

ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure

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CALPHAD modeling of properties of individual phases in multicomponent materials

$$\phi = {}^o\phi + \Delta\phi$$

$${}^o\phi = \sum x_i {}^o\phi_i$$

$$\Delta\phi = \Delta\phi_{conf} + \sum \sum x_i x_j \sum_{k=0}^k \phi_{i,j} (x_i - x_j)^k + \sum \sum \sum x_i x_j x_m \phi_{ijm}$$

Liu, *J. Phase Equilib. Diffus.*, 30 (2009), 517

Scaling of parameters in multicomponent systems

- Typical binary system: 10-30 parameters
- Al-Co-Ni-Y: ~200 parameters
- NIST Superalloy database (10 components): 2000+ parameters!
- What if one binary is remodeled?
 - Everything is connected
 - The entire parameter set may have to be re-optimized to be self-consistent

Inverse data pyramid of multicomponent materials

Ternary and multi-component systems

$$C_n^3 = \frac{n(n-1)(n-2)}{6}$$

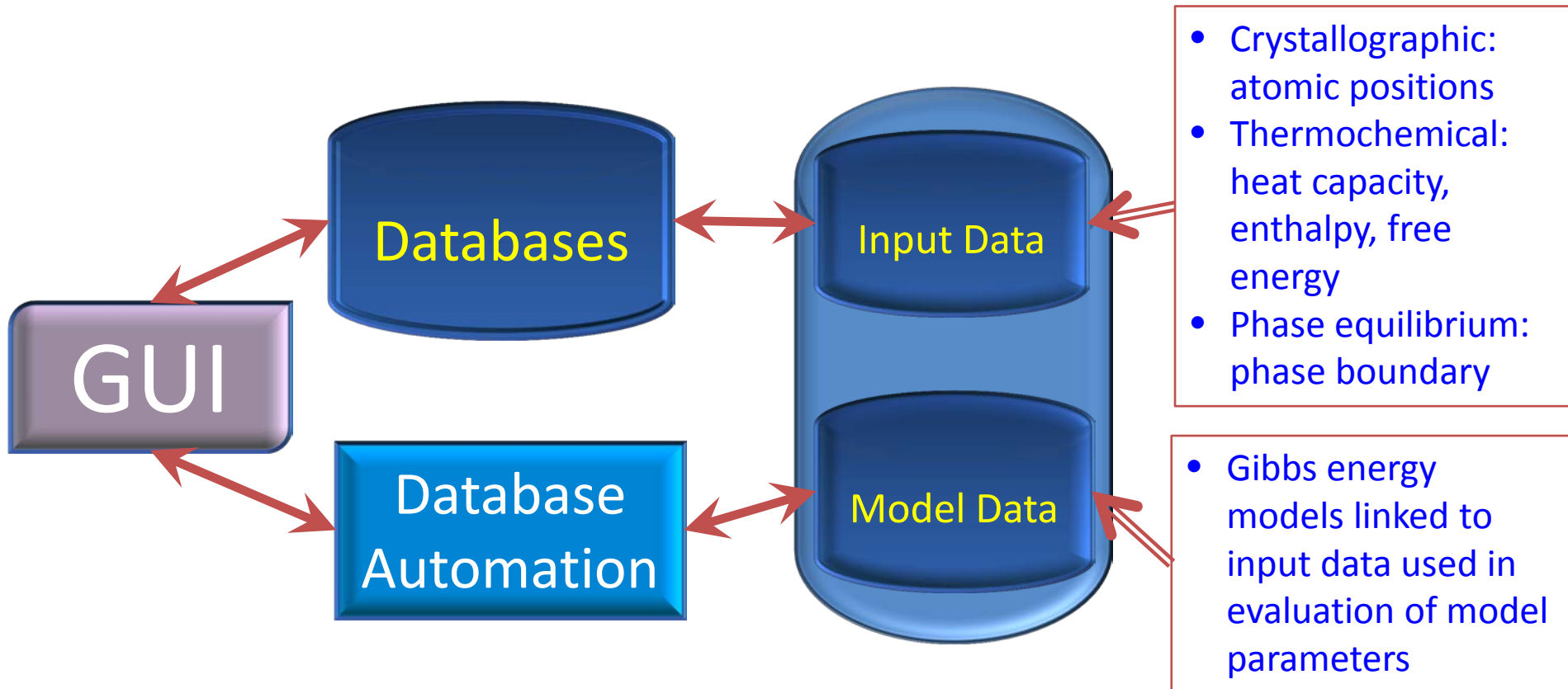
Binary systems

$$C_n^2 = \frac{n(n-1)}{2}$$

Unary

n components

ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure



ESPEI: integration of input data, model, and model parameters

- Input data
 - Thermochemical data from first-principles calculations
 - Thermochemical data from experiments
 - Phase equilibrium data from experiments
- Models
 - Stoichiometric phases: pure elements and end-members in sublattice models
 - Solution phases
- Model parameters
 - Coefficients of functions for stoichiometric phases
 - Interaction parameters of solutions phases in and between sublattices

Live Demo (Al-Mg)

ESPEI: Starting Window

The screenshot shows the ESPEI 1.3 software interface. The 'Automation' menu is open, with 'Automation for Ternary' selected. The main window displays a list of systems on the left and a detailed view of the Al-Cu-Mg-Zn system on the right.

System	Count
Al-Cu-Mg-Zn	4
Al-Mn-Mg	3
Ca-Mg-Sn	3
Ca-Mg-Sn	3
Mg-Y	2
Ca-Ce-Mg	3
Mg-Pr	2
Mg-Zn-Zr	3
Al-Ca-K-Li-Mg-Na	6
Al-Ca-Mg-Sr-Zn	5
Al-Cu-Mg-Zn	4
Al-Mg	2
B-C-Mg	3
B-C-Mg	3
B-C-Mg	3
Al-Mg	2
Al-Mg	2
As-Mg	2
B-Mg	2

```
$=====  
$  
$ Al-Cu-Mg-Zn System, alcumgzn.tdb  
$  
$ Last updated: 01-07-1997 by H. Liang  
$  
$ Based on: Al-Mg-Cu[96Chen], Al-Mg-Zn[96Liang], Al-  
Cu-Zn[96Liang],  
$           Cu-Mg-Zn[96Liang]  
$  
$ Quaternary: 29 phases  
$   6 quaternary phases: Liquid, FCC(Al,Cu), Hcp  
(Mg,Zn), EPS(Al,Cu,Mg,Zn),  
$           Sigma(Al,Cu,Zn)2Mg, T  
(Al,Cu,Zn)49Mg32  
$   9 ternary phases:  
$           S(Al2MgCu), Q(Al7Mg6Cu3), V(Al5Mg2Cu6) ---From  
Al-Cu-Mg  
$           Tao(Al3Zn2Cu5, Gamma(Al,Cu,Zn), Bcc(Al,Cu,Zn),  
$           GammaH(Al,Cu,Zn) ---From Al-Cu-Zn
```

Select This TDB

Al-Mg: Collect Thermodynamic Data

The screenshot shows the 'AutomationbyThermoCalc' software window. The title bar includes 'AutomationbyThermoCalc' and standard window controls. The menu bar contains 'File', 'Load', and 'Config'. Below the menu bar, there are tabs for 'Wizard' and 'UseTC'. The 'Wizard' tab is active, showing a 'Define System' section with a text input field containing 'Al-Mg' and a dropdown menu set to 'Ac'. Below this are four buttons: 'Collect Thermodynamic Data ...', 'Define Phases/Setup Gibbs Energy Model ...', 'Automation ...', and 'Feed Back to Database'. The main workspace has a tabbed interface with 'Phase Selecting' selected. Below the tabs is a table with the following columns: 'Select', 'Phase (NickName)', 'Solution or', 'No. of', 'Sublattice fraction', 'Sublattice formula', 'StrucID', and 'Stable Endmember'. The table body is currently empty. Below the table are two buttons: 'Run Optimizing' and 'Save Model to Database'. The bottom right corner of the image features a logo for 'ASES PSU' and the number '9'.

PEN

Al-Mg: Collected thermodynamic data

CollectingThermodynamicDataBinary

Thermodynamic Data | PhaseEquilibrium Data | ThermoChemical Data | Run Grid

OK Cancel Apply Save to excel file ...

Choose ThermoChemical Data

- All Data
- G or F
- H and S
- Cp, AC, H298 and S298

All found phases

StrucID	NickName
FCC_A1	FCC_A1
HCP_A3	HCP_A3
Liquid	Liquid
s244_a	ALMG_G...
s290	ALMG_EI...
s291	Al Mg RI...

phase with selected data

StrucID	NickName	EqTypeID	Eq
FCC_A1	FCC_A1	11	Entf
HCP_A3	HCP_A3	11	Entf
Liquid	Liquid	11	Entf
Liquid	Liquid	19	Acti
s244_a	ALMG_GAMMA	10	Entf
s244_a	ALMG_GAMMA	20	Gibt
s290	ALMG_EPS	10	Entf

System	TCID	NickName	weight	Element
Al-Mg	1	ALMG_EPS	2	Al
Al-Mg	1	ALMG_EPS	2	Mg
Al-Mg	2	ALMG_GAMMA	2	Al
Al-Mg	2	ALMG_GAMMA	2	Mg
Al-Mg	3	ALMG_BETA	2	Al
Al-Mg	3	ALMG_BETA	2	Mg
Al-Mg	4	Liquid	2	Al
Al-Mg	4	Liquid	2	Mg
Al-Mg	5	Liquid	2	Al
Al-Mg	5	Liquid	2	Mg
Al-Mg	6	Liquid	2	Al
Al-Mg	6	Liquid	2	Mg
Al-Mg	7	Liquid	2	Al

System	PEID	NickName	weight	Element	T	delta T	P	delta P
Al-Mg	1	Liquid	105	Al	724.700	1	101325.000	
Al-Mg	1	Liquid	105	Mg	724.700	1	101325.000	
Al-Mg	1	ALMG_BETA	105	Al	724.700	1	101325.000	
Al-Mg	1	ALMG_BETA	105	Mg	724.700	1	101325.000	
Al-Mg	2	Liquid	105	Al	736.300	1	101325.000	-20.335
Al-Mg	2	Liquid	105	Mg	736.300	1	101325.000	-22.121

Al-Mg: ESPEI single phase optimization model and model parameters

DefinePhaseFromThermodynamicDatabaseBinary

SetUp Model | Running DataGrids | Macros | tabPage4

Make Sublattice by

- TC
- TC+FP
- TC+FP+ESPEI

Define Initial Variables

- Define by user
- Load Thermchemical
- Load TC+First-principles
- Load TC+FP+ESPEI

Phase (NickName)	Solution(1) or not(0)	No. of sublattice	Sublattice fraction	Sublattice formula	StrucID	Stable Endmember
ALMG_BETA	0	2	140:89	Al; Mg;	S291	
ALMG_EPS	0	2	30:23	Al; Mg;	S290	
ALMG_GAMMA	0	3	5:12:12	Mg; Mg;Al; Al;Mg;	S244_A	
FCC_A1	1	1	1	Al;Mg;	FCC_A1	
HCP_A3	1	1	1	Al;Mg;	HCP_A3	
LIQUID	1	1	1	Al;Mg;	LIQUID	

ESPEI single phase optimization

ESPEI test

Phase	StrucID	Solution(or	No. of sublattice	Sublattice fraction	Sublattice formula	L0-1	L0-T	L0-T*Ln(L0-T**2	L0-T**3	L0-1/T	L0-1/T**2	L1-1	L1-T	L1-T*Ln(L1-T**2
ALMG_BETA	S291	0	2	140:89	Al;Mg	0.0	0.0									
ALMG_EPS	S290	0	2	30:23	Al;Mg	0.0	0.0									
ALMG_GAMMA	S244_A	0	3	5:12:12	Mg;Mg;Al	0.0	0.0									
ALMG_GAMMA	S244_A	0	3	5:12:12	Mg;Al;Al	0.0	0.0									
ALMG_GAMMA	S244_A	0	3	5:12:12	Mg;Mg;Al;Al	0.0	0.0									
ALMG_GAMMA	S244_A	0	3	5:12:12	Mg;Mg;Mg	0.0	0.0									
ALMG_GAMMA	S244_A	0	3	5:12:12	Mg;Al;Mg	0.0	0.0									
ALMG_GAMMA	S244_A	0	3	5:12:12	Mg;Mg;Al;Mg	0.0	0.0									
ALMG_GAMMA	S244_A	0	3	5:12:12	Mg;Mg;Al;Mg	0.0	0.0									
ALMG_GAMMA	S244_A	0	3	5:12:12	Mg;Al;Al;Mg	0.0	0.0									

Al-Mg: Results of single phase optimization

ESPEInonSt

ESPEI fitting | FPData | RunGrid

Fitting to J/Mol:

phase	EndMember	L	1	T	T*LN(T)	T**2	T**
s291	Al:Mg	0	-803385	105.238			
s290	Al:Mg	0	-170832	-8.047			
s244_a	MG:MG:MG	0	139371	-87.319			
s244_a	MG:MG:AL,MG	0	113100.01727	-14.5000152383			
s244_a	MG:MG:AL	0	-103596	22.121			
s244_a	MG:AL:MG	0	180556	-138.069			
s244_a	MG:AL:AL,MG	0	113100.01727	-14.5000152383			
s244_a	MG:AL:AL	0	8360	20.339			
Liquid	AL,MG	2	494.00013971				
Liquid	AL,MG	1	-1093.00080779	1.41200098462			
Liquid	AL,MG	0	-9019.000514	4.79400060994			
HCP_A3	AL,MG	2	-1963				
HCP_A3	AL,MG	1	-449	-0.135			
HCP_A3	AL,MG	0	4336	-2.836			
FCC_A1	AL,MG	2	-673				
FCC_A1	AL,MG	1	1014	-0.66			
FCC_A1	AL,MG	0	1593	2.149			

Al-Mg: Automation window

AutomationbyThermoCalc

File Load Config

Wizard Use TC

Phase Selecting | Parameter Optimizing | Expt. Data Sheet | Parameter Definition | Run Box | Set weight | Manual Optimization

Select	Phase (NickName)	Solutio or	No. of	Sublattice fraction	Sublattice formula	StrucID	Stable Endmember
<input checked="" type="checkbox"/>	ALMG_BETA	0	2	140:89	Al; Mg;	S291	
<input type="checkbox"/>	ALMG_EPS	0	2	30:23	Al; Mg;	S290	
<input type="checkbox"/>	ALMG_GAMMA	0	3	5:12:12	Mg; Mg,Al; Al,Mg;	S244_A	MG:Mg:AL
<input type="checkbox"/>	FCC_A1	1	1	1	Al,Mg;	FCC_A1	
<input type="checkbox"/>	HCP_A3	1	1	1	Al,Mg;	HCP_A3	
<input type="checkbox"/>	LIQUID	1	1	1	Al,Mg;	LIQUID	

Run Optimizing

Save Model to Database

Evaluate	Phase	Sublattice formula	fixed	L0-1	fixed	L0-T	fixed	L1-1	fixed	L1-T
<input checked="" type="checkbox"/>	S291	Al:Mg	<input type="checkbox"/>	-803385	<input type="checkbox"/>	105.238	<input type="checkbox"/>		<input type="checkbox"/>	
<input checked="" type="checkbox"/>	S290	Al:Mg	<input type="checkbox"/>	-170832	<input type="checkbox"/>	-8.047	<input type="checkbox"/>		<input type="checkbox"/>	
<input checked="" type="checkbox"/>	S244_A	Mg:Mg:Al	<input type="checkbox"/>	-103596	<input type="checkbox"/>	22.121	<input type="checkbox"/>		<input type="checkbox"/>	
<input checked="" type="checkbox"/>	S244_A	Mg:Al:Al	<input checked="" type="checkbox"/>	8360	<input checked="" type="checkbox"/>	20.339	<input type="checkbox"/>		<input type="checkbox"/>	
<input checked="" type="checkbox"/>	S244_A	Mg:Mg:Mg	<input checked="" type="checkbox"/>	139371	<input checked="" type="checkbox"/>	-87.319	<input type="checkbox"/>		<input type="checkbox"/>	
<input checked="" type="checkbox"/>	S244_A	Mg:Al:Mg	<input checked="" type="checkbox"/>	180556	<input checked="" type="checkbox"/>	-138.069	<input type="checkbox"/>		<input type="checkbox"/>	
<input checked="" type="checkbox"/>	S244_A	Mg:Mg:Al,Mg	<input checked="" type="checkbox"/>	113100.01...	<input checked="" type="checkbox"/>	-14.50001...	<input type="checkbox"/>		<input type="checkbox"/>	
<input checked="" type="checkbox"/>	S244_A	Mg:Al:Al,Mg	<input checked="" type="checkbox"/>	113100.01...	<input checked="" type="checkbox"/>	-14.50001...	<input type="checkbox"/>		<input type="checkbox"/>	
<input checked="" type="checkbox"/>	FCC_A1	Al,Mg	<input type="checkbox"/>	1593	<input type="checkbox"/>	2.149	<input type="checkbox"/>	1014	<input type="checkbox"/>	-0.66
<input checked="" type="checkbox"/>	HCP_A3	Al,Mg	<input type="checkbox"/>	4336	<input type="checkbox"/>	-2.836	<input type="checkbox"/>	-449	<input type="checkbox"/>	-0.135
<input checked="" type="checkbox"/>	LIQUID	Al,Mg	<input type="checkbox"/>	-9019.000...	<input type="checkbox"/>	4.7940006...	<input type="checkbox"/>	-1093.000...	<input type="checkbox"/>	1.41200

Load Model+Data

Calculate Equilibria

Reweight

Run Optimize

Automation

Clear TC Window

Quit ThermoCalc

Plot Phase Diagram

Plot Cp

Plot deltaH

Plot Gibbs Energy

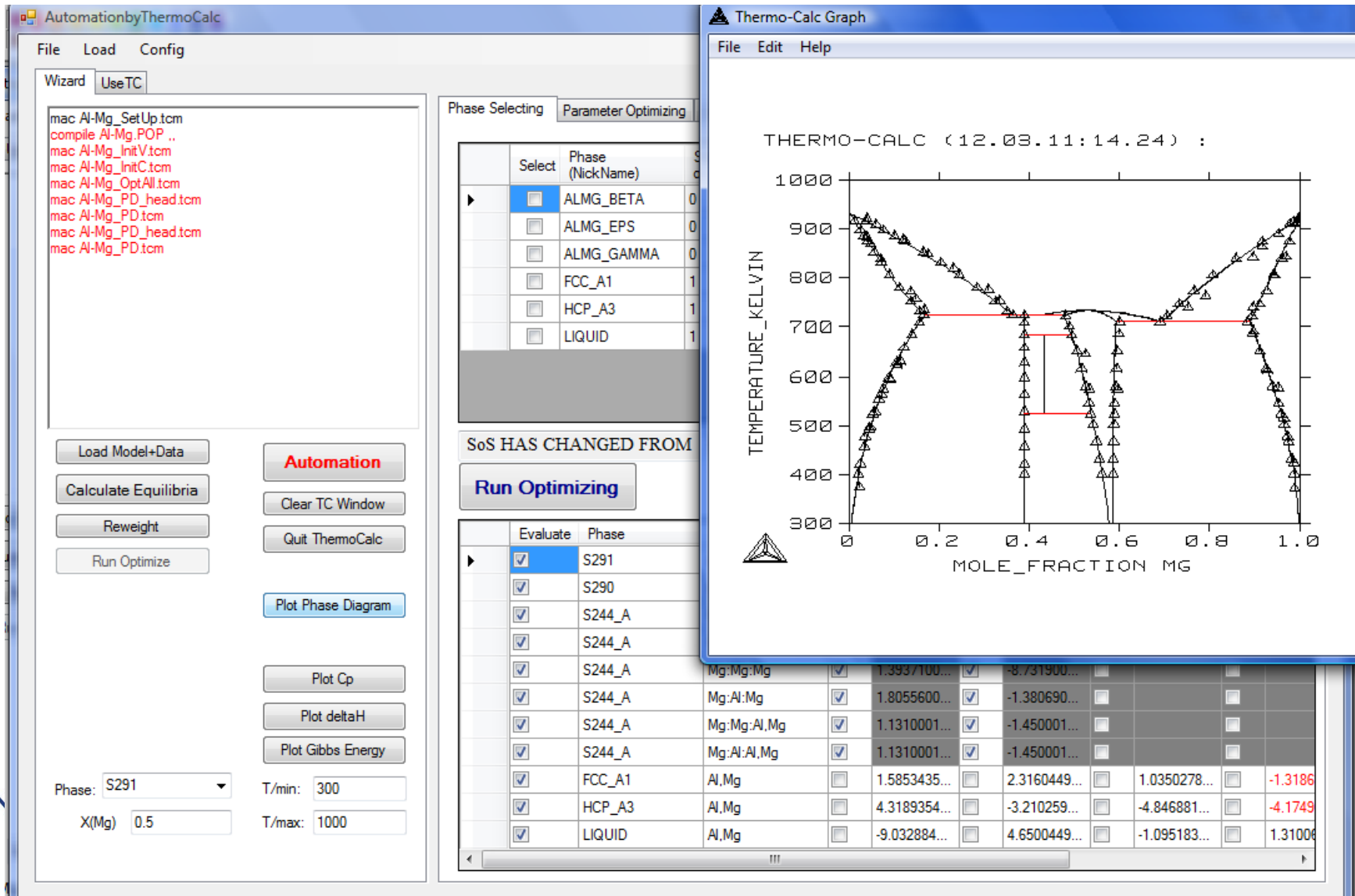
Phase: S291

X(Mg) 0.5

T/min: 300

T/max: 1000

Al-Mg: Results of automation



Al-Zn

AutomationbyThermoCalc

File Load Config

Wizard UseTC

```
mac Al-Zn_SetUp.tcm
compile Al-Zn.POP ..
mac Al-Zn_InitV.tcm
mac Al-Zn_InitC.tcm
mac Al-Zn_OptAll.tcm
mac Al-Zn_PD_head.tcm
mac Al-Zn_PD.tcm
mac Al-Zn_PD_head.tcm
mac Al-Zn_PD.tcm
```

Load Model+Data

Calculate Equilibria

Reweight

Run Optimize

Automation

Clear TC Window

Quit ThermoCalc

Plot Phase Diagram

Plot Cp

Plot deltaH

Plot Gibbs Energy

Phase: FCC_A1

X(Zn) 0.5

T/min: 300

T/max: 1000

Phase Selecting

Select	Phase (NickName)
<input type="checkbox"/>	FCC_A1
<input type="checkbox"/>	HCP_A3
<input type="checkbox"/>	LIQUID

SoS HAS CHANGED

Run Optimizing

Evaluate	Phase
<input checked="" type="checkbox"/>	FCC_A1
<input checked="" type="checkbox"/>	HCP_A3
<input checked="" type="checkbox"/>	LIQUID

Thermo-Calc Graph

File Edit Help

THERMO-CALC (12.03.11:14.34) :

TEMPERATURE_KELVIN

MOLE_FRACTION_ZN

SES

Mg-Zn

AutomationbyThermoCalc

File Load Config

Wizard UseTC

```

mac Mg-Zn_SetUp.tcm
compile Mg-Zn_POP ..
mac Mg-Zn_InitV.tcm
mac Mg-Zn_InitC.tcm
mac Mg-Zn_OptAll.tcm
mac Mg-Zn_PD_head.tcm
mac Mg-Zn_PD.tcm
mac Mg-Zn_PD_head.tcm
mac Mg-Zn_PD.tcm
        
```

Load Model+Data **Automation**

Calculate Equilibria Clear TC Window

Reweight Quit ThermoCalc

Run Optimize

Plot Phase Diagram

Plot Cp

Plot deltaH

Plot Gibbs Energy

Phase: HCP_A3 T/min: 300

X(Zn) 0.5 T/max: 1000

Thermo-Calc Graph

File Edit Help

THERMO-CALC (12.03.11:14.30) :

TEMPERATURE_KELVIN

MOLE_FRACTION_ZN

SoS HAS CHANGED FROM

Run Optimizing

Evaluate	Phase
<input checked="" type="checkbox"/>	S298
<input checked="" type="checkbox"/>	S301
<input checked="" type="checkbox"/>	S300
<input checked="" type="checkbox"/>	S299
<input checked="" type="checkbox"/>	S201
<input checked="" type="checkbox"/>	HCP_A3
<input checked="" type="checkbox"/>	LIQUID

	Mg,Zn						
			-1.194325...		3.8237763...		
			-1.600486...		7.6258598...		-3.8302
			-8.143781...		5.1821903...	<input checked="" type="checkbox"/>	-6.471000...
							2.6268