Article

Benchmark Database Containing Binary-System-High-Quality-Certified Data for Cross-Comparing Thermodynamic Models and Assessing Their Accuracy

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ABSTRACT: In the last two centuries, equations of state (EoSs) have become a key tool for the correlation and prediction of thermodynamic properties of fluids. They not only can be applied to pure substances as well as to mixtures but also constitute the heart of commercially available computer-aided-process-design software. In the last 20 years, thousands of publications have been devoted to the development of sophisticated models or to the improvement of already existing EoSs. Chemical engineering thermodynamics is thus a field under steady development, and to assess the accuracy of a thermodynamic model or to cross-compare two models, it is necessary to confront model predictions with experimental data. In this context, the importance of a reliable free-to-access benchmark database is pivotal and becomes absolutely necessary. The goal of this paper is thus to present a database, specifically designed to assess the accuracy of a thermodynamic model or cross-compare models, to explain how it was developed and to enlighten how to use it. A total of 200 nonelectrolytic binary systems have been selected and divided into nine groups according to the associating character of the components, i.e., their ability to be involved in a hydrogen bond (the nature and strength of the association phenomena are indeed considered a measure of the complexity to model the thermodynamic properties of mixtures). The methodology for assessing the performance of a given model is then described. As an illustration, the Peng—Robinson EoS with classical van der Waals mixing rules and a temperature-dependent binary interaction parameter (k_{ij}) have been used to correlate the numerous data included in the proposed database, and its performance has been assessed following the proposed methodology.
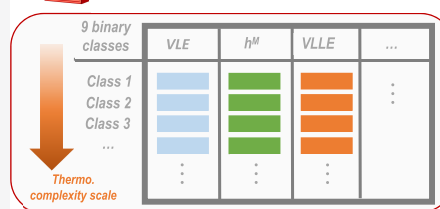
EVALUATION OF THERMODYNAMIC-MODEL PERFORMANCES

1. INTRODUCTION

Commercially available computer-aided-process-design software requires thermodynamic models to design, develop, analyze, and optimize chemical processes. As a result of their great potential, equations of state (EoSs) represent the cornerstone of thermodynamic models.[1] Indeed, combining an EoS and ideal-gas heat capacities enables one to calculate not only phase equilibria but also all of the thermodynamic properties needed for energy and exergy balances (enthalpy, entropy, exergy, heat capacities, etc.). It can be argued that in 2020, chemical engineering thermodynamics is a field under steady growth since new models are continuously under development. In the academic community, it is often assumed that the accuracy of incoming models is increasing over the years, as they become more sophisticated. However, the industry sometimes seems skeptical when weighing the value gained using a more complex model and rarely updates[2] or replaces its thermodynamic models with newer ones unless a clear advantage is evident. As a rule of thumb, it takes 10 years[3] for a new model to be conceived, developed, validated, and

accepted by the industry. It is believed that such a time lapse is extensive because, among other reasons, developers usually do not confront model predictions to experimental data that cover a wide range of compositions, temperatures, and pressures. Moreover, the comparison between experimental data and model predictions is often limited to phase equilibria, ignoring other properties like enthalpies and heat capacities. For a new model, the absence of serious validation seems to be the major obstacle to its industrialization. Although scientists spend a great deal of time building and revising EoS, and much journal space is dedicated to introducing these valuable tools, the
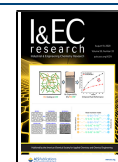
question of their accuracy inevitably arises because these models are, by definition, a simplification of reality.

In this paper, to address the relevant issue of model reliability, it was decided to build a high-quality reference database usable for assessing the accuracy of a thermodynamic model or to cross-compare the performances of two different models.

This work was conducted with the full support of the working party (WP) on thermodynamics and transport properties (https://wp-ttp.dk/) of the European Federation of Chemical Engineering (https://efce.info/). In 2010, this WP published[3] a paper entitled: "Industrial requirements for thermodynamics and transport properties" and one of the many conclusions, which fully justifies this work, was "new models are published very frequently, but unfortunately most, if not all, of these models are tested against only a few data sets. The issue of having large, standardized set of data against which all models may be tested is a very pertinent one that needs addressing and will be of great benefit, as it will allow models to be compared on equal footing."

In the first part of this paper devoted to the building of a benchmark database, a total of 200 nonelectrolytic binary systems was selected to cover all categories of mixtures and divided into nine groups according to the associating character of the components, i.e., to their ability to be involved in a hydrogen bond. The nature and strength of the association phenomena are indeed considered a measure of the complexity to model the thermodynamic properties of mixtures. In the second part of this paper, it is explained how to assess the accuracy of an EoS and to grade it with the proposed database. In particular, the exact procedure that has to be used to unambiguously calculate the deviations between model predictions and experimental data is discussed in detail and emphasis is given to the selection of specified and calculated variables. For illustration purposes, in the last part, the Peng–Robinson (PR) EoS with classical van der Waals mixing rules and a temperature-dependent k_{ij} is scored after being used to correlate the various data of the proposed database. The grades are then interpreted through a discussion dealing with the accuracy of such a thermodynamic model.

2. CRITERION TO BUILD A BENCHMARK DATABASE

2.1. Literature Review. Two databases that contain a vast number of experimental data points are widely used by researchers in the area of applied thermodynamics. The first one is the Dortmund Data Bank (DDB) (http://www.ddbst.com/ddb.html), which provides the largest data bank worldwide for thermophysical properties of pure components and their mixtures. In February 2020, the DDB contained 8.7 million data points for approximately 75 000 components from 88 200 references. The second one, provided by the National Institute of Standards and Technology (NIST), also contains pure-component and mixture data, divided into 90 Nation's Standard Reference Data (SRD) databases (https://www.nist.gov/srd). The trustworthiness of the data is assessed by experts, so that they can be used with confidence to make significant decisions.

Although extremely useful, such databases cannot be used as such to assess the accuracy of a thermodynamic model. First, they are so comprehensive that a model evaluation procedure accounting for all of the data would require an excessive amount of time. Second, the different types of systems (e.g., those that form ideal solutions, that contain size-asymmetric components, etc.) and data (e.g., vapor–liquid equilibrium (VLE) data, liquid–liquid equilibrium (LLE) data, etc.) are not equitably distributed; an evaluation over these data would lead to biased conclusions about the model efficiency. Our goal is thus to build a subdatabase from these very complete databases after a strict selection of the systems and data so that the diversity of molecular interactions and all kinds of fluid-phase behavior are represented.

To the best of our knowledge, the unique benchmark database for nonelectrolytic and nonpolymeric systems available in the literature is the one proposed by Danner and Gess in 1990.[4] This database that embeds data for 104 binary systems shows the following characteristics.

- Only subcritical VLE data are available.
- Data quality is ensured by performing consistency tests.
- Pure compounds are classified according to their polarity, from nonpolar to strongly polar, leading to the definition of nine classes of binary systems.
- For a given class, binary systems are categorized with respect to their deviations from ideality and there is an even distribution between ideal and nonideal systems.

In our opinion, such a database has many desirable features, including the classification scheme of the binary systems. However, several weak points can be pointed out: VLE data are limited to the subcritical domain and other types of phase equilibrium data, e.g., LLE, vapor–liquid–liquid equilibrium (VLLE), or derived properties like enthalpies and heat capacities are not included. Moreover, such a database was made available by their authors "on a 5 1/4 or 3 1/2 in. MS-DOS formatted floppy disk", and we cannot assert that it is still possible to get a copy or to read this support.

This short literature review makes it possible to conclude that the time has come to propose a revised version of the database developed by Danner and Gess,[4] which we hope will be widely adopted by others for assessing the accuracy of a thermodynamic model or cross-comparing two models. To guide the reader over the understanding of the choices we made to build this database, the following sections aim to address three questions.

1. Which thermophysical properties should be included?
2. Which binary systems?
3. How many systems and how many data?

2.2. Which Thermophysical Properties Should Be Included? To answer this question, we must be aware of the industrial needs. The paper by Hendriks et al.[3] explains that simultaneous description of different thermodynamic properties and phase equilibrium types (VLE, LLE, VLLE) is of great importance. It is also stated that thermodynamic modelers should no longer be satisfied with EoSs that are capable of reproducing VLE data with a reasonable accuracy at low pressures but are either untested or fail to reproduce other regions of the phase space and other properties.

As explained below, we followed these recommendations, but we have decided to go one step further in the selection of the thermophysical properties.

First, it is indisputable that a good reproduction of phase equilibrium data is mandatory to ensure that processes meet their compositional specifications. However, depending on the temperature and pressure conditions, phase equilibrium data may involve two subcritical compounds, a subcritical and a supercritical compound or possibly two supercritical compounds. In the two latter cases, binary critical points appear on

the corresponding phase diagrams. For some systems, azeotropic behavior and three-phase VLLE can occur as well. To consider such a diversity, it was decided to embed all kinds of phase equilibrium data in the developed database, i.e., VLE, LLE, VLLE, and azeotropic data points, and to cover a very wide range of compositions, temperatures, and pressures. Binary critical points were also included because we know by experience that a good representation of the critical lines[5] leads to an accurate restitution of phase diagrams on the entire temperature and pressure ranges. Such lines indeed fix the global topology[6] of the isothermal and isobaric phase diagrams for any fixed temperature or pressure, respectively. Convinced by the importance of critical points, special emphasis was given to binary systems for which such data were available.

A proper reproduction of energetic mixing properties (enthalpy and heat capacity changes on mixing) contributes to a good quantification of utility needs and energy losses in a chemical engineering process. Such knowledge is typically required for performing heat integration in chemical plants. Unlike phase equilibrium properties, the calculation of enthalpy and heat capacity changes on mixing (hereafter simply called mixing enthalpy and mixing heat capacity) with an EoS involves the derivative of the EoS expression with respect to the temperature. Consequently, h^M data help determine the temperature dependence of the phase equilibrium, which supports their value. As a matter of fact, a good reproduction of experimental phase diagrams does not ensure accurate estimations of mixing properties and, consequently, of energy-balance terms. The same conclusion was drawn by Agarwal et al.,[7] who wrote: "...if you are modeling a system with significant excess enthalpies and you have a good VLE fit, this does not automatically ensure you have a good overall model from an energy balance point of view." This highlights the necessity of considering mixing enthalpy and mixing heat capacity data for evaluating model performances. In his Ph.D. thesis, Qian[8] reached the same conclusion but also demonstrated that it was possible for the Peng−Robinson (PR) EoS with temperature-dependent binary interaction parameters (BIPs) to accurately correlate both fluid-phase equilibria and mixing properties if both types of data were included in the regression procedure. Eventually, we decided to include both mixing enthalpy and mixing heat capacity data in the proposed benchmark database.

To conclude this section, we want to emphasize that we intentionally did not incorporate excess volume data in the proposed database. This is because we know by experience that volume change on mixing is generally small (and often very small). As a direct consequence, the calculated density of a phase mainly depends on the accuracy with which the density of the pure components is calculated but is only slightly influenced by the mixing rules used. This implies that before grading a thermodynamic model with the proposed database, it is necessary to provide information on how the model behaves to correlate/predict the properties of pure compounds and in particular the vapor pressures, the liquid densities, the enthalpies of vaporization, and the liquid heat capacities.

It was also decided to exclude electrolytic systems and to only consider fluid-state binary systems, meaning that the proposed database does not include liquid−solid, solid−solid, or adsorption[9] equilibrium data.

2.3. Which Binary Systems Should Be Included? The Danner and Gess database retained our attention as it not only compiles experimental data but also provides a classification for

binary systems, revealing their thermodynamic complexity (here, thermodynamic complexity means a measure of the nonideal character of a system inducing difficulties for a model to reproduce thermodynamic macroscopic properties). In the paper by Danner and Gess, pure compounds were categorized with respect to their polarity and were classified as nonpolar, weakly polar, strongly polar, or very strongly polar. Such authors define polarity as the ability of a molecule to donate or accept a hydrogen atom and the presence of hydrogen bonding. Starting from these four categories of pure compounds, Danner and Gess defined nine classes of binary systems (nonpolar/nonpolar, nonpolar/weakly polar, etc.), and for each class, their database includes a variety of systems ranging from ideal to highly nonideal. We were totally convinced by this approach and decided to propose a somehow similar classification of binary systems but giving more emphasis on the associating character of the pure compounds, i.e., on their ability to be involved in a hydrogen bond, rather than on their polarity. Indeed, the various publications devoted to the CPA[10−12] or SAFT[13−24] EoSs clearly indicate that an actual scientific challenge for EoSs is their ability to properly describe the very complex association phenomena.

2.3.1. Definition of the "Associating Character" of a Pure Component. In this paper, "association" means association only by hydrogen bonding. In classical physical chemistry,[25] hydrogen bonds are defined as an attractive interaction between a hydrogen atom from a molecule or a molecular fragment A−H in which A is more electronegative than H and a highly electronegative atom (denoted B) in the same or a different molecule that possesses a lone pair of electrons. There is no strict cutoff for an ability to participate in hydrogen bonding, but nitrogen (N), oxygen (O), or fluor (F) atoms participate the most effectively. From the definition above, the formation of a hydrogen bond can be regarded as the electrostatic interaction between a partial positive charge (δ^+) located on the labile hydrogen atom and a partial negative charge (δ^-) located on B that possesses a lone pair of electrons (see Figure 1). The distance between the atoms H and B is classically taken as indication of the hydrogen-bond strength; it typically varies between 160 and 200 pm.
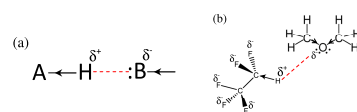
Figure 1. (a) Illustration of the definition of a hydrogen bond (red dashed line). The arrows indicate the more electronegative atom, i.e., the direction in which the shared pair of electrons (of the covalent bond) is shifted. (b) Case of the pentafluoroethane−dimethyl ether system.

To create an association by hydrogen bonding, it is needed the conjunction of (i) a labile hydrogen atom and (ii) a lone pair of electrons. It thus becomes possible to classify the pure components into four categories according to their associating character, i.e., depending on whether they have a labile hydrogen atom and/or a lone pair of electrons or none of them.

- Category 1 (associating character denoted NA for "nonassociating"): The molecule has neither a labile hydrogen atom nor a lone pair of electrons. It is

Table 1. . Definition of the 10 Families of Binary Systems and the 9 Corresponding Binary Association Codes (BACs)

component 1	component 2	binary association code (BAC)	type of exhibited association
nonassociating (NA) nonpolar	nonassociating (NA) nonpolar	1	
hydrogen-acceptor (HA) polar but nonassociating	nonassociating (NA) nonpolar	2	
hydrogen-donor (HD) polar but nonassociating	nonassociating (NA) nonpolar	3	mixtures without association
hydrogen-acceptor (HA) polar but nonassociating	hydrogen-acceptor (HA) polar but nonassociating	4	
hydrogen-donor (HD) polar but nonassociating	hydrogen-donor (HD) polar but nonassociating		
self-associating (SA) polar and associating	nonassociating (NA) nonpolar	5	mixtures in which self-association takes place (but tends to be broken)
hydrogen-donor (HD) polar but nonassociating	hydrogen-acceptor (HA) polar but nonassociating	6	mixtures in which cross-association takes place alone
self-associating (SA) polar and associating	hydrogen-donor (HD) polar but nonassociating	7	
self-associating (SA) polar and associating	hydrogen-acceptor (HA) polar but nonassociating	8	mixtures in which both cross-association and self-association take place
self-associating (SA) polar and associating	self-associating (SA) polar and associating	9	

nonpolar. Molecules like alkanes and monohalogenated compounds are included in this family. In short, this category includes nonpolar/nonassociating components.

- Category 2 (associating character denoted HA for "hydrogen-acceptor"): The molecule possesses a lone pair of electrons (on an electronegative atom) but no labile hydrogen atom. Consequently, the molecule is polar. Ketones, aldehydes, ether, and ternary amines belong to this family. In short, this category includes polar but nonassociating components.
- Category 3 (associating character denoted HD for "hydrogen-donor"): The molecule has a labile hydrogen atom but does not possess a lone pair of electrons and thus is polar. Di- or trihalogenated compounds or the ones with a terminal alkyne group belong to this family. The labile hydrogen earns its acidity from the electronegativity of its closest neighbors. In short, this category includes polar but nonassociating components.
- Category 4 (associating character denoted SA for "self-associating"): The molecule possesses both a labile hydrogen atom and a lone pair of electrons. It is strongly polar. Such molecules fulfill the two necessary and sufficient conditions to establish a hydrogen bond. They are thus self-associating. Water, alcohols, and carboxylic acids belong to this family. In short, this category includes polar and associating components.

Table S1 of the file ie0c01734_si_011.pdf which is part of the Supporting Information lists the 107 pure compounds included in the proposed database and indicates for each of them the corresponding associating character among nonassociating (NA), hydrogen-acceptor (HA), hydrogen-donor (HD), or self-associating (SA).

2.3.2. Definition of Binary Association Codes (BACs) to Describe Association in Solution. With this associating character coding, the binary systems in the database were immediately divided into the following ten families by performing all of the possible combinations (see Table 1), and a binary association code (BAC) was assigned to each family. From our experience, much less experimental data are reported for HA/HA and HD/HD binary systems than for any other family. The lack of experimental data on HD/HD binary systems can be explained by noticing that HD molecules are mostly refrigerants that are generally encountered as pure compounds in chemical processes. Therefore, it was decided to merge HA/HA and HD/HD families, which are both nonassociating mixtures, into a single family, thus reducing the number of BACs to nine.

From Table 1, it is possible to determine at a glance in which binary systems hydrogen bonds occur. Indeed, the requirement for the existence of a hydrogen bond remains to be the presence of both a labile hydrogen atom and a lone pair of electrons. In the case when the labile hydrogen atom and the lone pair of electrons originate from two different species, the hydrogen bond is said to be formed by "cross-association" between compounds 1 and 2. The last column of Table 1 highlights that all types of binary systems (those in which nonassociation, self-association, cross-association, or both cross-association and self-association are taking place) are included in the proposed database. In other words, four categories of binary systems based on the type of association they exhibit can be distinguished.

- Binary systems having a small BAC value (from 1 to 4) cannot exhibit association and are expected to be easily correlated by any sophisticated-enough thermodynamic model. In that sense, the BAC plays the role of a thermodynamic-complexity degree (for a small BAC value, the thermodynamic complexity is low, and this complexity increases with the BAC).
- In binary systems belonging to the BAC_5, an nonassociating (NA) component faces an self-associating (SA) component so that self-association (at least partially) persists in the mixture. The nonassociating molecules tend to break the hydrogen-bond network, while SA molecules tend to resist so that liquid-phase partial immiscibility is often observed in this family (these two compounds do not like being mixed together and often prefer to be each one in a separate liquid phase). In Table 1, such systems are thus considered as

Table 2. Overview of How the Deviations from Ideality Are Distributed Among the Nine Binary Association Codes (BACs) for the 200 Binary Systems of the Proposed Database[a]

binary association code (BAC)	deviations from ideality not assessed[b] (%)	ideal (%)	nonideal with enthalpic causes (%)	nonideal with entropic causes (%)	nonideal with enthalpic and entropic causes (%)	nonideal with nonassessed causes[c] (%)
1 (NA-NA)	38	15	15	4	19	8
2 (HA-NA)	29	29	13	4	17	8
3 (HD-NA)	10	30	15	0	10	35
4 (HA-HA or HD-HD)	32	32	14	5	9	9
5 (SA-NA)	33	11	22	0	22	11
6 (HD-HA)	28	16	4	0	28	24
7 (SA-HD)	44	0	6	25	25	0
8 (SA-HA)	23	15	27	4	23	8
9 (SA-SA)	9	30	22	9	17	13

[a]The abbreviations used for the associating character of a pure compound are NA for nonassociating, HA for hydrogen-acceptor, HD for hydrogen-donor, and SA for self-associating. [b]Nonavailability of subcritical VLE data (refer to Figure 2). [c]Nonavailability of h^M data (refer to Figure 2).

"mixtures in which self-association tends to be broken". All binary systems of water + alkane or alcohol + alkane types belong to this family.

- BAC_6 results from the mixing of a component that has a labile hydrogen atom with another component that possesses a lone pair of electrons, causing a cross-association phenomenon. The two components do not exhibit association when they are pure, but their mixture exhibits hydrogen bonding. Consequently, these two molecules are more attracted to each other in a mixture than when they are pure; therefore, such mixtures usually exhibit negative deviations from ideality.

- For binary association codes 7−9, more complex phenomena occur as a self-associating compound is mixed with another molecule likely to generate a hydrogen bonding with it. Therefore, it is not always possible to determine a priori how the mixture is going to behave (thermodynamically) and if the mixing leads to an intensification or a relaxation of hydrogen bonding.

2.3.3. Quantification of Deviations from Ideality. For each class of binary system, identified by its BAC, our motivation is to include in the proposed database a large variety of binary systems revealing the variety of deviation-from-ideality types. This section aims to explain how such deviations were sorted from both quantitative and qualitative viewpoints. Qualitatively, a system will be considered ideal if it is formed by molecules having (i) similar sizes, (ii) similar shapes, and (iii) showing similar energetic interactions (nature and strength), regardless of the temperature, pressure, and composition.[26] On the contrary, a system is considered nonideal if a noticeable departure from the three aforementioned criteria is observed. If deviations from ideality are the consequence of a difference in molecular sizes and/or shapes only, the excess enthalpy (h^E) is negligible and the solution is called athermal; consequently, the excess Gibbs energy is proportional to the mixture excess entropy ($g^E \approx Ts^E$) and it is said that deviations from ideality originate from entropic effects. In the same way, if deviations from ideality are solely caused by a difference in energetic interactions, the excess entropy (s^E) is negligible and the solution is called regular; consequently, $g^E \approx h^E$. In such a case, deviations from ideality are the consequence of enthalpic effects. Naturally, both effects may coexist in a nonideal solution and, in this case, it is said that deviations from ideality are the consequence of combined effects (of enthalpic and entropic natures). Such an overview of the possible causes of

deviations from ideality is important as many thermodynamic models are built by summing the contributions of an enthalpic (related to the energetic interactions in the system) and an entropic (related to the size of the molecules) term. To provide a benchmark database for EoS model evaluation, it is necessary to include mixture data spanning the whole range of departure-from-ideality types (from ideal to nonideal, including enthalpic, entropic, and combined effects). Doing so, our database will allow the identification of model failures in their enthalpic and/or entropic modeling patterns.

Quantitative information on how deviations from ideality were quantified and how the origin of such deviations was assessed is now detailed. To start, it is worth recalling that to determine the magnitude of the deviations from ideality, the activity coefficients have to be calculated from experimental VLE data. It can be done easily using the VLE relationship stemming from the $\gamma-\varphi$ approach:

$$\gamma_i(T, x) = P_{exp} \cdot y_{i,exp} / [P_i^{sat}(T_{exp}) \cdot x_{i,exp}] \quad (1)$$

Equation 1 however requires a correlation to estimate the vapor pressure of component i, so that only subcritical VLE data ($T < T_{c,i}$) can be used to estimate the deviations from ideality. In the case subcritical VLE data are not available for a system included in our database, the message deviations from ideality not assessed is reported for such a system in Table 2.

For each binary system for which subcritical VLE data were available, a set of four parameters (p_1, p_2, p_3, p_4) of the Margules excess Gibbs energy model was fit over both VLE data and enthalpy of mixing data (when available).

$$\begin{cases} \dfrac{g^E(T, \boldsymbol{x})}{RT} = x_1 \cdot x_2 \cdot A(T) \\ A(T) = p_1 - p_2 T - p_3 \ln T + P_4 \exp\left(\dfrac{1}{T}\right) \end{cases} \quad (2)$$

The p_i parameters were determined to minimize the mean average percent error (MAPE) between calculated and experimental VLE and h^M data. The mathematical expression of h^E (and thus h^M) can be straightforwardly derived from eq 2

$$h^E = g^E - T\left(\frac{\partial g^E}{\partial T}\right)_{\mathbf{X}} \quad (3)$$

For VLE calculations, the $\gamma-\varphi$ approach was used assuming that the gas phase is perfect and by neglecting the Poynting
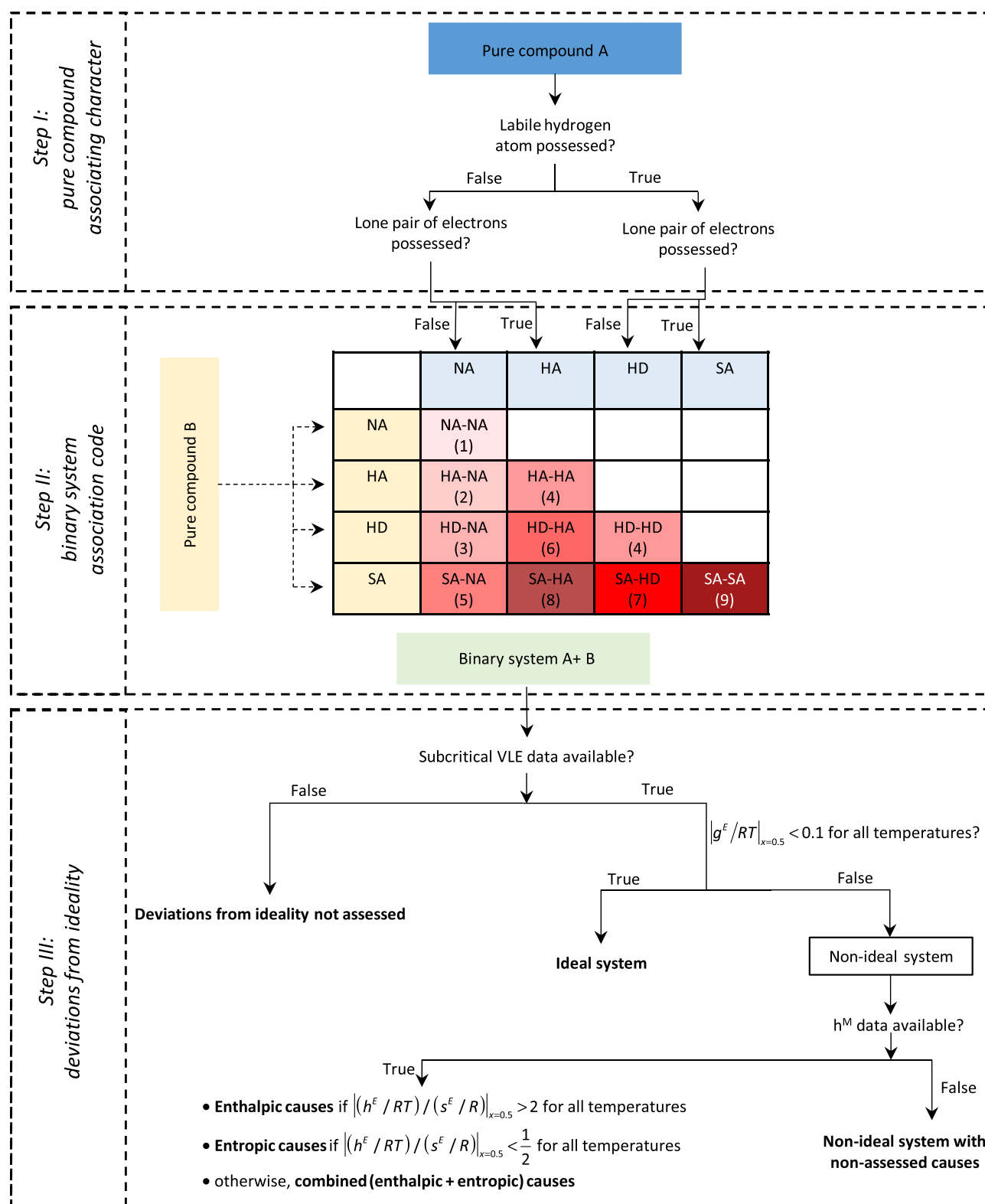
Figure 2. Procedure followed to build the proposed database.

factor. In other words, the following classical VLE relation, especially suitable to correlate subcritical data, was used:

$$P y_i = P_i^{sat} x_i \gamma_i \qquad (4)$$

The vapor pressures were calculated by means of correlations extracted from the DIPPR database.

Once the four parameters (p_1, p_2, p_3, p_4) have been fit, the magnitude of the deviations from ideality can be estimated. For each temperature involved in the regression procedure, g^E, h^E, and s^E were calculated at the unique composition $x_1 = 0.50$. Based on our experience, a binary system can be considered ideal (see Table 2) if $|g^E/RT|_{x = 0.5} < 0.1$ for each of the

Table 3. Overview of the Distribution of the Different Types of Experimental Data among the Nine Binary Association Codes (BACs) for the 200 Binary Systems of the Proposed Database[a]

binary association code (BAC)	subcritical liquid-phase[b] composition	subcritical vapor-phase (or second liquid phase[c]) composition	supercritical liquid-phase[b] composition	supercritical vapor-phase (or second liquid phase[c]) composition	azeotropic point	critical point	enthalpy of mixing	heat capacity of mixing	three-phase line	sum	%
1 (NA-NA)	1323	1336	2293	2203	11	252	1314	231	16	8979	18.8
2 (HA-NA)	1406	1406	1195	1148	22	319	1532	27	0	7055	14.7
3 (HD-NA)	1087	1087	306	306	44	49	258	30	0	3167	6.6
4 (HA-HA or HD-HD)	904	904	561	561	7	60	454	15	0	3466	7.2
5 (SA-NA)	1237	1219	343	378	35	130	1525	155	25	5047	10.5
6 (HD-HA)	1112	1112	410	410	18	63	466	99	0	3690	7.7
7 (SA-HD)	741	711	0	0	13	0	498	26	0	1989	4.2
8 (SA-HA)	2140	2119	915	881	42	193	1408	144	12	7854	16.4
9 (SA-SA)	2299	2287	149	149	33	50	1115	507	13	6602	13.8
sum	12 249	12 181	6172	6036	225	1116	8570	1234	66	47 849	
%	25.6	25.5	12.9	12.6	0.47	2.33	17.91	2.58	0.14		

[a]The abbreviations used for the associating character of a pure compound are NA for nonassociating, HA for hydrogen-acceptor, HD for hydrogen-donor, and SA for self-associating. [b]Liquid phase refers indifferently to a VLE or an LLE data point. For an LLE, it designates the composition of the α-liquid phase. [c]Second liquid phase designates the composition of the β-liquid phase in the case of an LLE.

considered temperatures. If not, the system is declared nonideal.

For nonideal systems, the origin of the deviations from ideality (entropic, enthalpic, or combined) was only evaluated when h^M experimental data were available and thus included in the regression procedure. We indeed noticed that the calculation of the excess enthalpy and entropy of a binary system could be very uncertain when the four p_i parameters were determined over VLE data only. For nonideal systems, when h^M data were lacking, the systems were thus declared (see Table 2): nonideal with nonassessed causes. In turn, when h^M data were available:

1. If $|(h^E/RT)/(s^E/R)|_{x = 0.5} > 2$ for all temperatures, it was considered that nonideality stemmed from enthalpic effects. In Table 2, the system is labeled nonideal with enthalpic causes.
2. If $|(h^E/RT)/(s^E/R)|_{x = 0.5} < 1/2$ for all temperatures, it was considered that nonideality stemmed from entropic effects. In Table 2, the system is labeled nonideal with entropic causes.
3. Otherwise, deviations from ideality are the consequence of combined effects, i.e., both enthalpic and entropic effects, and none is dominant. In Table 2, the system is labeled nonideal with enthalpic and entropic causes.

An overview of how the deviations from ideality are distributed among the nine BACs can be found in Table 2, whereas the different steps that were followed to build the proposed database are summarized in Figure 2.

2.4. How Many Systems and How Many Data Should Be Included? Commercial databases, especially the Dortmund Data Bank, report VLE data for tens of thousands of binary systems. It would be impractical to cross-compare EoS on such a huge number of data; therefore, our objective is to work with a much smaller number of wisely chosen binary systems to cover all categories of mixtures. For each of the nine families of binary systems—defined each by a distinct BAC—our objective is to consider systems, deemed as good representative of their family. Among these systems, our objective is to reach a distribution of one-fourth of systems containing high-pressure VLE data (for which deviations from ideality cannot be assessed), one-fourth of ideal systems, and

half of nonideal systems. The nonideal systems should include similar numbers of systems for which the origin of the deviations from ideality could not be assessed due to a lack of h^M data or stem from enthalpic, entropic, or (enthalpic + entropic) effects. To have a meaningful representation of such a diversity, it was found acceptable to include around 20 binary systems per BAC.

Another key point is to only retain high-quality-certified data explaining why the consistency of the data was checked with the help of four consistency tests: the point test,[27] the integral test,[28] the differential test, and the infinite-dilution test,[29] all performed with the Data Preparation Package (DPP), which is a software package for the regression of thermophysical property models commercialized by Dechema. It is however worth noting that the aforementioned tests only apply to VLE data when both compounds are subcritical. As a direct consequence, among the many data included in our benchmark database, only the quality of the subcritical data can be guaranteed. For an ideal binary system, passing the point test was considered as a sufficient consistency condition, while for nonideal systems, the point test and two of the three remaining tests had to be passed to keep the experimental data in our database. Indeed, as explained by Wisniak et al.,[30] the quality of the equilibrium data should be checked using simultaneously several of the available consistency tests.

In the end, the proposed database comprises 200 binary systems and contains about 30 000 experimental data points (around 18 000 VLE/LLE data points, 8500 h^M data, 1500 c_P^M data, and 2000 data points relative to critical points, azeotropic points, or three-phase lines).

2.5. Built Database. An extensive screening of thousands of binary systems was first realized, and a complex strategy was developed to only keep the 200 systems that met our criteria in terms of (i) types of association, (ii) deviations from ideality, and (iii) quality, quantity, and diversity of the experimental data. Indeed, as previously discussed, we made our best in order that the selected systems are such that phase equilibrium data (VLE, LLE, VLLE, azeotrope) and mixing properties (h^M, c_P^M) are abundant in large temperature, pressure, and composition ranges.

As previously stated, an overview of how the deviations from ideality are distributed among the nine BACs can be found in Table 2. Similarly, an overview of how the different types of data are distributed among the nine BACs can be found in Table 3. For each BAC, Tables 4−12 detail the list of the

Table 4. List of the 26 Binary Systems for Which the Binary Association Code Is BAC = 1 (NA-NA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	methane	propane	31−43
	methane	n-hexane	41, 44−51
	methane	n-heptane	41, 52−55
	nitrogen	ethane	56−63
	methane	n-decane	64−69
	ethane	n-heptane	70−75
	nitrogen	n-pentane	76−78
	nitrogen	n-decane	79, 80
	methane	n-tetracosane	81−84
	ethane	n-hexatriacontane	85−87
ideal	n-hexane	cyclohexane	88−100
	benzene	toluene	101−110
	propane	isopentane	111
	cyclohexane	methylcyclohexane	89, 110, 112−115
nonideal with nonassessed causes	ethane	propane	116−128
	methane	n-butane	41, 51, 129−133
nonideal with enthalpic causes	argon	methane	134−143
	n-heptane	monochlorobenzene	144−150
	cyclohexane	monochlorobenzene	113, 150−155
	1,2-dichloroethane	carbon tetrachloride	156−161
nonideal with entropic causes	1,2-dichloroethane	toluene	105, 162−166
nonideal with enthalpic and entropic causes	nitrogen	methane	61, 134, 142, 143, 167−175
	methane	ethane	39, 41, 60, 61, 176−180
	benzene	n-heptane	89, 110, 145, 181−197
	benzene	cyclohexane	91, 100, 191, 198−215
	ethylene	xenon	216−218

[a]Such a BAC corresponds to a binary system involving a nonassociating (NA) molecule + another nonassociating (NA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

selected binary systems, specify the origin of the deviations from ideality, and list the references in which the experimental data can be found. A scan of the 958 original references from which the data were extracted was realized, and the authors are committed to sending a copy of an article to any reader of this paper that would, e.g., necessitate more details on the used experimental setup.

Remark. Table 3 shows that the proposed database contains information for 225 azeotropic points. Some of them can however not be found in the original publications from which the data were extracted. We indeed decided on some azeotropic systems to interpolate the experimental VLE data

to determine the temperature, pressure, and composition of the azeotropic point.

Several Excel files are available as Supporting Information.

- The first one, named ie0c01734_si_001.xlsx, is a light Excel file that only contains the experimental data and the corresponding references. This file comprises 201 sheets. The first one, named "ReadMe", provides an overview of the database and explains how it is organized. The other 200 sheets each contain the data related to a given binary system.

- The nine others, one for each BAC, and named ie0c01734_si_002.xlsx (BAC$_1$), ie0c01734_si_003.xlsx (BAC$_2$), ie0c01734_si_004.xlsx (BAC$_3$), ie0c01734_-si_005.xlsx (BAC$_4$), ie0c01734_si_006.xlsx (BAC$_5$), ie0c01734_si_007.xlsx (BAC$_6$), ie0c01734_si_008.xlsx (BAC$_7$), ie0c01734_si_009.xlsx (BAC$_8$), ie0c01734_-si_010.xlsx (BAC$_9$) are large-size Excel files that provide figures to have a visualization of the experimental data (as a complement to data tables) and the singularities of the binary systems. These files contain several sheets. Here also, the first one, named ReadMe, provides an overview of the database and explains how it is organized, whereas the other sheets each contain the data related to a given binary system.

3. GRADING OF A THERMODYNAMIC MODEL BY MEANS OF THE PROPOSED DATABASE TO ASSESS ITS ACCURACY

This section focuses initially on the methodology that has to be followed to evaluate the deviations between model predictions and experimental data (in particular, which property of each data set must be specified and which property must be calculated from the thermodynamic model and compared to an experimental value). It is then explained how a thermodynamic model may be graded. The methodology described hereafter to assess the accuracy of a model is specific, but we believe this approach is necessary to fairly compare the scores obtained by two thermodynamic models. It is exactly what happens with the grading of students: the professor establishes a very detailed marking scheme before marking the examination papers.

3.1. Evaluation of the Deviations between Model Predictions and Experimental Data. To fairly cross-compare two thermodynamic models, we are convinced that the deviations between model predictions and experimental data have to be calculated in the same way, i.e., following the same procedure. However, in accordance with Gibbs's phase rule, there is no unique way to perform a fluid-phase equilibrium (VLE, LLE, VLLE, critical point, azeotropic point) calculation. It is always necessary to first determine the variance (also called the number of degrees of freedom) of the system and then to specify a number of intensive variables equal to the variance and finally to calculate the other intensive variables (those that will be compared to the experimental data). The variables that are specified and those that are calculated can however be freely chosen. To fix the ideas, let us consider the VLE calculation of a binary system for which the temperature T, pressure P, and composition of the liquid (x_1) and gas (y_1) phases were experimentally measured. For such a system, the number of degrees of freedom (the variance) is equal to 2 and it is thus necessary to specify two variables among (T, P, x_1, y_1) and to calculate the other two. The arbitrary

Table 5. List of the 24 Binary Systems for Which the Binary Association Code Is BAC = 2 (HA-NA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	carbon dioxide	toluene	219−233
	carbon dioxide	n-decane	234−245
	methane	carbon dioxide	35, 179, 246−255
	carbon dioxide	cyclopentane	256, 257
	nitrogen	carbon dioxide	58, 247−249, 253, 258−269
	methane	hydrogen sulfide	270−272
	carbon dioxide	n-dotriacontane	273−275
ideal	methyl *tert*-butyl ether	n-heptane	276−280
	ethyl acetate	toluene	281−284
	carbon tetrachloride	1,4-dioxane	285−290
	methyl ethyl ketone	benzene	291−294
	methyl *tert*-pentyl ether	n-heptane	295−298
	methyl *tert*-butyl ether	toluene	299−302
	1,2,3,4-tetrahydronaphthalene	quinoline	303, 304
nonideal with nonassessed causes	ethylene	carbon dioxide	305−311
	carbon dioxide	propane	35, 42, 127, 259, 312−320
nonideal with enthalpic causes	acetone	n-hexane	321−327
	n-pentane	acetone	321, 325, 327−329
	acetone	cyclohexane	98, 198, 330−337
nonideal with entropic causes	benzene	n-methyl-2-pyrrolidone	338−343
nonideal with enthalpic and entropic causes	carbon dioxide	ethane	179, 317, 344−353
	carbon dioxide	n-butane	127, 261, 306, 316−319, 354−361
	n-hexane	methyl ethyl ketone	187, 294, 362−365
	acetone	benzene	198, 286, 366−374

[a]Such a BAC corresponds to a binary system involving a hydrogen-acceptor (HA) molecule + a nonassociating (NA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 6. List of the 20 Binary Systems for Which the Binary Association Code Is BAC = 3 (HD-NA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	ethylene	dichloromethane	375
	nitrogen	chlorodifluoromethane	376−379
ideal	chloroform	benzene	105, 371, 380−386
	chloroform	1,2-dichloroethane	387−389
	chloroform	carbon tetrachloride	390−393
	1,1,1-trifluoroethane	2,3,3,3-tetrafluoropropene	394
	ethyl fluoride	1,1,1,2-tetrafluoroethane	395
	propylene	chlorodifluoromethane	396
nonideal with nonassessed causes	difluoromethane	propane	397−401
	trifluoromethane	ethane	402, 403
	carbon tetrafluoride	chlorodifluoromethane	404, 405
	pentafluoroethane	propane	398, 400, 406−408
	carbon tetrafluoride	trifluoromethane	409
	hexafluoroethane	1,1,1,2-tetrafluoroethane	396, 410
	decafluorobutane	1,1,1,3,3-pentafluorobutane	411
nonideal with enthalpic causes	chlorodifluoromethane	dichlorodifluoromethane	412−417
	dichloromethane	carbon tetrachloride	157, 160, 391, 418
	chloroform	n-hexane	419−425
nonideal with enthalpic and entropic causes	chloroform	n-heptane	419, 422, 423, 425−427
	dichloromethane	n-pentane	428−430

[a]Such a BAC corresponds to a binary system involving a hydrogen-donor (HD) molecule + a nonassociating (NA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

choice made in this paper is to specify T and P (i.e., to fix T and P to their experimental values) and to calculate, in turn, x_1 and y_1. There are thus no deviations between model predictions and experimental values of T and P but instead deviations over x_1 and y_1. Specifying T and P and calculating x_1 and y_1 are somehow similar to a T,P-flash calculation.[989] For

each property available in the proposed database, Table 13 reports the variance and the specified and calculated variables. In other words, Table 13 dictates the methodology that has to be strictly followed to evaluate the deviations between model predictions and experimental data by means of the proposed database.

Table 7. List of the 22 Binary Systems for Which the Binary Association Code Is BAC = 4 (HA-HA or HD-HD)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	carbon dioxide	dimethyl ether	431−433
	carbon dioxide	hydrogen sulfide	434−437
	carbon dioxide	ethyl acetate	438−442
	carbon dioxide	carbon disulfide	443, 444
	carbon dioxide	dimethyl carbonate	445−450
	carbon monoxide	carbon dioxide	451−453
	oxygen	carbon dioxide	264, 265, 454−457
ideal	pentafluoroethane	1,1,1,2-tetrafluoroethane	458−462
	chlorodifluoromethane	1,1,1,2-tetrafluoroethane	463, 464
	difluoromethane	1,1,1,2-tetrafluoroethane	458, 459, 461, 462, 465−469
	1,1,1,2-tetrafluoroethane	1,1-difluoroethane	396, 470, 471
	ethyl acetate	1,4-dioxane	285, 472−474
	dimethyl carbonate	diethyl carbonate	475−477
	1,2-epoxybutane	dimethyl carbonate	478
nonideal with nonassessed causes	dimethyl ether	sulfur dioxide	479−481
	trifluoromethane	chlorodifluoromethane	482, 483
nonideal with enthalpic causes	diethyl ether	acetone	383, 484, 485
	carbon disulfide	acetone	486−488
	triethylamine	1,4-dioxane	489, 490
nonideal with entropic causes	thiophene	sulfolane	491
nonideal with enthalpic and entropic causes	tetrahydrofuran	N,N-dimethylformamide	492, 493
	n-butyl acetate	N,N-dimethylformamide	494, 495

[a]Such a BAC corresponds to a binary system involving two hydrogen-acceptor (HA) molecules or two hydrogen-donor (HD) molecules. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 8. List of the 18 Binary Systems for Which the Binary Association Code Is BAC = 5 (SA-NA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	n-butane	water	496−500
	water	benzene	501−505
	ethane	1-propanol	506−511
	nitrogen	ammonia	512−514
	ethane	water	497
	nitrogen	water	515−525
ideal	diethylamine	benzene	145, 526, 527
	diethylamine	monochlorobenzene	145, 528
nonideal with nonassessed causes	ethane	methanol	508, 529−534
	propane	methanol	535−539
nonideal with enthalpic causes	1-propanol	benzene	200, 540−548
	ethanol	benzene	190, 193, 208, 380, 545, 548−558
	isopropanol	2,2,4-trimethylpentane	559−566
	2-butanol	cyclohexane	567−572
nonideal with enthalpic and entropic causes	1-propanol	n-hexane	573−579
	ethanol	n-heptane	580−596
	methanol	n-hexane	579, 588, 597−605
	methanol	benzene	545, 548, 555, 606−616

[a]Such a BAC corresponds to a binary system involving a self-associating (SA) molecule + a nonassociating (NA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 13 highlights that for systems of variance equal to 2 (two-phase equilibrium binary systems), we arbitrarily decided that temperature and pressure should be specified, whereas phase compositions should be calculated. For systems of unitary variance (binary critical point, binary azeotropic point, binary three-phase equilibrium), we decided that the temperature should be specified and that other variables (critical pressure and composition, azeotropic pressure and composition, three-phase pressure and compositions) should be calculated.

The calculation of the deviations between model predictions and experimental data for mixing properties does not need to make arbitrary choices on the specified and calculated variables; there is indeed a unique way to perform the calculation. For such properties, the temperature, pressure, global composition z_1, and h^M (or c_P^M) are experimentally determined. Depending on (T,P,z_1), the binary system can be either in a one-phase or in a two-phase region so that a T,P-flash calculation has to be first performed at a specified temperature, pressure, and global composition to determine the number of phases in equilibrium, their composition, and their proportions. Once done, h^M or c_P^M can be straightforwardly calculated for the specified (T,P,z_1) values.[990] It is worth noting that the experimentalists who performed h^M or c_P^M measurements do not mention systematically the pressure at which the measurements were conducted although such a value is required to perform the calculation from an EoS. This usually happens for mixing properties related to a liquid phase on which the pressure has a negligible influence. When this happened, the assumed experimental pressure was determined by trial and errors so that the calculated physical state of the system agrees with the experimentally observed state. The first guessed pressure is always the atmospheric pressure. In the 10 Excel files ie0c01734_si_001.xlsx (complete database),

Table 9. List of the 25 Binary Systems for Which the Binary Association Code Is BAC = 6 (HD-HA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	carbon dioxide	chlorodifluoromethane	376, 377, 483, 617
	carbon dioxide	1,1,1,2-tetrafluoroethane	618−621
	carbon dioxide	1,1,1,2,3,3,3-heptafluoropropane	622, 623
	trifluoromethane	carbon disulfide	483
	chloroform	diisopropyl ether	425, 490, 624, 625
	1,1,1-trifluoroethane	dimethyl ether	626
	chloroform	*n*-butyl ethyl ether	624, 627
ideal	carbon dioxide	difluoromethane	469, 628−630
	difluoromethane	dimethyl ether	631−633
	difluoromethane	sulfur dioxide	634
	ethyl acetate	trichloroethylene	635
nonideal with nonassessed causes	sulfur dioxide	1,1,1,2,3,3,3-heptafluoropropane	636
	chlorodifluoromethane	dimethyl ether	637
	chlorodifluoromethane	carbon disulfide	483
	pentafluoroethane	dimethyl ether	407, 638
	3-pentanone	1,1,2,2-tetrachloroethane	639
	dimethyl ether	1,1,1,3,3,3-hexafluoropropane	640, 641
nonideal with enthalpic causes	dichloromethane	carbon disulfide	642, 643
nonideal with enthalpic and entropic causes	acetone	chloroform	372, 374, 384, 420, 425, 490, 644−651
	chloroform	ethyl acetate	652−655
	chloroform	tetrahydrofuran	387, 425, 656−659
	chloroform	di-n-propyl ether	425, 624, 625, 627, 660, 661
	methyl acetate	chloroform	425, 652, 662, 663
	cyclopentanone	1,1,2,2-tetrachloroethane	664−666
	ethyl acetate	1,1,2,2-tetrachloroethane	667, 668

[a]Such a BAC corresponds to a binary system involving a hydrogen-donor (HD) molecule + a hydrogen-acceptor (HA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 10. List of the 16 Binary Systems for Which the Binary Association Code Is BAC = 7 (SA-HD)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	chloroform	1-butanol	382, 669, 670
	1-propanol	trichloroethylene	671, 672
	trichloroethylene	1-butanol	672, 673
	isopropanol	trichloroethylene	671, 674
	2-butanol	trichloroethylene	673, 674
	1-hexyne	acetonitrile	675, 676
	isopropanol	chloroform	670, 677, 678
nonideal with enthalpic causes	ethanol	1-heptyne	679, 680
nonideal with entropic causes	ethanol	chloroform	382, 427, 670, 681−686
	chloroform	acetic acid	687−691
	methanol	halothane	692−694
	trichloroethylene	2-methoxyethanol	695, 696
nonideal with enthalpic and entropic causes	chloroform	acetonitrile	697−702
	ethyl formate	chloroform	652, 654
	chloroform	1-propanol	383, 670, 703, 704
	n-propyl formate	1,1,2,2-tetrachloroethane	667, 705

[a]Such a BAC corresponds to a binary system involving a self-associating (SA) molecule + a hydrogen-acceptor (HA) Molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

ie0c01734_si_002.xlsx (BAC$_1$), ie0c01734_si_003.xlsx (BAC$_2$), ie0c01734_si_004.xlsx (BAC$_3$), ie0c01734_si_005.xlsx (BAC$_4$), ie0c01734_si_006.xlsx (BAC$_5$), ie0c01734_si_007.xlsx (BAC$_6$), ie0c01734_si_008.xlsx (BAC$_7$), ie0c01734_si_009.xlsx (BAC$_8$), ie0c01734_si_010.xlsx (BAC$_9$)—available as Supporting Information— that contain all of the experimental data, the experimental pressure appears as unknown and the assumed experimental pressure is indicated in parentheses. For clarity, an example is given in Figure 3. In this example, the unknown (not stated) experimental pressure has to be replaced by the atmospheric pressure (1.0132 bar).

Lastly, for any calculated property *X*, the mean absolute percentage error (MAPE) was selected to quantify the deviation between experimental and calculated data:

$$\mathrm{MAPE}_X(\%) = \frac{1}{N_{\mathrm{data}}} \sum_{i=1}^{N_{\mathrm{data}}} 100 \times \left| \frac{X_i^{\mathrm{EXP}} - X_i^{\mathrm{MODEL}}}{X_i^{\mathrm{EXP}}} \right| \tag{5}$$

3.2. Treatment of "Out-of-Model" Data Points. It may happen that the isothermal or isobaric phase diagram, calculated with the thermodynamic model we want to grade, does not have the expected topology. To fix the ideas, it may happen that a model does not predict the existence of a homogeneous azeotrope that is however experimentally observed. In such a case, the MAPE on P_{az} and x_{az} cannot be evaluated and the corresponding experimental data point is said to be out of model (not calculable by the model). When such a situation arises, the experimental data point must be rejected, i.e., not taken into account in eq 5 to evaluate the MAPE$_x$(%). In other words, we simply apply $N_{\mathrm{data}} = N_{\mathrm{data}} - 1$

Table 11. List of the 26 Binary Systems for Which the Binary Association Code Is BAC = 8 (SA-HA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	carbon dioxide	water	706−724
	carbon dioxide	ethanol	219, 242, 507, 579, 725−739
	ethanol	methyl tert-butyl ether	280, 740−744
	carbon dioxide	2-methyl-1-propanol	745−750
	carbon monoxide	methanol	751−753
	carbon dioxide	1-pentanol	242, 747, 754−757
ideal	diethylamine	ethyl acetate	473, 474
	diethylamine	triethylamine	758−761
	2-methyl-2-propanol	methyl tert-butyl ether	762−765
	acetonitrile	1,4-dioxane	766−768
nonideal with nonassessed causes	dimethyl ether	water	433, 769−772
	carbon dioxide	methanol	220, 221, 242, 433, 579, 731, 736, 739, 751, 773−783
nonideal with enthalpic causes	methanol	ethyl acetate	784−791
	isopropanol	diisopropyl ether	561, 742, 792, 793
	methanol	n-butyl acetate	789, 794−796
	diethyl ether	ethanol	797−799
	methanol	1,4-dioxane	800−805
	methanol	thiophene	606
	ethanol	di-n-butyl ether	799, 806−808
nonideal with entropic causes	methanol	diisopropyl ether	742, 809−811
nonideal with enthalpic and entropic causes	methanol	methyl tert-butyl ether	277, 279, 280, 741, 810, 812−816
	ethanol	ethyl acetate	786, 789, 790, 808, 817−824
	acetone	water	335, 610, 825−836
	ethanol	methyl ethyl ketone	291, 837−844
	ethanol	acetone	586, 845−850
	methanol	acetone	331, 335, 830, 851−856

[a]Such a BAC corresponds to a binary system involving a self-associating (SA) molecule + a hydrogen-acceptor (HA) Molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 12. List of the 23 Binary Systems for Which the Binary Association Code Is BAC = 9 (SA-SA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	water	ethylenediamine	857−859
	water	1-pentanol	860−863
ideal	methanol	1-butanol	610, 864−868
	ethanol	acetic acid	824, 869−872
	methanol	ethanol	655, 868, 873−879
	2-methyl-2-propanol	1-butanol	880−882
	ethanol	3-methyl-1-butanol	883−885
	methanol	3-methyl-1-butanol	885−887
	methanol	1-propanol	596, 833, 868, 878, 879, 888−891
nonideal with nonassessed causes	ammonia	water	892−901
	ammonia	acetonitrile	902
	water	allyl alcohol	903, 904
nonideal with enthalpic causes	water	phenol	905−911
	methyl formate	methanol	912−916
	ethyl formate	water	917, 918
	ethanol	ethyl formate	916, 919−921
	1-butanol	nitromethane	879, 922−926
nonideal with entropic causes	water	2-butoxyethanol	927−932
	water	propylene glycol monomethyl ether	928
nonideal with enthalpic and entropic causes	ethanol	water	817, 833, 874, 933−953
	water	acetonitrile	954−963
	methanol	water	830, 936, 950, 951, 964−981
	isopropanol	water	586, 938, 982−988

[a]Such a BAC corresponds to a binary system involving a self-associating (SA) molecule + another self-associating (SA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.
[b]The following part of this article (Section 3) aims at explaining how the proposed database should be used to grade a thermodynamic model to assess its accuracy. For illustrative purposes, Section 4 clarifies the grading of the thermodynamic model: {Peng−Robinson EoS + classical VdW mixing rules + a temperature-dependent BIP} and opens a discussion around its accuracy.

in eq 5. Below are detailed all of the cases in which out-of-model data points could appear.

Case 1. At specified T and P ($T = T_{exp}$ and $P = P_{exp}$), a two-phase system is experimentally observed, whereas the model predicts a one-phase system. All of the experimental data points for which the model predicts a one-phase system are declared out of model. This case is illustrated in Figure 4a.

Case 2. At specified T and P ($T = T_{exp}$ and $P = P_{exp}$), a two-phase system is experimentally observed and a two-phase system is also predicted by the model. However, it was experimentally found that $y_{1,exp} > x_{1,exp}$ (respectively, $y_{1,exp} < x_{1,exp}$), and the model predicts the wrong topology, i.e., predicts $y_{1,cal} < x_{1,cal}$ (respectively, $y_{1,cal} > x_{1,cal}$). All of these experimental data points are declared out of model. This case, which typically appears when the azeotropic composition

is not properly predicted by the model, is illustrated in Figure 4b.

Case 3. A homogeneous azeotrope is experimentally observed at $T = T_{exp}$, whereas the model predicts a different topology (a zeotropic behavior or a heterogeneous azeotrope). The experimental homogeneous azeotropic point is declared out of model. This case is illustrated in Figure 4b,c.

Case 4. A three-phase line (VLLE) is experimentally observed at $T = T_{exp}$, whereas the model does not predict such a behavior. The experimental three-phase line is thus declared out of model. This case is illustrated in Figure 4d.

Case 5. The number of calculated critical points at $T = T_{exp}$ is different from the number of critical points experimentally observed. For example, the binary system may exhibit two

Table 13. Specified and Calculated Variables for the Different Binary-System Properties Involved in the Database

property	variance	measured variables	specified variables	calculated variables (to be compared with experimental data values)
critical point		T, P, x_1	T	P, x_1
azeotropic point	1	T, P, x_1	T	P, x_1
three-phase equilibrium data (VLLE)		$T, P, x_1^\alpha, x_1^\beta, y_1$	T	$P, x_1^\alpha, x_1^\beta, y_1$
two-phase equilibrium data (VLE or LLE)	2	$\begin{cases} T, P, x_1, y_1 \text{ for VLE} \\ T, P, x_1^\alpha, x_1^\beta \text{ for LLE} \end{cases}$	T, P	$\begin{cases} x_1, y_1 \text{ for VLE} \\ x_1^\alpha, x_1^\beta \text{ for LLE} \end{cases}$
enthalpy of mixing	N.A.[a]	T, P, z_1, h^M	T, P, z_1	h^M
heat capacity of mixing		T, P, z_1, c_P^M	T, P, z_1	c_P^M

[a]Not applicable because global variables (here, global mole fractions z_1 and $z_2 = 1 - z_1$) are involved. Let us indeed recall that the phase rule that defines the variance only considers intensive variables specific to one of the phases.

```
-------------------- ---------------------------------------
Enthalpy of mixing (Methane + Ethane system)
-------------------- ---------------------------------------
Miller, R. C. - Staveley, L. A. K., Advances in Cryogenic Engineering. (1960) 493-500
T / K =            91.50
P / bar =          UNKNOWN (1.0132)
hᴹ / J.mol⁻¹       x₁
67.00              0.2825
80.00              0.4008
82.70              0.5105
84.90              0.6039
77.60              0.7044
65.80              0.7879
```

Figure 3. Notation used in the files database.xlsx and BACi with visualization of the data.xlsx ($i = 1-9$) when the experimental pressure is not mentioned.

experimental critical points, whereas 1 or 0 are returned by the model (see, e.g., Figure 4e). The opposite may also happen: the binary system exhibits a unique critical point, but 2 are returned by the model (see, e.g., Figure 4f). In such cases, the experimental critical points are all declared out of model.

3.3. Grading of a Thermodynamic Model. Our objective is to give a unique mark over 20 to a given thermodynamic model to immediately be able to benchmark its accuracy against the accuracy of other models. A grade of 20/20 is the highest attainable mark. It is obtained only if the model is able to exactly reproduce (with 0% deviation) all of the experimental data available in the proposed database. In all other cases, a score lower than 20 will be assigned to the model. Once the MAPEs are calculated (see eq 5), the scoring of a thermodynamic model starts by giving a mark over 20 to each of the nine families of binary systems, each identified by its BAC. Such a mark is actually an average over 10 marks (one for each of the 10 calculated properties defined in the last column of Table 13), which are:

(1) critical pressure,
(2) critical composition,
(3) azeotropic pressure,
(4) azeotropic composition,
(5) liquid-phase composition (x_1, x_1^α),
(6) gas-phase (or second liquid phase) composition (y_1, x_1^β),
(7) three-phase pressure,
(8) three-phase compositions,
(9) mixing enthalpy, and
(10) mixing heat capacity.

Once done, a thermodynamic model is characterized by nine marks (one for each BAC). In a second step, the number of marks is reduced from 9 to 4 by averaging the marks obtained by some BACs to only retain four categories of binary systems based on the type of association they exhibit.

- The marks obtained by $BAC_1 + BAC_2 + BAC_3 + BAC_4$ are averaged because all of these systems do not exhibit association (see Table 1). In eq 6, the resulting average mark is noted $mark_{NA}$ (where NA stands for no association).
- The mark obtained by BAC_5 is kept as a single mark because in this type of system, and only in this one, self-association tends to be broken (see Table 1). In eq 6, $mark_{BAC_5}$ is noted $mark_{SA}$ (where SA stands for self-association).
- The mark obtained by BAC_6 is kept as a single mark because in this type of system, and only in this one, cross-association without the presence of self-association is observed. BAC_6 refers to binary systems in which cross-association takes place alone (see Table 1). In eq 6, $mark_{BAC_6}$ is noted $mark_{CA}$ (where CA stands for cross-association).
- The marks obtained by $BAC_7 + BAC_8 + BAC_9$ are averaged because all of these systems exhibit both cross-association and self-association (see Table 1). In eq 6, the resulting average mark is noted $mark_{CA+SA}$ (where CA+SA stands for "cross-association + self-association").

The unique final mark given to a thermodynamic model is obtained by averaging the 4 marks (see eq 6) relative to (i)

Figure 4. Illustration of all of the cases in which out-of-model data points can appear. For such exp. data points, the MAPE cannot be evaluated. (a) Experimental two-phase data points that are found to be one phase by the model. (b) An azeotropic system is predicted as a zeotropic system so that the homogeneous azeotrope is declared as out of model. In addition, for small mole fractions, $y_{1,\exp} > x_{1,\exp}$, whereas the model predicts the opposite. (c) A homogeneous azeotrope is predicted as heterogeneous. (d) A three-phase line is not predicted by the model. (e) Two critical points that are not predicted by the model are experimentally observed. (f) The model predicts two critical points, whereas only one is experimentally observed.

systems without association, (ii) systems in which self-association tends to be broken, (iii) systems in which cross-association takes place alone, and (iv) systems in which both cross-association and self-association take place.

$$\begin{cases} \underset{\substack{\textit{Final mark} \\ \textit{of a thermodynamic model} \\ \textit{(over 20)}}}{} = \frac{1}{4} \times \left[\underbrace{mark_{NA}}_{\text{no association}} + \underbrace{mark_{SA}}_{\text{self-association}} + \underbrace{mark_{CA}}_{\text{cross-association}} + \underbrace{mark_{CA+SA}}_{\substack{\text{cross-association} \\ + \text{ self-association}}} \right] \\ \qquad\qquad\qquad\qquad\qquad \underbrace{\phantom{mark_{NA} + mark_{SA} + mark_{CA} + mark_{CA+SA}}}_{\text{average of 4 marks}} \end{cases} \tag{6}$$

$$with: \begin{cases} mark_{NA} = \dfrac{mark_{BAC_1} + mark_{BAC_2} + mark_{BAC_3} + mark_{BAC_4}}{4} \\ mark_{SA} = mark_{BAC_5} \\ mark_{CA} = mark_{BAC_6} \\ mark_{CA+SA} = \dfrac{mark_{BAC_7} + mark_{BAC_8} + mark_{BAC_9}}{3} \end{cases}$$

The procedure aimed at giving a mark over 20 to a given BAC ($mark_{BAC_i}$) is now detailed. As previously stated, such mark is, in itself, the average value of 10 marks (in liquid-phase composition x (or x^α), gas-phase (or second liquid phase) composition y (or x^β), three-phase pressure P_{LLV}, three-phase composition z_{LLV}, critical pressure P_c, critical composition x_c, azeotropic pressure P_{az}, azeotropic composition x_{az}, mixing enthalpy h^M, mixing heat capacity c_P^M), each defined below.

(1) Mark in the liquid-phase composition (x for VLE and x^α for LLE):

$$\text{Mark}_{x \text{ or } x^\alpha} = 20 - 0.5$$
$$\times \left[\frac{\text{MAPE on } x_1 \text{ or } x_1^\alpha \ (\%) + \text{MAPE on } x_2 \text{ or } x_2^\alpha \ (\%)}{2} \right] \tag{7}$$

where x_i (respectively, x_i^α) is the mole fraction of component i in the liquid phase (respectively, the α-liquid phase).

(2) Mark in the gas-phase (y) or second liquid-phase (x^β) composition:

$$\text{Mark}_{y \text{ or } x^\beta} = 20 - 0.5$$
$$\times \left[\frac{\text{MAPE on } y_1 \text{ or } x_1^\beta \ (\%) + \text{MAPE on } y_2 \text{ or } x_2^\beta \ (\%)}{2} \right] \tag{8}$$

where y_i (respectively, x_i^β) is the mole fraction of component i in the gas or second liquid phase.

Remark: Very small (or close to 1) mole fractions may lead to huge percent deviations. As an example, at $T/K = 377.59$ K and $P = 1.379$ bar, the solubility of n-butane in water is $x_{1,\exp} = 0.000002$. In the case a model calculates $x_1 = 0.000082$, the corresponding $1/2 \times$ (MAPE on x_1 + MAPE on x_2) relative to this unique data point is about 2000% even though the absolute deviation is extremely small ($|x_{1,\exp} - x_{1,cal}| = 0.00008$). Such a data point can thus have a huge influence on the calculated $\text{Mark}_{x \text{ or } x^\alpha}$ (or $\text{Mark}_{y \text{ or } x^\beta}$). To avoid such a bias, if

$$\begin{cases} z_{1,\exp} < 0.01 \text{ or } z_{1,\exp} > 0.99 \\ \\ \text{and simultaneously:} \\ \quad 1/2 \times (\text{MAPE on } z_1 + \text{MAPE on } z_2) \\ \quad > 45\% \end{cases} \tag{9}$$

where z_1 stands for the mole fraction of component 1 in the liquid or gas phase of a two-phase system (VLE or LLE), the corresponding data point is rejected (we here mean, it is not taken into account in eq 5 to annihilate its influence on the calculated $\text{Mark}_{x \text{ or } x^\alpha}$ (or $\text{Mark}_{y \text{ or } x^\beta}$)).

(3) Mark in the three-phase pressure, P_{LLV}:

$$\text{Mark}_{P_{\text{LLV}}} = 20 - 0.50 \times \text{MAPE on } P_{\text{LLV}} \ (\%) \qquad (10)$$

(4) Mark in the three-phase composition, z_{LLV}:

$$\text{Mark}_{z_{\text{LLV}}} = 20 - 0.5 \times$$

$$\sum_{i=1}^{2} \left[\frac{\text{MAPE on } x_i^\alpha \ (\%) + \text{MAPE on } x_i^\beta \ (\%) + \text{MAPE on } y_i \ (\%)}{6} \right] \qquad (11)$$

where x_i^α, x_i^β, and y_i are the mole fractions of component i in each of the three equilibrium phases.

(5) Mark in critical pressure, P_c:

$$\text{Mark}_{P_c} = 20 - 0.75 \times \text{MAPE on } P_c \ (\%) \qquad (12)$$

(6) Mark in critical composition, x_c:

$$\text{Mark}_{x_c} = 20 - 0.5 \times \left[\frac{\text{MAPE on } x_{1,c} \ (\%) + \text{MAPE on } x_{2,c} \ (\%)}{2} \right] \qquad (13)$$

where $x_{i,c}$ is the mole fraction of component i at the critical point.

(7) Mark in azeotropic pressure, P_{az}:

$$\text{Mark}_{P_{\text{az}}} = 20 - 0.50 \times \text{MAPE on } P_{\text{az}} \ (\%) \qquad (14)$$

(8) Mark in azeotropic composition, x_{az}:

$$\text{Mark}_{x_{\text{az}}} = 20 - 0.5$$
$$\times \left[\frac{\text{MAPE on } x_{1,\text{az}} \ (\%) + \text{MAPE on } x_{2,\text{az}} \ (\%)}{2} \right] \qquad (15)$$

where $x_{i,\text{az}}$ is the mole fraction of component i at the azeotropic point.

(9) Mark in mixing enthalpy, h^M:

$$\text{Mark}_{h^M} = 20 - 0.25 \times \frac{1}{n_{h^M}} \sum_{i=1}^{n_{h^M}} \frac{1}{2}$$
$$\left(100 \times \left| \frac{h_i^{M,\text{EXP}} - h_i^{M,\text{MODEL}}}{h_i^{M,\text{EXP}}} \right| + 100 \right.$$
$$\left. \times \left| \frac{h_i^{M,\text{EXP}} - h_i^{M,\text{MODEL}}}{h_i^{M,\text{MODEL}}} \right| \right) \qquad (16)$$

where n_{h^M} is the number of mixing enthalpy data points.

Remarks:

1. h^M goes to 0 when the mole fraction of the studied phase (z_1) goes to 0 or 1. In such cases, huge percent deviations and consequently very bad marks on h^M can be obtained. To avoid such a bias, if in eq 16

$$\frac{1}{2} \left(100 \times \left| \frac{h_i^{M,\text{EXP}} - h_i^{M,\text{MODEL}}}{h_i^{M,\text{EXP}}} \right| + 100 \right.$$
$$\left. \times \left| \frac{h_i^{M,\text{EXP}} - h_i^{M,\text{MODEL}}}{h_i^{M,\text{MODEL}}} \right| \right) > 80\%$$

this quantity is set to 80%.

2. Equation 16 highlights that we here decided to make the average between two MAPEs: one calculated with the classical definition (see eq 5) and one obtained by introducing $h_i^{M,\text{MODEL}}$ (i.e., the calculated value) at the denominator. This

procedure is selected to obtain the same mark when calculated values of h^M are n times (e.g., twice) smaller or n times larger than the experimental values. To fix the ideas, let us assume that $h^{M,\text{EXP}} = 100 \ \text{J·mol}^{-1}$. If the calculated value is 50 times too small, let us say $h^{M,\text{MODEL}} = 2 \ \text{J·mol}^{-1}$, then eq 5 returns a MAPE_{h^M} (%) of 98%. In contrast, if the calculated value is 50 times too large, i.e., $h^{M,\text{MODEL}} = 5000 \ \text{J·mol}^{-1}$, then eq 5 returns a MAPE_{h^M} (%) of 4900%. As a direct consequence, the classical MAPE definition favors the case where $h^{M,\text{MODEL}}$ is 50 times below $h^{M,\text{EXP}}$. However, for both cases ($h^{M,\text{MODEL}} = 2 \ \text{J·mol}^{-1}$ or $h^{M,\text{MODEL}} = 5000 \ \text{J·mol}^{-1}$), the average of the two MAPEs embedded in eq 16 is exactly the same. For the selected example,

$$\frac{1}{2} \left(100 \times \left| \frac{h_i^{M,\text{EXP}} - h_i^{M,\text{MODEL}}}{h_i^{M,\text{EXP}}} \right| + 100 \right.$$
$$\left. \times \left| \frac{h_i^{M,\text{EXP}} - h_i^{M,\text{MODEL}}}{h_i^{M,\text{MODEL}}} \right| \right) = 2499\%$$

3. In practice, h^M is used to evaluate molar enthalpies of the streams ($h_{\text{stream}} = z_1 h_1 + z_2 h_2 + h^M$) that are involved in the energy balance of a given process. The mark determined by eq 16 thus needs to capture the influence of h^M on such a balance. One possibility of reaching this target is to convert the difference $|h_i^{M,\text{EXP}} - h_i^{M,\text{MODEL}}|$ into terms of the temperature effect[990] ΔT_h through

$$\Delta T_h = \frac{|h_i^{M,\text{EXP}} - h_i^{M,\text{MODEL}}|}{c_P} \qquad (17)$$

where c_P is the molar isobaric heat capacity of the mixture. ΔT_h quantifies the error made in the estimation of the final temperature of a mixture obtained by mixing two pure compounds at isobaric and adiabatic conditions. From our experience in process simulation, we decided to consider that $\Delta T_h = 1.4 \ K$ was a good reference. In many cases, such a deviation is reached when h^M is estimated with a deviation of around 20%, and eq 16 is conceived so that with this deviation the mark is equal to 15/20.

(10) Mark in mixing heat capacity, c_P^M:

$$\text{Mark}_{c_P^M} = 20 - 0.10 \times \frac{1}{n_{c_P^M}} \sum_{i=1}^{n_{c_P^M}} \frac{1}{2} \left(100 \times \left| \frac{c_{P,i}^{M,\text{EXP}} - c_{P,i}^{M,\text{MODEL}}}{c_{P,i}^{M,\text{EXP}}} \right| \right.$$
$$\left. + 100 \times \left| \frac{c_{P,i}^{M,\text{EXP}} - c_{P,i}^{M,\text{MODEL}}}{c_{P,i}^{M,\text{MODEL}}} \right| \right) \qquad (18)$$

where $n_{c_P^M}$ is the number of mixing heat capacity data points. This mark was developed in a similar manner to Mark_{h^M} so that the following remarks apply.

Remarks:

1. Analogously to h^M, c_P^M goes to 0 when the mole fraction of the studied phase (z_1) goes to 0 or 1. In such cases, huge percent deviations and consequently very bad marks on c_P^M can be obtained. To avoid such a bias, if in eq 18

$$\frac{1}{2}\left(100 \times \left|\frac{c_{P,i}^{M,EXP} - c_{P,i}^{M,MODEL}}{c_{P,i}^{M,EXP}}\right| + 100 \right.$$

$$\left. \times \left|\frac{c_{P,i}^{M,EXP} - c_{P,i}^{M,MODEL}}{c_{P,i}^{M,MODEL}}\right|\right) > 200\%$$

this quantity is set to 200%.

2. The choice of eq 18 is based on the fact that for the data points embedded in the proposed database, we noticed that a deviation of 50% on c_P^M leads to an average deviation of only 2% on the molar isobaric heat capacity of the corresponding stream calculated as $c_{P,stream} = z_1 c_{P,1} + z_2 c_{P,2} + c_P^M$. As a consequence, eq 18 is developed so that a deviation of 50% on c_P^M leads to a good mark of 15/20.

Important remark: Any mark below 0 is raised to 0. Moreover, in the end:

$$\text{Mark}_{BAC_i} =$$

$$\text{average}\begin{pmatrix} \text{Mark}_{x \text{ or } x^\alpha}; \text{Mark}_{y \text{ or } x^\beta}; \text{Mark}_{P_{LLV}}; \text{Mark}_{z_{LLV}}; \text{Mark}_{P_c}; \\ \text{Mark}_{x_c}; \text{Mark}_{P_{az}}; \text{Mark}_{x_{az}}; \text{Mark}_{h^M}; \text{Mark}_{c_P^M} \end{pmatrix}$$

(19)

To conclude, 10 marks (at the most) are attributed to a given BAC. Obviously, when experimental data are missing for one or several properties, the corresponding mark(s) cannot be calculated and is(are) removed from eq 19. As an example, none of the binary systems embedded in BAC_2 contain three-phase equilibrium data so that $\text{Mark}_{P_{LLV}}$ and $\text{Mark}_{z_{LLV}}$ cannot be evaluated. For BAC_2, the given mark (eq 19) is the average of only 8 marks (instead of 10).

It is worth noting that the previous equations (from eq 7 to eq 18) give the greatest weight to the critical pressures that fix the topology of a binary system and are thus, in our view, extremely important, while less attention is given to mixing enthalpies and even less to mixing heat capacities. In practical terms, according to eq 12, a MAPE of 13% on the critical pressures leads to a Mark_{P_c} of 10/20 and a MAPE of 26% leads to a Mark_{P_c} of 0/20. By contrast, from eq 18, a similar MAPE of 13% on the mixing heat capacities leads to a $\text{Mark}_{c_P^M}$ of 18.7/20 and a MAPE of 26% leads to a $\text{Mark}_{c_P^M}$ of 17.4/20.

4. ILLUSTRATION: GRADING AND DISCUSSION AROUND THE ACCURACY OF THE PENG–ROBINSON EOS WITH CLASSICAL MIXING RULES AND A TEMPERATURE-DEPENDENT BIP

4.1. Model. In this section, it was decided to use the benchmark database developed in this study to assess the accuracy and to grade the Peng–Robinson[991,992] (PR) EoS with classical mixing rules and a temperature-dependent BIP (denoted k_{ij}). We found no reason to introduce a volume shift because all of the experimental properties contained in the database are unaffected by a temperature-independent volume translation.[993,994]

For a pure component, the PR EoS is

$$P = \frac{RT}{v - b_i} - \frac{a_i(T)}{v(v + b_i) + b_i(v - b_i)}$$

(20)

Although nonconsistent[995−997] at very high temperatures, it was decided to classically use the Soave-type[998] α-function

proposed by Peng and Robinson[991] in 1978. An updated version has however recently been developed by Pina-Martinez[999] and co-workers (including Peng). We thus used

$$\begin{cases} R = 8.314472 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1} \\[4pt] X = [1 + \sqrt[3]{4 - 2\sqrt{2}} + \sqrt[3]{4 + 2\sqrt{2}}\,]^{-1} \approx 0.253076587 \\[4pt] b_i = \Omega_b \dfrac{RT_{c,i}}{P_{c,i}} \text{ with } \Omega_b = \dfrac{X}{X + 3} \approx 0.0777960739 \\[4pt] a_i(T) = a_{c,i}\alpha_i(T) \text{ with } \begin{cases} a_{c,i} = \Omega_a \dfrac{R^2 T_{c,i}^2}{P_{c,i}} \text{ and} \\[4pt] \Omega_a = \dfrac{8(5X + 1)}{49 - 37X} \approx 0.457235529 \\[4pt] \alpha_i(T) = \left[1 + m_i\left(1 - \sqrt{\dfrac{T}{T_{c,i}}}\right)\right]^2 \end{cases} \\[4pt] \text{if } \omega_i \le 0.491 \text{ then } m_i = 0.37464 + 1.54226\omega_i - 0.26992\omega_i^2 \\[4pt] \text{if } \omega_i > 0.491 \text{ then } m_i = 0.379642 + 1.48503\omega_i - 0.164423\omega_i^2 \\ \qquad + 0.016666\omega_i^3 \end{cases}$$

(21)

where P is the pressure, R is the gas constant, T is the temperature, a_i and b_i are the cohesive parameter and the molar covolume of the pure component i, respectively, v is the molar volume, $T_{c,i}$ is the experimental critical temperature, $P_{c,i}$ is the experimental critical pressure, and ω_i is the experimental acentric factor of pure i. Such experimental properties were extracted from the DIPPR database, thus avoiding their estimation by group contribution methods.[1000]

To apply this EoS to a mixture, mixing rules are necessary to calculate the values of a and b of the mixture. Classical van der Waals one-fluid mixing rules[1001] are used in this study:

$$\begin{cases} a(T, z) = \displaystyle\sum_{i=1}^{N} \sum_{j=1}^{N} z_i z_j \sqrt{a_i(T) \cdot a_j(T)}\, [1 - k_{ij}(T)] \\[4pt] b(z) = \displaystyle\sum_{i=1}^{N} z_i b_i \end{cases}$$

(22)

where z_i represents the mole fraction of component i and N is the number of components in the mixture (in this work, $N = 2$). The $k_{ij}(T)$ parameter is the BIP characterizing the molecular interactions between molecules i and j. In this study, the equation that gives the changes of k_{ij} with respect to temperature (see eq 23) is the one used in the well-established PPR78[1002−1007] and PR$_2$SRK[1008] models and contains two parameters (A_{ij} and B_{ij}) for the binary system $i + j$.

$$k_{ij}(T) = \frac{A_{ij}\left(\dfrac{298.15}{T}\right)^{B_{ij}/A_{ij}-1} - \left(\dfrac{\sqrt{a_i}}{b_i} - \dfrac{\sqrt{a_j}}{b_j}\right)^2}{2 \times \dfrac{\sqrt{a_i}}{b_i} \times \dfrac{\sqrt{a_j}}{b_j}}$$

(23)

4.2. Fitting Procedure. The selected model is a correlative (i.e., nonpredictive) model, and for a given binary system, the two parameters involved in eq 23 have to be fitted against experimental data. In this work, it was decided that the two parameters would be determined, system by system, to ensure the best reproduction of the experimental data available in the proposed database by minimizing an objective function accounting for the deviations between experimental data (VLE data, LLE data, VLLE data, critical data, azeotropic

data, heat capacity of mixing data, and enthalpy of mixing data) and model predictions. The selected objective function expression is

$$F_{obj} = \frac{\begin{pmatrix} F_{obj,x \text{ or } x^{\alpha}} + F_{obj,y \text{ or } x^{\beta}} + F_{obj,P_{LLV}} + F_{obj,z_{LLV}} + F_{obj,P_c} \\ + F_{obj,x_c} + F_{obj,P_{az}} + F_{obj,x_{az}} + F_{obj,h^M} + F_{obj,c_P^M} \end{pmatrix}}{n_{x \text{ or } x^{\alpha}} + n_{y \text{ or } x^{\beta}} + 2n_{triph} + 2n_{crit} + 2n_{az} + n_{h^M} + n_{c_P^M}} \quad (24)$$

- $F_{obj,x \text{ or } x^{\alpha}}$ quantifies the deviations on the liquid-phase composition for VLE data and on the α-liquid phase for LLE data:

$$\begin{cases} F_{obj,x \text{ or } x^{\alpha}} = 100 \sum_{i=1}^{n_{x \text{ or } x^{\alpha}}} 0.5\left(\frac{|\Delta x|}{x_{1,exp}(\text{or } x_{1,exp}^{\alpha})} + \frac{|\Delta x|}{x_{2,exp}(\text{or } x_{2,exp}^{\alpha})} \right)_i \\ \text{with } |\Delta x| = |x_{1,exp}(\text{or } x_{1,exp}^{\alpha}) - x_{1,cal}(\text{or } x_{1,cal}^{\alpha})| \end{cases} \quad (25)$$

where $n_{x \text{ or } x^{\alpha}}$ is the number of data points for which the liquid-phase composition x_1 (VLE data) or the α-liquid phase composition x_1^{α} (LLE data) is known.

Remark: As previously explained, very small mole fractions may lead to huge percent deviations. When this happens, the fitting algorithm is going to change the parameters to reduce this huge deviation to the detriment of other compositions. To avoid such a bias, if $x_{1,exp} < 0.01$ (or $x_{1,exp} < 0.99$) and simultaneously $50\left(\frac{|\Delta x|}{x_{1,exp}(\text{or } x_{1,exp}^{\alpha})} + \frac{|\Delta x|}{x_{2,exp}(\text{or } x_{2,exp}^{\alpha})} \right) > 45\%$, the corresponding deviation was not included in the calculation of $F_{obj,x \text{ or } x^{\alpha}}$.

- $F_{obj,y \text{ or } x^{\beta}}$ quantifies the deviations on the gas-phase composition for VLE data and on the β-liquid phase for LLE data:

$$\begin{cases} F_{obj,y \text{ or } x^{\beta}} = 100 \sum_{i=1}^{n_{y \text{ or } x^{\beta}}} 0.5\left(\frac{|\Delta y|}{y_{1,exp}(\text{or } x_{1,exp}^{\beta})} + \frac{|\Delta y|}{x_{2,exp}(\text{or } x_{2,exp}^{\beta})} \right)_i \\ \text{with } |\Delta y| = |y_{1,exp}(\text{or } x_{1,exp}^{\beta}) - y_{1,cal}(\text{or } x_{1,cal}^{\beta})| \end{cases} \quad (26)$$

where $n_{y \text{ or } x^{\beta}}$ is the number of data points for which the gas-phase composition y_1 (VLE data) or the β-liquid-phase composition x_1^{β} (LLE data) is known.

Remark: Here also, to avoid bias, if $y_{1,exp} > 0.99$ (or $y_{1,exp} > 0.01$) and simultaneously $50\left(\frac{|\Delta y|}{y_{1,exp}(\text{or } x_{1,exp}^{\beta})} + \frac{|\Delta y|}{x_{2,exp}(\text{or } x_{2,exp}^{\beta})} \right) > 45\%$, the corresponding deviation was not included in the calculation of $F_{obj,y \text{ or } x^{\beta}}$.

- $F_{obj,P_{LLV}}$ quantifies the deviations on the three-phase pressure (VLLE data):

$$F_{obj,P_{LLV}} = 100 \sum_{i=1}^{n_{triph}} \left(\frac{|P_{LLV,exp} - P_{LLV,cal}|}{P_{LLV,exp}} \right)_i \quad (27)$$

where n_{triph} is the number of three-phase pressure data.

- $F_{obj,z_{LLV}}$ quantifies the deviations on the three-phase composition (VLLE data):

$$F_{obj,z_{LLV}} = 100$$

$$\sum_{i=1}^{n_{triph}} \frac{1}{6}\left(\frac{|\Delta x^{\alpha}|}{x_{1,exp}^{\alpha}} + \frac{|\Delta x^{\alpha}|}{x_{2,exp}^{\alpha}} + \frac{|\Delta x^{\beta}|}{x_{1,exp}^{\beta}} + \frac{|\Delta x^{\beta}|}{x_{2,exp}^{\beta}} + \frac{|\Delta y|}{y_{1,exp}} + \frac{|\Delta y|}{y_{2,exp}} \right)_i \quad (28)$$

$$\text{with} \quad \begin{cases} |\Delta x^{\alpha}| = |x_{1,exp}^{\alpha} - x_{1,cal}^{\alpha}| = |x_{2,exp}^{\alpha} - x_{2,cal}^{\alpha}| \\ |\Delta x^{\beta}| = |x_{1,exp}^{\beta} - x_{1,cal}^{\beta}| = |x_{2,exp}^{\beta} - x_{2,cal}^{\beta}| \\ |\Delta y| = |y_{1,exp} - y_{1,cal}| = |y_{2,exp} - y_{2,cal}| \end{cases}$$

n_{triph} being the number of three-phase composition data (VLLE data).

- F_{obj,P_c} quantifies the deviations on the critical pressure:

$$F_{obj,P_c} = 100 \sum_{i=1}^{n_{crit}} \left(\frac{|P_{c,exp} - P_{c,cal}|}{P_{c,exp}} \right)_i \quad (29)$$

where n_{crit} is the number of critical pressure data.

- F_{obj,x_c} quantifies the deviations on the critical composition:

$$F_{obj,x_c} = 100 \sum_{i=1}^{n_{crit}} 0.5\left(\frac{|\Delta x_c|}{x_{c1,exp}} + \frac{|\Delta x_c|}{x_{c2,exp}} \right)_i$$

$$|\Delta x_c| = |x_{c1,exp} - x_{c1,cal}| = |x_{c2,exp} - x_{c2,cal}| \quad (30)$$

where n_{crit} is the number of critical composition data.

- $F_{obj,P_{az}}$ quantifies the deviations on the azeotropic pressure:

$$F_{obj,P_{az}} = 100 \sum_{i=1}^{n_{az}} \left(\frac{|P_{az,exp} - P_{az,cal}|}{P_{az,exp}} \right)_i \quad (31)$$

where n_{az} is the number of azeotropic pressure data.

- $F_{obj,x_{az}}$ quantifies the deviations on the azeotropic composition:

$$F_{obj,x_{az}} = 100 \sum_{i=1}^{n_{az}} 0.5\left(\frac{|\Delta x_{az}|}{x_{az1,exp}} + \frac{|\Delta x_{az}|}{x_{az2,exp}} \right)_i$$

$$|\Delta x_{az}| = |x_{az1,exp} - x_{az1,cal}| = |x_{az2,exp} - x_{az2,cal}| \quad (32)$$

where n_{az} is the number of azeotropic composition data.

- F_{obj,h^M} quantifies the deviations on the mixing enthalpies:

$$F_{obj,h^M} = 100 \sum_{i=1}^{n_{h^M}} 0.5\left(\left| \frac{h_{exp}^M - h_{cal}^M}{h_{exp}^M} \right| + \left| \frac{h_{exp}^M - h_{cal}^M}{h_{cal}^M} \right| \right)_i \quad (33)$$

where n_{h^M} is the number of mixing enthalpy data points.

- F_{obj,c_P^M} quantifies the deviations on the mixing heat capacities:

$$F_{obj,c_P^M} = 100 \sum_{i=1}^{n_{c_P^M}} 0.5\left(\left| \frac{c_{P,exp}^M - c_{P,cal}^M}{c_{P,exp}^M} \right| + \left| \frac{c_{P,exp}^M - c_{P,cal}^M}{c_{P,cal}^M} \right| \right)_i \quad (34)$$

where $n_{c_P^M}$ is the number of mixing heat capacity data points.

Important remark: Section 3 of this paper, devoted to the grading of a thermodynamic model, dictates the methodology that has to be strictly followed to evaluate the deviations between model predictions and experimental data by means of

Table 14. Overview of the MAPE between Experimental Data and Values Calculated with the Model: {PR EoS + Classical Mixing Rules with a T-Dependent k_{ij}} for the 200 Binary Systems Included in the Proposed Database That Are Classified in Nine Binary Association Codes (BACs)^a

binary association code	type of association	MAPE on									
		x	y	P_{LLV}	z_{LLV}	P_c	x_c	P_{az}	x_{az}	h^M	c_P^M
		eq 25	eq 26	eq 27	eq 28	eq 29	eq 30	eq 31	eq 32	eq 33	eq 34
1 (NA-NA)		7.9%	7.9%	1.3%	42.7%	3.6%	12.9%	1.0%	5.0%	21.7%	34.7%
2 (HA-NA)	mixtures without association	8.8%	6.8%	-	-	2.4%	9.0%	1.0%	6.1%	16.3%	160.3%
3 (HD-NA)		6.9%	5.7%	-	-	5.2%	15.8%	0.6%	3.7%	12.5%	70.5%
4 (HA-HA or HD-HD)		7.5%	7.2%	-	-	4.0%	11.1%	5.6%	9.6%	13.5%	104.5%
5 (SA-NA)	mixtures in which self-association tends to be broken	40.0%	14.9%	5.2%	69.9%	10.9%	46.0%	4.9%	13.8%	32.4%	200%
6 (HD-HA)	mixtures in which cross-association takes place alone	6.0%	6.1%	-	-	3.5%	21.5%	2.0%	9.6%	23.6%	43.1%
7 (SA-HD)	mixtures in which both cross-association and self-association take place	15.2%	12.3%	-	-	-	-	2.5%	9.6%	84.4%	188.0%
8 (SA-HA)		24.9%	15.7%	24.5%	39.1%	13.0%	28.4%	3.9%	11.0%	37.2%	164.4%
9 (SA-SA)		33.9%	22.6%	6.4%	32.7%	5.5%	13.2%	1.1%	24.4%	39.7%	182.4%

^{a}The abbreviations used for the associating character of a pure compound are NA for nonassociating, HA for hydrogen-acceptor, HD for hydrogen-donor, and SA for self-associating.

the proposed database. If not, it becomes impossible to fairly compare two thermodynamic models.

In turn, the parameterization of the tested EoS (in the present case, the fitting procedure described above in Section 4.2) is not imposed and can be freely chosen. We are of the opinion that a researcher who wants to score a thermodynamic model (defined as the association of an EoS and a parameterization procedure) should be free to choose the number of adjustable parameters in the model, the experimental data to which such parameters are fitted, and the weighting given for each considered property during the fitting stage of the model parameters. In the previous section, a correlative model (the PR EoS with classical mixing rules and a T-dependent k_{ij}) was selected so that the experimental data of the proposed database were used to fit the parameters of eq 23. If our goal were to assess the accuracy of a predictive thermodynamic model in which the binary interaction parameters are determined by group contribution (e.g., PSRK,[1009,1010] VTPR,[1011,1012] UMR-PRU,[1013,1014] PPR78,[1002] MHV1-UNIFAC,[1015] etc.), the experimental data of the proposed database would not have been used for parameterization purposes.
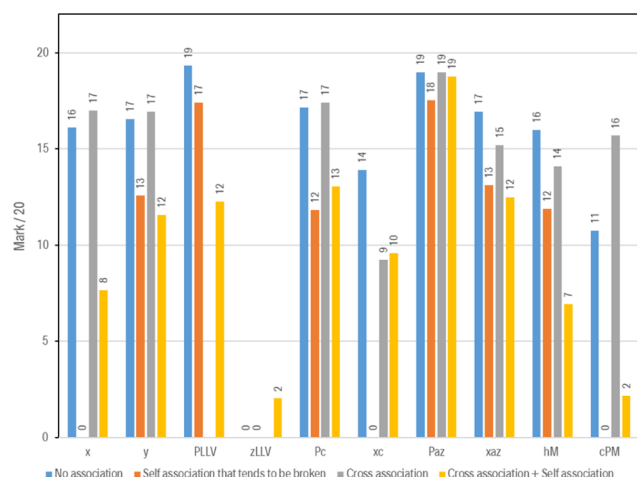
From the above, an <mark>EoS may thus get different grades depending on its parameterization</mark>. For example, it would be possible in this paper to grade the PR EoS by setting all k_{ij} to 0. By doing so, a lower score than with temperature-dependent k_{ij} would be obtained. In short, <mark>a grade is in fact always given to a model, i.e., to the association of both {an equation of state + a selected parameterization}</mark>. The proposed database can thus be used to test the influence of the parameterization on EoS performance, and we know by experience[1016] that such an influence may be huge.

4.3. System-by-System Results of the Fitting Procedure. A system-by-system analysis of the {PR EoS + classical mixing rules with a T-dependent k_{ij}} performances to correlate the data included in the proposed database can be found in Table S2 of the file ie0c01734_si_011.pdf, available as Supporting Information. This very detailed analysis (over 1000 pages) includes the following.

1. Information on how the system deviates from ideality.
2. Values of the A and B optimal parameters (see eq 23).
3. Values of the numerical values of the average deviations between experimental data and model correlation for the ten calculated properties. In the file ie0c01734_-si_011.pdf of the Supporting Information,
   - MAPE on x refers to $F_{obj, \, x \, or \, x^\alpha}/n_{x \, or \, x^\alpha}$ (see eq 25)
   - MAPE on y refers to $F_{obj, \, y \, or \, x^\beta}/n_{y \, or \, x^\beta}$ (see eq 26)
   - MAPE on P_{LLV} refers to $F_{obj, \, P_{LLV}}/n_{triph}$ (see eq 27)
   - MAPE on Z_{LLV} refers to $F_{obj, \, Z_{LLV}}/n_{triph}$ (see eq 28)
   - MAPE on P_c refers to $F_{obj, \, P_c}/n_{crit}$ (see eq 29)
   - MAPE on x_c refers to $F_{obj, \, x_c}/n_{crit}$ (see eq 30)
   - MAPE on P_{az} refers to $F_{obj, \, P_{az}}/n_{az}$ (see eq 31)
   - MAPE on x_{az} refers to $F_{obj, \, x_{az}}/n_{az}$ (see eq 32)
   - MAPE on h^M refers to $F_{obj, \, h^M}/n_{h^M}$ (see eq 33)
   - MAPE on c_P^M refers to $F_{obj, \, c_P^M}/n_{c_P^M}$ (see eq 34)
4. The so-called global phase equilibrium diagram (GPED), calculated by the PR EoS, enabling one to immediately identify the binary system class according to the scheme proposed by van Konynenburg and Scott.[6]
5. All of the experimental data with the corresponding references.
6. All of the deviations between experimental data and model correlation graphically illustrated by hundreds of figures. Explanations on "how to read the charts" are available at the beginning of the file ie0c01734_-si_011.pdf, available as Supporting Information..

4.4. Grading of the Model: {PR EoS + Classical Mixing Rules with a T-Dependent k_{ij}}. For each binary association code, the MAPEs on liquid-phase composition x, gas-phase composition y, three-phase pressure P_{LLV}, three-phase composition z_{LLV}, critical pressure P_c, critical composition x_c, azeotropic pressure P_{az}, azeotropic composition x_{az}, mixing enthalpy h^M, and mixing heat capacity c_P^M are resumed in Table 14. Such MAPEs make it possible to give a score over 20 to

each of the nine BACs by averaging the 10 marks in x, y, P_{LLV}, z_{LLV}, P_c, x_c, P_{az}, x_{az}, h^M, and c_P^M (see eq 19). Such marks can be found in Table 15. At the end, as previously explained, the marks obtained by BACs 1−4 and BACs 7−9 are averaged to only retain four categories (BAC$_1$−BAC$_4$; BAC$_5$; BAC$_6$; BAC$_7$−BAC$_9$) of binary systems based on the type of association they exhibit. By averaging the marks of these four categories of binary systems (see eq 6), the model {PR EoS + classical mixing rules with a T-dependent k_{ij}} receives the final mark of 12.3/20.

4.5. Discussion around the Accuracy of the Model: {PR EoS + Classical Mixing Rules with a T-Dependent k_{ij}}. At this step, it is possible to analyze the results obtained with the PR EoS coupled to classical mixing rules and a T-dependent k_{ij}. The marks reported in Table 15 are plotted in Figure 5 for each category of binary systems based on the type of association they exhibit.

Figure 5 and Table 15 highlight that with an excellent mark of 15.6/20, the binary systems that exhibit cross-association alone are those that are correlated with the highest accuracy by the model {PR EoS + classical mixing rules with a T-dependent k_{ij}}. For such binary systems, the two molecules form hydrogen bonds after mixing, thus stabilizing the liquid phase and preventing phase splitting. As a general rule, mixtures of this family exhibit negative deviations from ideality and belong to type-I in the classification scheme of van Konynenburg and Scott.

With the poorest rating of 8.4/20, binary systems belonging to BAC$_5$ cannot be accurately correlated with the PR EoS even when temperature-dependent BIPs are used. Three marks are equal to 0. In such systems, a nonassociating component is mixed with a self-associating compound so that self-association (partially) persists in the mixture. The nonassociating molecules tend to break the hydrogen-bond network, but the self-associating compounds withstand so that liquid-phase splitting is often observed in this family. As previously stated, such systems were thus classified as "mixtures in which self-association tends to be broken". As a general rule, they exhibit positive deviations from ideality and three-phase equilibrium at low temperature. Many of them belong to type-III systems in the classification scheme of van Konynenburg and Scott. All binary systems of water + alkane or alcohol + alkane belong to this family. They are generally considered by model developers as the most difficult systems to correlate. It can be reasonably thought that either the addition of an association term or the use of more-sophisticated mixing rules could help the PR EoS quantitatively reproduce the behavior of such systems.

Mixtures in which both cross-association and self-association take place fall into the middle scoring range by receiving a mark of 9.8/20. This is the result of two antagonistic effects: on the one hand, hydrogen bonds between two identical self-associating molecules are broken by dilution effect and this behavior is highly difficult to describe with the model {PR EoS + classical mixing rules with a T-dependent k_{ij}}, while, on the other hand, new hydrogen bonds are formed by cross-association; this latter behavior can be modeled accurately with the selected model, as explained above. Many of these systems belong to type-I systems in the classification scheme of van Konynenburg and Scott (although some may fall into type-III).

As expected, systems that do not exhibit association received a very good mark of 15.5/20. The identified weakness is the inaccurate correlation of the composition of the phases in

Table 15. Rating of the Nine Binary Association Codes to Finally Grade the Model {PR EoS + Classical Mixing Rules with a T-Dependent k_{ij}}[a]

binary association code (BAC)	type of association	mark on										binary association code mark	mark (over 20) by type of association	final mark of the PR EoS with classical MR and T-dependent BIPS
		x	y	P_{LLV}	z_{LLV}	P_c	x_c	P_{az}	x_{az}	h^M	c_P^M			
		eq 7	eq 8	eq 10	eq 11	eq 12	eq 13	eq 14	eq 15	eq 16	eq 18	eq 19	eq 6	eq 6
1 (NA-NA)	mixtures without association	16.0	16.1	19.3	0.0	17.3	13.6	19.5	17.5	14.6	16.5	15.0	$\text{Mark}_{NA} = 15.5$ (no association)	12.3/20
2 (HA-NA)		15.6	16.6			18.2	15.5	19.5	16.9	15.9	4.0	15.3		
3 (HD-NA)		16.5	17.2			16.1	12.1	19.7	18.2	16.9	13.0	16.2		
4 (HA-HA or HD-HD)		16.2	16.4			17.0	14.4	17.2	15.2	16.6	9.6	15.3		
5 (SA-NA)	mixtures in which self-association tends to be broken	0.0	12.6	17.4	0.0	11.8	0.0	17.5	13.1	11.9	0.0	8.4	$\text{Mark}_{SA} = 8.4$ (self–association)	
6 (HD-HA)	mixtures in which cross-association takes place alone	17.0	16.9			17.4	9.2	19.0	15.2	14.1	15.7	15.6	$\text{Mark}_{CA} = 15.6$ (cross−association)	
7 (SA-HD)	mixtures in which both cross-association and self-association take place	12.4	13.9					18.8	15.2	0.0	1.2	10.2	$\dfrac{\text{Mark}_{CA+SA}}{\text{cross−association+self−association}} = 9.8$	
8 (SA-HA)		7.5	12.2	7.7	0.45	10.3	5.8	18.0	14.5	10.7	3.6	9.1		
9 (SA-SA)		3.1	8.7	16.8	3.6	15.8	13.4	19.5	7.8	10.1	1.8	10.0		

[a]The abbreviations used for the associating character of a pure compound are NA for nonassociating, HA for hydrogen-acceptor, HD for hydrogen-donor, and SA for self-associating.

Figure 5. Overview of the accuracy of the model {PR EoS + classical mixing rules with a T-dependent k_{ij}} by plotting the marks in 10 properties for the four categories of binary systems based on the type of association they exhibit.

equilibrium when the system exhibits a three-phase line. This weakness highlights the difficulty in simultaneously correlating VLE and LLE data with a unique set of adjustable parameters. Nonassociating systems often belong to type-I systems but some fall into type-III, especially when the two compounds show a high size-asymmetry.

This analysis allows one to conclude that, with an overall score of 12.3/20, the PR EoS with classical mixing rules and a temperature-dependent k_{ij} can be safely used in process and product design applications as long as systems in which hydrogen bonds are broken without the possibility of forming new ones are not involved.

A similar analysis is possible from the viewpoint of system ideality.

Figure 6 shows that except for the liquid-phase composition (including the critical composition), all of the other properties are correlated with a similar accuracy for both ideal and nonideal systems. It is observed that deviations on mixing enthalpies can become huge when the deviations from ideality
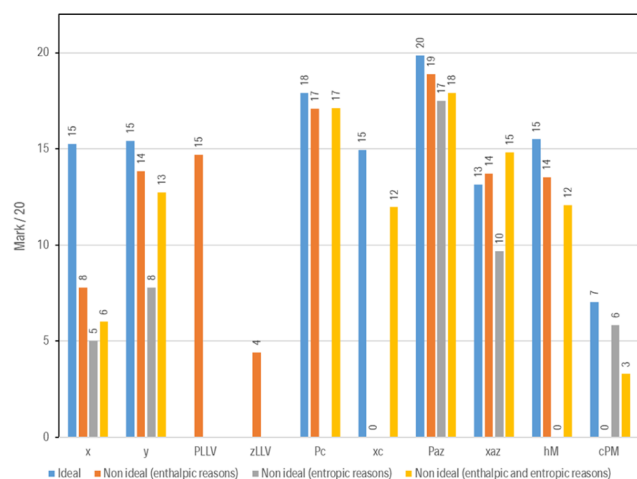
originate from entropic effects, but this result is not significant because in such a case experimental and calculated h^M values are both low.

It is thus possible to conclude that deviations from ideality are not the key parameters to be accounted for when highlighting the strengths and the weaknesses of a model. A classification of the binary systems based on the type of association they exhibit, as the one proposed in this paper, is much more pertinent.

5. CONCLUSIONS

A benchmark database is presented in this paper to enable a proposed-standardized assessment of the performance of a given thermodynamic model or to compare two models. To classify a database's systems on the basis of their thermodynamic complexity, 107 pure components were first divided into four categories according to their associating character and nine classes of binary systems were defined combining these four pure-component categories. Each of these classes is identified by a binary association code (BAC). We are indeed convinced that binary systems must be classified according to the type of association they exhibit. For each class of systems, the proposed database includes a variety of binary systems ranging from ideal to highly nonideal. In the end, the proposed database embeds 200 binary mixtures uniformly distributed among the nine BACs and includes for each system both phase equilibrium data (VLE, LLE, VLLE, azeotropic data, critical data) and energetic data (h^M and c_P^M data). For each property, a detailed procedure explaining how deviations between model predictions and experimental data have to be estimated is provided.

Finally, the performances of the Peng–Robinson EoS with classical van der Waals mixing rules and a temperature-dependent binary interaction parameter were evaluated over the full database. In light of the obtained results, a discussion about the strengths and weaknesses of the model was conducted. Such a thermodynamic model got an overall respectable score of 12.3/20. Its main drawback is the poor correlation of systems in which hydrogen bonds are broken without the possibility of forming new ones. For such complex systems, the addition of an association term to the EoS and the selection of more sophisticated mixing rules could help improve the model efficiency.

Last but not the least, we hope that the proposed database will be widely adopted by the scientific community to identify the strengths and weaknesses of the many published thermodynamic models and to identify the remaining scientific obstacles that need to be overcome. We also hope that such a database will be used by model developers to test a new concept. As an example, experimental data of binary systems, the BAC of which is 7, 8, or 9, could be very useful to test the influence of various association schemes.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.iecr.0c01734.

Numerical values of the experimental data included in the proposed database with the corresponding references (light Excel file named: ie0c01734_si_001.xlsx) (XLSX)

Figure 6. Marks in eight properties calculated for five categories of binary systems based on how they deviate from ideality (marks on VLLE data are not shown due to a lack of information on some categories of binary systems).

Numerical values of the experimental data included in the proposed database with the corresponding references and with a visualization of the experimental data through graphs. Nine large-size Excel files (one for each BAC) are provided:

1. ie0c01734_si_002.xlsx (BAC_1) (XLSX)
2. ie0c01734_si_003.xlsx (BAC_2) (XLSX)
3. ie0c01734_si_004.xlsx (BAC_3) (XLSX)
4. ie0c01734_si_005.xlsx (BAC_4) (XLSX)
5. ie0c01734_si_006.xlsx (BAC_5) (XLSX)
6. ie0c01734_si_007.xlsx (BAC_6) (XLSX)
7. ie0c01734_si_008.xlsx (BAC_7) (XLSX)
8. ie0c01734_si_009.xlsx (BAC_8) (XLSX)
9. ie0c01734_si_010.xlsx (BAC_9) (XLSX)

List of the 107 pure compounds included in the proposed database with their corresponding associating character: NA, Non-Associating; HA, Hydrogen-Acceptor; HD, Hydrogen-Donor; SA, Self-Associating. Provided in Table S1 of the file ie0c01734_si_011.pdf (PDF)

System-by-system analysis of the {PR EoS + classical mixing rules with a T-dependent k_{ij}} performances to correlate the data included in the proposed database. Provided in Table S2 of the file ie0c01734_si_011.pdf (PDF)

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Notes

The authors declare no competing financial interest.

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