Physical Properties of Hydrocarbons

VOLUME 2

R. W. GALLANT

CARL L. YAWS

THIRD EDITION

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PREFACE

The objective of this book is to provide the working engineer with all the essential data to design and run production facilities. The data are presented in graphs covering a wide temperature range to enable the engineer to quickly determine the information he needs at the desired temperature.

The literature has been carefully searched for experimental data. When several sources give different values, the authors made a judgment as to the most reliable source. To enable the engineer to go back to the original article for additional information, the sources of all data are documented.

For many compounds, experimental results are available only over a narrow temperature span. In these cases, estimation methods have been used to extend the data over a wider temperature range. When estimation methods are used, the method and expected accuracy are explained. Thus, the user is aware of the reliability of the graphical values. Reference to the original work is provided for those wishing to study the method further.

The physical properties normally needed in design and production are vapor pressure, heat of vaporization, density, surface tension, heat capacity and thermal conductivity. For chemical reactions, enthalpy of formation and Gibb's free energy of formation are helpful. Also, the boiling point, freezing point, molecular weight, critical properties, lower explosion limit in air and solubility in water are tabulated for each compound. This latter property data are helpful in safety and environmental engineering.

In this edition, special attention is paid to improving the accuracy of estimation techniques. Improved methods of extending data and new experimental data are included.

The SI and metric units are used for all properties except vapor pressure, both because these units are becoming increasingly used in production plants and because conversion is generally easier. Each graph displays a conversion factor providing English units. The temperature scale in all graphs is Centigrade.

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DISCLAIMER

This handbook presents a variety of thermodynamic and physical property data. It is incumbent upon the user to exercise judgment in the use of the data. The authors and publisher do not provide any guarantee, express or implied, with regard to the general or specific applicability of the data, the range of errors that may be associated with any of the data, or the appropriateness of using any of the data in any subsequent calculation, design or decision process. The authors and publisher accept no responsibility for damages, if any, suffered by any reader or user of this handbook as a result of decisions made or actions taken on information contained herein.

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Volume 2/Third Edition

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CONTENTS

Chapter 1

C₁ TO C₄ NORMAL ALDEHYDES

Robert W. Gallant, Carl L. Yaws, Xiaoyan Lin and Randy J. McDonald

PHYSICAL PROPERTIES - Table 1-1

Physical, thermodynamic and transport property data from the literature (3,4,6-8,14-23,25-27,30-36,38-39,44-55,61-78) are given in Table 1-1. The critical constants are from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available. Results from the DIPPR (Design Institute for Physical Property Research) project (5) and recent data compilations by Yaws and co-workers (44-60) were consulted extensively in preparing the tabulation.

The property data in the top and middle parts of the tabulation are helpful in process engineering. The property data in the lower part of the tabulation are helpful in safety and environmental engineering.

VAPOR PRESSURE - Figure 1-1

Results from the DIPPR project (5) were selected. These results are applicable for vapor pressure from very low temperatures to the critical point. Correlation of vapor pressure as a function of temperature was accomplished using the equation:

$$\ln P = A + B/T + C \ln T + D\, T^E \tag{1-1}$$

where
P = vapor pressure
T = temperature

Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 1-2

Results from the data compilation of Yaws and co-workers (44,52) were selected. Data for heat of vaporization were correlated using the Watson equation:

$$\Delta H_{vap} = A\, (1 - T_r)^{0.38} \tag{1-2}$$

where
ΔH_{vap} = heat of vaporization
T_r = reduced temperature, T/T_C

Reliability of results is good with errors of about 5% or less.

For the DIPPR project (5), data for heat of vaporization were correlated using a modified Watson

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equation with extended terms in the exponent:

$$\Delta H_{vap} = A (1 - T_r)^{[B + C T_r + D T_r^2 + E T_r^3]}$$

(1-2a)

LIQUID DENSITY - Figure 1-3

Results from the data compilation of Yaws and co-workers (44,54) were selected. A modified Rackett equation was used for correlation of the data:

$$\rho = A B^{-(1 - T_r)^{2/7}}$$

(1-3)

where
ρ = saturated liquid density
T_r = reduced temperature, T/T_C

Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

For the DIPPR project (5), a slightly different Rackett equation was used for correlation of the data:

$$\rho = A B^{-(1 - T/C)^D}$$

(1-3a)

SURFACE TENSION - Figure 1-4

Results from the data compilation of Yaws and co-workers (44,55) were selected. Using data from the literature, surface tension over the full liquid range was achieved by the modified Othmer equation:

$$\sigma = A (1 - T_r)^{11/9}$$

(1-4)

where
σ = surface tension
T_r = reduced temperature, T/T_C

Accuracy is good with errors being about 5% or less in most cases.

For the DIPPR project (5), surface tension was correlated by a slightly different Othmer equation:

$$\sigma = A (1 - T_r)^{[B + C T_r + D T_r^2 + E T_r^3]}$$

(1-4a)

HEAT CAPACITY - Figures 1-5 and 1-6

Results from the data compilation of Yaws and co-workers (44) were selected for heat capacity of ideal gas. Correlation of data was accomplished using a series expansion in temperature:

$$C_P = A + B T + C T^2 + D T^3$$

(1-5)

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where C_P = heat capacity of ideal gas
                       T = temperature

Results are in favorable agreement with data. Errors are about 1% or less in most cases.

For the DIPPR project (5), two different equations were used for correlation of the data for heat capacity of ideal gas:

$$C_P = A + B \exp[-C/T^D] \tag{1-5a}$$

$$C_P = A + B\,[(C/T)/\sinh(C/T)]^2 + D\,[(E/T)/\cosh(E/T)]^2 \tag{1-5b}$$

Results from the data compilation of Yaws and co-workers (44,59) were selected for heat capacity of liquid. Data were correlated with a series expansion in temperature:

$$C_P = A + B\,T + C\,T^2 \tag{1-6}$$

where C_P = heat capacity of liquid
                       T = temperature

Results are in favorable agreement with data. Errors are about 10% or less using the equation. To provide wider coverage, the temperature range was extended using thermodynamic principles.

For the DIPPR project (5), the following equation was used for heat capacity of liquid:

$$C_P = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4 \tag{1-6a}$$

VISCOSITY - Figures 1-7 and 1-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data were correlated using the equation:

$$\eta_{gas} = \frac{A\,T^B}{1 + C/T + D/T^2} \tag{1-7}$$

where η_{gas} = viscosity of gas
                       T = temperature

Results are in favorable agreement with data. Errors are about 10% or less in most cases.

For the data compilation of Yaws and co-workers (31), a series expansion in temperature was used for viscosity of gas:

$$\eta_{gas} = A + B\,T + C\,T^2 \tag{1-7a}$$

Results from the DIPPR project (5) were selected for viscosity of liquid. Data were correlated using the de Guzman - Andrade equation with extended terms:

$$\ln \eta_{liq} = A + B/T + C \ln T + D\,T^E \tag{1-8}$$

where $\quad \eta_{liq}$ = viscosity of liquid
$\quad\quad\quad T$ = temperature

Correlation results and data are in rough agreement with errors being about 25% or less.

For the data compilation of Yaws and co-workers (31), a modified de Guzman - Andrade equation was used for viscosity of liquid:

$$\log \eta_{liq} = A + B/T + C\,T + D\,T^2 \tag{1-8a}$$

THERMAL CONDUCTIVITY - Figures 1-9 and 1-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data were correlated using the equation:

$$\lambda_{gas} = \frac{A\,T^B}{1 + C/T + D/T^2} \tag{1-9}$$

where $\quad \lambda_{gas}$ = thermal conductivity of gas
$\quad\quad\quad T$ = temperature

Reliability of results is good with errors of about 10% or less in most cases.

For the data compilation of Yaws and co-workers (31), a series expansion in temperature was used for thermal conductivity of gas:

$$\lambda_{gas} = A + B\,T + C\,T^2 + D\,T^3 \tag{1-9a}$$

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. Data were correlated using the equation:

$$\lambda_{liq} = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4 \tag{1-10}$$

where $\quad \lambda_{liq}$ = thermal conductivity of liquid
$\quad\quad\quad T$ = temperature

Results are in favorable agreement with data. Errors are about 5% or less in most cases.

For the data compilation of Yaws and co-workers (31), a series expansion with less terms was used for thermal conductivity of liquid:

$$\lambda_{liq} = A + B\,T + C\,T^2 \tag{1-10a}$$

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ENTHALPY OF FORMATION - Figure 1-11

Results from the data compilation of Yaws and co-workers (44,45) were selected. The correlation for enthalpy of formation of the ideal gas is a series expansion in temperature:

$$\Delta H_f = A + B\,T + C\,T^2 \tag{1-11}$$

where ΔH_f = enthalpy of formation of ideal gas
T = temperature

Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 1-12

Results from the data compilation of Yaws and co-workers (44,46) were selected. The correlation for Gibb's free energy of formation of the ideal gas is a series expansion in temperature:

$$\Delta G_f = A + B\,T + C\,T^2 \tag{1-12}$$

where ΔH_f = Gibb's free energy of formation of the ideal gas
T = temperature

Results from the correlation are in favorable agreement with data.

CORRELATION CONSTANTS FOR EQUATIONS

The A, B, C, D and E in the above equations are correlation constants for the specific property under discussion. The correlation constants which have distinct values for individual compounds maybe used in the above equations to calculate the specific property value at the temperature of interest.

Table 1-1 Physical Properties

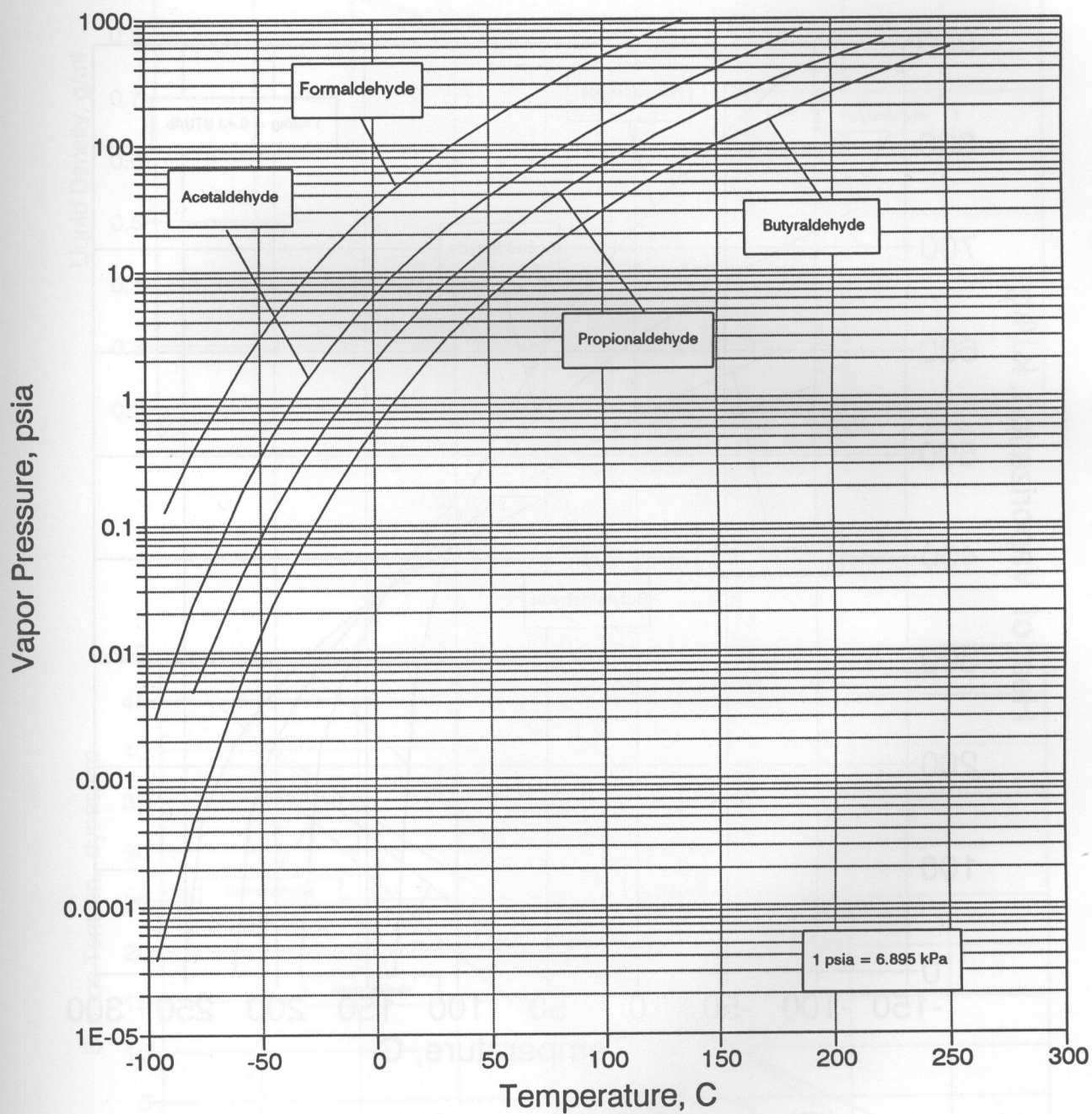| 1. Name	Formaldehyde	Acetaldehyde	Propion-aldehyde	Butyr-aldehyde
2. Formula	CH2O	C2H4O	C3H6O	C4H8O
3. Molecular Weight, g/mol	30.026	44.053	58.080	72.107
4. Critical Temperature, K	408.00	461.00	496.00	525.00
5. Critical Pressure, bar	65.861	55.500	46.600	40.000
6. Critical Volume, ml/mol	105.00	157.00	210.00	263.00
7. Critical Compressibility Factor	0.204	0.227	0.237	0.241
8. Acentric Factor	0.2816	0.3167	0.3015	0.3445
9. Melting Point, K	181.15	150.15	193.15	176.75
10. Boiling Point @ 1 atm, K	254.05	293.55	321.15	347.95
11. Heat of Vaporization @ BP, kJ/kg	758.15	584.45	487.89	436.89
12. Density of Liquid @ 25 C, g/ml	0.732	0.770	0.779	0.785
13. Surface Tension @ 25 C, dynes/cm	15.16	20.42	29.30	24.17
14. Heat Capacity of Gas @ 25 C, J/g K	1.18	1.24	1.35	1.42
15. Heat Capacity of Liquid @ 25 C, J/g K	------	1.39	2.25	2.17
16. Viscosity of Gas @ 25 C, micropoise	117.74	86.04	78.32	69.90
17. Viscosity of Liquid @ 25 C, centipoise	------	0.213	------	------
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.016	0.012	0.011	0.010
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.188	0.176	0.160	0.145
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-115.87	-166.38	-192.10	-205.08
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-110.00	-133.45	-130.67	-115.04
22. Flash Point, K	220.00	235.37	243.15	266.48
23. Autoignition Temperture, K	703.15	458.15	480.37	503.15
24. Lower Explosion Limit in Air, vol %	7.0	1.6	2.6	2.5
25. Upper Explosion Limit in Air, vol %	73.0	10.4	16.1	12.5
26. Solubility in Water @ 25 C, ppm(wt)	total	total	404,700	83,720

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Figure 1-1 Vapor Pressure

The chart shows Vapor Pressure (psia) on the y-axis (logarithmic scale from 1E-05 to 1000) versus Temperature, C on the x-axis (from -100 to 300). Curves are labeled: Formaldehyde, Acetaldehyde, Propionaldehyde, Butyraldehyde.

1 psia = 6.895 kPa

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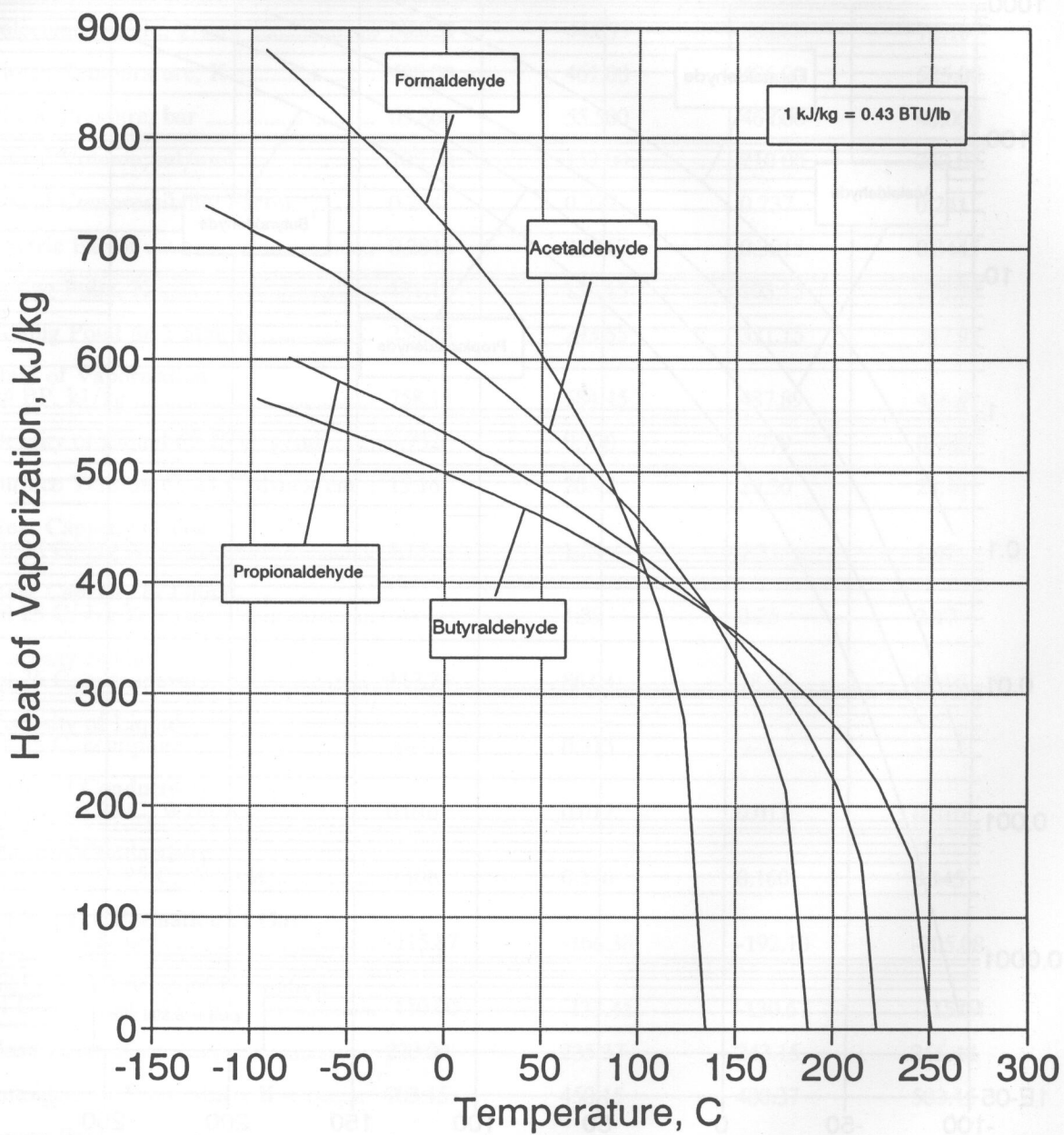
Figure 1-2 Heat of Vaporization

The figure plots Heat of Vaporization (kJ/kg) on the vertical axis (0 to 900) against Temperature, C on the horizontal axis (-150 to 300) for: Formaldehyde, Acetaldehyde, Propionaldehyde, and Butyraldehyde.

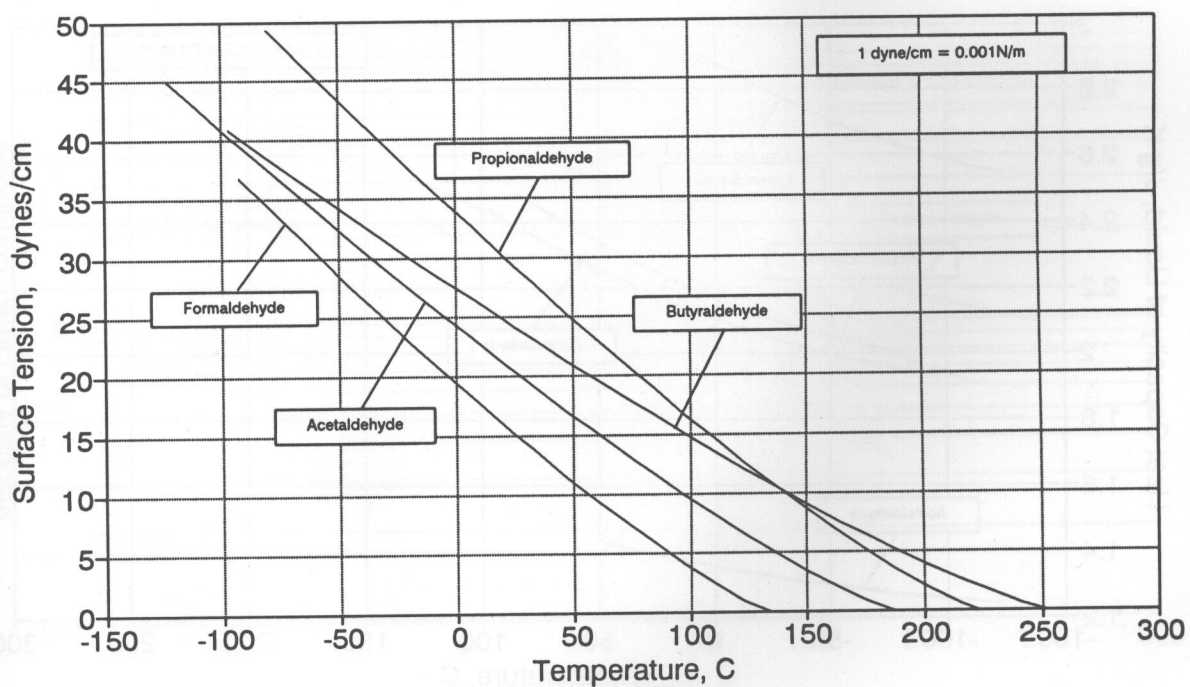1 kJ/kg = 0.43 BTU/lb
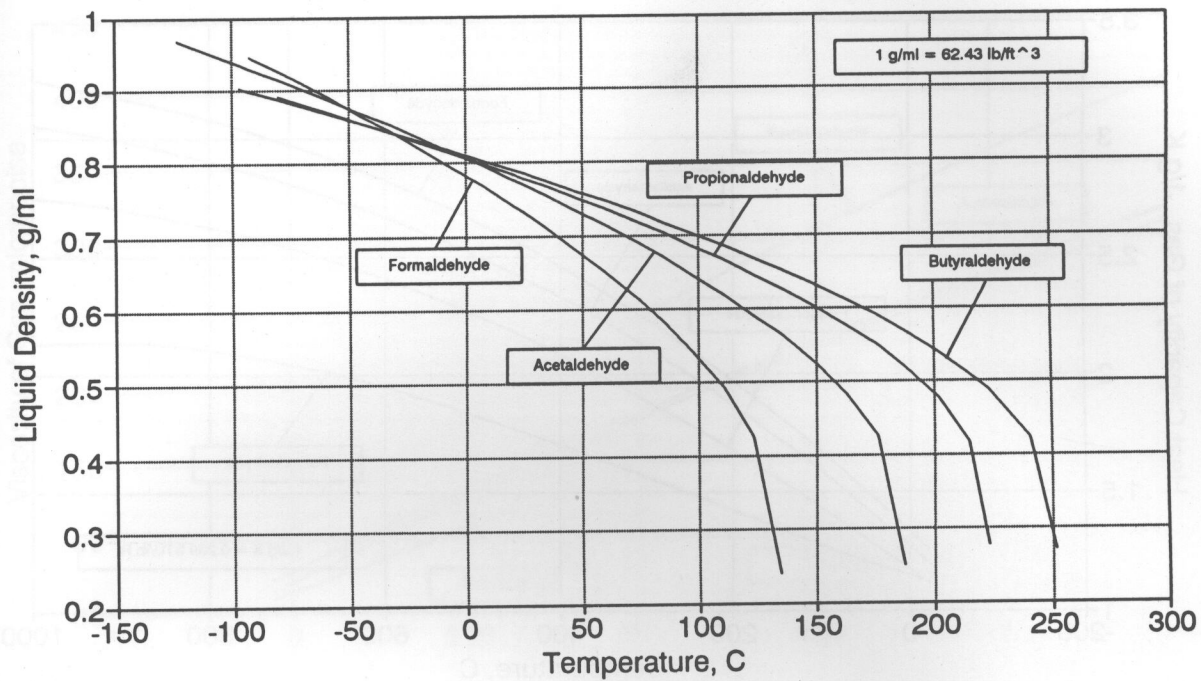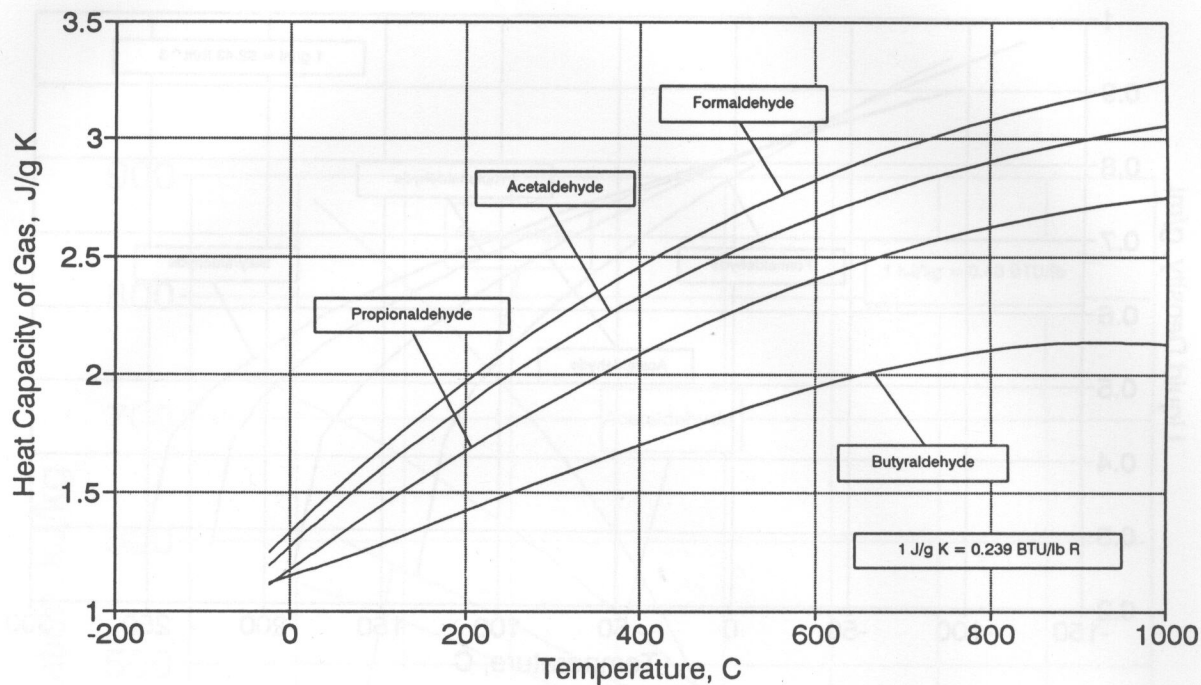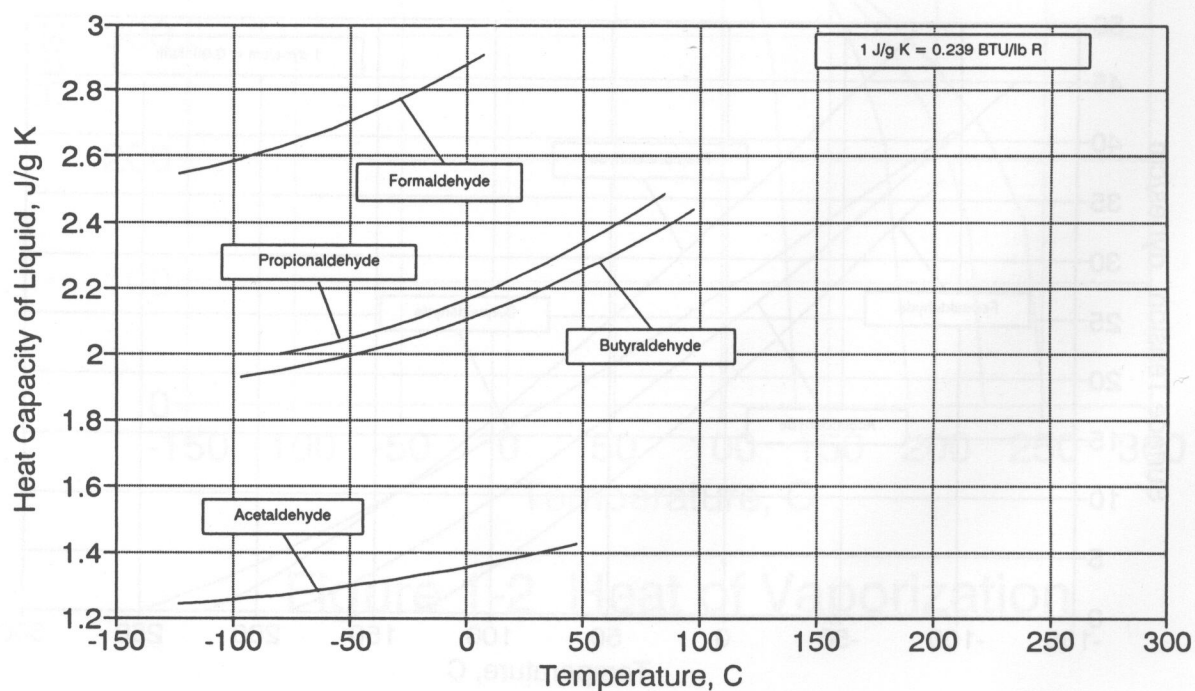
Figure 1-3 Liquid Density

Figure 1-4 Surface Tension

Figure 1-5 Heat Capacity of Gas

Figure 1-6 Heat Capacity of Liquid