

MATHEMATICAL MODELLING OF FLUID PROPERTIES

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Abstract

In a study of a complex thermal system where fluids are used as working media, it is always necessary to calculate thermo-physical properties of the fluids involved. When such a study is conducted by computer simulation, tabulated data of fluid properties are inconvenient to use, especially if variations of the fluid properties are encountered. A better approach is to make use of mathematical models representing the fluid in the form of mathematical equations. This paper will outline the procedure which may be used to obtain such equations. A particular case of Refrigerant 12 is presented to illustrate the modelling approach. Some important equations for determining R12 properties are also presented. These equations are highly accurate as compared with the data published by ASHRAE and IIR.

แบบจำลองทางคณิตศาสตร์ของคุณสมบัติของของไหล

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บทคัดย่อ

ในการศึกษาระบบความร้อนที่ซับซ้อน มักจะมีความจำเป็นต้องคำนวณหาค่าคุณสมบัติของของไหลอยู่เสมอ ซึ่งส่วนใหญ่ในเอกสารหรือตำราทั่วไปจะบอกอยู่ในรูปของตารางหรือกราฟการใช้ข้อมูลในลักษณะเช่นนี้จะเป็นการไม่สะดวก โดยเฉพาะอย่างยิ่งในการศึกษาโดยการจำลองสถานการณ์โดยคอมพิวเตอร์ และในกรณีที่ต้องคำนวณหาคุณสมบัติต่าง ๆ บ่อยครั้ง วิธีการที่สะดวกกว่าก็คือการใช้แบบจำลองทางคณิตศาสตร์ของคุณสมบัติในรูปของสมการบทความนี้จะกล่าวถึงวิธีการสร้างสมการเพื่อหาคุณสมบัติของของไหล โดยจะใช้ตัวอย่างกรณีของสารทำความเย็น R12 และเสนอสมการสำหรับคุณสมบัติของ R12 ที่ใช้กันมากเพื่อประโยชน์ของผู้สนใจได้นำไปใช้ต่อไป สมการคุณสมบัติของ R12 ที่เสนอนี้มีความแม่นยำสูงมากเมื่อเปรียบเทียบกับข้อมูลของ ASHRAE และ IIR

1. Introduction

As part of the heat pump research conducted at the University of Melbourne, Australia, mathematical models for predicting the thermodynamic and physical properties of Refrigerant 12 were required. Refrigerant 12 (Dichlorodifluoromethane) was Tabulated data of these properties are available in the literature but they are not suitable for use in a computer simulation. The most common approach in dealing with this situation is to obtain equations describing the fluid properties of interest by either referring to the

empirical equations available or curve-fitting of the generally accepted published data. Curve-fitting technique is generally good for a narrow range of independent variables whereas empirical equations generally cover a wider range of data. In this paper both approaches were adopted to model the properties of R12.

2. Thermodynamic Properties of Refrigerant 12 at Saturation

The most commonly used data of R12 include pressure, temperature, and enthalpies of vapour and liquid. The following equations represent these properties respectively.

$$P = -7747.90 + 102.36693T - 462.6415 \times 10^{-3}T^2 + 717.0089 \times 10^{-6}T^3; \quad |\epsilon| < 0.16\% \quad (1)$$

$$T = 103.1045 + 49.408151 \log(P) - 6.98746[\log(P)]^2 + 0.618201[\log(P)]^3; \quad |\epsilon| < 0.005\% \quad (2)$$

$$h_v = 198.0127 + 6.660140T - 3.43036 \times 10^{-2}T^2 + 8.576819 \times 10^{-5}T^3 - 8.165573 \times 10^{-8}T^4; \quad |\epsilon| < 0.0007\% \quad (3)$$

$$h_l = -90.25694 + 1.562328T - 3.199744 \times 10^{-3}T^2 + 5.0167 \times 10^{-6}T^3; \quad |\epsilon| < 0.008\% \quad (4)$$

where P = absolute pressure at saturation (kPa)
 T = absolute temperature at saturation (K)
 h_v = enthalpy of vapour refrigerant at saturation (kJ/kg)
 h_l = enthalpy of liquid refrigerant at saturation (kJ/kg)
 ϵ = percentage error

These equations were curve-fitted by the author using the data of ASHRAE for the range of saturation temperatures of -20°C to 60°C . This range of temperature was selected because in usual operations a refrigerating machine or a heat pump using R12 operates within these limits.

It should be noted that in Eq.(1) - Eq.(4) represents the maximum discrepancy of predicted data from the original tabulated data of ASHRAE. Evidently these four equations are very accurate. Better results may be obtained by curve-fitting the data for a shorter range of saturation temperatures, but the benefit to be gained should be weighed against the increasing number of equations required to cover the range of interest. It should also be noted that at saturation P and T are dependent; Eq.(1) and Eq.(2) are therefore an alternative form of each other.

3. Thermodynamic Properties of Superheated Refrigerant 12

At some stages in the operation of a heat pump, the refrigerant is superheated. Two independent refrigerant properties are pressure, temperature, specific volume and enthalpy. The first three properties are related by the equation of state which may be written as,

$$P = \frac{RT}{(v-L)} + \frac{A+BT+Ce^{-KT}}{(v-L)^2} + \frac{D+ET+Fe^{-KT}}{(v-L)^3} + \frac{G}{(v-L)^4} + HT + Ie^{-KT} \quad (5)$$

where R, A, B, C, D, E, F, G, H, I, K and L are constants, v is the specific volume, and, P and T have the same meanings as before. The enthalpy of superheated vapour, h_v , may be represented as,

$$h_v = aT + bT^2 + cT^3 + dT^4 + ePv + \left[\frac{f}{v-L} + \frac{g}{(v-L)^2} + \frac{h}{(v-L)^3} \right] + (1+iT)e^{-KT} \left[\frac{j}{v-L} + \frac{k}{(v-L)^2} + \frac{l}{(v-L)^4} + x \right] \quad (6)$$

where a, b, c, d, e, f, g, h, i, j, k, l and x are constants. Eq.(5) and Eq.(6) were obtained from those given by Downing (1974). The equations have been greatly simplified by deleting irrelevant terms and combining constants. The constants of the original equation, quoted in the British system of units, are also given by Downing. These original constants were converted by the author to give new constants in S.I. units, as tabulated in Table 1 and Table 2, for use with Eq.(5) and Eq.(6), respectively. Eq.(5) and Eq.(6) are highly accurate, giving predictions in excellent agreement with the published data of the International Institute of Refrigeration (IIR) (1981). For enthalpy prediction in the range of saturation temperatures of interest, -20°C to 60°C , with levels of superheat ranging from 0°C to 20°C , Eq.(6) gives identical results with those of IIR. For given values of pressures and temperatures within the same range, Eq.(6) predicts the specific volumes with deviations of less than 0.025% from those given by IIR.

In most cases, the use of Eq.(5) and Eq.(6) requires iteration. The Newton-Raphson method of solving implicit equations has been found to be very effective for the purpose.

4. Physical Properties of Refrigerant 12

Besides the thermodynamic properties, physical and thermal properties are generally needed for computer simulation. For the sake of completeness of this paper in describing the most commonly used properties of Refrigerant 12, the following equations representing some common thermal and physical properties of Refrigerant 12 are given.

Table 1 : Constants for use with Eq. (5)

R = -0.0687481266	A = -0.0916214328	B = .000077113996
C = -1.5254249926	D = 1.0105029x10 ⁻⁴	E = 5.6754304x10 ⁻⁷
F = 2.1998419x10 ⁻³	G = -5.746455x10 ⁻⁸	H = 4.0819805x10 ⁻¹⁴
I = -1.6630913x10 ⁻¹⁰	J = -1.42220352x10 ⁻²	K = 4.063681x10 ⁻⁴

Table 2 : Constants for use with Eq.(6)

a = 0.03389	b = 0.0012535	c = -1.091502x10 ⁻⁶
d = 4.10434x10 ⁻¹⁰	e = 1.000017	f = -9.1623022x10 ⁻²
g = 5.0526023x10 ⁻⁵	h = -1.9155x10 ⁻⁸	i = 1.42220352x10 ⁻²
j = -1.525276385	k = 1.099940048x10 ⁻³	l = -4.1578004x10 ⁻¹¹
x = 255.9458		

$$\rho_l = 1397.30329 - 3.2607T - 8.758x10^{-3}T^2 \quad (7)$$

$$\rho_v = P/[R_v(273.17 + T)] \quad (8)$$

$$R_v = 6.26376x10^{-2} - 1.3412x10^{-4}T - 9.5059x10^{-4}T^2 \quad (9)$$

$$C_{pl} = 0.93078 + 1.3441x10^{-3}T + 1.0299x10^{-5}T^2 + 2.60882x10^{-7}T^3 \quad (10)$$

$$C_{pv} = 0.64815 + 2.7147x10^{-3}T + 1.35427x10^{-5}T^2 + 1.6502x10^{-7}T^3 \quad (11)$$

$$k_l = 7.83039x10^{-5} - 3.661x10^{-7}T \quad (12)$$

$$k_v = 8.3365x10^{-5} + 5.14867x10^{-8}T + 8.8162x10^{-11}T^2 \quad (13)$$

$$\mu_l = 2.6657x10^{-5} - 2.456x10^{-6}T + 2.1088x10^{-8}T^2 - 1.2629x10^{-10}T^3 \quad (14)$$

$$\mu_v = 1.1855x10^{-5} + 4.0627x10^{-8}T - 3.4042x10^{-10}T^2 + 8.5054x10^{-12}T^3 \quad (15)$$

T = refrigerant temperature at saturation (°C)

ρ_l = liquid density (kg/m³)

ρ_v = vapour density (kg/m³)

R_v = parameter given by Eq.(9)

C_{pl} = liquid specific heat (kJ/kg°C)

C_{pv} = vapour specific heat (kJ/kg°C)

k_l = liquid thermal conductivity (kW/m°C)

k_v = vapour thermal conductivity (kW/m°C)

μ_l = liquid dynamic viscosity (Pas)

μ_v = vapour dynamic viscosity (Pas)

These physical and thermal properties of R12 have been curve-fitted by Flemming using IIR (1981) data over the range of -30°C to 50°C

Although the physical property equations were originally curve-fitted for the temperature range of -30°C to 50°C, they can be used for greater temperature of up to 60°C with deviations of less than 0.2% from the data given by IIR.

5. Properties of subcooled liquid

The properties of subcooled liquids are not usually published for refrigerants. However, as discussed by Martin (1959), at temperatures well below the critical value, properties of common use such as specific volume and enthalpy of subcooled liquid may be taken to be the same as those of saturated liquid at the same temperature. This is because pressure has little effect on these properties of liquid refrigerants.

Physical properties such as viscosity, thermal conductivity and specific heat depend principally on temperature. These properties for both subcooled liquids and superheated vapours may be taken to be those of saturated values of the respective phases at the same temperature.

6. Discussion and Conclusion

Techniques commonly used in mathematical modelling of fluid properties have been outlined with particular emphasis on Refrigerant 12. Equations representing a range of common properties of Refrigerant 12 have also been presented. These equations are highly accurate and very suitable for use in computer modelling and simulation. The techniques may also be used in modelling properties of other fluids provided that data or equations are available. Curve-fitting of the available data in a simple mathematical functional form such as a polynomial is very useful when a small range of data are required. The use of a complex equation such as Eq.(5) and Eq.(6) normally requires iteration which may result in excessive computer time. The decision to adopt a more simple or complex equation depends on the accuracy required and whether the additional accuracy is justified by using a more complex form of equation.

REFERENCE

1. ASHRAE Handbook of Fundamentals. Ch.17, pp. 17.5-17.7, 1985
2. Fleming, M.G., Aspects of modelling two phase refrigerant evaporating flow in horizontal tubes. Ph.D. Thesis, University of Melbourne, 1988.
3. Downing, R.C., Refrigerant equations. ASHRAE Transactions, Vol.80, Part 2, pp.158-168, 1974.
4. Martin, J.J., Correlations and equations used in calculating the thermodynamic properties of refrigerant. Thermodynamic and Transport Properties of Gases, Liquids, and Solids, ASME, pp. 111-122.