



# Critical and maximum temperatures of coexistence of liquid and gas phase in hydrocarbons binary mixtures. II. Maximum temperatures of coexistence of liquid and gas phase in alkane binary mixtures



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## ABSTRACT

This work systematizes the data published to date on the maxcondentherm for 27 binary mixtures of alkanes (first component – C<sub>1</sub>–C<sub>4</sub> and second component – C<sub>2</sub>–C<sub>10</sub> and the mixtures which contain 2-methylpentane, 2-methylhexane, 2-methylheptane and 2-methyloctane). The abilities of combination methods and limits of their use were defined in application to prediction of the maxcondentherm for binary mixtures of alkanes.

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## 1. Introduction

In our previous article [1] we reviewed the available literature data on critical temperatures of alkane binary mixtures. Recommendations on the use of some of the methods of their prediction were given.

This article deals with maximum temperatures of coexistence of liquid and gas phases (maxcondentherm or  $T_{\max,m}$ ) in alkane binary mixtures. Maxcondentherm is one of the end points on the phase (liquid–vapor) diagram of the binary mixture and is characterized by smaller density value and greater temperature value as compared to the critical point.

## 2. Methods

To determine the comparability of the experimental data within each system, we used the Redlich–Kister equation [2], similarly as for critical temperatures:

$$T_{\max,m} = x_i \cdot T_{ci} + x_j \cdot T_{cj} + x_i x_j (A_1 + A_1(x_i - x_j) + A_3(x_i - x_j)^2), \quad (1)$$

where  $x_i, x_j$  – mole fractions of mixture components;  $T_{ci}, T_{cj}$  – critical temperature of the mixture components (K);  $A_1, A_2, A_3$  – coefficients obtained from the experimental data processing.

Silverman and Thodos [3] suggest an empirical correlation based approach to maxcondentherm prediction:

$$T_{\max,m} = x_1 \cdot T_{c1} + x_2 \cdot T_{c2} + x_1 x_2 \cdot (A + B \cdot x_1 + C \cdot x_1^2 + D \cdot x_1^3), \quad (2)$$

where  $x_i, x_j$  – mole fractions of mixture components;  $T_{c1}, T_{c2}$  – critical temperature of the mixture components (K); the coefficients  $A, B, C$  and  $D$  are calculated using the equations:

$$A = -0.60 + 202.2 \cdot (\tau - 1) + 32.2 \cdot (\tau - 1)^2 + 78.0 \cdot (\tau - 1)^3 \quad (3)$$

$$B = 1.61 + 158.3 \cdot (\tau - 1) - 238.4 \cdot (\tau - 1)^2 + 448.2 \cdot (\tau - 1)^3 \quad (4)$$

$$C = 0.76 - 104.6 \cdot (\tau - 1) + 0.10 \cdot (\tau - 1)^2 - 496.2 \cdot (\tau - 1)^3 \quad (5)$$

$$D = 1.47 + 124.8 \cdot (\tau - 1) + 271.9 \cdot (\tau - 1)^2 + 1022.1 \cdot (\tau - 1)^3, \quad (6)$$

where  $\tau = T_{b2}/T_{b1}$  is the relation of normal boiling temperatures of the components.

Eqs. (2)–(6) were obtained on the basis of experimental data for 10 systems: ethane + *n*-butane, ethane + *n*-heptane, ethane + cyclohexane, ethane + benzene, ethane + *n*-heptane, *n*-butane + *n*-heptane, methane + propane, methane + *n*-butane,

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**Table 1**  
Maxcondentherm of binary mixtures of alkanes accumulated to date.

$X_1$	$X_2$	$\Delta T_{c(ij)}$ (K)	Lit.
Methane	Propane	179.2	8, 7
	<i>n</i> -Butane	234.5	9
	<i>n</i> -Pentane	279.1	10
	<i>n</i> -Heptane	349.6	28
	<i>n</i> -Decane	427.1	24
Ethane	<i>n</i> -Butane	119.8	11
	<i>n</i> -Pentane	164.4	12
	<i>n</i> -Heptane	234.9	13
	<i>n</i> -Decane	312.4	25
	Cyclohexane	248.5	14
Propane	<i>n</i> -Butane	55.3	15, 16
	Neopentane	64	17
	<i>n</i> -Pentane	99.9	15
	2,2-Dimethylbutane	119.2	18
	2,3-Dimethylbutane	130.2	18
	2-Methylpentane	127.9	18
	3-Methylpentane	134.8	18
	<i>n</i> -Hexane	137.8	18, 19
	<i>n</i> -Heptane	170.4	19
	<i>n</i> -Octane	198.9	20
<i>n</i> -Butane	<i>n</i> -Decane	247.9	26
	<i>n</i> -Pentane	44.6	21
	<i>n</i> -Hexane	82.5	21
	<i>n</i> -Heptane	115.1	22
	<i>n</i> -Octane	143.6	20
2-Methylpentane	<i>n</i> -Decane	192.6	27
	2-Methylhexane	32.7	23
	2-Methylheptane	62	23
2-Methylhexane	2-Methyloctane	85.1	23
	2-Methylheptane	29.2	23
2-Methylheptane	2-Methylheptane	29.2	23
	2-Methyloctane	52.4	23
2-Methylheptane	2-Methyloctane	23.2	23

propane + *n*-butane, propane + *n*-pentane [3]. The authors tested the method on the data for the mixtures including methane + ethane, methane + isobutane, methane + *n*-pentane, methane + *n*-decane, acetylene + propylene, acetylene + propane, ethane + propylene, propane + isopentane, butane + *n*-heptane, hydrogen sulphide + propane, and those used for identification of coefficient values for Eqs. (2)–(6). As the result it was determined that the method is applicable for binary mixtures of aliphatic hydrocarbons, excluding the systems which contain methane. Silverman and Thodos explain the abnormal deviations for the methane mixtures by considerable differences between physical properties, size and shape of the molecules in these systems.

We have used a slightly different method of prediction, which is based on the critical properties of individual components, and the correlation which demonstrated good applicability for critical temperatures [1].

$$T_{\max,m} = \theta_i \cdot T_{ci} + \theta_j \cdot T_{cj} + \theta_i \cdot \theta_j \cdot \Delta T, \quad (7)$$

where  $T_{ci}$ ,  $T_{cj}$  are critical temperature of the mixture components (K);  $\Delta T$  – coefficient of binary interaction which is obtained experimentally;  $\theta_i$ ,  $\theta_j$  – surface fractions of the low-boiling and the high-boiling components calculated by the equation:

$$\theta_i = \frac{x_i V_{ci}^{2/3}}{x_i V_{ci}^{2/3} + x_j V_{cj}^{2/3}}, \quad (8)$$

where  $x_i$ ,  $x_j$  are mole fractions of mixture components;  $V_{ci}$ ,  $V_{cj}$  critical volume of the mixture components ( $\text{sm}^3/\text{mol}$ ). Critical volumes for *n*-alkanes are taken from [4], for cyclic and branched alkanes – from [5], for 2-methylpentane, 2-methylhexane, 2-methylheptane, and 2-methyloctane – from [6].

### 3. Database

The experimental data on the maxcondentherm of binary mixtures of alkanes accumulated to date present in Table 1.

Information on maxcondentherm of alkane mixtures for the whole range of components is represented by systems with one  $C_1$ – $C_4$  component and the other component  $C_2$ – $C_8$  [7–22], and for mixtures containing 2-methylpentane, 2-methylhexane, 2-methylheptane and 2-methyloctane [23]. Mixtures of lower alkanes with *n*-decane are studied for a narrow range of concentrations and are limited to four systems: methane + *n*-decane [24], ethane + *n*-decane [25], propane + *n*-decane [26], and *n*-butane + *n*-decane [27]. In all cases the maxcondentherm and critical temperatures were determined simultaneously by building a phase diagram on the basis of experimental data.

Some works do not provide primary data, and contain only the result of experimental data processing for selected mixtures [7–10,12,16]. These studies were carried out by the same research group and provide information on  $C_1 + C_3$ – $C_6$ ,  $C_2 + n$ – $C_5$  and  $C_3 + n$ – $C_4$  mixtures. This data was excluded from further analysis of the applicability of prediction methods.

Experimental data on maxcondentherm of alkane binary mixtures, accumulated at present, are represented in Table 2.

### 4. Results

Maxcondentherm for most alkane mixtures can be adequately described by Eq. (1), with average absolute deviations not exceeding 1 K (see Table 2). Therefore, Eq. (1) can be used to test the quality of experimental data when calculating maxcondentherm.

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