Three approximate approaches to determine the total pressure and gas-phase composition in water–hydrogen peroxide (HP) two-phase systems depending on solution composition and temperature are presented. Chemical composition is assumed to vary (e.g., due to HP decomposition) slowly as compared with the rate of physical relaxation processes. Although the approaches are based on different prerequisites, all of them are in a good agreement with each other in terms of predictions of total pressure, activity coefficients and equilibrium gas-phase composition. The approaches have been generalized on three- and four-component systems containing low-volatility (non-solvable jet propulsion fuel (JPF)) and high-volatility (air) components. The results are discussed in view of the dual-fuel concept of pulse detonation engine (PDE) for advanced propulsion.

### Introduction

The operational ability of an air-breathing liquid-fueled PDE is dependent on the fuel used. In authors’ previous publications, a concept of a dual-fuel PDE has been suggested and substantiated\(^1\)\(^-\)\(^3\). The concept particularly implies the use of two liquid energetic materials: conventional JPF and HP. In terms of the critical initiation energy, the gas-phase JPF–air mixtures with 5% and 20% of HP vapor were shown to be equivalent to stoichiometric ethylene–air and hydrogen–air mixtures, respectively.\(^4\)\(^-\)\(^6\). As the dual-fuel air-breathing PDE\(^1\)\(^-\)\(^3\) implies the use of liquid sprays of JPF and HP, it is important to know thermodynamic properties (activity coefficients, gas-phase composition, etc.) of the multiphase multi-component mixture containing JPF, aqueous solution of HP, and air at high temperature and pressure. There is no general approximation that would be readily applicable to such two-phase systems\(^4\)\(^-\)\(^6\).  

This paper suggests three approximate analytical approaches for calculating total pressure \(P(x,T)\) and activity coefficients of the \(\text{H}_2\text{O}_2\)–\(\text{H}_2\text{O}\) two-phase systems. The effect of JPF and air on the total pressure is also considered.

1. **Liquid–Vapor Phase Equilibrium Curves for Individual Components**

For individual components, a two-parameter approximation\(^7\)\(^-\)\(^9\) of pressure vs. temperature dependence along the phase equilibrium curve is used:

\[
P(T) = \left( \frac{T_0}{\alpha} \right)^{1/8} - A \tag{1}\]

where \(T\) is temperature in K, \(P\) is pressure in atm, \(\alpha\) and \(A\) are parameters. Equation (1) provides very accurate results at relatively high pressure, including the critical point. Parameters \(\alpha\) and \(A\) are determined by using experimental data for saturated vapor pressure vs. temperature. Equation (1) differs from other available approximations of the \(TP\)-curve by its simplicity and a possibility to resolve it in terms of a simple temperature vs. pressure dependence:

\[
T(P) = \alpha[Z + A]^{8}, \quad Z = \left( \frac{P}{P_0} \right)^{1/8}, \quad P_0 = 1 \text{ atm} \tag{2}\]

For water, HP, and \(n\)-tetradecane (to simulate JPF), the liquid–vapor phase equilibrium curves have the following explicit formulae:

\[
P_w(T) = \left[ \frac{2.8836 \cdot 10^6 T}{\alpha} - 12.4575 \right]^{8} \tag{3}\]

\[
P_{HP}(T) = \left[ \frac{2.6566 \cdot 10^6 T}{\alpha} - 12.5302 \right]^{8} \tag{4}\]

\[
P_{JPF}(T) = \left[ \frac{7.5324 \cdot 10^6 T}{\alpha} - 10.8701 \right]^{8} \tag{5}\]

Parameters \(\alpha\) and \(A\) for water and \(n\)-tetradecane were determined by using tables of thermodynamic data\(^10\),\(^11\); for HP they were calculated by using nonlinear regression and 8 points on a 4-parameter \(P(T)\)-curve approximation\(^12\):
Table 1: Comparison between liquid – vapor phase equilibrium curves (Eqs. (3) to (5)) and experimental data\textsuperscript{10,11} for water and \textit{n}-teradecane, and with the approximation of experimental data\textsuperscript{13} by Eq. (6) for HP. \(\Delta P / P\) is the error of approximation. Last columns correspond to the critical points.

<table>
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<th>(n)-tetradecane</th>
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\[ \log P_{HP} \text{ (mm Hg)} = C_0 + C_1/T + C_2 \log T + C_3 T \] \hfill (6)\n
where \(C_0 = 44.5760, C_1 = -4025.3, C_2 = -12.996, C_3 = 0.0046055\).\n
Table 1 shows the accuracy of Eqs. (3) to (5) as compared to the experimental data (for water and \textit{n}-tetradecane) and to Eq. (6) (for HP). The error of the approximations at pressure \(0.003 \text{ atm} \leq P \leq P_c\) (\(P_c\) is the critical pressure) is typically a fraction of percent.

2. Calculation of the Total Pressure of Two-Phase System at Isotherms

2.1 Correlation Based on Redlich–Kister Method

To provide the correlation for the total pressure \(P(x, T)\), the authors\textsuperscript{13} use the formula:

\[ P(x, T) = \gamma_{HP} P_{HP}(T) x + \gamma_w P_{w}(T) X \] \hfill (7)

where \(x\) and \(X = 1 - x\) are the molar fractions of HP and water, respectively, \(\gamma_{HP}\) and \(\gamma_w\) are the corresponding activity coefficients. To calculate \(\gamma_{HP}\) and \(\gamma_w\), the following relationships\textsuperscript{14} are used:

\[ \gamma_w = \exp\left(\frac{X^2}{RT}\right) B_0 + B_1 (3 - 4X) + B_2 (1 - 2X)(5 - 6X) \] \hfill (8)

\[ \gamma_{HP} = \exp\left(\frac{X^2}{RT}\right) B_0 + B_1 (3 - 4X) + B_2 (1 - 2X)(1 - 6X) \] \hfill (9)

Parameters \(B_0, B_1,\) and \(B_2\) in Eqs. (8) and (9) were determined by fitting the results provided by Eq. (7) with the experimental data. For this purpose, total pressure of aqueous solutions of HP at several values of \(x\), at 5 isothersms \((T = 317.65 K, 333.15, 348.15, 363.15,\) and 378.15 K) was measured\textsuperscript{13}. The data for phase equilibrium curves \(P_{HP}(T)\) and \(P_{w}(T)\) have been taken from literature. As a result, the following expressions for \(B_0, B_1,\) and \(B_2\) have been obtained (dimension in cal/mol):

\[ B_0 = -1017 + 0.97 T, \quad B_1 = 85, \quad B_2 = 13 \] \hfill (10)

When substituting Eqs. (8) and (9) for \(\gamma_w\) and \(\gamma_{HP}\) and Eqs. (3) and (4) for \(P_{w}(T)\) and \(P_{HP}(T)\) into Eq. (7) and using Eqs. (10), one obtains the explicit analytical dependence \(P(x, T)\). Application of Eqs. (8) and (9), that are based on low-temperature data \((T \leq 378 K)\), to high temperatures can be considered as extrapolation. Its accuracy can be estimated by comparing the results obtained by different methods (see below).
2.2 Correlation Based on Similarity of Component Properties

For systems containing components with like thermodynamic properties the values of $\alpha$ and $A$ in Eq. (1) appear close (e.g., for water and HP they differ by 8.5% and 0.6%, respectively). It is reasonable to assume that for such systems Eq. (1) can be used for estimating $P(x,T)$. In this case, parameters $\alpha$ and $A$ in Eq. (1) can be approximated as linear combinations:

$$\alpha(x) = \alpha_1(1-x) + \alpha_2 x, \quad A(x) = A_1(1-x) + A_2 x$$

with indices 1 and 2 corresponding to components of a binary solution, and $1-x$ and $x$ representing their molar fractions. Within this approximation, Eqs. (1) and (2) provide isothermal dependence of pressure and isobaric dependence of temperature on solution composition, respectively. Application of Eqs. (1) and (11) to aqueous solutions of HP results in the following approximation for $P(x,T)$:

$$P(x,T) = \left[\frac{T}{\alpha(x)}\right]^{1/8} - A(x),$$

$$\alpha(x) = 3.4679 \cdot 10^{-7}(1-x) + 3.7642 \cdot 10^{-7} x$$

$$A(x) = 12.4575(1-x) + 12.5302 x$$

2.3 Correlation Based on Boiling Temperature of Binary Solution

The other approach for estimating $P(x,T)$ is based on Eq. (2). If one knows the dependence $T_b(x,P)$ of the solution boiling temperature $T_b$ on solution composition at $P = const$, then the procedure of determining $P(x,T)$ is straightforward.

Figures 1a and 1b show the measured dependencies of $T_b$ on HP concentration in aqueous solutions at total pressure $P = 0.04$ atm (Fig. 1a) and $P = 1$ atm (Fig. 1b). It follows from Fig. 1 that function $T_b(x,P)$ at $P = const$ is almost linear, at least within the range $P = 0.04$–1 atm. This finding allows one to assume that isobaric function $T_b(x,P)$ remains approximately linear for higher pressures. Although this assumption is insufficiently substantiated due to the lack of available experimental data, a general trend of evening up the thermodynamic properties of liquids and dense gases with temperature can serve as the indirect indication of its validity. With this in mind, function $T_b(x,P)$ is represented as a linear combination:

$$T_b(x,P) = T_w(P)(1-x) + T_{HP}(P)x$$

where $T_w(P)$ and $T_{HP}(P)$ are given by (see Eq. (2)):

$$T_w(P) = 3.4679 \cdot 10^{-7}[Z + 12.4575]^8$$

$$T_{HP}(P) = 3.7642 \cdot 10^{-7}[Z + 12.5302]^8$$

$$Z = \left(\frac{P}{P_0}\right)^{1/8}, \quad P_0 = 1 \text{ atm}$$

Substituting Eqs. (14) into Eq. (13) results in equation relating $T_b$, $P$, and $x$. Thus, for a given $T = T_b$ one obtains the equation determining $P(x,T)$ implicitly:

$$T = 3.4679 \cdot 10^{-7}[Z + 12.4575]^8(1-x) + 3.7642 \cdot 10^{-7}[Z + 12.5302]^8 x$$
3. Results of Total Pressure Calculations

Figure 2 shows the example of total pressure calculations at isotherm \( T = 573 \) K for aqueous solutions of HP. The curves are marked with abbreviations corresponding to various approximations: RK stands for Redlich–Kister approach (Eqs. (7) to (10)); CS for “Component Similarity” approach (Eqs. (12)), and BT for “Boiling Temperature” approach (Eqs. (15)). To distinguish between curves CS and BT, the CS curve is plotted as dashed curve. In addition, “Ideal Solution” – IS curve is plotted in Fig. 2. Within the ideal solution approximation, the total pressure is determined by Eq. (7) with \( \gamma_w = \gamma_{HP} = 1 \), i.e.

\[
P(x, T) = P_{HP}(T)x + P_P(T)X
\]  

(16)

Figure 2: Predicted dependencies of total pressure on the mole fraction of HP in aqueous solution at \( T = 573 \) K.

The difference between the calculated results for nonideal solutions attains a maximum value at \( x \approx 0.3–0.4 \) for all isotherms within the temperature range \( 373 \) K \( \leq T \leq 623 \) K. The maximum difference in the total pressure predicted by the approaches of Sections 2.1 to 2.3 is 13% at \( T = 373 \) K, 8% at \( T = 423 \) K, 5% at \( T = 573 \) K, 3.5% at \( T = 523 \) K, 3% at \( T = 573 \) K, and 2.6% at \( T = 623 \) K. The remarkable feature of the comparison is that a good agreement between the predicted values of total pressure exists even at \( 573 \) K and \( 623 \) K, i.e., in the domain where the gas-phase density is high and interaction between molecules in the gas phase becomes significant. Equations (12) and (15) provide almost identical dependencies \( P(x, T) \). The maximum difference of less than 2% is attained in the vicinity of \( x = 0.3 \).

The value of total pressure predicted by the ideal-solution relationship (16) differs considerably from the values provided by other approaches.

4. Calculation of Activity Coefficients and Gas-Phase Composition

Parameters \( B_0, B_1, \) and \( B_2 \) entering Eqs. (8) and (9) for the activity coefficients were obtained based on the limited set of low-temperature (\( T \leq 378 \) K) experimental data on the total pressure of binary water–HP system for several values \( (x, T) \). As Sections 2.2 and 2.3 provide the approximate expressions for \( P(x, T) \) that are applicable at temperatures ranging from 330–370 K to \( T \leq T_c \), it becomes possible to determine \( B_0, B_1, \) and \( B_2 \) more precisely for the extended temperature range. For this purpose, Eq. (7) combined with Eqs. (3) and (4) was applied to determine \( B_0, B_1, \) and \( B_2 \) by attaining the best least square fit with the \( P(x, T) \)-dependence of Eq. (12). Two approximations were used: in the first (referred to as II-parameter approximation), parameter \( B_2 \) in Eqs. (8) and (9) was taken zero; in the second (III-parameter approximation), all three parameters \( B_0, B_1, \) and \( B_2 \) were determined. It was found that the dependencies of \( B_0, B_1, \) and \( B_2 \) on \( T \) are very regular. The following exponential interpolations were obtained for the II-parameter approximation:

\[
B_0^{(II)} = -431.31 - 225 \exp \left( -2253.1 - 31.43 \right) x
\]

\[
B_1^{(II)} = 201.0 + 247.1 \exp \left( 423.15 - T \right)
\]

\[
B_2^{(II)} = 0
\]

and for the III-parameter approximation:

\[
B_0^{(III)} = -376.69 - 197.41 \exp \left( 438.39 - T \right)
\]

\[
B_1^{(III)} = 99.21 + 110.77 \exp \left( 445.66 - T \right)
\]

\[
B_2^{(III)} = -106.62 - 189.07 \exp \left( 438.58 - T \right)
\]

(17)

(18)
Maximum interpolation errors are 0.2% for $B_0^{(II)}$ and 0.7% for $B_1^{(II)}$ (Eqs. (17)), and 0.2% for $B_0^{(III)}$, 0.2% for $B_1^{(III)}$ and 0.8% for $B_2^{(III)}$ (Eqs. (18)).

Equations (8) and (9) in combination with Eqs. (17) or (18) can be used for calculating $\gamma_{HP}$ and $\gamma_w$. Then, one can determine the equilibrium composition of gas phase in the water–HP system by applying the following formulae:

\[ Y = \frac{\gamma_w P_w(T) X}{P(x,T)} \]  
\[ y = \frac{\gamma_{HP} P_{HP}(T) x}{P(x,T)} \]  

where $Y$ and $y$ are the molar fractions of water and HP vapor, respectively.

Alternatively, for gas phase obeying the Dalton’s law, $y$ can be obtained directly (i.e., without calculating $\gamma_{HP}$ and $\gamma_w$) using the Duhem’s equation:

\[ \frac{\partial \ln P}{\partial y} = \frac{y - x}{y(1 - y)} \]  

If the total pressure $P$ is known as a function of $y$ (along the isotherm) then Eq. (21) provides algebraic or transcendental dependence $y(x)$ at a given $T$. Usually, total pressure is known as a function of solution composition, $x$. By changing variables from $y$ to $x$ in Eq. (21), one can arrive at the differential equation for water concentrations in the two-phase water–HP system:

\[ \frac{dY}{dx} = \frac{Y(1 - Y)}{(Y - X)} Z(X,T), \quad Z(X,T) = \left( \frac{\partial \ln P}{\partial X} \right)_T \]  

To find a unique integral curve of Eq. (22), it is necessary to specify a point on the curve. For this purpose one can chose a singular point at the edge of interval $0 \leq X \leq 1$, where the molar fraction of one component in solution and in gas phase is zero. It can be shown that the singular point $X = 0$, $Y = 0$ is of saddle type and Eq. (22) should be integrated from this point.

The accuracy of approximation given by Eqs. (23) in relation to the numerical solution of Eq. (22) is illustrated in Figs. 4 and 5. Solid curves in Fig. 4 show

\[ \gamma_w = \gamma_w^{(II)} + \gamma_w^{(III)}, \quad \gamma_{HP} = \gamma_{HP}^{(II)} + \gamma_{HP}^{(III)} \]  

Figure 3: Predicted dependencies of water activity coefficient $\gamma_w$ on the mole fraction of HP in aqueous solution at $T = 523$ K.
the results of calculations of $\gamma_w$ and $\gamma_{HP}$ based on function $Y(X)$ obtained by direct integration of Eq. (22) along isotherm $T = 523$ K. Dashed curves in Fig. 4 correspond to approximation given by Eqs. (23). Solid curve in Fig. 5 shows the results of direct integration of Eq. (22). Dotted curve in Fig. 5 corresponds to approximation given by Eqs. (23); dashed curve corresponds to ideal solution approximation.

It follows from Fig. 4 that at $x > 0.02$, mean and maximum discrepancies $|\Delta Y|/Y_i$ are, respectively, fractions of percent and 4%-6%. However, gas-phase HP concentrations determined by Eqs. (20) and (23) differ from those obtained by direct integration of Eq. (22) no more than by 0.011 at $T = 423$ K and 0.006 at $T = 523$ K at all $0 \leq x \leq 1$ (see Fig. 5). Such accuracy allows one to apply Eqs. (20) and (23) for practical calculations of gas-phase composition at given $x$ and $T$ rather than directly integrate the Duhem’s equation (22).

5. Ideal solution approximation

The fact that coefficients $\gamma_w$ and $\gamma_{HP}$ can be considerably less than unity (see Figs. 3 and 4) indicates that aqueous solutions of HP do not obey the ideal solution laws, in particular at small $x$ or $X$. Nonideality of the solutions has a relatively insignificant effect on the total pressure. Nevertheless, it results in a considerable variation of the deficient gas-phase component, i.e., the component that can be considered as a small additive in the gas phase. With increasing temperature the activity coefficients tend to unity. The accuracy of formulae used for evaluation of $\gamma_w$ and $\gamma_{HP}$ decreases with the gas-phase density and, correspondingly, with the degree of gas phase departing from the ideal-gas law. However, as the gas-phase density approaches the liquid density along the phase equilibrium curve one can expect that realistic activity coefficients are closer to unity than the estimated values.

6. Ternary system

**water – hydrogen peroxide – air**

Consider the effect of air on the phase equilibrium of aqueous solutions of HP. When the volume $V_G$ occupied by a three-component gas phase is large as compared to the volume $V_L$ occupied by the liquid solution, and air pressure $P_A$ is not too high (e.g., $V_G > V_L$ and $P_A < 10$ atm), the fraction of air solved in the solution is negligibly small as compared to both the mole fraction of air in the gas phase and to mole fractions of other components. Due to low compressibility of liquid, variation of gaseous pressure caused by the presence of air does not affect significantly the thermodynamic state of solution and, in particular, the chemical potentials of main solution components. Chemical potentials of main components in the gas phase remain also unaffected if the mo-
lar fraction of air is small or if the total pressure does not exceed several dozens of atmospheres. If the chemical potentials of main components in the solution and in the gas phase are independent of the air partial pressure, all above formulae and equations determining \( \Pi(x, T, \rho_A) \) within the ideal-gas approximation will be given as a sum:

\[
\Pi(x, T, \rho_A) = P(x, T) + P_A, \quad P_A = \frac{P_A^0RT}{\mu_A}
\]

where \( \rho \) is the density, \( \mu \) is the molecular mass, and index \( A \) denotes properties of air.

7. Ternary system
water – hydrogen peroxide – jet propulsion fuel

Herein, JPF is modeled by \( n \)-tetradecane (NTD). NTD differs from water and HP by low volatility. For example, at temperature \( T = 423 \) K the saturated vapor pressure of NTD is 34.6 mm Hg, that is 103 times less than the corresponding water vapor pressure and 22 times less than HP vapor pressure. NTD is not soluble in aqueous solutions of HP and may form emulsions similar to water-in-oil emulsions. In such emulsions, NTD affects thermodynamics of the water–HP binary subsystem through the gas-phase pressure (with the accuracy of the order of inter-phase surface effects in emulsion), as the partial pressure of NTD vapor contributes to the total pressure. However, taking into account the above examples for the vapor pressure of individual components, this contribution is insignificant and the effect of NTD on the equilibrium composition of the water–HP subsystem is negligible. As for the effect of water and HP vapors on the phase equilibrium of NTD itself, it is also insignificant, at least at \( T \leq 523 \) K. At \( T = 523 \) K, the density of gas phase in the water–HP system is approximately two orders of magnitude less than the liquid density, and the Dalton’s law relating the partial pressures of components is still valid. However at higher temperatures and, correspondingly, higher densities of the gas phase the chemical potential of NTD vapor changes considerably (increases) due to intermolecular interaction (with domination of repulsive forces). As a result, phase equilibrium of NTD is shifted towards lower vapor pressure. Quantitative description of these effects is beyond the scope of this paper.

Concluding Remarks

Approximate approaches to estimate the total pressure in water–HP system are presented. Chemical composition of the system is assumed to be either “frozen” or varying slowly as compared with the rate of physical relaxation processes. Although the approaches are based on different prerequisites, they are in a good agreement with each other in terms of predictions of total pressure, activity coefficients and equilibrium gas-phase composition. In the approach of Section 2.1, total pressure was calculated as a sum of partial pressures of water and HP vapors. In Sections 2.2 and 2.3, the concept of partial pressure was not used at all. The expression for the total pressure derived in Section 2.2 does not incorporate the ideal-gas approximation and is applicable within the entire temperature range where each of the solution components exists in both liquid and gas phases. It is hardly possible that a good agreement (within a wide temperature range including the critical temperature of water) between the predictions is occasional. More preferably, all the approaches give realistic approximations for \( P(x, T) \). The extended validity of the approach of Section 2.1 (based on the ideal-gas law) for calculating \( P(x, T) \) is most probably caused by compensation of errors in the approximations for the binary system under consideration.

The activity coefficients and the equilibrium gas-phase composition have been calculated by using relationships based on the Dalton’s law. This also applies to the Duhem’s equation in the form of Eq. (22). For water–HP system this approach is approximately valid at \( T \leq 520 \) K. Comparison of activity coefficients and gas-phase composition obtained within the Redlich–Kister approximations and by numerical integration of Eq. (22) indicates that the modified approach of Eq. (23) agrees well with the solution of Eq. (22). With this modification, Eqs. (8), (9), (17), (18), and (23) provide the explicit and fairly accurate dependencies of activity coefficients on solution composition and temperature. Based on the activity coefficients, gas-phase composition can be readily obtained by using the approximations for the total pressure and Eqs. (3) and (4). Application of these formulae for estimating activity coefficients and gas-phase concentrations at higher temperatures \( T > 520 \) K.
should be considered as extrapolation. The accuracy of this extrapolation can be worse as compared to total pressure calculations.

The approaches for calculating equilibrium gas-phase composition in a two-phase system containing aqueous solution of HP, air and JPF are also suggested. The further step in evaluating the performance of the dual-fuel air-breathing PDE1–3 is to incorporate chemical kinetics of HP decomposition and JPF oxidation. Preliminary results on simulation of JPF (or HP) liquid drop ignition and combustion in air with HP (or JPF) vapor have been reported16.

References