

# ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure for Magnesium Alloys

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## Abstract

In order to store and use thermodynamic knowledge in materials design, we develop a user-friendly, extensible, self-optimizing phase equilibrium software package: ESPEI, which integrates databases (crystallographic, phase equilibrium, thermochemical, and modeled Gibbs energy data, etc) and database development (automation of thermodynamic modeling) with GUI (graphical user interface) designed mainly by Microsoft C# and SQL (structured query language). We establish the data infrastructure for storing input data used for thermodynamic modeling and output data for thermodynamic analyses. The infrastructure of experimental data storage as well as the automation of database development is unique for ESPEI. In this report, the features of ESPEI are demonstrated for the Al-Mg system.

## Introduction

In comparison to the conventional trial-and-error method in materials development, computational thermodynamics, as one of the computational materials approaches, is emerging as a key technology to accelerate the pace of material research and development, and reduces the design-to-manufacturing cycle time. Computational thermodynamics, based on CALPHAD (calculation of phase diagrams) technique [1-4], possesses the abilities to model and numerically solve a vast number of materials-related problems linking to phase equilibrium, phase stability, and phase transformation, etc, implemented by the well developed CALPHAD software [5], such as Thermo-Calc [6], FactSage [7], and PANDAT [8], wherein the modeled thermodynamic databases are prerequisite for thermodynamic analyses [9]. However, the experimental and predicted thermodynamic data used as inputs for thermodynamic modeling (i.e., database development) are scattered in the literature, requiring significant amount of work to collect and analyze them. Unfortunately, those data are not kept electronically after the thermodynamic database is developed, which is not only a loss of valuable data, but also make the revision of multicomponent thermodynamic databases an extremely daunting task. Furthermore, thermodynamic modeling (database development) itself is a procedure that requires considerable experience and skill [10]. To the best of our knowledge, the thermodynamic databases of experimental data and the automation of database development are absent currently, and thus motivate the present work. Here, we develop a user-friendly, extensible, self-optimizing phase equilibrium infrastructure (ESPEI) [11], applied for Mg alloys currently. The software ESPEI (current version is 1.1) is designed to fill out the gaps between experimental data and modeled databases, making the material research and development more efficient. Herein, the selection of Mg alloys is due to their great promise as future vehicle structural materials with light weight, since Mg has a density that is two-third of aluminum and one-quarter of steel.

## Overall Infrastructure of ESPEI

The overall infrastructure of ESPEI is shown in Fig. 1, including three parts, (i) the GUI (graphical user interface) part in client side, (ii) the database part in the server side, storing databases as detailed below, and (iii) the database development part in connection with the third party code (Thermo-Calc [6] is mainly used in ESPEI) in order to generate/model new thermodynamic data for the system of interest. Wherein the databases are stored and managed by Microsoft SQL, the GUI and the communications between different parts are designed by the Microsoft C#. The ESPEI is designed as a user-friendly, extensible, self-optimizing phase equilibrium computer program with its uniqueness being the experimental data storage and the automation of database development (thermodynamic modeling).

Figure 2 illustrates the GUI features of ESPEI. We use two kinds of databases: (i) the TargetData to store input data for thermodynamic modeling and (ii) the ModelData to store output data for thermodynamic analyses (see next section for details of databases). In order to analyze and generate thermodynamic database, we use the external (e.g., Thermo-Calc [6]) and internal CALPHAD tools. In addition, the GUI part also gives the interfaces to (i) manage the databases, (ii) analyze and collect the TargetData and ModelData, (iii) communicate with internal and external CALPHAD codes, (iv) perform automation of database development, and (v) save the modeled data, etc.

Figure 3 shows the starting window of ESPEI, including the usual menus of File, Edit, Search, Automation, Tool, View, and Help (some of their functions are yet to be implemented). The window body of ESPEI includes the tabs of "TDB Specific (Mg)": available TDB files including Mg (modeled data in Thermo-Calc format); "Structure": available structures defined by ESPEI; and "All TDB imported": all available TDB files.

## Databases implemented in ESPEI

In ESPEI, two kinds of databases are used, i.e., the TargetData and the ModelData (see Fig. 2). Figure 4 shows that the TargetData includes the crystallographic data, phase equilibrium data, and thermochemical data from both first-principles calculations and experimental investigations. The extensible crystallographic data implemented in ESPEI are used to define a phase by considering the convenience and uniqueness, including the characters of (i) Pearson's symbol, (ii) space group (only its number will be used for simplify), (iii) Strukturbericht designation, (iv) crystal type, and (v) nick name (if available). Examples of phase names in the Al-Mg system [12] are shown in Table 1, containing Al, Mg, Al<sub>12</sub>Mg<sub>17</sub>, and Al<sub>2</sub>Mg. In order to use the crystallographic information for phase of interest (e.g., space group, Wyckoff positions, and lattice parameters), or to setup the Gibbs energy model for database development, or to setup the

structure file for first-principles calculations, the PaulingFile [13] (it needs separate license) was transferred into SQL format and linked to ESPEI. Figure 5 shows the PaulingFile in ESPEI with the selected  $\text{Al}_{12}\text{Mg}_{17}$  as an example. In addition, the GUI also gives user options to append new crystallographic information based on measurements, first-principles calculations, and empirical estimations.

Regarding the storing of thermodynamic TargetData, we use multi-rows to store the phase equilibrium data (identified by PEID) and the thermochemical data (TCID). As shown in Fig. 6, the phase equilibrium data include the eutectic reaction, peritectic reaction, solidus, liquidus, and tie line, etc, under the conditions of compositions (X), pressure (P), and temperature (T). For example, Table 2 gives phase equilibrium data structure for the congruent melting in Al-Mg system [12]. The same PEID indicates these data are for the same equilibrium. "StrucID" indicates the ID number of structures (phases), where 288 represents the liquid phase and 291 the  $\beta\text{-Al}_{140}\text{Mg}_{89}$  phase. The symbol  $\Delta$  ( $\Delta T$ ,  $\Delta P$ ,  $\Delta X$ ) gives the uncertainty of the corresponding datum. "EqTypeID" gives the ID number of the thermodynamic equilibrium, here the "8" indicates the congruent melting. "RefID" represents the ID number of reference used herein. "PaulingID" is one of the recommended ID numbers in PaulingFile for the current phase.

For the thermochemical data in TargetData (see Fig. 4), as shown in Fig. 7, we store the enthalpy of formation, enthalpy of mixing, heat capacity, entropy of formation, etc, under the conditions of reference states, X, P, and T. Table 3 gives an example of thermochemical data: the enthalpy of formation (EqTypeID 10) in Al-Mg system [12]. The same TCID indicate these thermochemical data are for the same equilibrium. Besides the items explained in Table 2, more items are shown in Table 3. "Value" gives the value of thermochemical data with the uncertainty of  $\Delta\text{Value}$ , "Operator" gives the operator (>, <, =, etc) of this value. "DrivingF" lists the driving force of this phase with the default value of zero. "RefStateID" gives the ID numbers of reference states of this thermochemical datum. "MagID" is the ID number of magnetic contribution.

Figure 8 illustrates the sources for inputting TargetData, including the published data and the assessments by user. In Fig. 9, we show a window to input thermochemical data in ESPEI. This window can be opened from "Tool" (see Fig. 3)  $\rightarrow$  "DataInput"  $\rightarrow$  "ThermoChemical". The meaning for each column has been explained in Table 3. In Fig. 9, we can click the symbol "+" to add a new data record, and click "X" to delete a data record. Note that: each input datum will link to the existing tables of ESPEI and the default value for each datum will be available in next version of ESPEI (version 1.2). For the safety of the database, user can only input new data and modify his/her just inputted data.

Regarding the ModelData (see Fig. 4), we store the available Gibbs energy models (e.g., sublattice model and quasichemical model, etc), modeling results (e.g., the TDB file for Thermo-Calc [6]), weights of the used TargetData, steps of modeling, and other files (e.g., pop, exp files for Thermo-Calc [6]).

For all the above data tables in TargetData and ModelData, ESPEI gives the options to edit them. Figure 10 shows the "TableEditor" interface, opened from "Tool" (see Fig. 3)  $\rightarrow$  "Edit Table ...". In Fig. 10, the ModelData is in the middle part. "ModelID" links to

the model used herein (e.g., 1 is the sublattice model). "GibbsEnergy" is the main table to save the modeled results. "FormulaID" gives the ID number of formula of the corresponding model. "FormationID" connects to the formation of enthalpy of compound or end member. "ExtraGibbsID" shows the ID number linking to extra Gibbs energy.

Besides the stored TargetData and ModelData, the GUI of ESPEI also provides interfaces to input, output, browse, and analyze these data. Figure 11 shows the general features of data output in ESPEI.

### Database Development in ESPEI

Database development (automation) is another key feature of ESPEI, the full functions will be available in next version of ESPEI (version 1.2). Figure 12 gives the interface to develop a new database or to update a pre-existed one, by using the TargetData described above.

Besides the Database and Database Development, ESPEI provide options to plot phase diagram and thermodynamic functions in connection with the third party code (Thermo-Calc [6] is mainly adopted by ESPEI).

### Summary

The software ESPEI (version 1.1), a user-friendly, extensible, self-optimizing phase equilibrium infrastructure, has been developed and applied in magnesium alloys currently. ESPEI integrates databases (crystallographic, phase equilibrium, thermochemical, and modeled Gibbs energy data) and database development (automation of thermodynamic modeling) with GUI designed mainly by Microsoft C# and SQL, filling out the gaps between experimental data and modeled thermodynamic database, making the material research and development more efficient. The storing of experimental data as well as the automation of database development is unique for ESPEI.

### Acknowledgement

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### References

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Table 1: Examples of the phase names defined in the Al-Mg system [12] (see text part for the meanings).

Material	Phase name
Al	cF4-225-A1-cubic-fcc
Mg	hP2-194-A3-hexagonal-hcp
Al <sub>2</sub> Mg	cF24-227-C15-cubic-Laves
Al <sub>12</sub> Mg <sub>17</sub>	cI58-217-A12-cubic-Gamma

Table 2: Thermodynamic TargetData: phase equilibrium data of congruent melting in Al-Mg system [12].

PEID	StrucID	Elem.	T	$\Delta T$	P	$\Delta P$	X	$\Delta X$	EqTypeID	RefID	PaulingID	CommentID
1	288	Al	724.7	1	1e5				8	1		1
1	288	Mg	724.7	1	1e5		0.385		8	1		1
1	291	Al	724.7	1	1e5				8	1	1521010	1
1	291	Mg	724.7	1	1e5		0.385		8	1	1521010	1

Table 3: Thermodynamic TargetData: thermochemical data of enthalpy of formation in Al-Mg system [12].

TCID	StrucID	Elem.	T	$\Delta T$	P	$\Delta P$	X	$\Delta X$	EqTypeID	Value	$\Delta Value$	Operator
1	290	Al	298			1e5			10	-175090		=
1	290	Mg	298			1e5	0.434		10	-175090		=

(continue the columns)

DrivingF	DeltaDF	RefStateID	MagID	RefID	PaulingID	CommentID
0		1		1	1251260	1
0		2		1	1251260	1

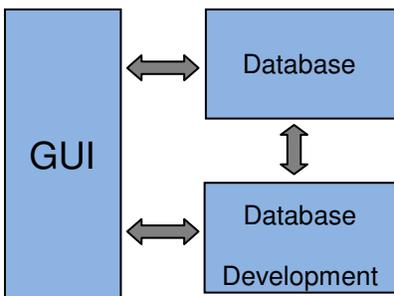


Figure 1: Overall infrastructure of ESPEI.

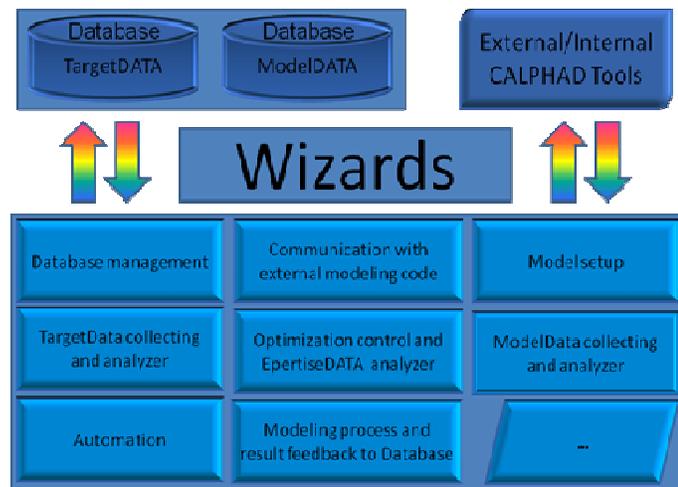


Figure 2: GUI features of ESPEI.

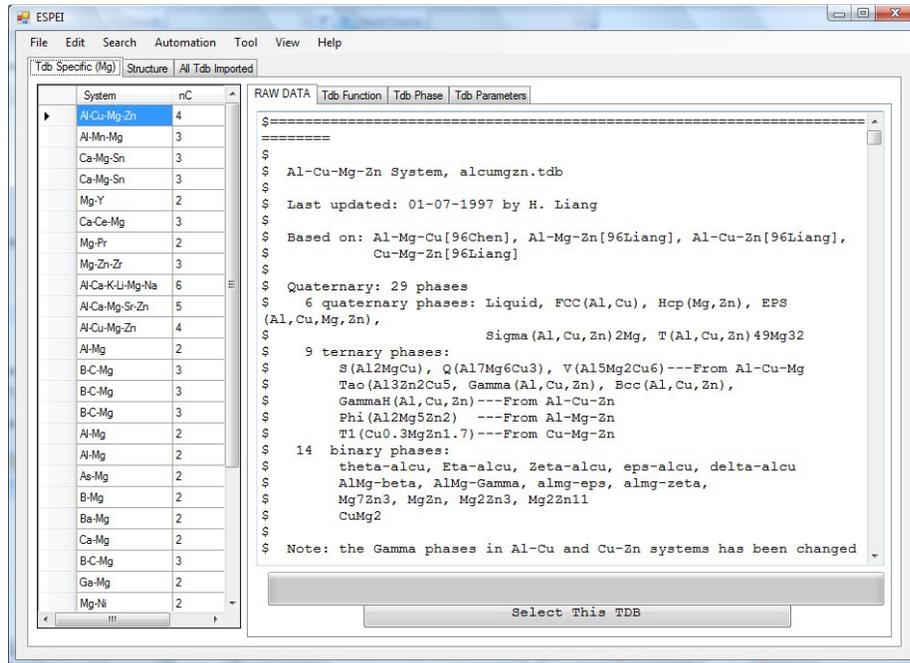


Figure 3: The starting window of ESPEI.

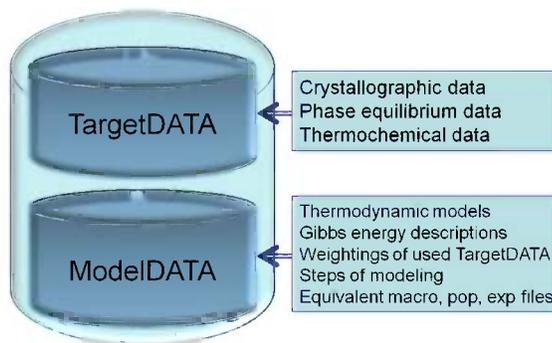


Figure 4: Databases implemented in ESPEI.

SearchPaulingDataStruc

Option:

- All Records
- Exact
- Under With
- Above With
- Under+Above

Al-Mg

1 Sys

System nC

Al-Mg 2

SENTRYNUMBER	a	b	c	alpha	beta	gamma	V
105438	1 05438	1 05438	1 05438	90	90	90	1 1722

SENTRYNUMBER	x	y	z	Wyck Mul	Wyck Pos	Elem
1250992	0 0954	0 0954	0 2725	24	g	Al
1250992	0 3582	0 3582	0 0393	24	g	Mg
1250992	0 324	0 324	0 324	8	c	Mg
1250992	0	0	0	2	a	Mg

Option:

- All Records
- Exact
- Under With
- Above With
- Under+Above

3 Cpds

SENTRYNUMBER	System	Compound	SG Symbol	SG #	Component #	Mark	Resource
452072	Al-Mg	Al <sub>23</sub> Mg <sub>77</sub>	hP2	194	2	IRF	TMSAAB,196
455193	Al-Mg	Al <sub>63</sub> Mg <sub>37</sub>	cF1832	227	2	IRF	MENAP,197
456265	Al-Mg	Al <sub>2</sub> 40Mg <sub>97</sub> 60	hP2	194	2	IRF	PHRVAO,198
456938	Al-Mg	Al <sub>7</sub> Mg <sub>93</sub>	hP2	194	2	IRF	PHMAA4,198
457996	Al-Mg	Al <sub>1</sub> Mg <sub>9</sub>	hP2	194	2	IRF	TAIMAF,198
458490	Al-Mg	Al <sub>19</sub> Mg <sub>1</sub>	cF4	225	2	IRF	ZTEFA3,198
534312	Al-Mg	Al <sub>23</sub> Mg <sub>2</sub>	cF4	225	2	IRF	JIMEAP,195
1250992	Al-Mg	Al <sub>12</sub> Mg <sub>17</sub>	cI68	217	2	TYP	NATWAY,19
1251010	Al-Mg	Al <sub>61</sub> 64Mg <sub>33</sub> 36	cF1832	227	2	TYP	ACCRA9,196
1251260	Al-Mg	Al <sub>56</sub> 60Mg <sub>43</sub> 40	hR159	148	2	TYP	ACBCAR,196

Figure 5: PaulingFile linked by ESPEI (Al<sub>12</sub>Mg<sub>17</sub> as an example).

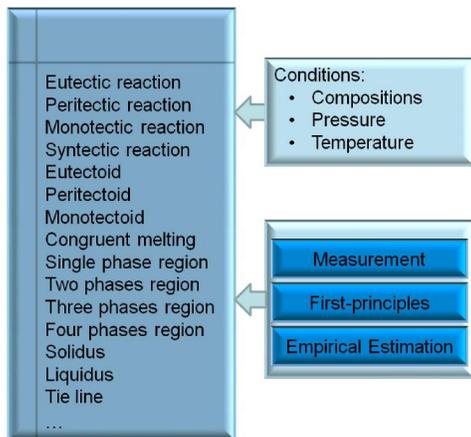


Figure 6: Phase equilibrium data of TargetData.

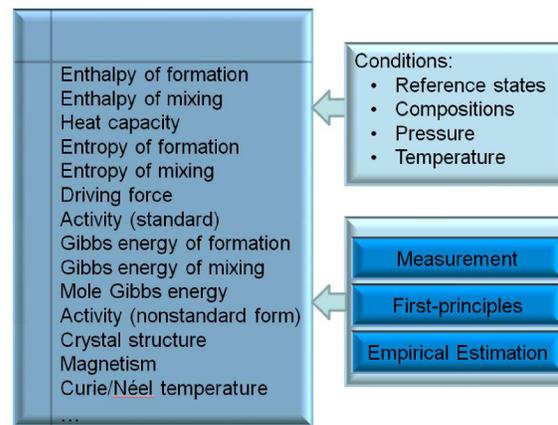


Figure 7: Thermochemical data of TargetData.

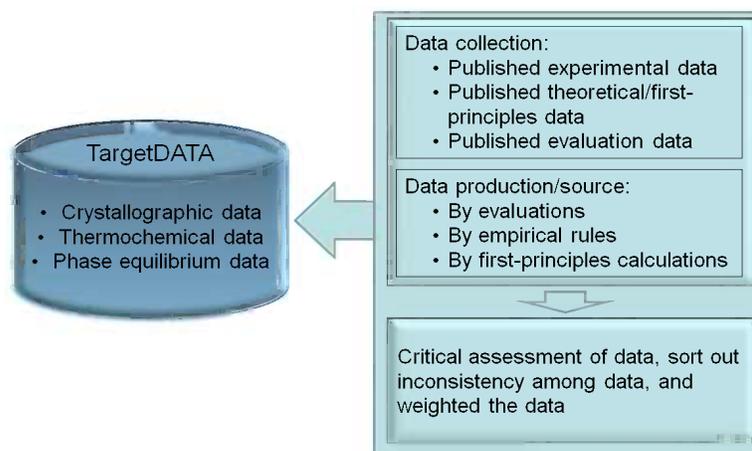


Figure 8: Sources for inputting TargetData.

ThermoChemicalDI

TCID: 120    Operator: <    T: 273.150    Notes: 313

Struc ID: 295    Value:    delta T: 0.000

Element: Mn    delta V:    P: 101325.000

Eq Type ID: 18    Driving F: -0.001    delta P:    X:   

Mag ID:    Delta DF: 0.001    delta X:   

SENTRYNUMBER: 1100355    Ref State ID:   

Comment ID: 41

TCID	StrucID	Element	T	deltaT	P	deltaP	X	deltaX	EqTypeID	Value	deltaV	Operator	Driving
120	296	Mn	273.150	0.000	101325.000				18			<	-0.001
120	295	Al	273.150	0.000	101325.000				18			<	-0.001
120	295	Mn	273.150	0.000	101325.000				18			<	-0.001
121	294	Al	273.150	0.000	101325.000				18				
121	294	Mn	273.150	0.000	101325.000				18				
121	296	Al	273.150	0.000	101325.000				18				
121	296	Mn	273.150	0.000	101325.000				18				
121	288	Al	273.150	0.000	101325.000				18			<	-0.001
121	288	Mn	273.150	0.000	101325.000				18			<	-0.001
121	293	Al	273.150	0.000	101325.000				18			<	-0.001
121	293	Mn	273.150	0.000	101325.000				18			<	-0.001
121	295	Al	273.150	0.000	101325.000				18			<	-0.001
121	295	Mn	273.150	0.000	101325.000				18			<	-0.001
121	297	Al	273.150	0.000	101325.000				18			<	-0.001
121	297	Mn	273.150	0.000	101325.000				18			<	-0.001
121	292	Al	273.150	0.000	101325.000				18			<	-0.001
121	292	Mn	273.150	0.000	101325.000				18			<	-0.001
122	296	Al	273.150	0.000	101325.000				18				
122	296	Mn	273.150	0.000	101325.000				18				
122	297	Al	273.150	0.000	101325.000				18				
122	297	Mn	273.150	0.000	101325.000				18				

Figure 9: Data input window for thermochemical data in ESPEI.

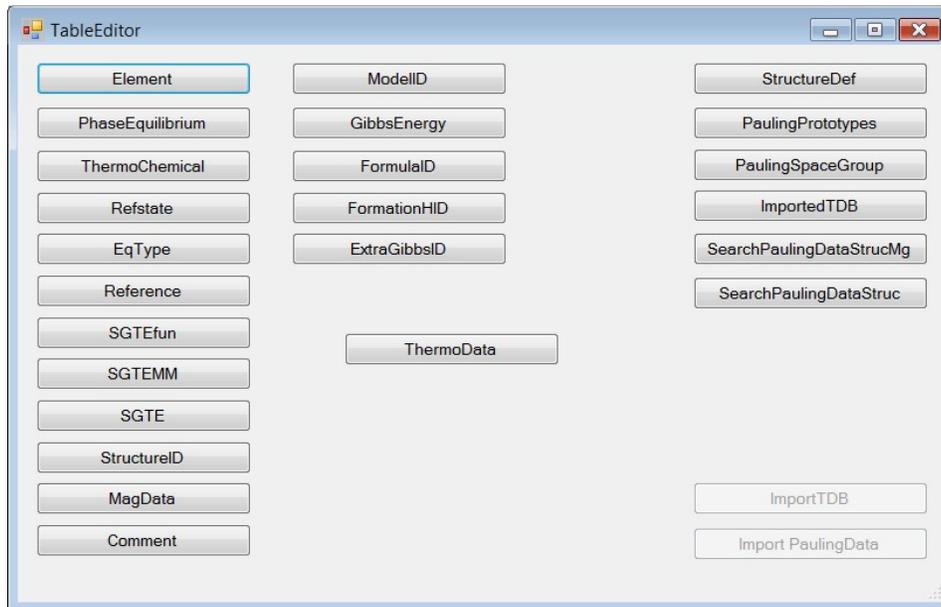


Figure 10: Edit data tables in EPSEI.

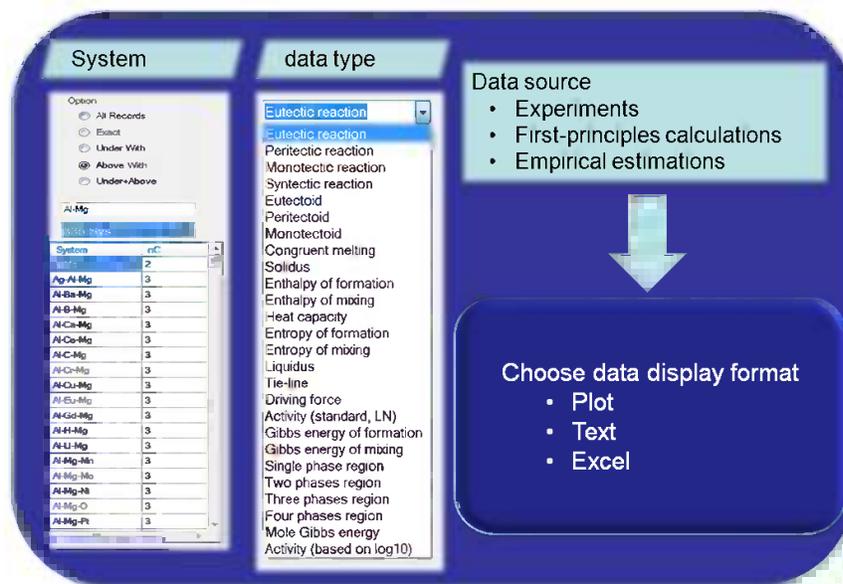


Figure 11: Data output in ESPEI.

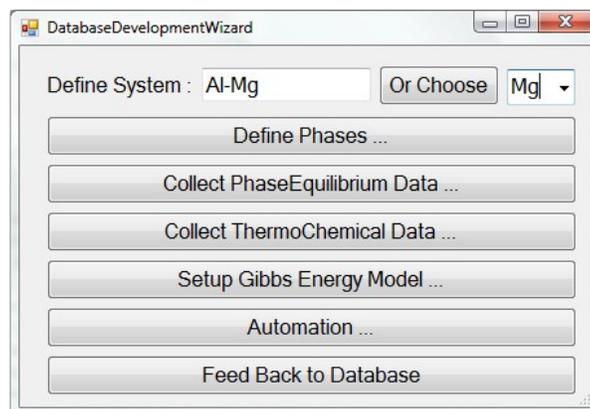


Figure 12: Database development of ESPEI.