelling approaches have been presented. Since the focus of this study is to model a single-effect absorption chiller, other absorption chiller configurations were not considered. However, the same fundamentals of constructing heat and mass transfer and energy balance relationships apply to other absorption chiller cycle configurations.

In order to accurately predict the performance of single-effect absorption systems in MERIT; to typify their dynamic behaviour under various disturbances, under start-up, shut-down, part load and periodic operations, a realistic mathematical modelling approach is required. The models presented in this chapter, apart from the first most basic model; provide sufficient modelling ability for absorption chillers but for application in MERIT, they display various challenges.

Two kinds of mathematical models are needed in MERIT: a mathematical model capable of determining the cooling capacity and COP achievable from an amount of available heat supply under a specified cooling water inlet temperature into the absorber; another to determine the amount of driving or supply heat required and the COP achievable for an amount cooling demand and cooling water inlet temperature into the absorber. Also, it was desirable that these models are generic and applying to any capacity or size of single-effect absorption chillers.

One real challenge lies in forming a generic mathematical model capable of simulating all capacities or sizes of single-effect absorption chillers. A literature survey on absorption chiller modelling and existing commercial and open source packages for absorption chiller simulation shows that no generic mathematical model exists.

However, the approach of forming mathematical expressions through curve fits of performance data from manufacturing catalogs or reliable experimental data has been adopted [36, 38, 47] and used in TRNSYS. However, this requires a supporting database to hold the different commercial absorption chiller performance characteristics from different manufacturers.

It is therefore not possible to make a conclusion that any of the models presented in this chapter can meet the modelling needs specific to MERIT. If not a novel one, any of the models presented here would have to be adapted and reengineered in some way to make it compatible with the fundamental purpose of MERIT. This is what the next chapter is about.

The steady state model with heat transfer across external fluids was adapted. It was coded into Engineering Equation Solver (EES) and executed several times for several runs to generate sufficient data representing the characteristics of the thermodynamic heat transfer models, mass and energy balance models, and thermophysical properties of the working pair.

Chapter 4

Model Development, Implementation and Application

4.1 Introduction

This chapter is a presentation of the outcomes of this thesis. It begins with drawing the reader's attention to the nature of mathematical models used for accomplishing simulations in MERIT before undertaking a detailed description of the developed absorption chiller models. Validation results of the developed absorption chiller models against the actual physical model solved using EES are presented. These models are then implemented using Microsoft Visual Studio C++, the integrated development environment for MERIT to allow absorption chiller simulations.

4.2 The software development concept for MERIT

The approach taken by this thesis in obtaining the suitable single-effect absorption chiller models for simulating the absorption chiller can be easily followed by first understanding the premise on which software development for MERIT is based. It is focused on ensuring that a wide range of energy technologies are made available in the MERIT user interface to aid the accomplishment of unlimited demand and supply matching simulations. In the core program code, simple explicit mathematical models are implemented to represent the performance behaviour of specific energy technologies.

Thus the models used to model energy technologies in MERIT take the form of high level mathematical statements that can describe the output of a particular energy technology given certain inputs. Moreover, MERIT computation capabilities are not limited to this. Algorithms for accomplishing permutations and comparisons of various choices of technology combinations have been implemented and are executed when energy supply and demand profile combinations are selected.

The simulations of absorption chillers based on the theoretical physical model however entail solving a large system of simultaneous equations, a capability MERIT lacks. An attempt to implement a solver algorithm for absorption chillers in MERIT may lead to a need to overhaul the entire package as well as its design philosophy. Therefore, the problem of developing a model describing the behaviour of any energy technologies for inclusion in MERIT should be in line with the software development philosophy for

MERIT. Therefore in the development of the single-effect absorption chiller simulation models presented in this thesis, it was necessary to adhere to this strict condition so that the developed models would be compatible with the existing programming structure.

4.3 Assumptions on operating conditions and machine parameters

In order to arrive at the models presented here, it was assumed that if the physical-mathematical models presented under subsection 3.2.2 are coded into EES and solved at various operating temperatures, an operating map is generated. Appropriate curve fits representing the general characteristics of the system of mass, energy balance and heat transfer models and the thermophysical properties of the working pair can then be formed from this operating map.

Following the above assumption, a system of 100 equations composed of mass balance, energy balance and heat transfer expressions were coded in EES and solved simultaneously over a range of inputs as will be described in the specific sections of each model. The single-effect absorption chiller parameters and operating conditions assumed and used in this thesis were adopted from Harold et al.[13] and are as shown in Table 4.1 and Table 4.2.

Parameters	*Value*
Condenser UA	1.2 kW/K
Evaporator UA	2.25 kW/K
Absorber UA	1.8 kW/K
Generator UA	1.0 kW/K
Solution heat exchanger effectiveness	64%

Table 4.1: Chiller parameters

Parameters	*Value(kg/s)*
Cooling water flow rate	0.28
Chilled water flow rate	0.4
Hot water flow rate	1.0
Strong solution flow rate	0.05

Table 4.2: Chiller operating conditions

4.4 Model development

Two kinds of simulation models were required which would ultimately be included in MERIT as two absorption chiller operation modes. Mode 1, to predict the cooling load achievable from an amount of available waste heat for a specified cooling water temperature and mode 2 to predict the amount of driving or supply heat required to meet an amount of cooling load at a specified cooling water temperature. In both cases, the cooling load and the driving heat could be time varying profiles. The next sections present the explicit mathematical models developed using results obtained by solving the physical-mathematical models described in subsection 3.2.2 in EES.

4.4.1 Explicit models for mode 1

This simulation mode determines the generator driving heat supply required to meet a specified cooling demand at a specified cooling water temperature. The first step was to simulate the physical models in EES and the second was to use the data generated by EES to construct explicit expressions. To obtain the data for this mode the variables of interest i.e. COP, generator temperature, cooling water temperature, lithium bromide concentrations, cooling capacity, chilled water temperature and generator heat input were arranged into a parametric table in EES. For this mode, the chilled water supply temperature was maintained at 6^{o}C as generator and cooling water temperatures were varied.

For each round of parametric table runs in EES, the generator driving heat temperature was varied between 90°C and 100°C while the cooling water temperature was varied from 24°C and 31°C because within this range, aqueous LiBr concentrations of the weak and strong solutions would stay in the range 50% to 65% thus avoiding entering the crystallisation limit. 2338 data sets were obtained. These data sets were transferred into MATLAB curve fitting toolbox to obtain the following explicit surface-fitting models:

$$t_g = a_0 + a_1 Q_e + a_2 t_c \quad {}^{*}\mathbf{R^2 = 0.6261} \tag{4.1a}$$

where Q_e is the cooling load (in kW) to be met by the absorption chiller, t_g is the generator heat supply temperature, t_c is the cooling water temperature; and

$24°\mathrm{C} < t_c < 31°\mathrm{C}$ and $4\,\mathrm{kW} < Q_e < 12\,\mathrm{kW}$.

Using equation (4.1a), the required generator heat input temperature to satisfy a known cooling load at a known cooling water temperature can be calculated. Once t_g is calculated it is used together with t_c in the calculation of *COP* as given by,

$$COP = b_0 + b_1 t_c + b_2 t_g + b_3 t_c^2 + b_4 t_c t_g\,,\ (95°\mathrm{C} < t_g < 100°\mathrm{C}) \quad {}^{*}\mathbf{R^2 = 0.9995} \tag{4.1b}$$

$$COP = c_0 + c_1 t_c + c_2 t_g + c_3 t_c^2 + c_4 t_c t_g + c_5 t_g^2\,,\ (94°\mathrm{C} < t_g < 95°\mathrm{C}) \quad {}^{*}\mathbf{R^2=0.9929} \tag{4.1c}$$

$$COP = d_0 + d_1 t_c^2 + d_2 t_c^3 t_g\,,\ (92°\mathrm{C} < t_g < 94°\mathrm{C}) \quad {}^{*}\mathbf{R^2 = 0.9246} \tag{4.1d}$$

$$COP = k_0 t_c t_g + k_1 t_c^2 t_g\,,\ (90°\mathrm{C} < t_g < 92°\mathrm{C}) \quad {}^{*}\mathbf{R^2 = 0.9415} \tag{4.1e}$$

Values of the constants a_n, b_n, c_n, d_n and k_n are given in Table 4.3.

Once the COP is calculated, the quantity of heat input into the generator required to meet the cooling load can be determined by the relation,

$$Q_g = \frac{Q_e}{COP} \tag{4.1f}$$

index	*0*	*1*	*2*	*3*	*4*	*5*
a_n	-0.6714	3.986	2.171	-	-	-
b_n	2.965	-0.06561	-0.02557	-0.0005307	0.0009152	-
c_n	18.6	-0.1013	-0.3469	-0.001199	0.001731	0.001578
d_n	0.6262	0.0005581	-0.0000001692	-	-	-
k_n	0.0006114	-0.00001176	-	-	-	-

Table 4.3: Values of constants used in for equations 4.1

4.4.2 Explicit models for mode 2

This simulation mode determines the cooling load that can be supplied from a specified amount of driving heat for a specified cooling water temperature. Here, the physical models were simulated in EES by varying the chilled water supply set point from 2.5ºC to 6ºC with fixed generator heat supply temperature of 90ºC. 795 data sets were obtained. These data sets were transferred into MATLAB curve fitting toolbox to obtain the following explicit surface-fitting models:

$$t_e = p_0 + p_1 Q_g + p_2 t_c + p_3 Q_g t_c + p_4 t_c^2 + p_5 Q_g t_c^2 + p_6 t_c^3, \ {}^*\mathbf{R^2 = 0.9999} \tag{4.2a}$$

where Q_g is the driving heat supply to the absorption chiller (in kW), t_e is the chilled water supply temperature, t_c is the cooling water temperature; and

$$24°\text{C} < t_c < 31°\text{C} \quad \text{and} \quad 8\,\text{kW} < Q_g < 12\,\text{kW}$$

With equation (4.2a), the chilled water supply temperature that can be delivered by the absorption chiller for a known quantity of heat input and cooling water temperature can be calculated. Once t_e is calculated it is used together with t_c in the calculation of *COP* as given by,

$$COP = q_0 + q_1 t_e + q_2 t_c + q_3 t_e^2 + q_4 t_c t_e + q_5 t_c^2 + q_6 t_c t_e^2 + q_7 t_c^2 t_e + q_8 t_c^3 \text{, } ^*\mathbf{R^2 = 1} \quad (4.2b)$$

where

$$3°C < t_e < 14°C \text{.}$$

Values of the constants p_n and q_n are given in Table 4.4.

Once the COP is calculated, the cooling load that can be supplied for a known heat input and cooling water temperature can be determined by the relation,

$$Q_e = Q_g \cdot COP \qquad (4.2c)$$

index	*0*	*1*	*2*	*3*	*4*	*5*	*6*	*7*	*8*
p_n	-91.36	3.521	2.608	-0.01412	-0.01537	1.16E-5	1.049E-4	-	-
q_n	0.988	1.964E-2	-2.878E-2	5.53E-4	-1.479E-3	1.219E-3	-2.415E-5	3.86E-5	-2.134E-5

Table 4.4: Values of constants used in equations 4.2

4.5 Significance of these simulation models

Steady state simulations and theoretical performance studies of single-effect absorption chillers have been performed by many researchers as has been reviewed in chapter 3. However the interest in these studies is often focused at analysing the effect of various machine parameters on performance. For example the temperature at which heat is supplied to the generator is altered to see how this may impact on COP and cooling capacity. Although this type of analysis can be handy for performing various studies, it can not be applied to MERIT in this way because it involves solving many equations simultaneously which would necessitate an equation solver.

Simulations in MERIT are based on simpler explicit mathematical models that relate one or more independent variables to a single output variable. Thus the models presented in the preceding sections can accomplish a big step as far as simulation of a single-effect absorption chiller in MERIT is concerned.

4.6 Verification of the model results against EES results

The explicit mathematical models presented in the previous sections were verified against the results obtained from the EES physical model and the obtained results were comparable and are discussed in the next sections.

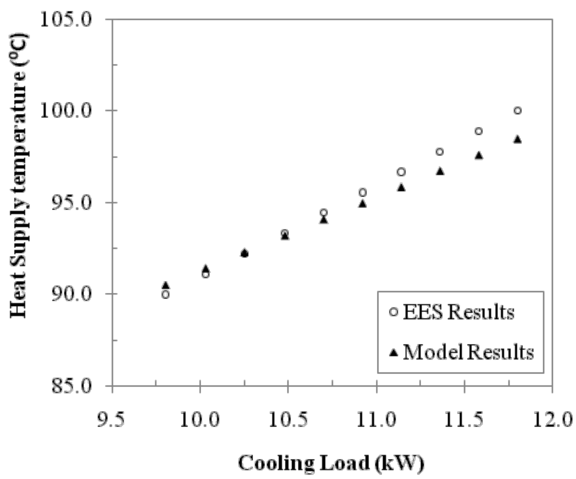
4.6.1 Models for mode 1

Mode 1 predicts the generator heat input required to meet a specified cooling load with cooling water temperature as the operating condition. To achieve this, the temperature at which the heat must be supplied to the generator is calculated first as an intermediate variable from the provided cooling load profile at a known cooling water temperature.

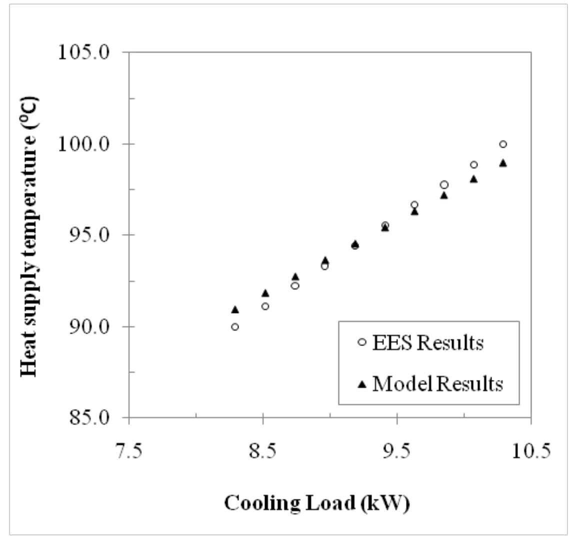
Prediction of generator heat input temperature

Fig 4.1 is a comparison of prediction results obtained with EES and the explicit mathematical model of equation 4.1a. Three different cooling water temperatures are considered with the chilled water supply temperature set to 6^{o}C in all cases.

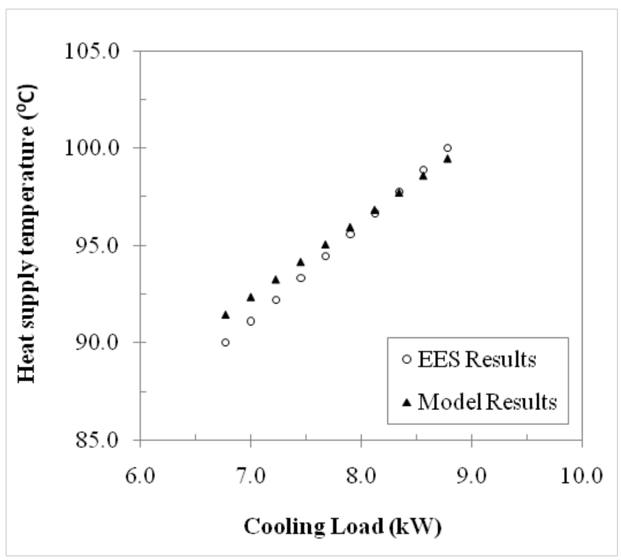
With both models, an almost perfectly linear relationship is displayed between the variables and both models show that higher cooling loads can be satisfied by an absorption chiller when operated at low cooling water temperatures for the same generator heat supply temperature.



(a) Cooling water temperature (24^oC) and chilled water supply temperature (6^oC).



(b) Cooling water temperature (27^oC) and chilled water supply temperature (6^oC).



(c) Cooling water temperature (30^oC) and chilled water supply temperature (6^oC).

Fig 4.1: Comparison of prediction of generator heat input temperature

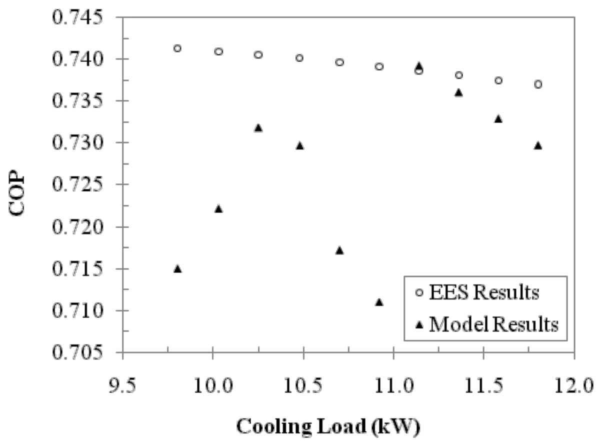
In Fig 4.1a, the model results closely compare with EES results at low cooling loads, converge at some value of cooling load and then diverge off predicting low values with an error of about 1% as compared to EES results. This same behaviour is seen to persist at cooling water temperatures of 27°C and 30°C as shown in Fig 4.1b and Fig 4.1c respectively with Fig 4.1b showing the closest match between the two models. This behaviour can be largely attributed to the poor correlation that was obtained for equation 4.1a.

Prediction of coefficient of performance

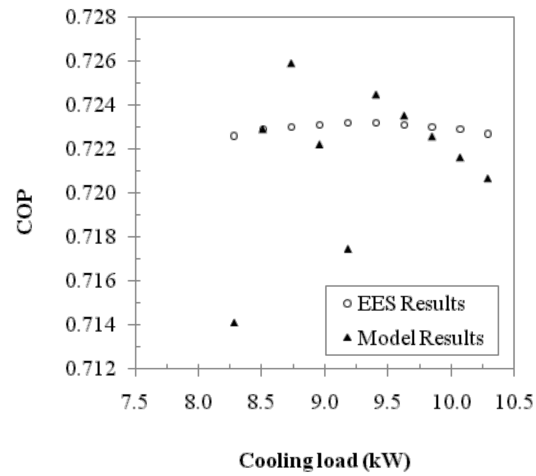
Once the generator input temperature is calculated, it is used together with cooling water temperature to predict the COP at which the cooling load would be met. Because the data obtained from EES had numerous discontinuities and divergences, it was divided into 4 groups in which the data pattern was systematic to obtain 4 COP expressions shown in equations 4.1b through 4.1e.

Fig 4.2 is a comparison of prediction results obtained with EES and the explicit mathematical relations stated in equations 4.1b through 4.1e. Again three different cooling water temperatures are considered with the chilled water supply temperature set to 6°C in all cases.

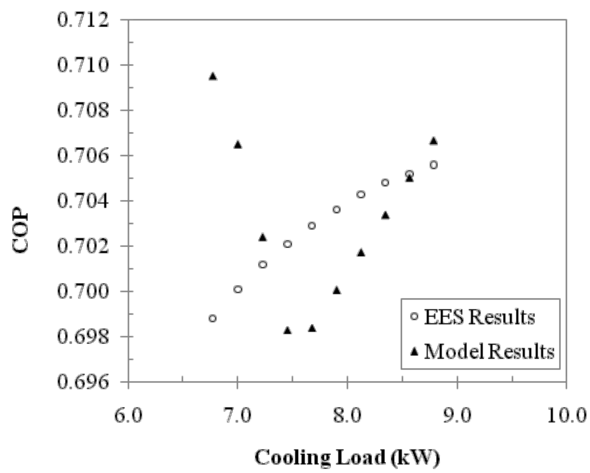
For small cooling loads at cooling water temperature of 24°C (Fig 4.2a) the developed mathematical model does not predict accurately with a maximum error of 3.9%. The maximum prediction error becomes 1.2% at cooling water temperature of 27°C (Fig 4.2b) and 1.5% at cooling water temperature of 30°C (Fig 4.2c).



(a) Cooling water temperature (24^oC) and chilled water supply temperature (6^oC).



(b) Cooling water temperature (27^oC) and chilled water supply temperature (6^oC).

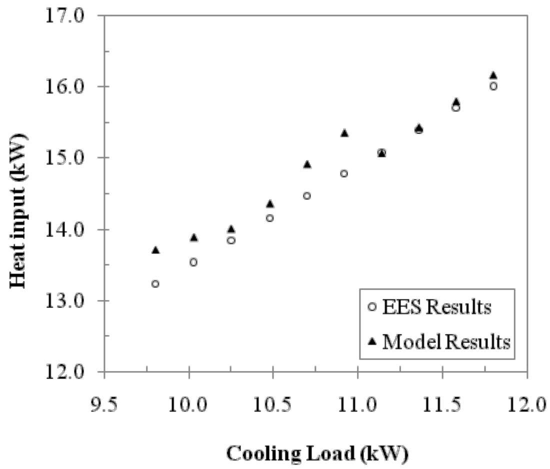


(c) Cooling water temperature (30^oC) and chilled water supply temperature (6^oC).

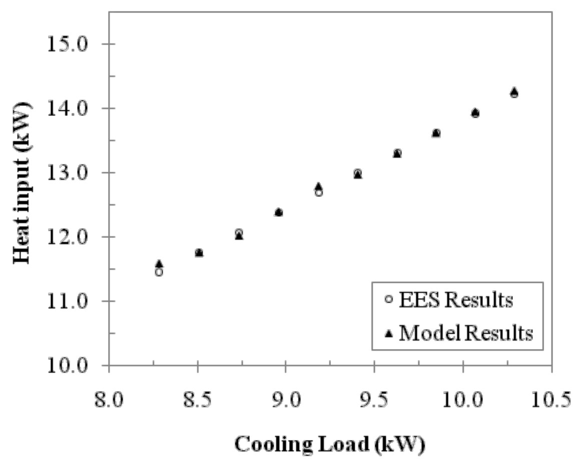
Fig 4.2: Comparison of prediction of COP

Prediction of quantity of generator heat input

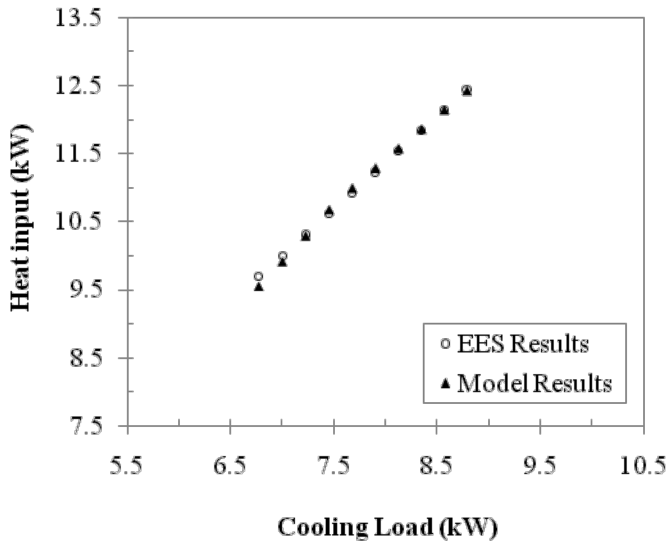
With the COP calculated in subsection 4.4.2, the quantity of generator heat input is calculated using equation 4.1f to generate the results shown in Fig 4.3. It can be seen that although COP looked so dispersed in Fig 4.2, good agreement is obtained between results from the developed model and EES at cooling water temperature of 27^{o}C (Fig 4.3b) and 30^{o}C (Fig 4.3c). The poor prediction at low cooling loads for the cooling water temperature of 24^{o}C is more vivid in Fig 4.3a with a maximum error of 3.7%.



(a) Cooling water temperature (24^{o}C) and chilled water supply temperature (6^{o}C).



(b) Cooling water temperature (27^{o}C) and chilled water supply temperature (6^{o}C).



(c) Cooling water temperature (30^{o}C) and chilled water supply temperature (6^{o}C).

Fig 4.3: Comparison of prediction of generator heat input

4.6.2 Models for mode 2

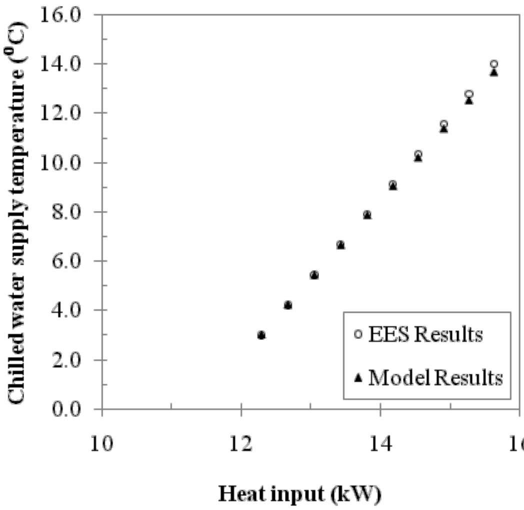
This mode predicts the cooling load that can be satisfied by a specified amount of heat input into the generator with cooling water temperature as the operating condition. To achieve this, the chilled water supply temperature is calculated first as an intermediate variable using the provided heat input profile and the known cooling water temperature as independent variables.

Prediction of chilled water supply temperature

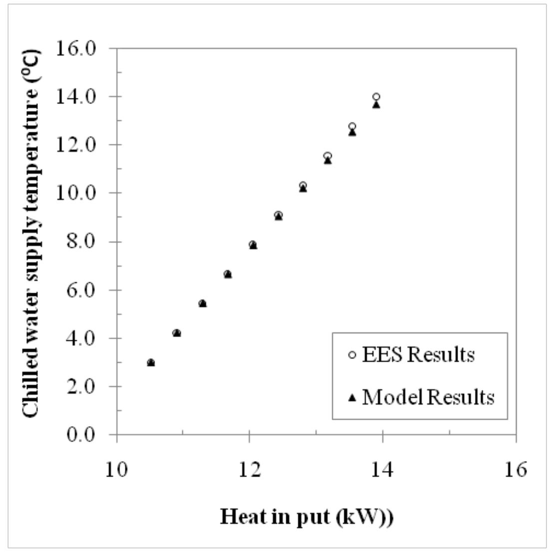
Fig 4.4 compares chilled water supply temperature prediction results obtained with EES and the explicit mathematical model of equation 4.2a. Three different cooling water temperatures are considered with the generator heat input temperature set to 90°C in all cases.

Both the physical model results from EES and the results from equation 4.2a show a linear relationship between the variables. For each individual graph, it can be seen that for a fixed cooling water supply temperature, as the heat input increases the chilled water temperature also increases. This trend is valid for single-effect absorption chillers due to the tendency for them to become unstable at high generator temperatures which increase the risk of crystallisation. As the heat input increases, more effective cooling of the absorber and the condenser are required if the machine is to continue operating properly. Under the assumptions made during the development of the explicit models, it can be seen that if the cooling water temperature is higher, and all mass flow rates remain constant, the heat input should be decreased to avoid the overheating of the absorber and condenser as well as the risk of crystallisation at the exit of the solution heat exchanger.

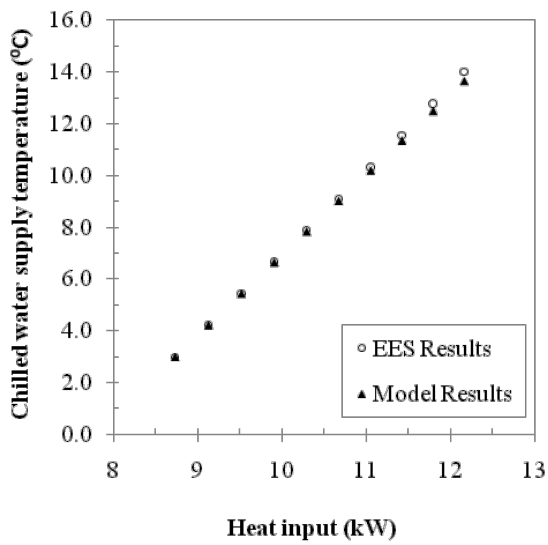
Fig 4.5 further reinforces the fact that lower cooling water temperatures result in a higher coefficient of performance and Fig 4.6 sums up by showing that higher cooling loads can be satisfied by an absorption chiller when operated at low cooling water temperatures for the same generator heat supply temperature.



(a) Cooling water temperature (24^oC) and generator heat supply temperature (90^oC).



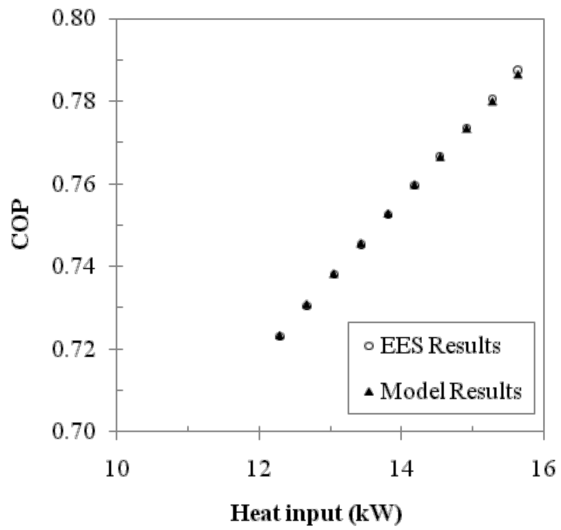
(b) Cooling water temperature (27^oC) and generator heat supply temperature (90^oC).



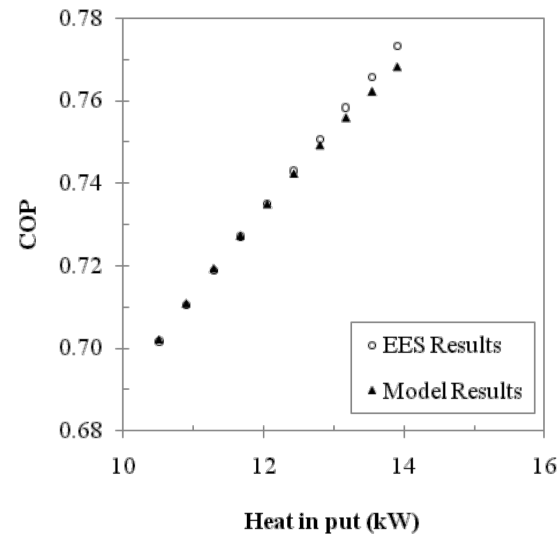
(c) Cooling water temperature (30^oC) and generator heat supply temperature (90^oC).

Fig 4.4: Comparison of prediction of generator heat input

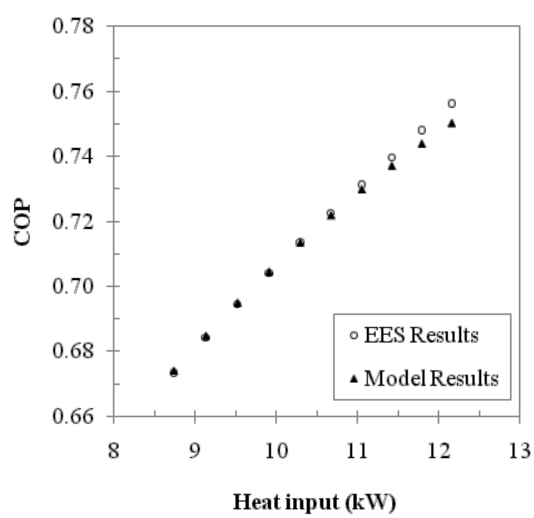
Prediction of coefficient of performance



(a) Cooling water temperature (24^{o}C) and generator heat supply temperature (90^{o}C).



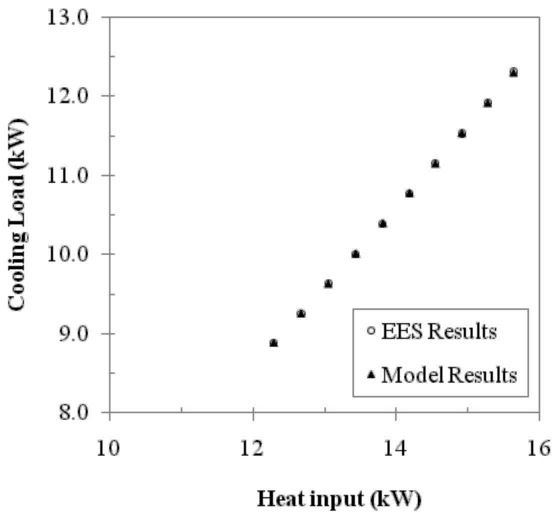
(b) Cooling water temperature (27^{o}C) and generator heat supply temperature (90^{o}C).



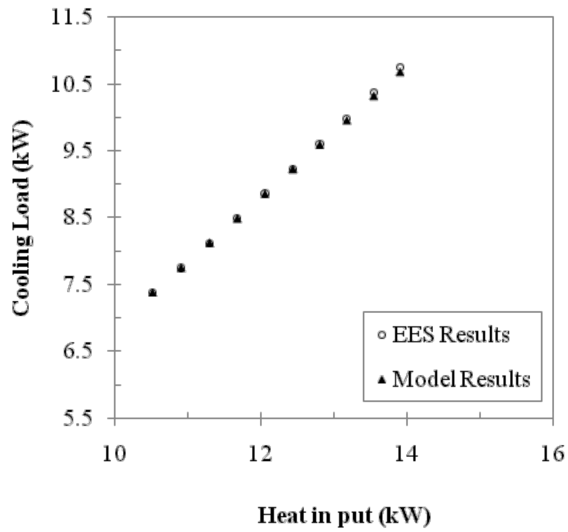
(c) Cooling water temperature (30^{o}C) and generator heat supply temperature (90^{o}C).

Fig 4.5: Comparison of prediction of COP

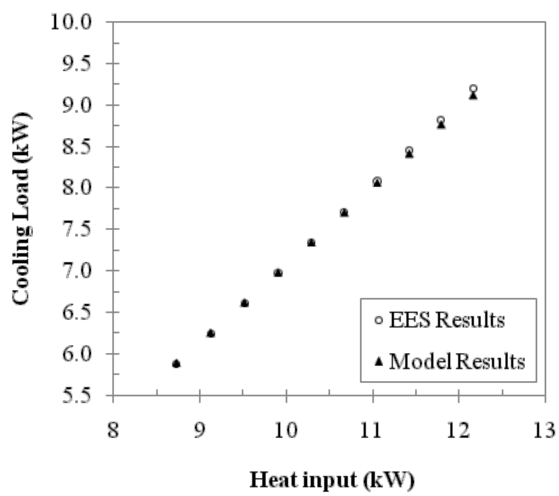
Prediction of quantity of cooling capacity



(a) Cooling water temperature (24°C) and generator heat supply temperature (90°C).



(b) Cooling water temperature (27°C) and generator heat supply temperature (90°C).



(c) Cooling water temperature (30°C) and generator heat supply temperature (90°C).

Fig 4.6: Comparison of prediction of cooling capacity

4.7 Implementation and simulation results

The two modes have been implemented in MERIT to expand on the auxiliary energy supply technologies available to users. Based on the developed mathematical models, an 8kW single-effect absorption chiller was implemented. Implementation was done using Microsoft Visual C++, the programming IDE for MERIT.

Three operation modes were implemented as "standard mode", "follow heating" and "follow cooling". The standard mode provides the most basic simulation option where the coefficient of performance and all the heat flows are assumed constant through time. This idealistic option was provided in the user interface but not implemented – so it is currently not operational. Focus was directed toward the remaining two modes.

Like any other simulation in MERIT, the simulation period needs to be selected first. This can be any period ranging from hours to years as required by the user but a shorter period is much better to allow for visual clarity and less computation time. Depending on which absorption chiller operating mode the user is interested in, either a demand/cooling load profile or a heat supply profile is selected next. The single-effect absorption chiller can then be loaded by selecting it from the list of technologies available under the CHP auxiliary tab. For the results presented in this thesis a simulation period of two weeks of May from 01/05/1972 to 14/05/1972 was used.

4.7.1 Implementation and simulation results for the follow heating mode

The follow heating mode provides the option for viewing the cooling capacity profile that can be derived from any selected heat supply profile. Because of the risk of freezing the chilled water supply pipe work, the chilled water temperature is not allowed to go below 3^{o}C and for useful cooling to be accomplished, it is not allowed to go above 14^{o}C.

Fig 4.7 is the implementation concept diagram showing the inputs required, the intermediate variables calculated within the program and the output. Q_g is the heat supply profile that must be input by the user and Q_e is the output cooling effect that is predicted by the model.

For the *follow heating* mode, the user loads the cooling load profile, the heat supply profile and the single-effect (SE) absorption chiller into the thermal match view interface (Fig 4.8). The single-effect absorption chiller is then selected together with the heat supply profile to predict the cooling effect that can be provided by the absorption chiller running on the selected heat supply profile (Fig 4.9). This predicted cooling effect profile can then be matched with the known cooling load profile from any facility (Fig 4.10).

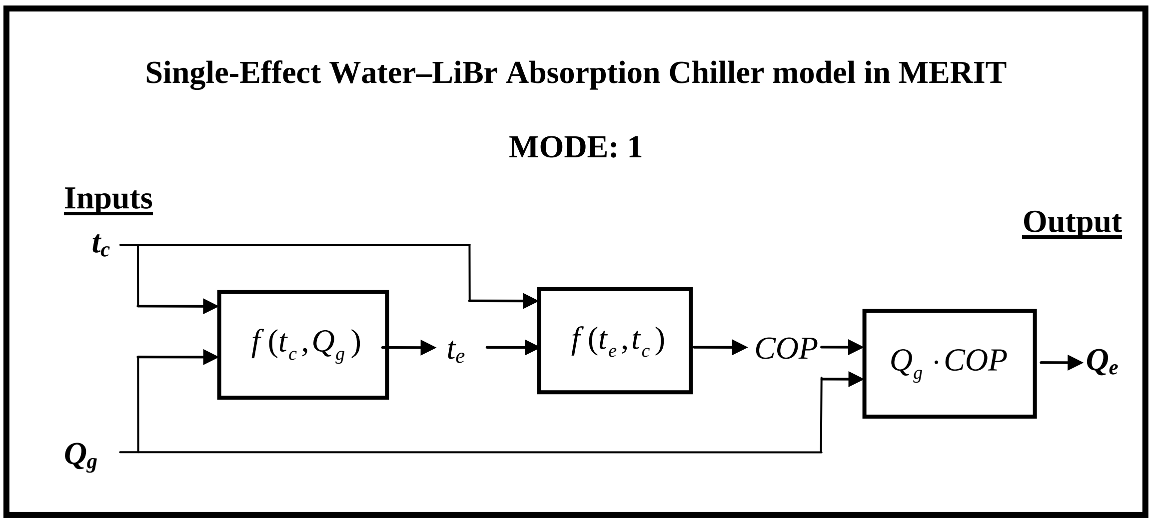


Fig 4.7: Implementation concept for mode 1 (Follow heating)

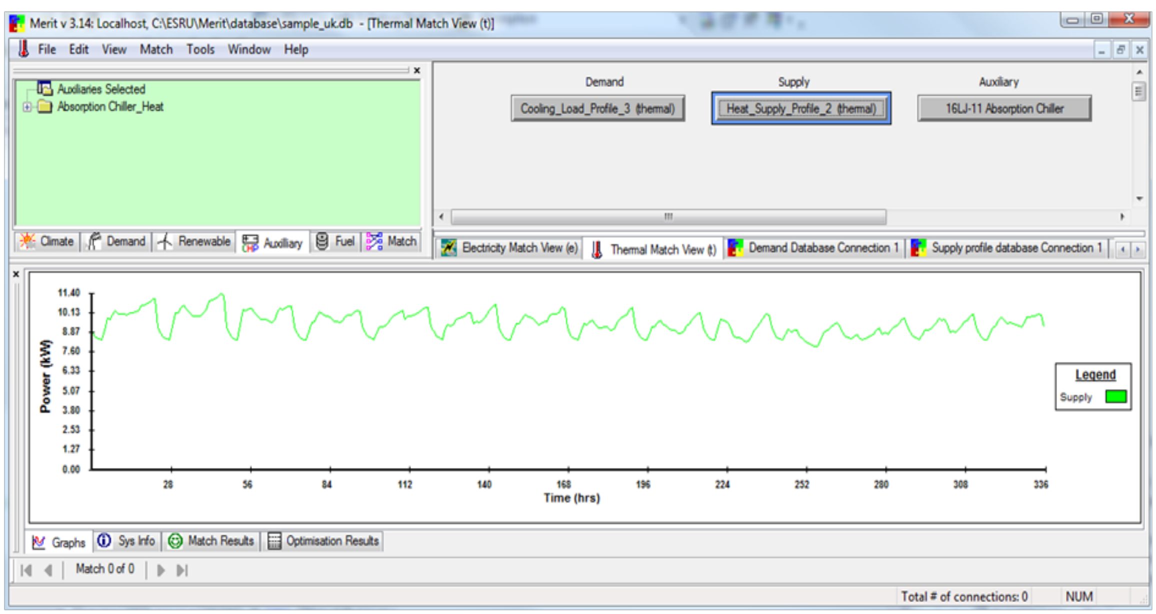


Fig 4.8: Thermal profiles (cooling load and heat supply profiles) and the 8kW SE absorption chiller

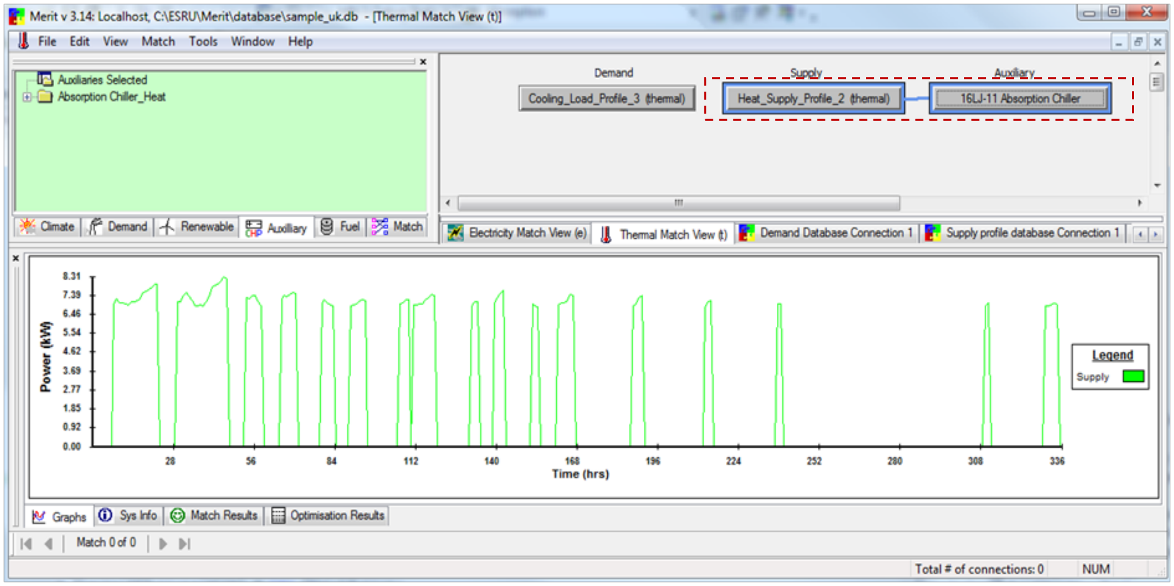


Fig 4.9: Cooling effect predicted by using the 8kW SE absorption chiller

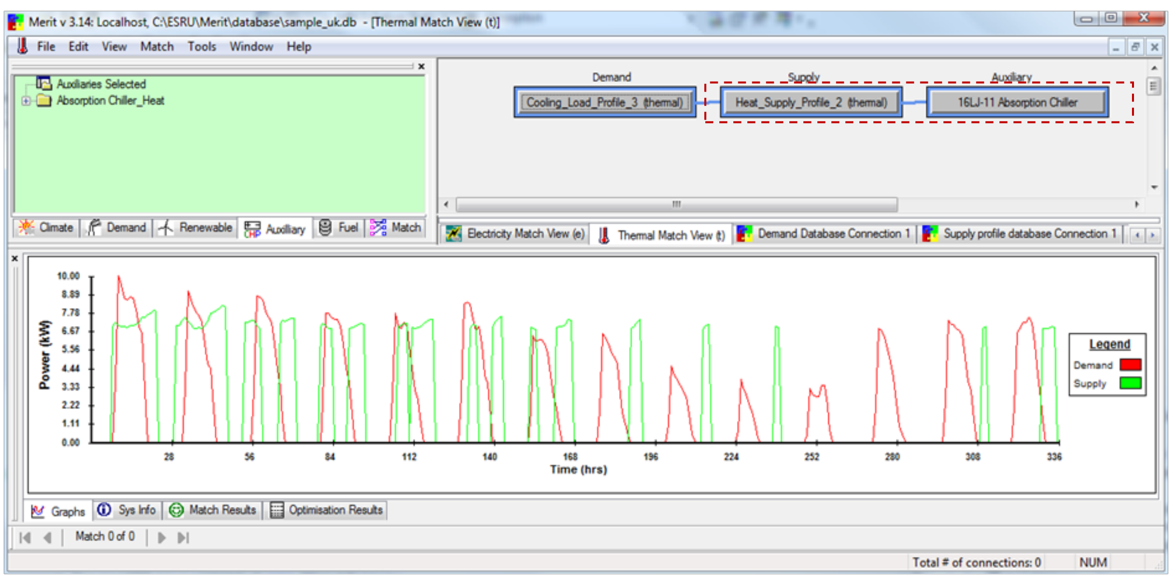


Fig 4.10: Graphical match between the predicted cooling effect and the actual cooling demand

Discussion of mode 1 (follow heating) results

The discussion focuses on Fig 4.9 and Fig 4.10. In Fig 4.9 the cooling effect delivered by the 8kW SE absorption chiller under the follow heating operating mode is shown. This profile is calculated by MERIT upon selecting the heat energy supply profile and the absorption chiller together. Because the heat energy available at certain times is very low, the absorption chiller is switched off at these times which results in gaps on the graph. The calculated cooling effect profile can be matched against the cooling energy demand as shown in Fig 4.10. MERIT calculates additional parameters as shown in Table 4.5 to give a clearer picture on how well the heating energy profile can meet cooling demand while using the 8kW SE absorption chiller.

Parameter	**Value**
Total cooling demand (kWh)	722.46
Total AuxSupply (kWh)	731.13
Match Rate (%)	46.22
Correlation Coefficient (-)	0.15
Energy Delivered (kWh)	263.94
Energy Surplus (kWh)	453.74
Energy Deficit (kWh)	445.70

Table 4.5: Computed values relating to Fig 4.10

Here, display of the heating energy contained in the heat supply profile shown in Fig 4.8 is not provided but this value can easily be obtained by selecting it together with the cooling demand profile. When this is done, 3.18 MWh of heat energy supply is obtained. So out of 3.18 MWh of heat energy supply, Table 4.5 shows that 731.13 kWh of cooling effect can be supplied by the 8kW SE absorption chiller. This information is however not sufficient to calculate the COP since some of the heat energy is not used.

Nevertheless, information in Table 4.5 can be used to perform the heat energy supply technology appraisal. In this particular example, the heat energy supply technology is not good because with it, only 263.94 kWh of useful cooling is delivered, and 453.74 kWh of cooling is actually wasted leaving a deficit of 445.70 kWh.

4.7.2 Implementation and simulation results for mode 2 (follow cooling)

In the case of the *follow cooling* mode, MERIT predicts the heat supply profile that will be required to meet any selected cooling load profile. Because of the risk of crystallisation the heat supply temperature is not allowed to exceed 100°C and to ensure continuous operation of the single-effect absorption chiller, it is not allowed to go below 75°C.

In addition, it is important to recognise that if any absorption chiller was set to operate in the *follow cooling* mode, it would only follow to a certain extent. It would go off for very low cooling loads because it can only be under loaded by a small percentage below its rated capacity but it would only be overloaded by a small percentage above its rated capacity. For purposes of this simulation cooling load fluctuation was allowed at 20% for both under load and overload. Thus, an 8kW rated SE absorption chiller was assumed to operate continuously under the *follow cooling* mode as long as the cooling load profile stays equal or greater than 6.4kW. For the case of operation above rated capacity, the 8kW SE absorption chiller delivers only up to 9.6kW.

Fig 4.11 is the implementation concept diagram showing the inputs required, the intermediate variables calculated within the program and the output. Q_e is the cooling load profile that must be input by the user and Q_g is the heat supply profile predicted by the model.

The user loads the cooling load profile, the heat supply profile and the single-effect absorption chiller into the thermal match view interface. Unlike in the *follow heating* mode, selecting the absorption chiller under this mode, displays 2 buttons (shown inside the red dots in Fig 4.12) into the thermal match view interface. The absorption chiller button in the auxiliary column of the thermal match view interface simulates the mathematical models while the absorption chiller button in the demand column of the thermal match view interface displays the predicted heat profile which is required to meet the cooling load profile.

When the cooling load profile button is selected together with the absorption chiller button under the auxiliary column (Fig 4.13), the *follow cooling* mode is simulated and data representing the heat profile required to meet the selected cooling load profile is saved into the data base. This data is retrieved by selecting the absorption chiller button under the demand column of the thermal match view interface (Fig 4.14) to allow the user perform another simulation to select appropriate heat supply technologies represented by buttons under the supply column of the thermal match view interface (Fig 4.15).

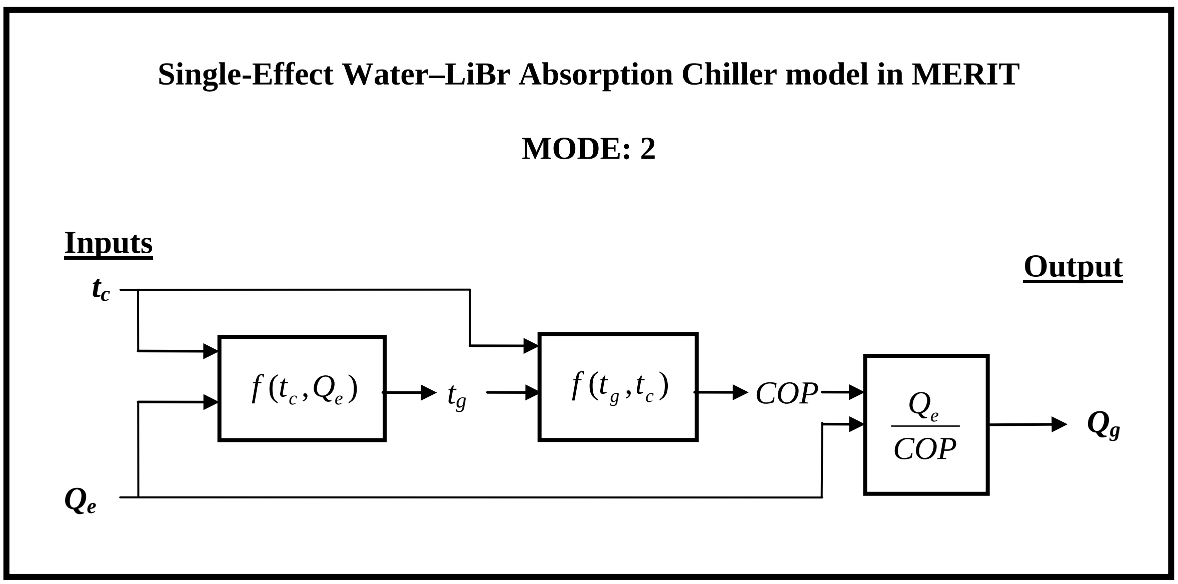


Fig 4.11: Implementation concept for mode 2 (Follow cooling)

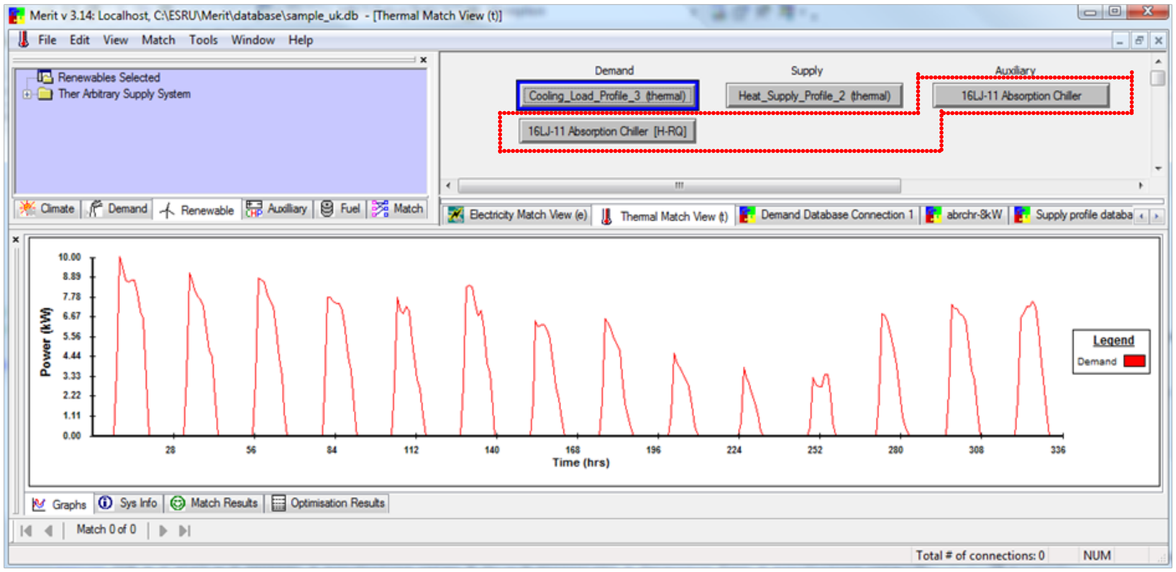


Fig 4.12: Thermal profiles (cooling load and heat supply profile) and the 8kW SE absorption chiller

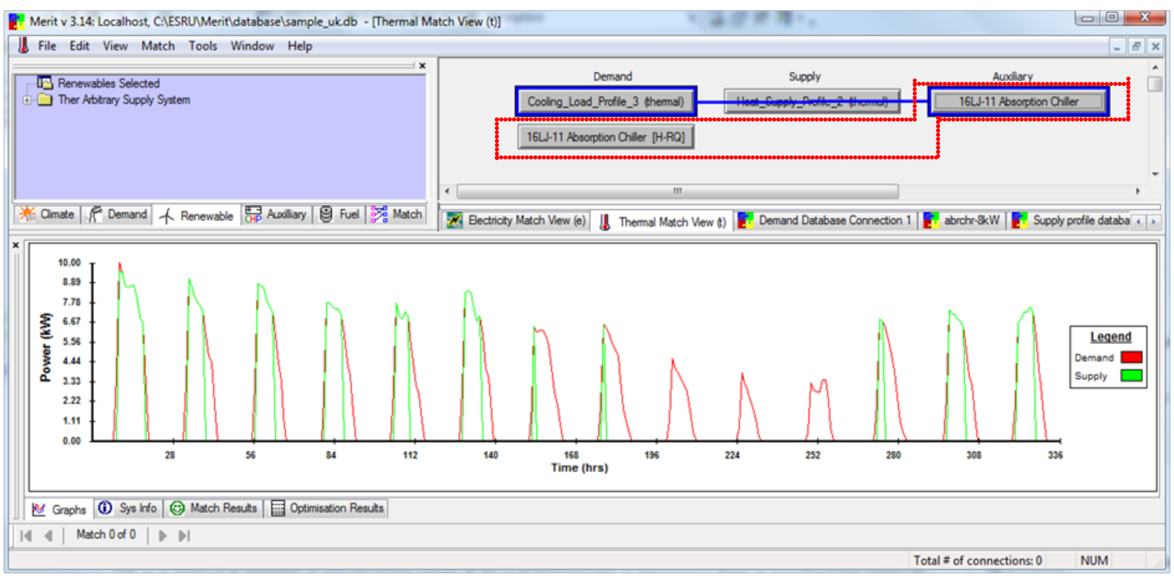


Fig 4.13: Cooling load following capability of the 8kW SE absorption chiller

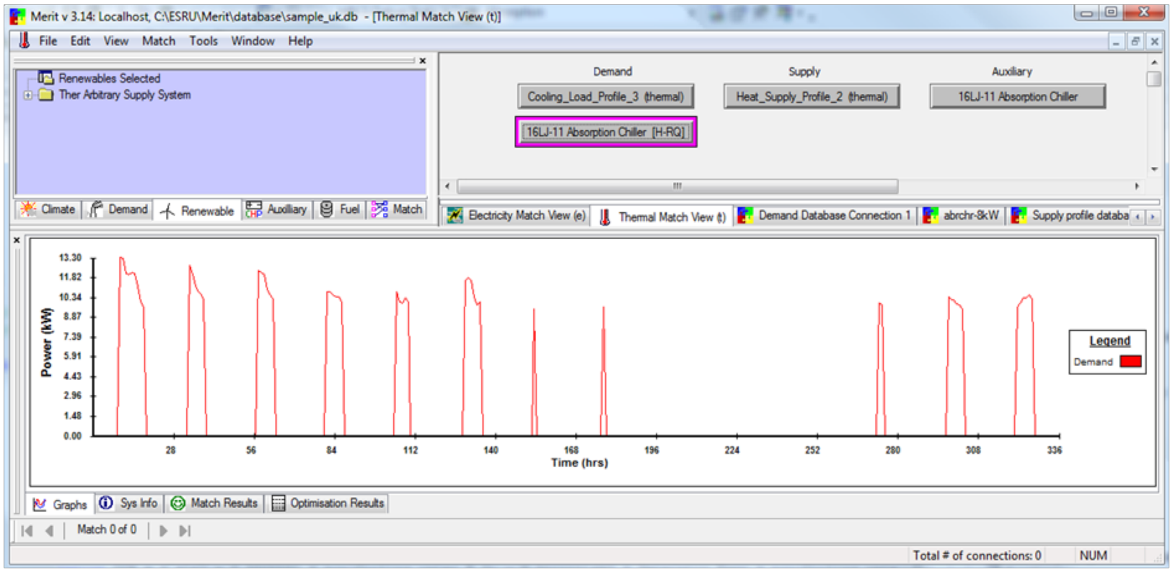


Fig 4.14: Heat profile predicted by using the 8kW SE absorption chiller

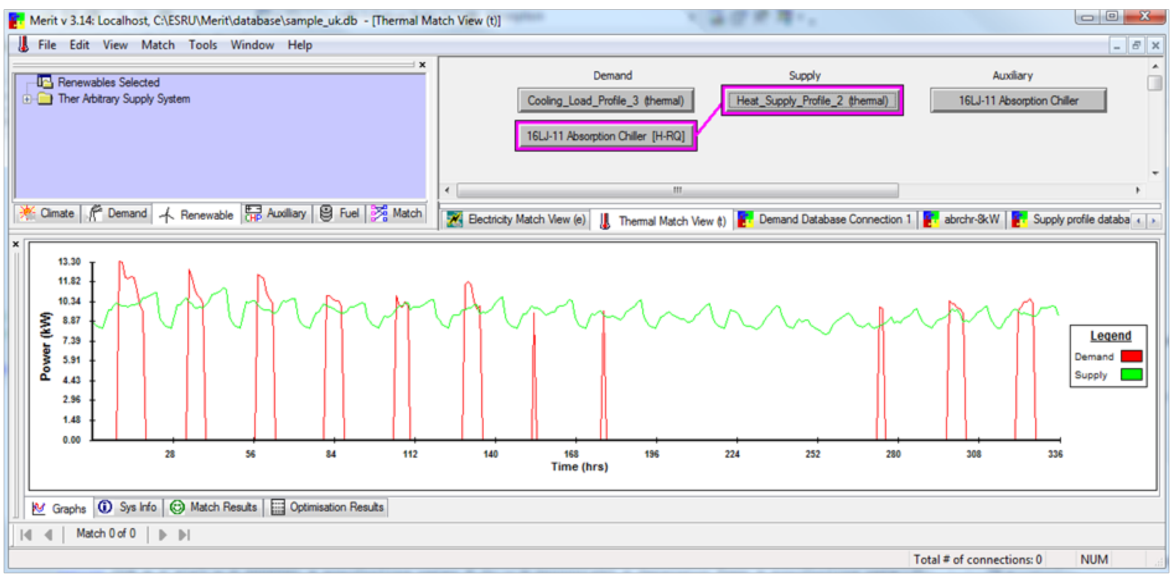


Fig 4.15: Graphical match between the predicted heat profile and the available heat supply

Discussion of mode 2 (follow cooling load) results

The discussion focuses on Fig 4.13, Fig 4.14 and Fig 4.15. In Fig 4.13 the 8kW SE absorption chiller (green graph) is seen to follow the cooling load profile closely. The cooling load is not allowed to exceed the capacity of the absorption chiller beyond 9.6kW. The absorption chiller is also not allowed to be under loaded below 6.4kW. When the cooling load exceeds 9.6kW, the absorption chiller only delivers 9.6kW and when the cooling load goes below 6.4kW, the absorption chiller switches off. This traces out a cooling effect supply profile as shown by the green graph. Table 4.6 shows the cooling load following characteristics of Fig 4.13 as computed by MERIT.

Characteristic	**Value**
Total demand (kWh)	722.46
Total AuxSupply (kWh)	413.61
Match Rate (%)	70.96
Correlation Coefficient (-)	0.82
Energy Delivered (kWh)	413.61
Energy Surplus (Wh)	0.00
Energy Deficit (kWh)	308.86

Table 4.6: Values computed relating to Fig 4.13

Using the cooling effect supply profile in the green graph of Fig 4.13, the corresponding heat supply profile is computed as shown in Fig 4.14. This would be the demand for heating that be met by any available heat supply technologies. Fig 4.15 shows the matching between the heat supply available from one heat supply technology and the heat demanded by the absorption chiller to supply the cooling load profile shown in Fig 4.12. Table 4.7 shows the match results.

Characteristic	Value
Total demand (kWh)	584.95
Total ReSupply (kWh)	3180.00
Match Rate (%)	37.57
Correlation Coefficient (-)	0.24
Energy Delivered (kWh)	529.34
Energy Surplus (kWh)	2600.00
Energy Deficit (kWh)	50.17

Table 4.7: Values computed relating to Fig 4.15

A look at the figures in Table 4.6 and Table 4.7 shows that out of the cooling energy demand of 722.46 kWh the 8kW SE absorption chiller is able to supply 413.61 kWh under the *follow cooling* operating mode. For the absorption chiller to supply this amount of cooling capacity, a heat energy input of 584.95kWh is required which gives a COP of 0.707. Matching this absorption chiller heat energy demand with some heat energy supply technologies gives allows an appraisal of waste heat sources as shown in Table 4.5 and Fig 4.15. Certainly, the heat energy supply technology that was used for this appraisal is way off the mark, so other profiles can be tried to find the best match.

Chapter 5

Concluding Highlights and Areas of Further Study

5.1 Thesis highlights

The current concerns about global warming require appropriate energy conservation technologies to ensure that the waste heat generated by some technologies is utilised in accomplishing a useful task. Single-effect H_2O-LiBr absorption chillers can utilise waste heat from appropriate sources to provide cooling for air conditioning but the extent of their usability need to be carefully studied. MERIT provides a suitable platform for accomplishing energy technology performance appraisals which can be extended to single-effect H_2O-LiBr absorption chillers.

In this thesis, the steady state modelling approach has been used to develop simple explicit curve fit expressions that allow absorption chiller simulation in MERIT. The thesis has expanded on the current energy resource technologies that can be assessed in the demand and supply matching simulations with MERIT in the effort to search for the best hybrid renewable energy technology combinations that can be deployed together.

Absorption chiller steady state modelling and simulation studies in literature have seldom considered ideas relating to how the absorption chiller can better be utilised to meet the available cooling load or how it can be better made flexible to utilise most if not all of the waste heat available at a site. This could be partly because most studies focus on larger absorption chillers for commercial applications where the cooling loads are largely stable.

In domestic applications however, cooling loads change significantly hour by hour. With the formulations in this thesis, it can be possible to study the cooling demand following as well as the heat supply following characteristics of a single-effect absorption chiller. In this way, possibilities of maximum utilisation of the absorption chiller to supply the required cooling demand and maximum utilisation of available driving heat can be investigated and suitable application found.

5.2 Areas of Further Study

The commonly used working pairs in absorption chillers are H_2O-LiBr and NH_3-H_2O. The current models have considered a single-effect absorption chiller that uses H_2O-LiBr as the working pair. The performance characteristics of the same type of absorption chiller that uses the NH_3-H_2O working pair are significantly different. Therefore, simulation of the NH_3-H_2O single-effect absorption chiller requires the development of and implementation of suitable models.

Different types of absorption chillers exist apart from the single-effect type and their use in the HVAC-R sector is increasing. These types include the more efficient but highly energy intensive double-effect absorption chillers. To take the absorption chiller simulation capabilities to the level of double-effect absorption chillers and their working pairs, other models need to be developed and implemented in MERIT.

Energy storage technologies can show significant improvement of absorption chiller performance. These technologies can come in form of chilled water storage, phase change materials or hot water storage. To support absorption chiller simulations with energy storage technologies, suitable models and appropriate C++ function routines need to be developed.

5.3 Lessons learnt

Besides the fact that this project enhanced the authors' technical understanding of vapour absorption technologies, some additional lessons were learnt. First, the author recognised that the idea of rapid prototyping in software development would have enabled quick completion of this thesis.

Second MERIT is not an energy system design tool but rather an energy system evaluation tool. While it would be an easy thing to setup a steady state physical theoretical model of absorption chiller as (described in chapter 3), such a model would be of no utility in MERIT because the software development concept for MERIT does not take solution of many non linear simultaneous equation into account. In fact, such a solver would make the whole programming activity complex and MERIT would require huge computation power to accomplish even a few simulation time steps.

Manufacturers' performance data can provide the quickest way of obtaining suitable mathematical models for simulating absorption chillers in MERIT. Some research studies were found that used performance data published in manufacturers' catalogs or data obtained from experiments. Setting up an absorption chiller test rig for experimental performance data acquisition would be an expensive venture. Whereas, manufacturers' performance data has been used in some studies, it is not easy to obtain and most manufacturers conceal it outside the public domain. In addition, if manufacturer's performance data is obtained, it was often not used independently since it can be highly optimistic. More often, such data is combined with experimental data to obtain more realistic absorption chiller performance maps.

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