

Validation of a Computerised Analytical Model for Evaluating Natural Hydrocarbon Mixtures as Alternative Refrigerants

M.M. El-Awad

Department of Mechanical Engineering, Faculty of Engineering, University of Khartoum, P.O. Box 321, Khartoum, Sudan,
E-mail: mmelawad09@gmail.com

Abstract: This paper describes a computer-based thermodynamic model that evaluates the performance of hydrocarbon (HC) mixtures as alternative refrigerants to conventional synthetic refrigerants. By estimating the refrigeration effect, compressor work, and coefficient of performance, the analytical tool helps to optimize the system's design to suit a particular HC mixture or to identify the best HC mixture to be used as a drop-in refrigerant for an existing conventional system. The model is validated against experimental data that compared the performance of liquefied petroleum gas (LPG) to that of refrigerant R12 for domestic refrigeration. The results obtained show that the model correctly predicts the differences observed in the experiment. In agreement with the experimental data, the model's estimates show an improved performance for LPG compared to R12.

Keywords: Global warming, hydrocarbon refrigerants, natural refrigerants, ozone-layer depletion, thermodynamic model.

1. Introduction

Interest in natural refrigerants, such as hydrocarbons and CO₂, has been renewed in recent years because of the environmental problems associated with synthetic chlorofluorocarbon (CFC) and hydrochlorofluorocarbon (HCFC) refrigerants. Because of their ozone-layer depletion and global warming effects, synthetic refrigerants are being gradually phased out in accordance with the international protocols that aim to protect the environment. Hydrocarbon (HC) refrigerants, such as propane and butane, are being considered as potential substitutes for synthetic fluids in residential, commercial and automotive refrigeration and air-conditioning systems as well as heat-pumps. Sattar et al [1] compared the performance of a domestic refrigerator using pure iso-butane, butane and their blends as refrigerants with that of HCFC R134a. Their results showed that the compressor consumed 3% and 2% less energy than that of R134a when iso-butane and butane were used as refrigerants, respectively. Chang et al [2] studied the performance of four pure hydrocarbon refrigerants (propane, butane, iso-butane and propylene) and their blends as alternatives to HCFC R22 in a heat pump system. Their results also showed that the system's coefficient of performance (COP) with both propane and propylene was higher than that with R22.

The transformation to natural refrigerants would be more attractive if they could be used to replace synthetic refrigerants in existing refrigeration and air-conditioning systems without costly modifications. Unfortunately, the physical characteristics of HC refrigerants are different from those of synthetic refrigerants. For example, propane has a higher saturation pressure at a given temperature compared to R134a, while butane and iso-butane have lower pressures [3]. Therefore, a mixture of HC refrigerants, rather than a single pure one, can be a more practical solution because the thermodynamic properties of a HC mixture can be closer than those of a single gas as a drop-in substitute for a synthetic refrigerant. Wongwises et al [4] conducted an experimental investigation of hydrocarbon mixtures to replace R134a in an automotive air-conditioning system. The air-conditioner was charged and tested with four different ratios of hydrocarbon mixtures. Their results showed that propane/butane/isobutane (50%, 40%, 10%) was the most appropriate alternative refrigerant to replace R134a.

The cost and availability of the HC mixture is an important factor that influences the selection of the suitable HC substitute. In this respect, liquefied petroleum gas (LPG) is a HC mixture that is easier and cheaper to obtain than pure propane

or pure butane. Akash and Said [5] performed an assessment of LPG as a possible alternative to R12 in a domestic refrigerator. The composition of LPG was 30% propane, 55% butane and 15% iso-butane. Their results showed that the cooling capacity of LPG was about three to four times higher than that of R12, leading to a higher COP. The need to suppress their flammability is yet another practical reason for mixing HC refrigerants with inert refrigerants. Mixtures of HC with synthetic refrigerants have been considered with the synthetic fluid acting as a flame suppressant [6]. For the same reason, Sarkar and Bhattacharyya [7] assessed the performance of blends of CO₂ (R744) with butane (R600) and isobutene (R600a) as alternative working fluids for CFC R114 in heat pump applications. Their results showed that the blend R744/R600a can be the best alternative to R114 for high-temperature heating due to superior COP compared to pure R600 and R600a.

Considering the wide range of applications for refrigeration, air-conditioning and heat-pump systems and the many refrigerant mixtures that are potentially suitable, it is clear that selecting the best mixture for a particular application is not a trivial task. Researchers and engineers around the globe are trying to evaluate the performance of different mixture compositions for given system designs or different system designs for given mixture compositions. Compared to experimental investigations, theoretical models offer greater flexibility and lower cost. The present paper presents a computer-based thermodynamic model that can be used to compare the performance of mixtures of HC refrigerants with that of conventional refrigerants. The model is validated against the experimental data provided by Akash and Said [5] that assessed the performance of a household refrigerator designed for CFC R12 with LPG used as a drop-in refrigerant. The model's estimates for the refrigeration effect, compressor work, and coefficient of performance are compared with the measured values at a condenser temperature of 47°C and various evaporator temperatures.

2. The vapour-compression cycle

Figure 1a shows the main components of the vapour-compression refrigeration system which include the evaporator, compressor, condenser, and expansion valve. A suction-line heat exchanger (SLHX) is included to facilitate heat transfer between the hot refrigerant at the condenser's exit with the cold fluid leaving the evaporator. Domestic refrigerators usually replace the SLHX and expansion valve with a capillary tube in close

thermal contact with the compressor suction line. Figure 1b shows a T - s diagram of the ideal refrigeration cycle. Pressure drops in the condenser and evaporator tube are assumed to be negligible so that the evaporation and condensation processes can be treated as constant-pressure processes. Figure 1.b shows the ideal isentropic compression process (1-2s) and the actual compression processes (1-2). Discharged at a high temperature from the compressor, the refrigerant enters the condenser where it emits heat to the surroundings (process 2-3-4). After the condenser, the refrigerant is sub-cooled (process 4-5) before entering the expansion valve where it undergoes an adiabatic expansion process that takes it to the saturated liquid-vapour phase (process 5-6). The saturated refrigerant then passes through the evaporator where it absorbs heat from the refrigerated space to vaporize (process 6-7). More heat is then absorbed so that the refrigerant enters the compressor as superheated vapour.

The important performance parameters in the vapour-compression refrigeration cycle are:

(a) Refrigeration effect (q)

$$q = (h_7 - h_6) \quad (1)$$

(b) Compressor's specific work (w)

$$w = (h_2 - h_1) \quad (2a)$$

$$w = \frac{(h_{2s} - h_1)}{\eta} \quad (2b)$$

(c) Coefficient of performance (COP)

$$COP = \frac{q}{w} \quad (3)$$

(d) Mass flow rate (\dot{m})

$$\dot{m} = \frac{Ca}{q} \quad \text{for a given } Ca \quad (4a)$$

$$\dot{m} = \frac{Po}{w} \quad \text{for a given } Po \quad (4b)$$

(e) Compressor volume displacement (\dot{V})

$$\dot{V} = \dot{m}v_1 \quad (5)$$

where, h is the enthalpy in kJ/kg, η is the compressor's isentropic efficiency, Ca is the refrigeration capacity in kW ($Ca = \dot{m}q$),

Po is the compressor input power in kW ($Po = \dot{m}w$), and v_1 is the specific volume of the superheated refrigerant at state 1 on Figure 1b in m^3/kg .

3. The Theoretical Model

Certain simplifying assumptions were frequently made in previous studies that used theoretical models to analyse the

performance of HC and synthetic refrigerants. One of these simplifications is to neglect the effects of refrigerant sub-cooling and super-heating [3, 8-9]. However, a model that neglects these effects will not be able to investigate the effect of adding a suction-line heat exchanger. The present model, which allows for a suction-line heat exchanger, defines its effectiveness (ε) as:

$$\varepsilon = (T_1 - T_7)/(T_4 - T_7). \quad (6)$$

Given the values of T_4 , T_7 and ε , Eq. (6) is used to determine the compressor's suction temperature (T_1). Once T_1 is determined, the temperature T_5 can be found from the first-law of thermodynamics. Neglecting the changes in kinetic and potential energies across the SLHX, conservation of energy dictates:

$$(h_1 - h_7) = (h_4 - h_5) \quad (7)$$

Using constant specific heats, Eq. (7) becomes:

$$Cp_7 (T_1 - T_7) = Cp_4 (T_4 - T_5) \quad (8)$$

where, Cp_4 and Cp_7 are values of the specific-heat taken as those of the saturated refrigerant at point 4 and point 7 on Fig. 1.b, respectively.

Another common simplification of theoretical models is to adopt the polytropic relationship ($Pv^k = C$) for modelling the compression process [8,9]. However, the polytropic model leads to erroneous estimates of the compressor's work-input and discharge temperature [10]. Therefore, the present model determines the temperature after an isentropic compression (T_{2s}) by making use of the temperature-entropy relationship in the superheated region for two points at the same pressure. The isobaric temperature-entropy relationship determines T_{2s} from the saturation temperature T_3 :

$$T_{2s} = T_3 \times e^{(s_{2s} - s_3)/Cp_{avr}} \quad (9)$$

where, Cp_{avr} is the average specific heat given by:

$$Cp_{avr} = 1/2 (Cp_3 + Cp_{2s}) \quad (10)$$

In the ideal adiabatic compression, the entropy at point 2s is the same as that at point 1 (i.e. $s_{2s} = s_1$). Since T_{2s} is not known in advance, the average specific heat is initially taken as that at point 3 on the saturation line. The calculated T_{2s} is then used to obtain a value for Cp_3 , and the average value of the specific heat from Eq. (10) is then used in Eq. (9) to obtain a corrected value of T_{2s} . El-Awad [10] showed that this method yields more accurate estimates of the compressor's discharge temperature than the polytropic relationship that assumes ideal-gas behaviour and constant specific heats.

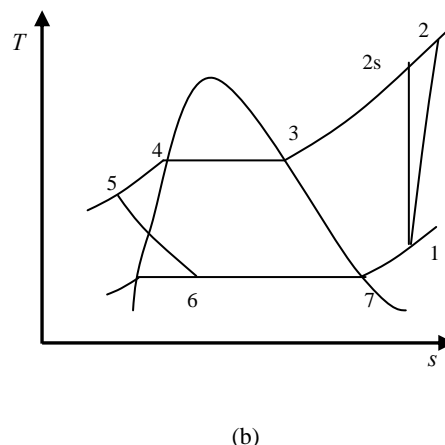
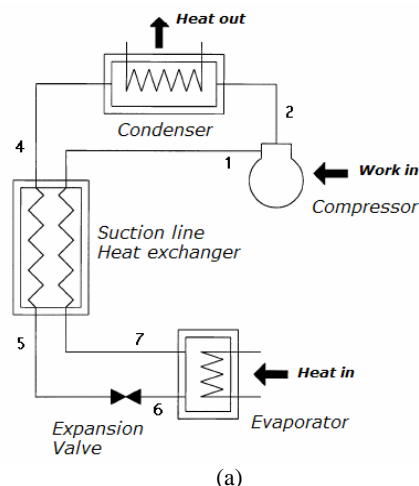


Figure 1. The vapour-compression refrigeration system: (a) schematic diagram, (b) T - s diagram of the ideal cycle.

4. The Computer Program

The computer program developed for the present model extends the MATLAB program described earlier [10-11] to allow for refrigerant mixtures as well as pure refrigerants. Given the evaporator and condenser temperatures (or pressures), the program calculates the following cycle parameters:

1. The evaporator and condenser pressures (or the temperatures if pressures are given)
2. The refrigeration effect and compressor's specific work
3. The mass flow rate and compressor volume displacement
4. The compressor discharge temperature
5. The compressor power (or cooling capacity)
6. The coefficient of performance

The computer code offers its user the choice to compare the refrigerants performance, with or without a suction-line heat exchanger. If a suction-line heat exchanger is included, the program requires as input the SLHX effectiveness. If a suction-line heat exchanger is not included, the program requires as input the degrees of superheat and sub-cooling (both of which can be zero). The program can be used to compare the refrigerants' performance on a new design with a specified capacity (Ca) or compressor power (Po). When Ca is specified, the required mass flow rate for each refrigerant is calculated using Eq. (4a). In this case, the compressors of different refrigerants will have different power inputs. Alternatively, if Po is given instead of Ca , Eq. (4b) is used to calculate the mass flow rate. Then, different refrigerants will give different refrigeration capacities. In both cases the compressor displacement volumes will be different.

4.1 Properties of Pure Refrigerants

The model needs the refrigerant properties at the different states along the cycle. Since the properties in the saturated region depend on temperature (or pressure) only, they are easier to store than those in the superheated region which depend on both temperature and pressure. Properties of three synthetic refrigerants (R12, R134a and R22) and three hydrocarbons (propane, n-butane, and iso-butane) as saturated liquid and saturated vapour at selected temperatures were extracted from ASHRAE Handbook-Fundamentals [12]. For a given temperature, these included the saturation pressure, specific volumes, enthalpies, entropies, and specific heats (C_p and C_v) as saturated liquid and saturated vapour. To find the properties at temperatures other than the selected values, MATLAB built-in function (**interp1**) is used. The enthalpy in the sub-cooled region (h_s) is approximated by the saturated liquid value at the given temperature, i.e. h_f at T_s . The refrigerant properties in the superheated region, which depend on both temperature and pressure, are not easy to store. Therefore, the model uses property relations to determine them as discussed by El-Awad [10].

4.2 Properties of Refrigerants' Mixtures

At various stages of the refrigeration cycle, the HC mixture exists in compressed-liquid phase, saturated mixture, as well as superheated vapour phase. Treatment of superheated vapours (as a mixture of ideal gases) is simple, but treatment of saturated mixtures is usually more complex. Fortunately, the only property needed in the liquid-vapour phase is h_6 , which can be substituted by h_5 since process 5-6 is an adiabatic throttling process. For the superheated vapour, the specific enthalpy of the refrigerant mixture (h_m) is obtained from the ideal-gas mixture relation [13]:

$$h_m(T, y_i) = \sum y_i h_i \quad (11)$$

where, h_i and y_i stand for the specific enthalpy and mass fraction of the i^{th} component of the mixture. Similar relations are used for the mixture's entropy (s_m), molar mass (M_m),

specific heat at constant pressure (C_p) and specific heat and constant volume (C_v).

The saturation pressure of a mixture at a given evaporator or condenser temperature is also taken as the mass-weighted summation of the saturation pressures of each component corresponding to that temperature, i.e.

$$P_{sat,m}(T, y_i) = \sum y_i P_{sat,i} \quad (12)$$

where, $P_{sat,i}$ is the saturation pressure of the i^{th} component at a given temperature. For liquid mixtures of similar molecules such as hydrocarbons, a simplified ideal model similar to that for ideal-gas mixtures is adopted. Thus the enthalpy at point 5 on Figure 1b is obtained using Eq. (11), where h_i is now that of the HC component as a compressed liquid. In its present form the computer program can deal with a mixture of three hydrocarbons (propane, n-butane and iso-butane) as well as different conventional refrigerants.

5. Validation of the Model

Akash and Said [5] assessed the performance of LPG on a domestic 240-litre refrigerator designed to work with R12. Their LPG consisted of 30% propane, 55% n-butane and 15% iso-butane fractions by mass. Their experimental data, which were obtained for a condenser temperature of 47°C and variable evaporator temperatures, are used here for validating the present analytical model. Akash and Said [5] measured the refrigeration effect, compression work, COP and mass flow rate for both R12 and LPG. Unfortunately, the degrees of sub-cooling and superheating were not reported. In the present analysis, a 10°C sub-cooling and a 10°C superheating were assumed for the base refrigerant, R12. For LPG, the degrees of sub-cooling and superheating were calculated from the respective values of R12, taking into consideration the differences in thermal conductivities, specific heats and mass flow rates. Accordingly, sub-cooling and superheating degrees of 17.7°C and 18.7°C, respectively, were used for LPG.

Akash and Said [5] tested three charges of LPG, 50, 80 and 100 g. Optimum performance was obtained with the 80 g charge, which is used here for comparison with the present theoretical model. Figure 2 compares the results of the model for the refrigeration effect with the experimental data. Note that the refrigeration effect of LPG is more than twice that of R12. The model's results are shown with and without including the effect of superheating for both refrigerants. Figure 2.a shows that including the superheating effect slightly increases the model's estimations for R12. Better agreement with experimental data is obtained without including the superheating effect. However, excluding the superheating effect significantly reduces the refrigeration effect for LPG as shown on Figure 2.b. This discrepancy could be attributed to the differences between the values of the degrees of superheating and sub-cooling used in the model and the experimental values.

Figure 3 compares the compression work predicted by the present model with the experimental data. The model (Equation 2b) needs the value of the compressor's isentropic efficiency (η). Although different values of η should be used for different refrigerants, it is common practice to use the same value [3,9]. Kilicarslan and Muller [9] used values of η in the range 0.5-0.9, but Fatouh and El Kafafy [3] used a single value of 0.75. Figure 3 shows estimates of the present model for three values of η , 0.75, 0.80, and 0.90. While an efficiency of 0.80 gave the best results for LPG, the steeper increase in compression work for R12 as the evaporator temperature decreases made it difficult to use a constant value for η . Also, note that the compression work per kg for LPG is almost three times that for R12. Figure 4 shows the calculated values of the

COP compared with those of the experiment. The model's results shown are for η of 0.80. As the figure shows, the model's estimates compare very well with the experimental data for both refrigerants over the range of evaporator temperatures. The model's estimates show an improved COP for LPG compared to R12, which agrees with the experimental data.

6. Conclusions

The results of the present theoretical model show that it can be used to compare the performance of HC mixtures and synthetic refrigerants with reasonable accuracy. However, the model needs to be extended or improved in a number of aspects

so that it can take into account the effects of important practical factors that it presently ignores. In its present form, the model mainly analyses the thermodynamic performance of the refrigerants. Hydrocarbons, such as LPG, also have different thermal and hydrodynamic properties compared to R12 and other synthetic refrigerants. The model needs to take these differences into consideration. Another factor that the present model ignores is the pressure drop and temperature glides through the condenser and evaporator tubes which are characteristic of zeotropic refrigerant mixtures. Finally, the accuracy of the model can be enhanced by making use of the available property software such as REFPROP [14], which will also extend its range of application.

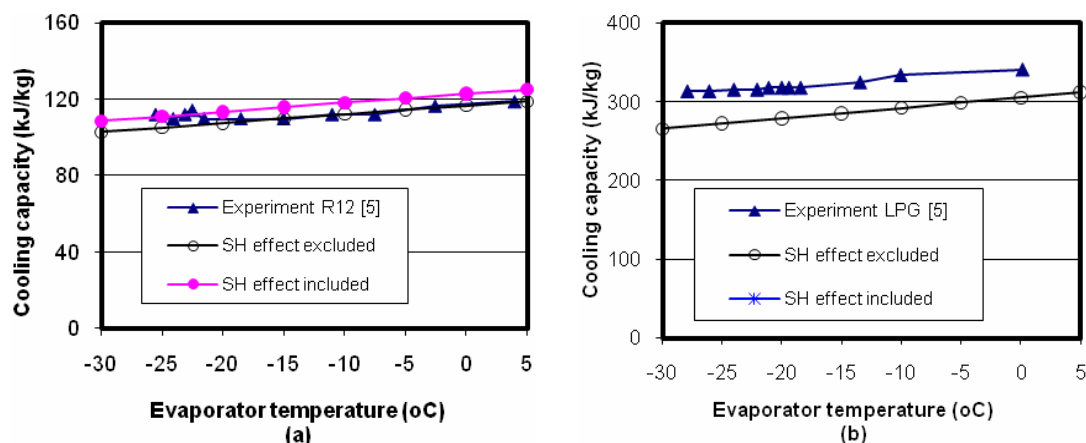


Figure 2. Comparison of model's estimation and experimental data for the refrigeration effect: (a) R12 and (b) LPG.

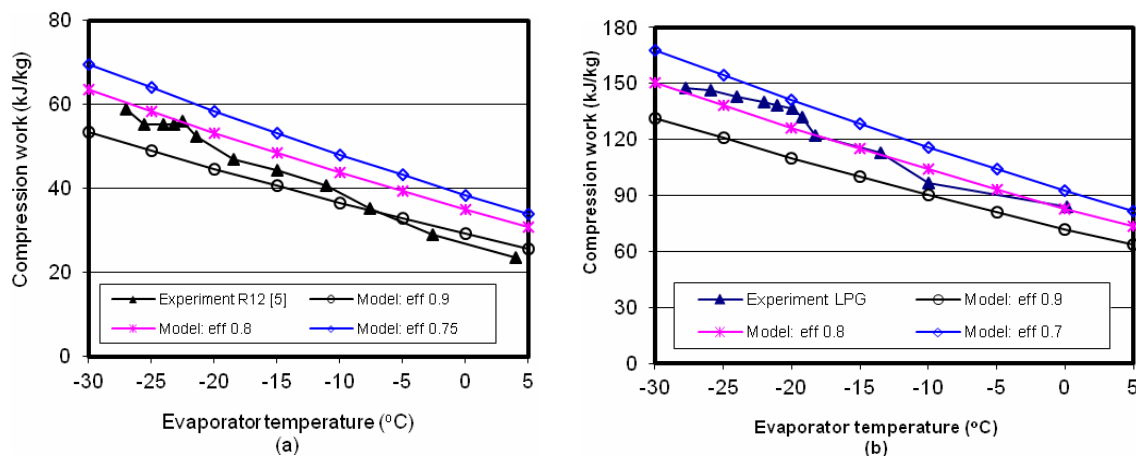


Figure 3. Comparison of model's estimation and experimental data for compression work: (a) R12 and (b) LPG.

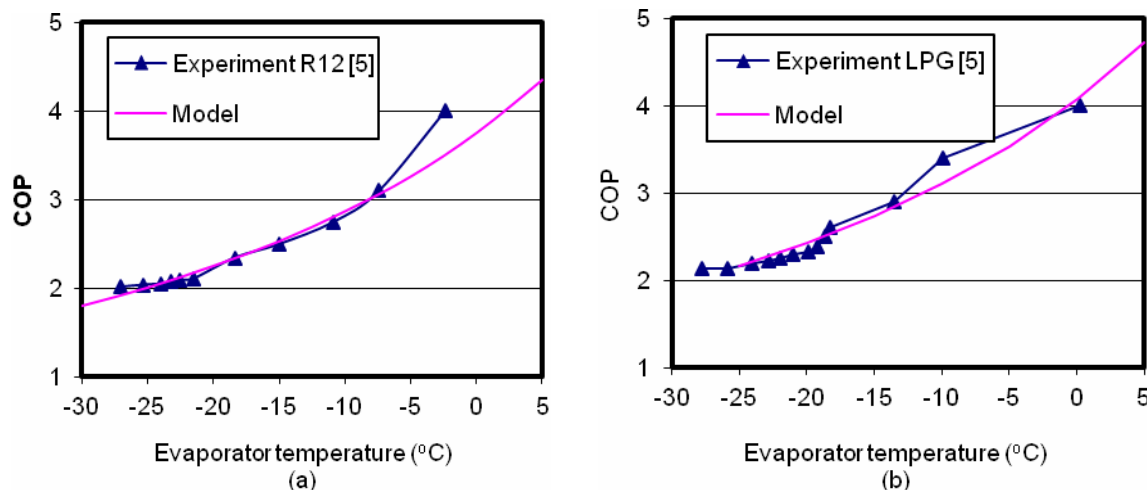


Figure 4. Coefficient of performance for: (a) R12 and (b) LPG.

References

- [1] Sattar MA, Saidur R, Masjuki HH, Performance investigation of domestic refrigerator using pure hydrocarbons and blends of hydrocarbons as refrigerants, *Proc. World Academy of Science, Engineering and Technology* (2007) 223-228.
- [2] Chang YS, Kim MS, Ro ST, Performance and heat transfer characteristics of hydrocarbon refrigerants in a heat pump system, *International Journal of Refrigeration* 23 (2000) 232-242.
- [3] Fatouh M, El Kafafy M, Assessment of propane/commercial butane mixtures as possible alternatives to R134a in domestic refrigerators, *Energy Conversion and Management* 47 (2006) 2644-2658.
- [4] Wongwises S, Kamboon A, Orachon B, Experimental investigation of hydrocarbon mixtures to replace HFC-134a in an automotive air conditioning system, *Energy Conversion and Management* 47/11-12 (2006) 1644-1659.
- [5] Akash BA, Said SA, Assessment of LPG as a possible alternative to R-12 in domestic refrigerators, *Energy Conversion and Management* 44 (2003) 381-388.
- [6] Hichens RK, Dlugogorski BZ, Kennedy EM, Flammability properties of mixtures of hydrocarbon blends with CF₃I and C₃HF₇, *Proceedings, Halon Options Technical Working Conference* (2000) Albuquerque.
- [7] Sarkar J, Bhattacharyya S, Assessment of blends of CO₂ with butane and isobutene as working fluids for heat pump applications, *International Journal of Thermal Sciences* 48 (2009) 1460-1465.
- [8] Boumaza M, Performance assessment of natural refrigerants as substitutes to CFC and HCFC in hot climate, *Proceedings of the International Engineering Conference in Hot Arid Regions (IECHAR 2010)* (2010) 371-374 Al-Ahsa, KSA.
- [9] Kilicarslan A, Muller N, A comparative study of water as a refrigerant with some current refrigerants, *Int. J. Energy Res* 29 (2005) 947-959.
- [10] El-Awad MM, A computerized analytical model for evaluating hydrocarbon fluids as natural alternative refrigerants, *The World Journal of Modelling and Simulation* 5/3 (2009) 232-240.
- [11] El-Awad, MM, Effects of a suction-line heat exchanger on the performance of pure hydrocarbon fluids as alternative refrigerants (2009) Presented at the Global Conference on Global Warming (GCGW09) Istanbul, Turkey.
- [12] ASHRAE, *Handbook-Fundamental* (1997) American Society of Heating, refrigeration and Air Conditioning (ASHRAE), Atlanta, USA.
- [13] Sonntag RE, Borgnakke C, Van Wylen GJ, *Fundamentals of Thermodynamics* (2003) Six Edition, John Wiley & Sons, Inc.
- [14] Lemmon EW, Huber ML, McLinden MO, NIST Standard Reference Database 23, *NIST Reference Fluid Thermodynamic and Transport Properties- REFPROP Version 8.0, User's Guide* (2007) National Institute of Standards and Technology, Physical and Chemical Properties Division, Boulder, Colorado 80305.