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Data-driven study of the enthalpy of mixing in the liquid phase

Guillaume Deffrennes^{a,*}, Bengt Hallstedt^b, Taichi Abe^c, Quentin Bizot^a, Evelyne Fischer^a, Jean-Marc Joubert^d, Kei Terayama^{e,f}, Ryo Tamura^{g,h,**}

^a Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, F-38000, Grenoble, France

^b Institute for Materials Applications in Mechanical Engineering (IWM), RWTH Aachen University, Augustinerbach 4, 52062, Aachen, Germany

^c Research Center for Structural Materials, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki, 305-0047, Japan

^d Univ. Paris Est Creteil, CNRS, ICMPE, UMR 7182, 2 rue Henri Dunant, 94320, Thiais, France

^e Graduate School of Medical Life Science, Yokohama City University, 1-7-29, Suehiro-cho, Tsurumi-ku, Kanagawa, 230-0045, Japan

^f MDX Research Center for Element Strategy, Tokyo Institute of Technology, 4259, Nagatsuta-cho, Midori-ku, Yokohama, Kanagawa, 226-8501, Japan

^g Center for Basic Research on Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan

^h Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwa-no-ha, Kashiwa, Chiba, 277-8561, Japan

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ABSTRACT

The enthalpy of mixing in the liquid phase is a thermodynamic property reflecting interactions between elements that is key to predict phase transformations. Widely used models exist to predict it, but they have never been systematically evaluated. To address this, we collect a large amount of enthalpy of mixing data in binary liquids from a review of about 1000 thermodynamic evaluations. This allows us to clarify the prediction accuracy of Miedema's model which is state-of-the-art. We show that more accurate predictions can be obtained from a machine learning model based on LightGBM, and we provide them in 2415 binary systems. The data we collect also allows us to evaluate another empirical model to predict the excess heat capacity that we apply to 2211 binary liquids. We then extend the data collection to ternary metallic liquids and find that, when mixing is exothermic, extrapolations from the binary systems by Muggianu's model systematically lead to slight overestimations of roughly 10 % close to the equimolar composition. Therefore, our LightGBM model can provide reasonable estimates for ternary alloys and, by extension, for multicomponent alloys. Our findings extracted from rich datasets can be used to feed thermodynamic, empirical and machine learning models for material development. Our data, predictions, and code to generate machine learning descriptors from thermodynamic properties are all made available.

1. Introduction

The enthalpy of mixing provides basic information on the nature, attractive or repulsive, of the interactions between elements in solutions. Therefore, it provides important information for understanding chemical-related issues in materials, such as the glass-forming ability of metallic glasses [1]. Moreover, it is an essential property for predicting phase transformations in materials. Generally, deep eutectics, solid solutions and compounds are found in systems where mixing in the liquid phase is exothermic, e.g., Au-Sn [2], whereas miscibility gaps form in those where mixing is endothermic, e.g., Ag-Ni [3]. The enthalpy of mixing in the liquid phase is used to determine the stability of liquids by thermodynamic calculations using the Calphad technique [4], which is

important for the processing and design of a large variety of alloys [5]. In addition, several empirical rules for alloy design are based on this property [6–8]. Besides, the thermodynamic properties of mixing in the liquid phase are important features for machine learning (ML) models to predict phase equilibria such as binary liquidus [5], ternary isothermal sections [9], or phase formation in high-entropy alloys [10–12].

At present, the most reliable way [13] to estimate the enthalpy of mixing in the liquid phase is to use the semi-empirical model established by Miedema *et al.* in 1980 [14]. It is remarkable that no better model has been developed since then. Miedema's model is widely used in ML models for predicting phase equilibria [5,10–12], and sometimes used in Calphad models in systems where experimental data is not available [15, 16]. However, since it has never been systematically evaluated, the

* Corresponding author.

** Corresponding author. Center for Basic Research on Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan.

E-mail addresses: Guillaume.DEFFRENNES@cnrs.fr (G. Deffrennes), TAMURA.Ryo@nims.go.jp (R. Tamura).

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accuracy that can be expected from it is not well known, except for binary systems of magnesium [17].

In multicomponent liquids, data are scarce. Therefore, in ML [5, 10–12], empirical [6–8] and high-throughput [18,19] approaches, their enthalpy of mixing is extrapolated from the binary systems. This can be done by different geometric models [20], but the most widely used is the one proposed by Muggianu *et al.* [21] because of its simplicity. Again, the accuracy of this extrapolation has never been systematically studied.

In recent studies [18,19], the enthalpy of mixing in solid solutions was studied through high-throughput density functional theory calculations. It was approximated in binary systems from a single calculation performed at the equimolar composition. The underlying assumption is that the enthalpy of mixing is symmetrical with respect to composition and reaches its extremum at the equimolar composition. This introduces an error of unknown magnitude.

High-throughput *ab initio* approaches are currently not available to study the enthalpy of mixing of liquids. ML approaches represent an unexplored alternative. In a recent study, an ensemble of graph neural networks was developed to predict the zeroth-order parameter of the Redlich-Kister expansion used in Calphad models to describe the enthalpy of mixing in the liquid phase [22]. This study is based on a dataset of 524 Calphad models of different binary systems for which it was not checked whether the parameters are well constrained by experimental measurements. For solid solutions, a model was trained on data from density functional theory calculations to predict the enthalpy of mixing in the body-centered cubic phase for Fe-Cr-based alloys [23]. A neural network was developed to reproduce the enthalpy of mixing in binary and ternary face-centered cubic solutions obtained from a Calphad commercial database for high entropy alloys [24].

In this work, the enthalpy of mixing in the liquid phase is systematically studied using large datasets collected from a review of about 1000 thermodynamic Calphad assessments. First, we evaluate Miedema’s model, and we develop a machine learning model that performs better. Second, we evaluate the performance of Witusiewicz and Sommer’s empirical model [25] for predicting the temperature dependence of the enthalpy of mixing, i.e., the excess heat capacity. Third, we evaluate how accurately the enthalpy of mixing of ternary metallic liquids can be extrapolated from their binary subsystems by Muggianu’s model. An overview of this work is presented in Fig. 1.

2. Methods

2.1. Datasets

About 1000 Calphad-type thermodynamic evaluations of binary systems were reviewed, and enthalpy of mixing data were collected in 375 binary systems from Refs. [2,3,26–335] in composition domains where the models are supported by experimental measurements with steps of 1 at%. 94 % of these data are supported by direct calorimetric measurements. The remaining 6 % are supported by activity or chemical potential data at different temperatures separated by at least 350 K (the contribution from the configurational entropy is then more than 2 kJ/mol), or data on both the liquidus and the thermodynamic properties of the solid phases involved. Calphad model parameters were retrieved from various sources: mainly NIMS CPDDB [336] and compilations by the authors, but also TDBDB [337], NUCLEA [132], and publications. When the liquid phase was described using a substitutional solution model, the enthalpy of mixing was calculated directly from the Redlich-Kister coefficients. For cases involving an associate or ionic model, the Pandat software [338] was used. When the enthalpy of mixing is temperature dependent, it is calculated at the composition-weighted average melting point of the elements.

Excess heat capacity data were obtained from measurements of the enthalpy of mixing at different temperatures that were digitized from figures found in publications. Data were collected in 43 binary systems for which it was found that a clear and consistent trend emerged from the experimental data. They were collected from Refs. [2,26–60, 339–344] at the composition where the enthalpy of mixing is at its maximum in absolute value, or at the closest composition where experimental data are available.

Data on ternary liquids were collected from Refs. [26–29,61–68, 345–383] in which a substitutional solution model is proposed based on experimental data covering a large part of a ternary system.

2.2. Miedema’s model and descriptors

Miedema’s theory is presented in detail elsewhere [14,384,385]. The equations of the model and the origin of the parameters used in this work are given in the appendix.

58 descriptors are obtained from composition-weighted mean and

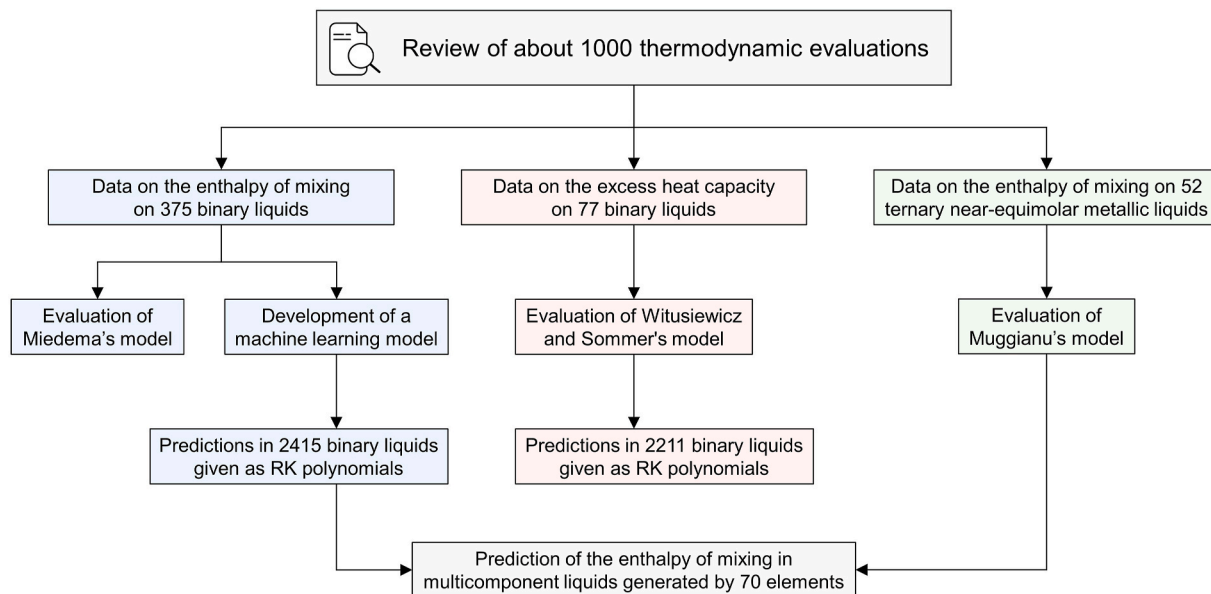


Fig. 1. Overview of this work on the prediction of the enthalpy of mixing in the liquid. RK stands for Redlich-Kister. Our datasets and predictions are made available as detailed in “Data availability.”

average deviation of the properties of the pure elements. They are listed in Table S1. The melting and thermodynamic properties of the pure elements are obtained from the SGTE unary database [386] in its 5.0 version, and other properties are calculated from magpie [387] using matminer [388].

2.3. Machine learning methods

Three algorithms are used: LightGBM [389], a gradient boosting decision tree, Gaussian process (GP) implemented using PHYSBO [390], and artificial neural network (ANN) with two to three hidden layers comprising 10 to 1200 nodes implemented using TensorFlow [391]. For LightGBM and ANN, the target variable is the error of Miedema's model from which the enthalpy of mixing is recalculated, and for GP it is the enthalpy of mixing directly and Miedema's model is used as a descriptor, since this leads to better results.

First, feature selection is performed based on a 5-fold group cross-validation (CV), with data for a binary system forming a group that cannot be split between the training and validation sets. For LightGBM and ANN, a preliminary hyperparameter tuning is performed using Optuna [392]. For LightGBM, recursive feature elimination is performed: starting from all 58 descriptors, the least important feature is dropped. This is repeated until only two features remain. For ANN and GP, sequential feature selection is performed: starting from a single-descriptor model, descriptors are tested one by one, and the one that leads to the model with the smaller RMSE is selected. This is repeated until a model based on all 58 or 59 descriptors is obtained for ANN or GP, respectively. This method requires a relatively high computation time, which is why feature selection was carried out as a first step on the whole dataset. The set of features that minimizes the RMSE is selected.

Second, a nested CV is performed as schematized in Fig. S3 of Ref. [5]. The advantage of this approach is that model performance is evaluated over the entire dataset. For LightGBM and ANN, a 5-fold group CV is performed in the inner loop to determine the best hyperparameters using Optuna [392]. A 12-fold group CV is performed in the outer loop to evaluate model performance.

2.4. Redlich-Kister substitutional solution model

For each binary system, the enthalpy of mixing is calculated at every at% from the value predicted by Miedema's model and the error on this value predicted by machine learning. Then, it is fitted by a Redlich-Kister polynomial:

$$H_{mix}^{liq} = x_A x_B \sum_{\nu} a_{A,B} (x_A - x_B)^{\nu} \quad (1)$$

with H_{mix}^{liq} the enthalpy of mixing in the A-B binary liquid phase, x_A and x_B the atomic fraction of A and B, and $a_{A,B}$ the parameter of order ν . Starting from the order 0, additional parameters are iteratively added up to the order 3 if the RMSE between the predicted and the fitted enthalpy of mixing is higher than 0.5 kJ/mol. In systems where the maximum absolute value of the enthalpy of mixing is predicted to be less than 10 kJ/mol, no more than two parameters of order 0 and 1 are used to avoid overfitting.

In a multicomponent liquid composed of n elements, the binary contributions to the enthalpy of mixing can be calculated using Muggianu's model [21] by summing Eq. (1) over all binaries without weighting compositions:

$$H_{mix}^{bin,liq} = \sum_{i=1}^{n-1} \sum_{j=i+1}^n x_i x_j \sum_{\nu} a_{i,j}^{\nu} (x_i - x_j)^{\nu} \quad (2)$$

The excess heat capacity predicted by Witusiewicz and Sommer's model [25] using our LightGBM/RK model, melting points from the SGTE unary database [386], a temperature set to the

composition-weighted average melting point of the elements, and boiling points from magpie [387] as inputs is fitted and can be extrapolated using the same formalism as Eqs. (1) and (2).

3. Results

3.1. Prediction of the enthalpy of mixing in binary liquid phases

Reliable enthalpy of mixing data were collected in 375 binary liquids after a review of about 1000 systems. Data coverage is shown per binary system in Fig. 2, and per element in Fig. S1. In general, our dataset covers many binary systems of base alloy elements such as Al or Mg, low melting point metals such as Ga or Sn, and between elements of groups 10 to 14. In contrast, our dataset contains little information, if any, on binaries of refractory elements such as C or W, and of elements of groups 3 to 6 besides with elements of groups 8 to 14.

First, the performance of the Miedema model was evaluated on our dataset. The relation between the observed and predicted values is shown in Fig. 3, and a mean absolute error (MAE) of 4.2 kJ/mol is obtained. In systems where the enthalpy of mixing is exothermic, it generally gives values that are not sufficiently negative.

Next, we developed an ML model based on LightGBM to predict the enthalpy of mixing. It is based on 30 descriptors selected from the 58 descriptors considered in this work to obtain a better accuracy (Fig. S3). Its performance is evaluated on the entire dataset using a nested cross-validation approach, and the results are shown in Fig. 3. The values predicted by the LightGBM model are slightly noisy (Fig. S2) and fitting by a Redlich-Kister (RK) polynomial smooth them out without any significant impact on performance. The combination of the LightGBM and RK models is referred to as LightGBM/RK. The MAE of this model is of 3.0 kJ/mol in systems for which no data is included in the training set, which is better than that obtained with Miedema's model, while training data are reproduced closely with a training MAE of 0.4 kJ/mol for the final LightGBM/RK model. The mean absolute percentage error (MAPE) is an intuitive metric, but it is only meaningful for large values that are not close to zero. It is evaluated on data greater than 10 kJ/mol in absolute value from 199 binary systems. An error of 22 % is obtained with our LightGBM/RK model in systems where it has seen no data, compared with 34 % for Miedema's model. The LightGBM/RK model performs slightly better than the artificial neural network (ANN) and gaussian process (GP) models (Table 1). The MAE of the LightGBM/RK model is shown per element in Fig. S1. Predictions are relatively inaccurate for group 16 elements. However, the LightGBM/RK model still tends to outperform Miedema's model: its MAE over the 21 binaries of Te in the dataset is of 6.4 kJ/mol compared to 10.4 kJ/mol for Miedema's model. Excluding group 16 elements, the MAE of the LightGBM/RK model decreases to 2.6 kJ/mol.

There are 120 binary systems in our dataset for which the extremum in the enthalpy of mixing is well-defined in the sense that it is greater than 5 kJ/mol in absolute value and that experimental data are available over the whole compositional range. In these systems, the composition of the extremum differs from the equimolar composition by 8.6 at% in average, and by up to 30 at%. Miedema's model generally fails to account for an asymmetry with respect to composition (Fig. 4), with an MAE on the composition of the extremum of 7.4 at% on these 120 systems. While our ML model show some potential to correct this (Fig. 4), this MAE is only reduced to 6.7 at% on these systems when they are not included in the training set.

The enthalpy of mixing is then predicted in all the 2415 binary systems generated by 70 elements using our LightGBM/RK model. The extremum value obtained in each system is shown in Fig. 5. The enthalpy of mixing is predicted from the LightGBM/RK model to be most exothermic in binary systems between an element of groups 2 to 4 with an element of groups 9 to 16. For instance, extremum values of -150 kJ/mol are predicted in carbon - rare earths systems. It is most endothermic in binary systems between an alkali metal and an element of groups 3 to

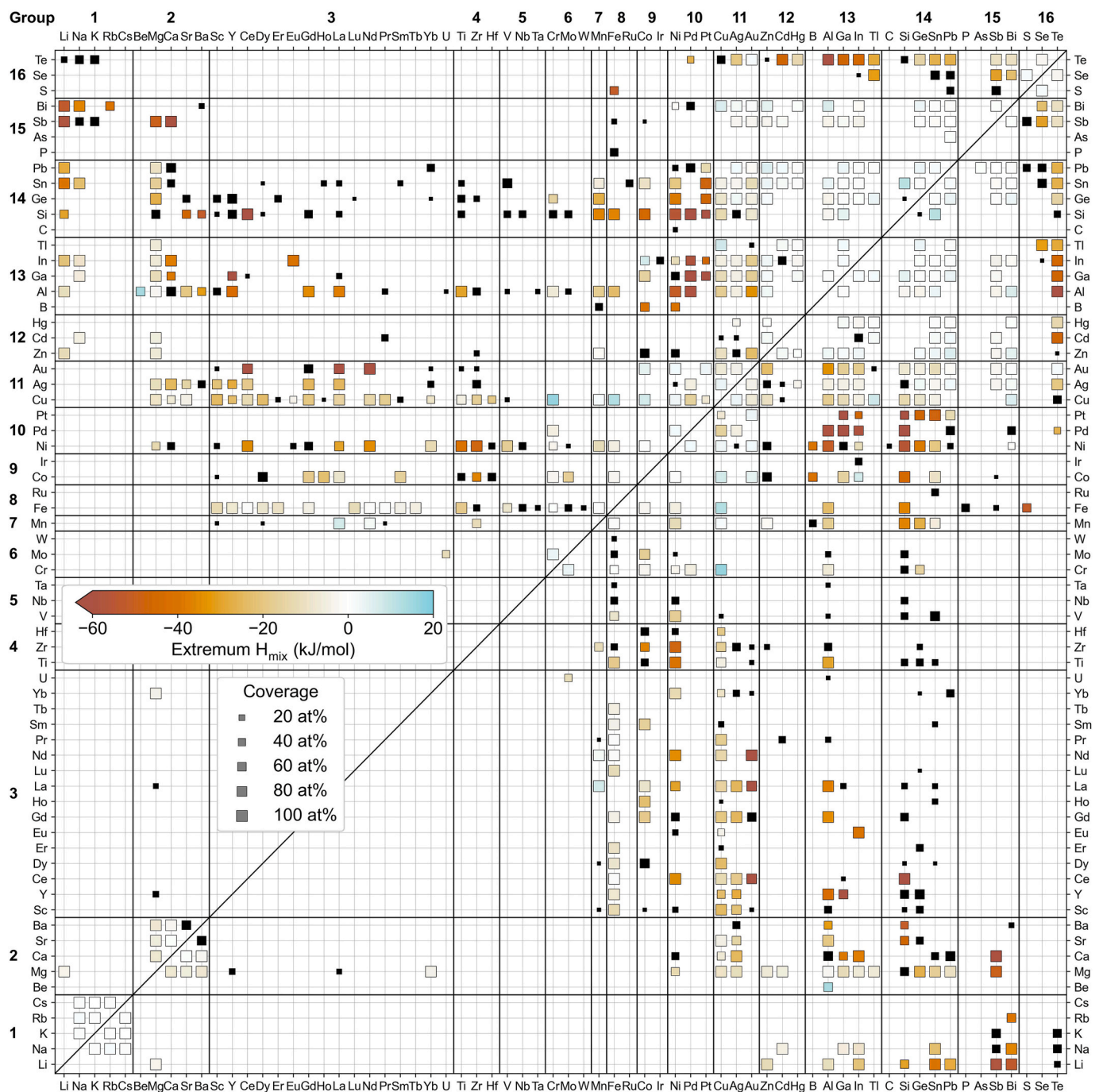


Fig. 2. Overview of our dataset on the enthalpy of mixing in binary liquid phases. For each of the 375 binary systems included, symbol size corresponds to the span of compositions over which reliable data have been found, and symbol color to the extremum value of the enthalpy of mixing. Symbols are black when the extremum is not well-defined.

8. Mg and Be tend to behave more like Au and Zn, which are their neighbors in an ordering by Mendeleev number, than other alkaline-earth metals. In binary systems between two elements of the same group, the enthalpy of mixing tends to be small and no larger than 30 kJ/mol in absolute value.

3.2. Temperature dependence of the enthalpy of mixing in the liquid phase

The excess heat capacity is the temperature derivative of the enthalpy of mixing. It can be predicted from Witusiewicz and Sommer's empirical model [25] whose MAE on experimental data from 77 binary systems is of 3.7 J/K/mol (Fig. 6a). It takes the enthalpy of mixing as

input, and using our LightGBM/RK model predictions can be made with greater accuracy than using Miedema's model, especially in systems included in its training set (Fig. 6b). The results obtained this way in 2016 binary systems suggests that the excess heat capacity and the enthalpy of mixing are strongly correlated (Fig. 6c). As discussed in Ref. [393], they are in most cases of opposite signs, which means that temperature brings liquids closer to ideality. However, experimental evidence is lacking in systems where mixing is endothermic, such as Ag-Pb where measurements suggest an exception to this rule [28]. In 90 % of the binary systems, the extremum value of the enthalpy of mixing is predicted to decrease by 3.5–9.7 % in absolute value over 100 K (Fig. 6c).

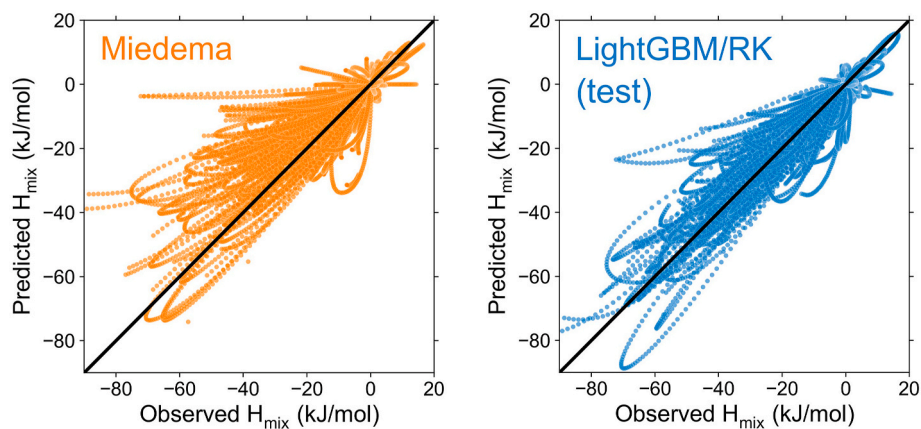


Fig. 3. Scatter plots showing the performance on data from 375 binaries of Miedema’s model [14] and of our ML model (in test) after fitting by a Redlich-Kister substitutional solution model. The diagonal line represents perfect agreement.

Table 1

Performance metrics obtained on data from 375 binary systems for different models for predicting the enthalpy of mixing in binary liquids. RMSE stands for root mean squared error.

Model	MAE (kJ/mol)	RMSE (kJ/mol)
Miedema’s model	4.2	7.5
LightGBM/RK (on test)	3.0	4.9
ANN (on test)	3.2	5.2
GP (on test)	3.3	5.1

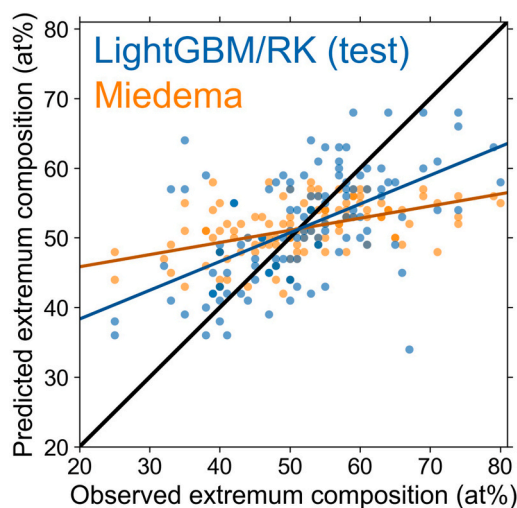


Fig. 4. Performance of Miedema’s model and our ML model (on test) for predicting the composition of the extremum n data from 120 binaries for which the extremum is well-defined. Linear regression lines are plotted to guide the eye.

3.3. Extrapolation from the binary systems in ternary metallic liquids

In multicomponent liquids, the main contribution to the enthalpy of mixing comes from the binary contributions. The extent of higher-order contributions has never been studied systematically. To address this, we collected experimental data on 52 ternary metallic liquids close to the equimolar composition. We find that the enthalpy of mixing extrapolated from the binary systems by Muggianu’s model [21] is reasonable, with an MAE of 1.6 kJ/mol. In liquids where mixing is exothermic, the extrapolations are systematically too negative (Fig. 7). The overestimation is of the order of 10 % (Fig. S5). In liquids where mixing is endothermic, more data is necessary to draw conclusions.

4. Discussion

We developed an ML model to predict the enthalpy of mixing in binary liquid phases. It is significantly more reliable than Miedema’s model [14]. The prediction results obtained in all the 2415 binary systems generated by 70 elements are fitted by a substitutional solution model whose parameters are provided. From these parameters, the main contribution to the enthalpy of mixing can be easily calculated in multicomponent liquids using Eq. (2) or the open-access notebook linked in the Data availability section. In ML models for alloys, the enthalpy of mixing in the liquid phase is an important descriptor not only for predicting phase equilibria [5,9–12], but also properties of the alloys such as the Young’s modulus [394] or the Vickers hardness [395]. Our ML model is used as an input to Witusiewicz and Sommer’s model [25] to predict the excess heat capacity in 2016 binary liquids. Data on the excess heat capacity are scarce, so in thermodynamic evaluations it is common practice to set it to zero and to adjust the excess entropy to model the temperature dependence of the Gibbs energy. Instead, relying on the reasonable excess heat capacity estimates provided here should in most cases lead to a better description of the entropy and of the interactions at high temperature. Therefore, our predictions can be used as an input to thermodynamic, empirical and ML models for the development of a variety of materials.

We took a data-driven approach to evaluate different sources of error in estimation of the enthalpy of mixing in binary and multicomponent liquids: model error to predict its binary contributions, neglecting its temperature dependence, and neglecting its ternary contributions. The same type of approach should be applied to solid solutions, but similar deviations may be expected. The uncertainty from measurements or calculations is difficult to evaluate systematically and is not discussed. Our findings can be summarized as follows. First, the enthalpy of mixing predicted by Miedema’s model in binary liquids where mixing is exothermic is in most cases not sufficiently negative. This is not the case with our LightGBM/RK model for which an MAE of 3.0 kJ/mol, or an MAPE of 22 %, can be expected in systems not included in its training set. However, its accuracy in predicting the composition of the extremum remains limited in systems for which no data is included in the training set, with an MAE of 6.7 at% obtained over 120 binaries. Second, neglecting the temperature dependence of the enthalpy of mixing can lead to an error of roughly 5 % per 100 K on the extremum value (Fig. 6c). Third, in metallic liquids where mixing is exothermic, close to ternary equimolar compositions, the enthalpy of mixing extrapolated from the binary systems by Muggianu’s model is systematically overestimated, i.e., too negative, by roughly 10 %. The same is observed for the faced-centered cubic phase of the Co-Cr-Fe-Mn-Ni system [396], which strengthens this observation and suggests that it

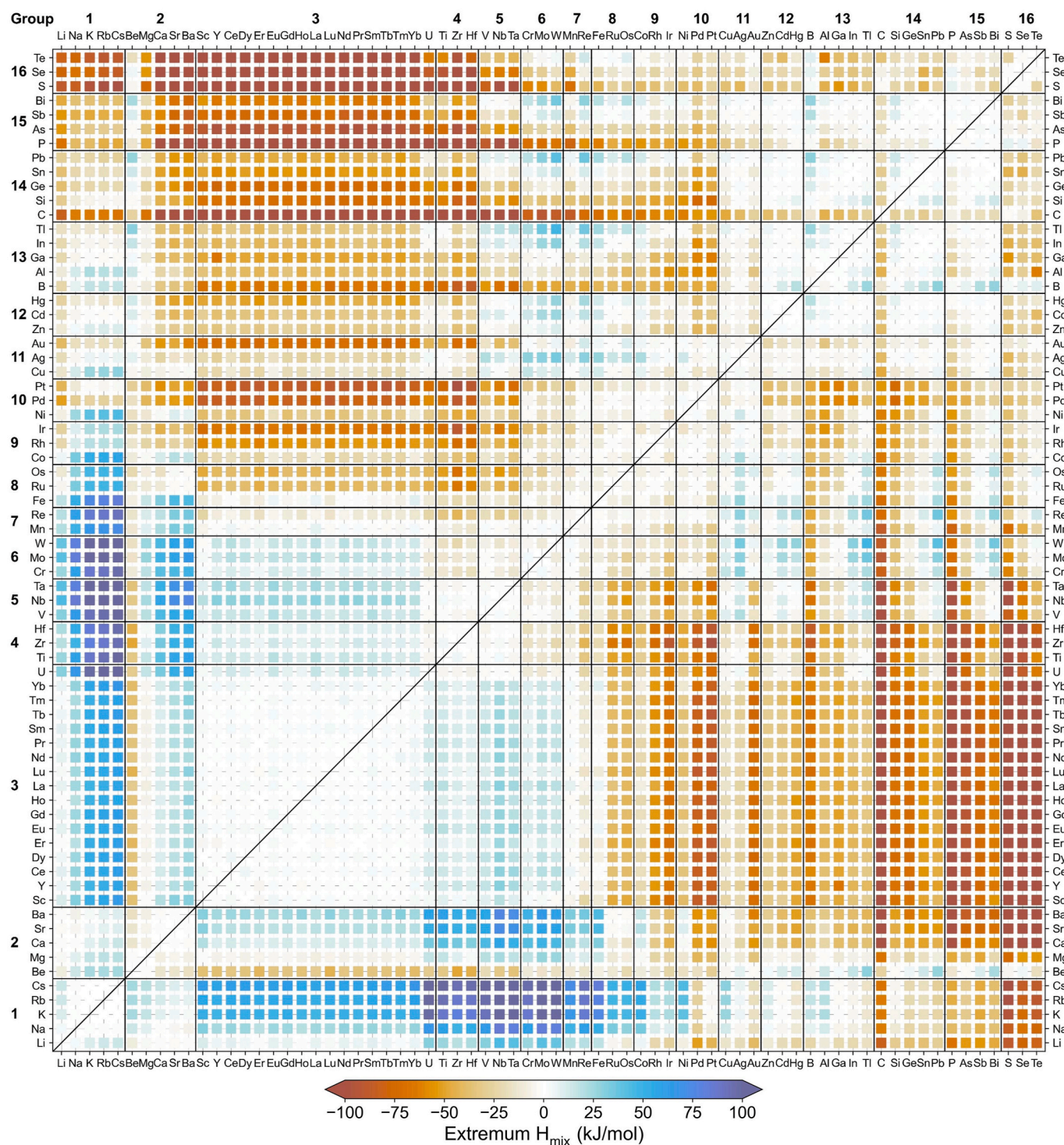


Fig. 5. Extremum value of the enthalpy of mixing in the liquid phase predicted using the LightGBM/RK model over all the 2415 binary systems generated by 70 elements.

may also holds for solid solutions. It is concluded that none of these errors is negligible, but when estimating the enthalpy of mixing of complex concentrated alloy, the prediction of its binary contributions remains the most important source of error.

The quality of our results depends on that of our datasets. They were obtained from Calphad assessments whose reliability was critically evaluated on a case-by-case basis. The advantages of this approach were discussed in Ref. [5]. It enabled us to collect an unprecedentedly large amount of data supported by direct and indirect measurements. Our

dataset on the enthalpy of mixing in binary liquids is centered on metals (Fig. 2). The LightGBM/RK model performs relatively poorly on group 16 elements. On test, this can be explained by the fact they tend to form complex liquids with strong short-range ordering that are underrepresented in the dataset. Their enthalpy of mixing has a characteristic V-shape, but an enthalpy with a U-shape is predicted as in metallic liquids (Fig. S2). On training, the problem comes from the use of a substitutional solution model (Eq. (1)) that is not well suited for these liquids. In immiscible systems where the enthalpy of mixing is

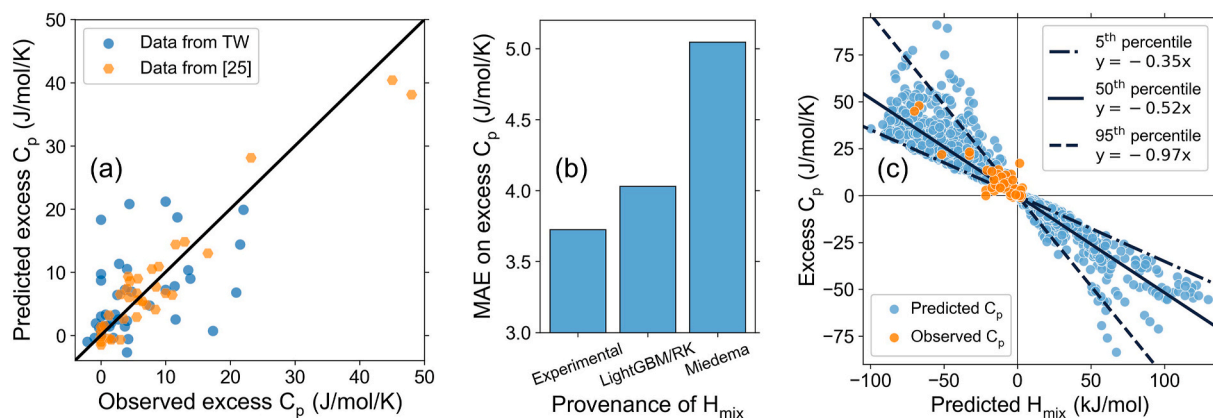


Fig. 6. Performances over data on 77 binary liquids of Witusiewicz and Sommer's model [25] using (a) experimental and (b) experimental or predicted values for the input enthalpy of mixing. (c) Relationship between the excess heat capacity and the enthalpy of mixing over 2016 binary liquids generated by 64 elements of groups 1 to 15 at the composition where the enthalpy of mixing reaches its extremum. Excess heat capacity predictions for As, C and P are abnormal due to their boiling points being lower than their melting points and are not plotted. Percentile regression lines are obtained from absolute values.

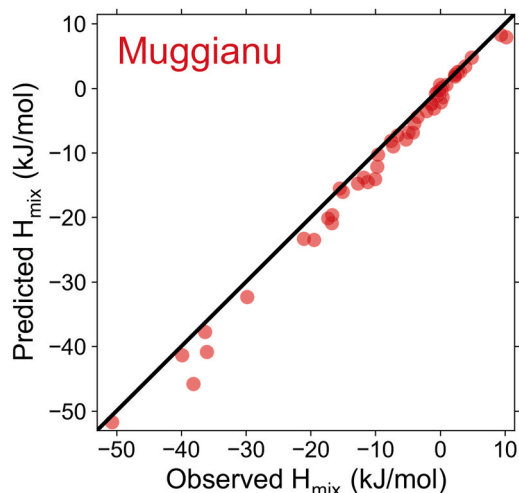


Fig. 7. Scatter plot showing the enthalpy of mixing extrapolated from the binary systems by Muggianu's model [21] against experimental data on 52 ternary near-equimolar metallic liquids.

endothermic, measurements are difficult [3], and the model is only supported by a limited number of data all below 20 kJ/mol (Fig. 3). Our data on the enthalpy of mixing in binary liquids are within or close to experimental uncertainty. However, our data on the ternary contributions to the enthalpy of mixing are less reliable because they depend on the choice made regarding binary contributions. For example, in the Ag-Ga-Sn system, the maximum ternary contributions can vary from +4.8 to +2 kJ/mol on the basis of the same experimental data but a different description of the Ag-Ga binary [360,397]. Besides, data on the excess heat capacity are also less reliable since they are derived from two experimental data at different temperatures.

Model training time may be reduced without significantly decreasing performance by selecting a composition step higher than 1 at%. Model performance will be more sensitive to step size in systems where the enthalpy of mixing has a V-shape than a U-shape. Model training speed and interpretability can also be improved by using less features. Our LightGBM model is based on a set of 30 features to maximize accuracy, but comparable performance can be achieved with sets of 20–58 features (Fig. S3). A Pearson's correlation analysis between these 30 features and the error of Miedema's model as well as the enthalpy of mixing is shown in Fig. S4. There is a positive correlation between the enthalpy of mixing and the error of Miedema's model because it generally gives values that

not sufficiently negative (Fig. 3). Our features derived from the thermodynamic properties of the elements before and after melting are important for predicting the enthalpy of mixing in the liquid and to correct Miedema's model (Table S1), particularly for our LightGBM model for which they represent 7 of the 10 most important features (Fig. S4). In a future work, we plan to develop a more interpretable model with better performance based on an improved dataset.

CRedit authorship contribution statement

Guillaume Deffrennes: Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Bengt Hallstedt:** Writing – review & editing, Methodology, Data curation, Resources. **Taichi Abe:** Writing – review & editing, Data curation, Resources. **Quentin Bizot:** Writing – review & editing, Formal analysis. **Evelyne Fischer:** Writing – review & editing, Data curation, Resources. **Jean-Marc Joubert:** Writing – review & editing, Visualization, Methodology. **Kei Terayama:** Writing – review & editing, Methodology. **Ryo Tamura:** Writing – original draft, Visualization, Methodology, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Our datasets on the excess heat capacity and on the enthalpy of mixing in ternary liquids are shared as supplementary materials. Our dataset on the enthalpy of mixing in binary liquids is shared in an open access data repository [398]. The parameters of our LightGBM/RK model obtained in the 2415 binary systems generated by 70 elements are shared as supplementary materials and in the same data repository. The binary contributions to the enthalpy of mixing in the liquid phase can be calculated in J/mol from these using Eqs. (1) and (2). The parameters to calculate the excess heat capacity in J/mol/K in 2211 binary liquids generated by 67 elements based on Witusiewicz and Sommer's model [25] are shared as supplementary materials. Descriptors for machine learning studies of alloys can be easily generated from our models and from the thermodynamic properties of pure elements using the open-access notebook at <https://colab.research.google.com/drive/1XRqgvP11JuU8pxHqJpkZQChAJ5tvLdVWV>.

Dataset on the enthalpy of mixing in binary liquids (Original data)

(Mendeley Data)

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.calphad.2024.102745>.

Appendix. Prediction of the enthalpy of mixing in the liquid phase using Miedema's model

The enthalpy of mixing in a binary A-B liquid is predicted by Miedema's model by following steps S1 to S5:

$$c_B^s = \frac{x_B V_B^{2/3}}{x_A V_A^{2/3} + x_B V_B^{2/3}} \quad (S1)$$

with x_B , V_B and c_B^s the molar fraction, molar volume, and surface fraction of B.

$$\left(V_A^{2/3}\right)_{alloy} = V_A^{\frac{2}{3}} \left(1 + a_A c_B^s (\varphi_A - \varphi_B)\right) \quad (S2)$$

with a_A a parameter for A, φ_B the so-called work function of B, and $\left(V_A^{2/3}\right)_{alloy}$ the molar volume of A accounting for changes upon alloying.

$$\left(c_B^s\right)_{alloy} = \frac{x_B \left(V_B^{2/3}\right)_{alloy}}{x_A \left(V_A^{2/3}\right)_{alloy} + x_B \left(V_B^{2/3}\right)_{alloy}} \quad (S3)$$

with $\left(c_B^s\right)_{alloy}$ the surface fraction of B corrected as recommended in Ref. [399].

$$H_{inter}(A \text{ in } B) = \frac{\left(V_A^{2/3}\right)_{alloy} \left(-P(\varphi_A - \varphi_B)^2 + Q\left(n_{wsA}^{1/3} - n_{wsB}^{1/3}\right)^2 + 0.73R_A R_B\right)}{\frac{1}{2} \left(\frac{1}{n_{wsA}^{1/3}} + \frac{1}{n_{wsB}^{1/3}}\right)} \quad (S4)$$

$H_{inter}(A \text{ in } B)$ is the interfacial enthalpy of solving 1 mol of A in B obtained for the liquid phase. P is a parameter equal to 14.2, 12.35 or 10.7 [385] for alloys of two transition metals, a transition metal with a non-transition metal, and two non-transition metals, respectively. Fig. 33 of Ref. [14] details which elements are considered transition metals and which are not. n_{wsA} is the averaged electron density at the boundary of the Wigner-Seitz cell of A. R is another parameter, and 0.73 is a reducing factor used for the liquid phase. The ratio of Q over P equals 9.4.

The enthalpy of mixing in the A-B liquid, H_{mix} , is finally obtained in step 5:

$$H_{mix} = c_A c_B^s H_{inter}(A \text{ in } B) \quad (S5)$$

For elements of group 1 to 15, parameter values are taken from matminer [388] and checked against Refs. [14,384]. The R parameter for Ag is corrected from 0.3 to 0.15, and the a parameter for Eu and Yb are corrected from 0.1 to 0.07, which is the recommended value for trivalent metals [14]. For elements of group 16, parameter values are taken from Ref. [400]. The model is not straightforward to use. We have verified for a few systems that the values obtained in this work were the same as those obtained in Ref. [399]. Significantly different results can be obtained with other calculators proposed in the literature due to errors in parameters or possibly equations.

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