

## VALIDATION OF A COMPUTERISED ANALYTICAL MODEL FOR EVALUATING NATURAL HYDROCARBON MIXTURES AS ALTERNATIVE REFRIGERANTS

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### ABSTRACT

Refrigeration systems using natural hydrocarbon (HC) refrigerants have a favourable direct impact on the environment. However, their total contribution can match that of the corresponding systems using synthetic refrigerants if they are less efficient. Considering the added costs due to safety considerations, the energy efficiency of HC systems is crucial for their acceptability. This paper describes a theoretical computer model developed for evaluating propane-butane mixtures as natural alternative refrigerants. The model, which compares the performance of these refrigerants with that of conventional synthetic refrigerants, is validated against experimental data that compared LPG to R12 for domestic refrigeration. Results of the present model show that it correctly predicts the differences observed in the experiment. The model shows that an 8% increase in the refrigeration capacity can be achieved with LPG as compared to R12.

### INTRODUCTION

Refrigeration systems have direct as well as indirect contributions to global warming. The direct contribution is due to the leakage of the refrigerant itself. The indirect contribution is due to the emission of carbon-dioxide by consuming the energy which is obtained by combustion of fossil fuels. Since indirect contributions from refrigerant emissions dominate their direct contributions, refrigeration systems must be energy efficient [1,2]. Particularly in developing countries, the transformation to HC refrigerants would be more attractive if they could be used to replace synthetic refrigerants in existing refrigeration and air-conditioning systems without affecting their performance. 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 R12 or R134a, while n-butane and iso-butane have lower pressures. Other properties which are critical to the performance of the system,

such as the specific volume and thermal conductivity, are also different. Therefore, to get the best performance from HC refrigerants, the refrigeration system must be specially designed to suit their particular properties. The performance of a system originally designed for a synthetic refrigerant may suffer by using a single HC refrigerant as a “drop-in” substitute without suitably modifying the system [3,4]. In this case, a mixture of HC refrigerants can be more suitable than a single gas. Any analytical tool that helps the designer to identify the best HC mixture for an existing system, or to optimize the system’s design to suit a particular HC mixture, will be of great value.

### NOMENCLATURE

$Ca$	[kW]	Refrigeration capacity
$C_p$	[kJ/kg.K]	Specific heat at constant pressure
$C_v$	[kJ/kg.K]	Specific heat at constant volume
$h$	[kJ/kg]	Specific enthalpy
$k$	[-]	Ratio of specific heats of gas
$\dot{m}$	[kg/s]	Mass flow rate
$P$	[kPa]	Pressure
$P_o$	[kW]	Power
$q$	[kJ/kg]	Refrigeration effect
$R_u$	[kJ/kmol.K]	Universal gas constant
$s$	[kJ/kg.K]	Entropy
$T$	[K]	Temperature
$\dot{V}$	[m <sup>3</sup> /s]	Compressor's volume displacement
$v$	[m <sup>3</sup> /kg]	Specific volume
$\tilde{v}$	[m <sup>3</sup> /kmol]	Molar specific volume
$w$	[kJ/kg]	Specific work
$y$	[-]	Mass fraction
Special characters		
$\eta$	[-]	Adiabatic efficiency of compressor
Subscripts		
$avr$		Average value
$m$		Mixture property
$sat$		Saturation property

## 2 Topics

A number of experimental studies compared the performance of single HCs and HC mixtures with that of synthetic refrigerants [4-6]. A fair comparison requires optimising the system for each refrigerant, which is costly. Theoretical models can be of great help in this respect. Unfortunately, most of the theoretical studies applied severe simplifying assumptions in their theoretical basis by using ideal-gas laws for modelling the compression process or by neglecting the effects of sub-cooling and super-heating [7-10]. El-Awad [11, 12] described a computer-based thermodynamic model that can be used to compare the performance of pure HC refrigerants with that of conventional refrigerants in vapour-compression systems without the above simplifications. The present study extends the model to deal with hydrocarbon mixtures as well as single HC refrigerants. The paper validates the model against the experimental data provided by Akash et al [5] for the performance of a household refrigerators designed for R12 with liquefied petroleum gas (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.

### THE THEORETICAL MODEL

Figure 1.a shows the main components of the vapour-compression refrigeration system which include the compressor, evaporator, condenser, and expansion valve. The suction-line heat exchanger (SLHX) is included to facilitate heat transfer between the hot refrigerants at the condenser's exit with the cold fluid entering the compressor. Domestic refrigerators usually replace the SLHX and expansion valve by using a capillary tube in close thermal contact with the compressor suction line. Figure 1.b shows a  $T$ - $s$  diagram of the ideal refrigeration cycle, in which 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.

The refrigerant enters the compressor at point 1 where it is compressed to the condenser pressure (process 1-2). Discharged at a high temperature, the refrigerant enters the condenser where it rejects heat to the surroundings (process 2-3-4). After the condenser, the refrigerant is sub-cooled in the SLHX (process 4-5) before entering the expansion valve where it undergoes an adiabatic expansion process that takes it to state 6 in the saturated liquid-vapour mixture (process 5-6). The saturated refrigerant at point 6 then passes through the evaporator where it absorbs heat from the refrigerated space to vaporize (process 6-7). More heat is absorbed in the SLHX so that the refrigerant becomes superheated at the compressor inlet. The important performance parameters in the vapour-compression refrigeration cycle are:

(a) Refrigeration effect ( $q$ )

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

(b) Mass flow rate ( $\dot{m}$ )

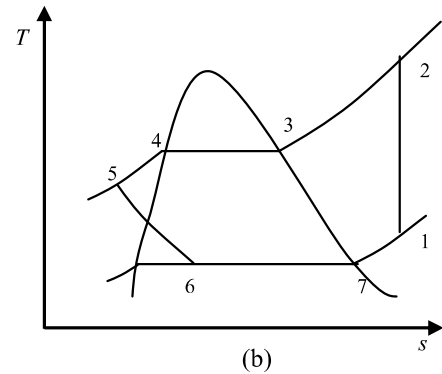
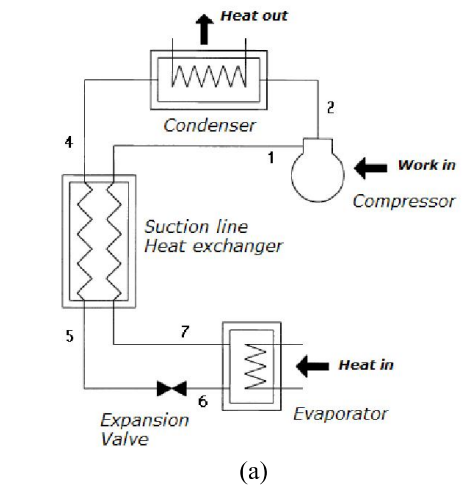


Fig. 1. The vapour-compression refrigeration system: (a) schematic diagram, (b)  $T$ - $s$  diagram of the ideal cycle.

$$\dot{m} = \frac{Ca}{q} \quad \text{for a given } Ca \quad (2.a)$$

$$\dot{m} = \frac{Po}{w} \quad \text{for a given } Po \quad (2.b)$$

(c) Compressor volume displacement ( $\dot{V}$ )

$$\dot{V} = \dot{m}v_1 \quad (3)$$

(d) Compressor power input ( $P_o$ )

$$P_o = \dot{m}w \quad (4)$$

(e) Coefficient of performance ( $COP$ )

$$COP = \frac{q}{w} \quad (5)$$

where,  $h$  is the enthalpy in kJ/kg,  $Ca$  is the refrigeration capacity in kW,  $v$  is the specific volume in  $\text{m}^3/\text{kg}$  and  $w$  is the compressor's specific work in kJ/kg. Note that Equation (1) excludes the superheating effect in the SLHX from the refrigeration effect. The model presented here extends that described previously [11,12] by treating hydrocarbon mixtures. The important submodels and extensions are discussed below.

### Modelling the Compression Process

The compression process in real systems does not normally follow the ideal isentropic process shown on Figure 1.b. Figure 2 shows the actual processes (1-2a) compared to the ideal isentropic process (1-2s). As the figure shows, the compressor's discharge-temperature and work input in the actual process can be significantly different from those of the isentropic process. Modelling the compression process, which takes place in the superheated region, is an important aspect of the computerised model.

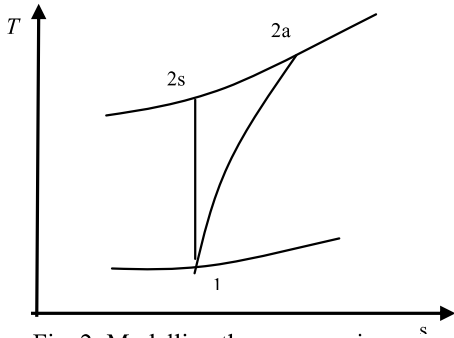


Fig. 2: Modelling the compression process.

The temperature after isentropic compression ( $T_{2s}$ ) is determined by making use of the temperature-entropy relationship in the superheated region. In the ideal adiabatic compression, the entropy at point 2s is the same as that at point 1 (i.e.  $s_{2s} = s_1$ ). Using the isobaric temperature-entropy relationship,  $T_{2s}$  can be found from:

$$T_{2s} = T_3 \times e^{(s_1 - s_3) / C_{p_{avr}}} \quad (6.a)$$

where,  $C_{p_{avr}}$  is the average specific heat given by:

$$C_{p_{avr}} = \frac{1}{2} (C_{p_3} + C_{p_{2s}}) \quad (6.b)$$

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  $C_{p_3}$ , which is then used in Eq. (6.a) to obtain a corrected value of  $T_{2s}$ .

Treating the compression process as adiabatic, and neglecting the minor effects of potential and kinetic-energy changes, the first law of thermodynamics reduces to the following simple equation that gives the compressor's isentropic work ( $w_{1-2s}$ ):

$$w_{1-2s} = h_{2s} - h_1 \quad (7.a)$$

The actual compression work ( $w_{1-2a}$ ) is then obtained from:

$$w_{1-2a} = w_{1-2s} / \eta \quad (7.b)$$

where,  $\eta$  is the compressor's isentropic efficiency. By calculating  $w_{1-2s}$  from the first law, this method does not assume any particular behaviour of the refrigerant's vapour. El-Award [11] showed that this method yields more accurate estimates of the compressor's volume displacement, discharge temperature and work input, than those of the frequently used polytropic

model ( $Pv^k = C$ ) that assumes ideal-gas behaviour and constant specific heats.

The refrigerant's specific volume is required by the calculation of the compressor volume displacement. When the suction point approaches the saturation line, the values obtained by applying the ideal-gas equation of state depart significantly from the actual values. The present model reduces the error by applying the Soave-Redlich-Kwong equation of state [13]:

$$P = \frac{R_u T}{\tilde{v} - b} - \frac{a\alpha}{\tilde{v}(\tilde{v} + b)} \quad (8)$$

where,  $R_u$  is the universal gas constant,  $\tilde{v}$  is the molar specific volume, and  $T$  is the absolute temperature. The constants  $a$ ,  $b$  and  $\alpha$  depend on the refrigerant's pressure and temperature at the critical point. Equation (8) leads to a third order non-linear equation in  $\tilde{v}$  which requires a numerical solution. The present model solves the equation by using Newton-Raphson method.

### Treatment of Refrigerants' Mixtures

The present model deals with a mixture of three hydrocarbons (propane, n-butane and iso-butane) as well as different conventional refrigerants. 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 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. By placing point 1 in the superheated region, the model only requires the properties at the saturated liquid and superheated vapour.

For the superheated vapour, the specific enthalpy of the hydrocarbon mixture ( $h_m$ ) was obtained from the following relation [13]:

$$h_m(T, x_i) = \sum y_i h_i \quad (9)$$

where,  $h_i$  and  $y_i$  stand for the specific enthalpy and mass fraction of the  $i^{\text{th}}$  components of the mixture. Similar relations were 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 hydrocarbon mixture at a given evaporator or condenser temperature was also taken as the mass-weighted summation of the saturation pressures of each component corresponding to that temperature, i.e.

$$P_{sat,m}(T, y_i) = \sum y_i P_{sat,i} \quad (10)$$

where,  $P_{sat,i}$  is the saturation pressure of the  $i^{\text{th}}$  component at the given temperature. Figures 3 compares the estimation of  $P_{sat,m}$ , for propane-butane mixtures, obtained by Equation (10) with measured data [14]. The values shown for the pressure are gauge values. For liquid mixtures of similar molecules such as hydrocarbons, a simplified ideal model similar to that for ideal-gas mixtures could be adopted. Thus the enthalpy at point 5 on Fig. 1.b was obtained using Equation (9), where  $h_i$  is now that of the HC component as compressed liquid.

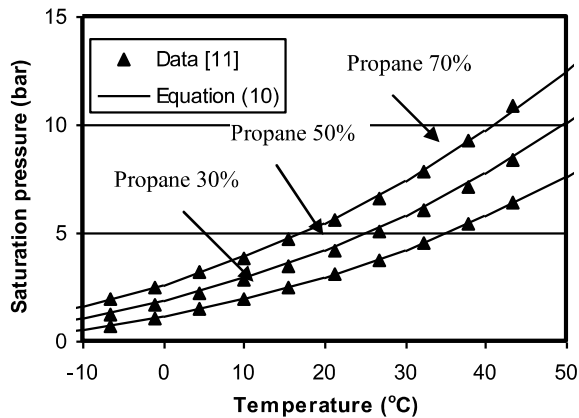


Fig. 3: Saturation pressure of propane-butane mixtures

### THE COMPUTERISED MODEL

The theoretical model described above has been coded in a MATLAB computer program. The computer code offers its user the choice to compare the refrigerants performance, with or without a suction-line heat exchanger. 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

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. (2.a). In this case, the compressors of different refrigerants will have different power inputs and displacement volumes. Alternatively, if  $Po$  is given instead of  $Ca$ , Eq. (2.b) is used to calculate the mass flow rate. Then, different refrigerants will give different refrigeration capacities and the compressor displacement volumes will also be different.

Properties of R12, R134a and R22 and the three hydrocarbons (propane, n-butane, and iso-butane) as saturated liquid and saturated vapour were extracted from ASHRAE Handbook-Fundamentals [15]. For a given temperature, these included the saturation pressure, specific volumes, enthalpies, entropies, and specific heats ( $Cp$  and  $Cv$ ) as saturated liquid and saturated vapour. The enthalpy in the sub-cooled region ( $h_7$ ) was approximated by the saturation value at the given

temperature, i.e.  $h_f(T_7)$ . Verification of the computerised model is reported in [11, 12].

### 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 about 30% propane, 55% n-butane and 15% iso-butane by mass fraction. Assessment was made for a condenser temperature of 47°C and variable evaporator temperatures. Reported measurements included the refrigeration effect, compression work, COP and mass flow rate for both R12 and LPG. Unfortunately, Akash and Said [5] didn't report direct measurements of the condenser and evaporator pressures. Also, the degrees of sub-cooling and superheating were not reported. Therefore, it is not clear whether their refrigeration effects and COPs took the effects of sub-cooling and superheating into consideration. In the present simulation, a 10°C sub-cooling and a 10°C superheating are assumed for the original refrigerant, which is 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, are used for LPG.

Akash and Said [5] tested three charges of LPG, which were 50, 80 and 100g. Optimum performance was obtained with the 80g charge, which is used here for comparison with the present theoretical model. Fig. 4 compares the results of the present model for the refrigeration effect with the experimental data. The model's results are shown with and without including the effect of superheating for both refrigerants. Fig. 4.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 Fig. 4.b. This discrepancy could be attributed to a difference between the values of the degrees of superheating and sub-cooling used in the model and the experimental values. Note that the refrigeration effect of LPG is more than twice that of R12.

Fig. 5 compares the compression work predicted by the present model with the experimental data for three values of the compressor's efficiency ( $\eta$ ): 80%, 85%, and 90%. While an efficiency of 85% gives the best results for LPG, the steeper increase in compression work for R12 as the evaporator temperature decreases makes it difficult to use a constant value for  $\eta$ . Also, note that the compression work per kg for LPG is almost three times that for R12. Fig. 6 shows the calculated values of the COP compared with those of the experiment. The model's results are shown only for  $\eta$  of 85%, which gave good results for LPG but underestimated the COP for R12 at the high end of evaporator temperatures. The model's estimates compare very well with the experimental data for both refrigerants over the range of evaporator temperatures.

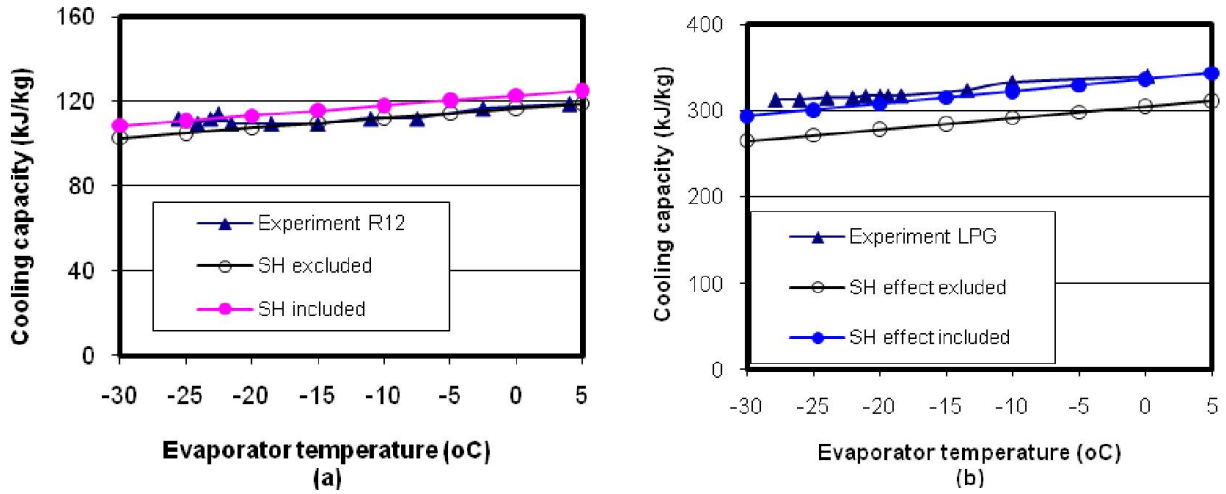


Fig. 4: Comparison of model's estimation and experimental data for the refrigeration effect: (a) R12 and (b) LPG.

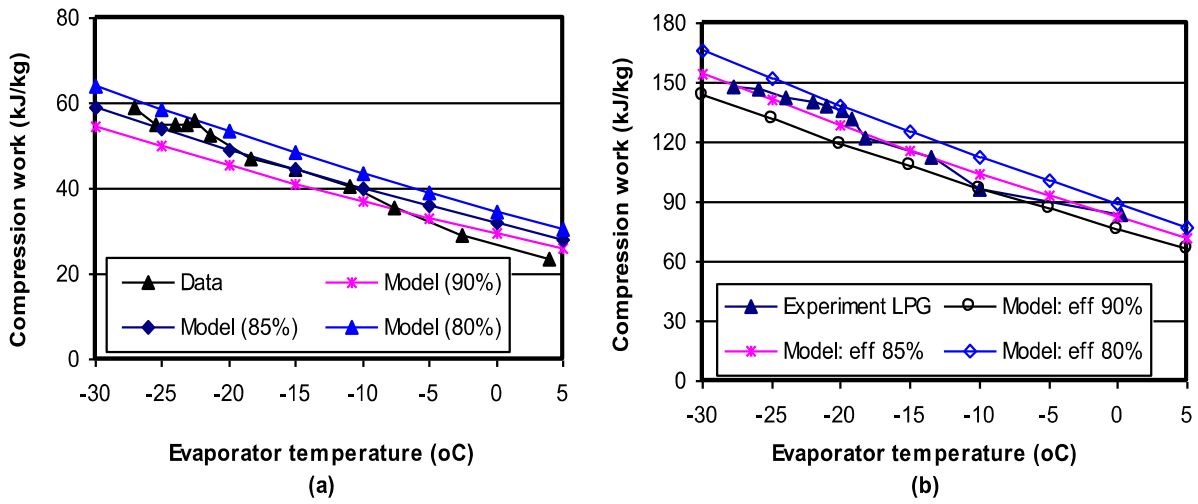


Fig. 5: Comparison of model's estimation and experimental data for compression work: (a) R12 (b) LPG.

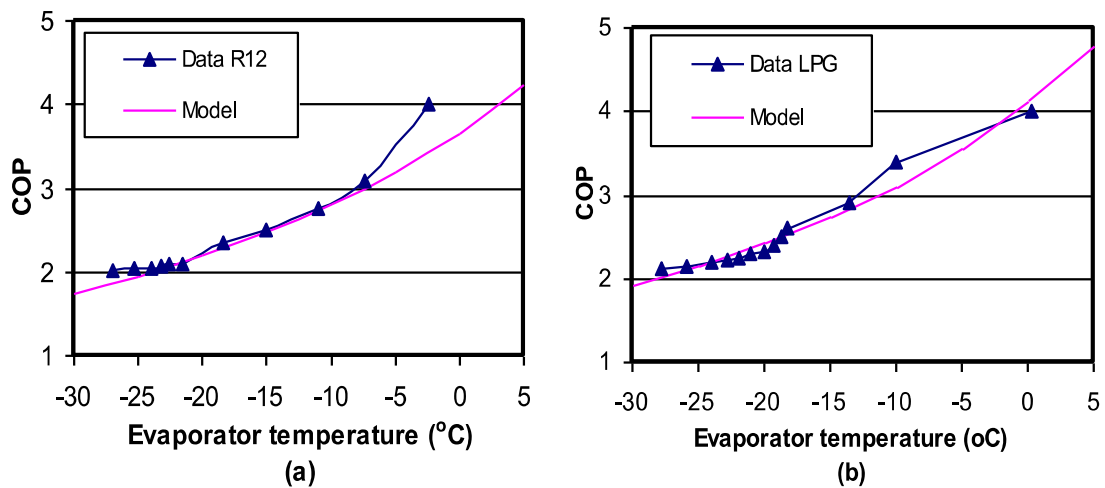


Fig. 6: Coefficient of performance for: (a) R12 and (b) LPG.



**CONCLUSION**

Although the results presented here show that the present model can be used to compare the performance of HC mixtures and synthetic refrigerants with reasonable accuracy, the model needs further refinements and extensions in a number of aspects. One important aspect is that of evaluating refrigerants' properties, particularly in the sub-cooled and superheated regions. At present, these properties are interpolated from a limited number data points and need to be evaluated more accurately. The model should also be extended to take into account the effects of important practical factors that it presently ignores, such as the pressure drop and temperature glide through the condenser and evaporator tubes. Further validation of the model against experimental data is needed to test the viability of the model's techniques adopted for the different processes involved. The two most important aspects is those of the suction-line heat exchanger and the isentropic efficiency of the compression process.

A theoretical model, such as the one presented here, can also be used to investigate the effectiveness of different blends of hydrocarbon and non-hydrocarbon mixtures. For example, a hydrocarbon refrigerant can be mixed with a non-hydrocarbon refrigerant as a flame suppressant. The performance of such a mixture can be analysed using the present model without the cost and time required by an experimental investigation. However, it should be stressed that, in its present form, the theoretical 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. Previous studies reported that these differences were in favour HC refrigerants. Therefore, in order to give more accurate results, the model needs to take these differences into consideration.

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