ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure

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CALPHAD modeling of properties of individual phases in multicomponent materials

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

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

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

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

National Research Council

"Integrated Computational Materials Engineering," page 71-73

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

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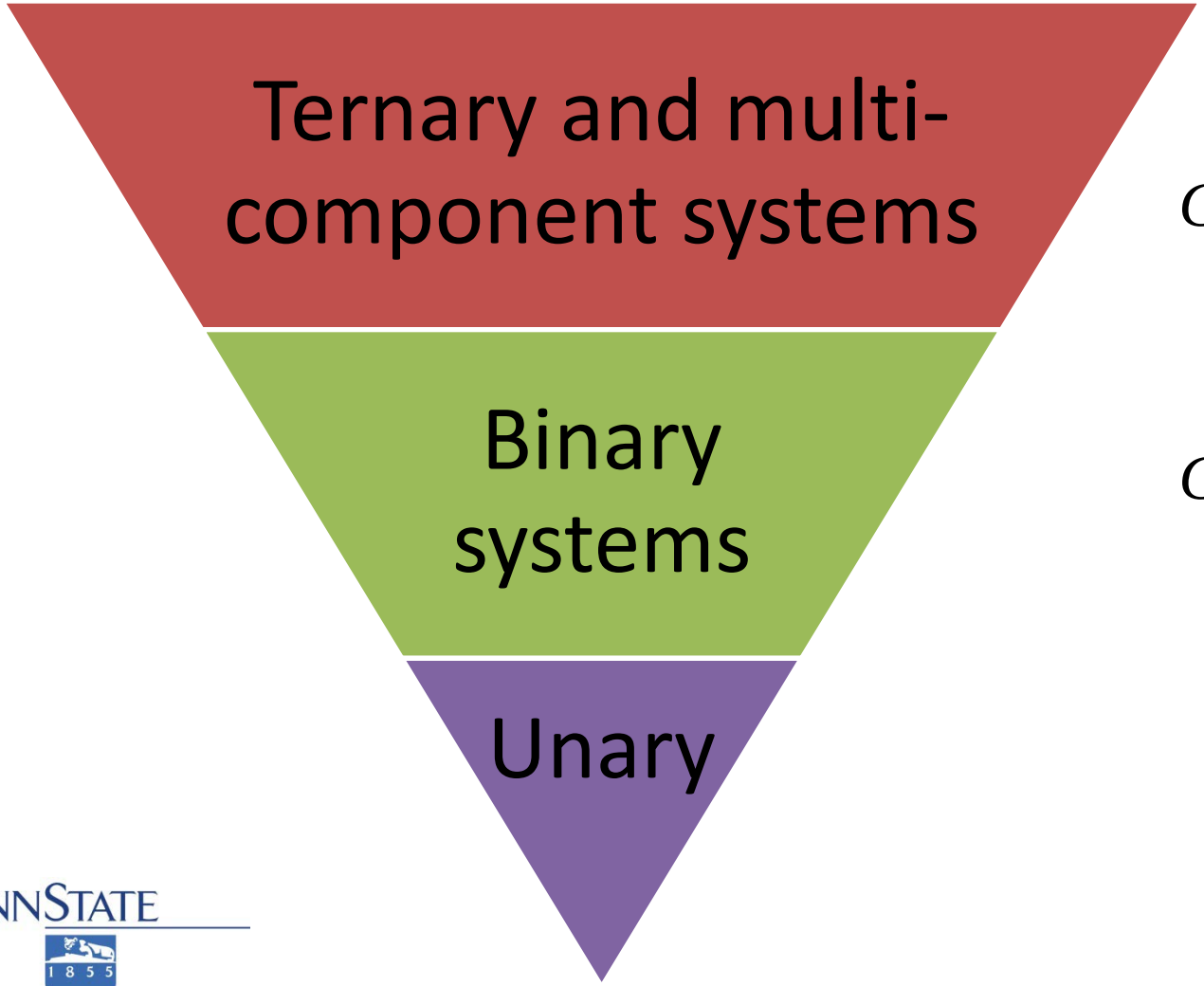
Inverse data pyramid of multicomponent materials



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

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

n components

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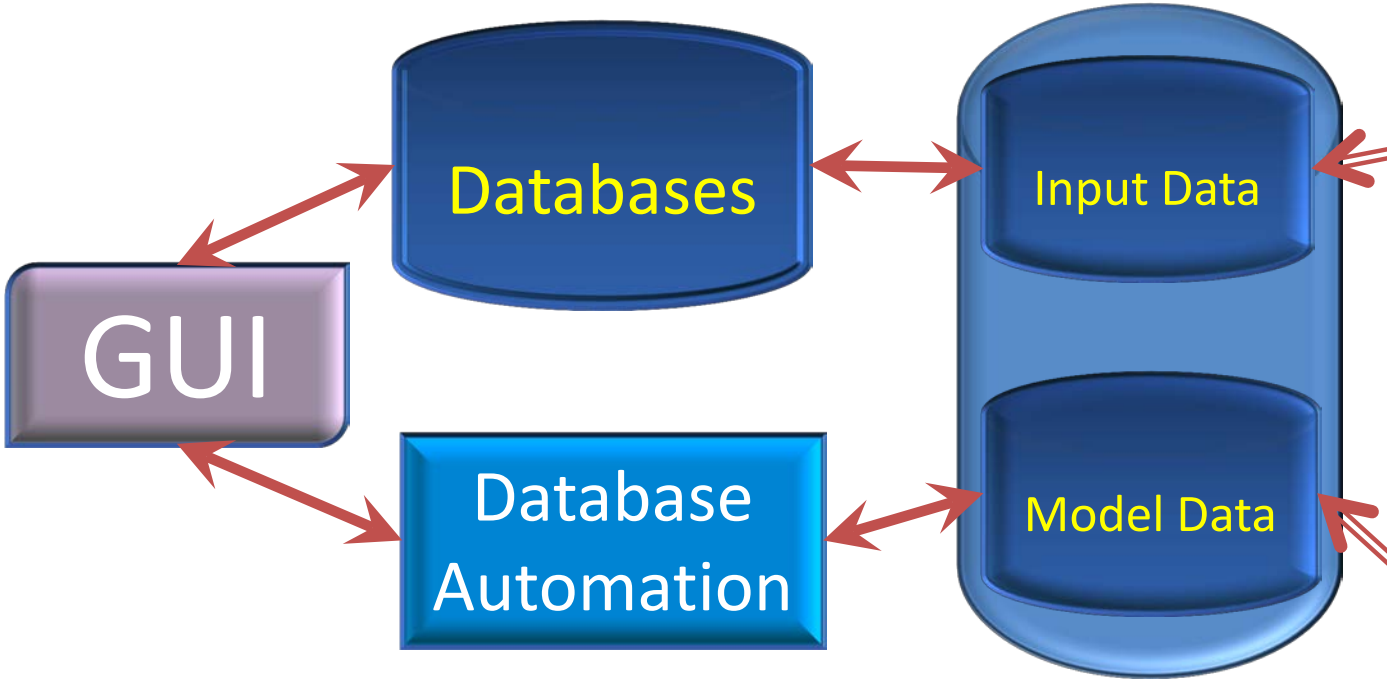

- Crystallographic: atomic positions
- Thermochemical: heat capacity, enthalpy, free energy
- Phase equilibrium: phase boundary

- Gibbs energy models linked to input data used in evaluation of model parameters

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Shang, Wang, Liu, Magnesium Technology 2010, p. 617

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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

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Live Demo (Al-Mg)

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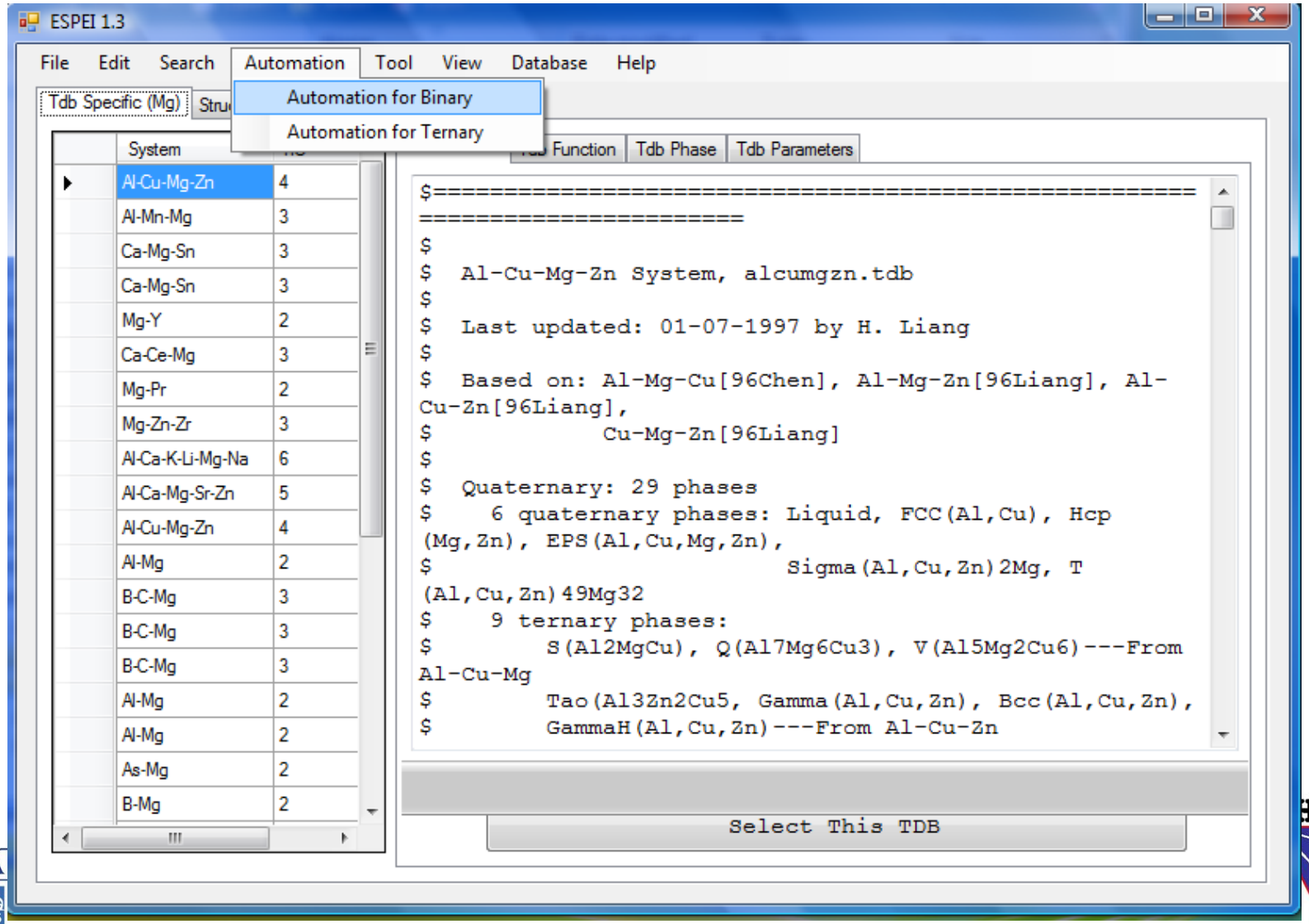
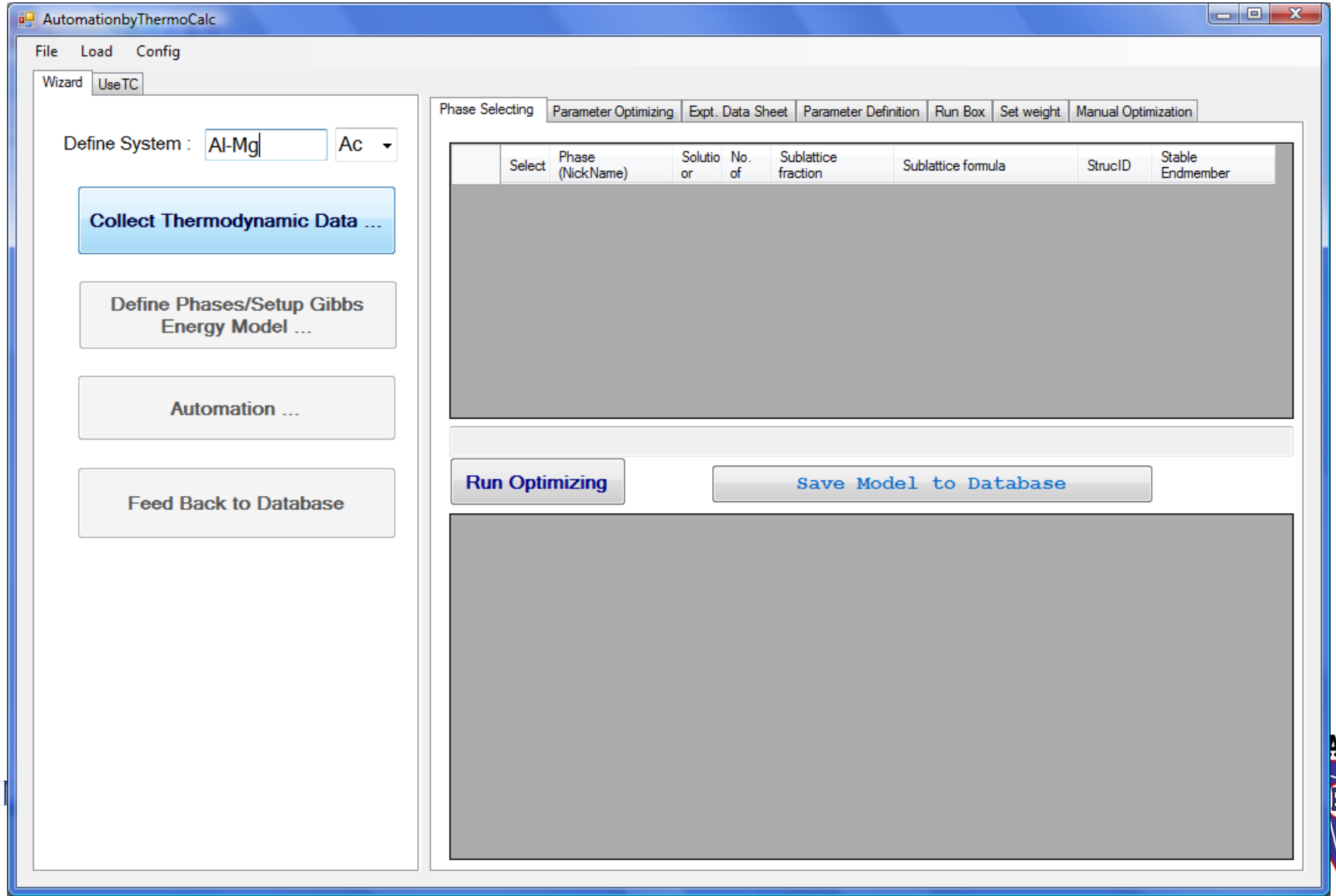
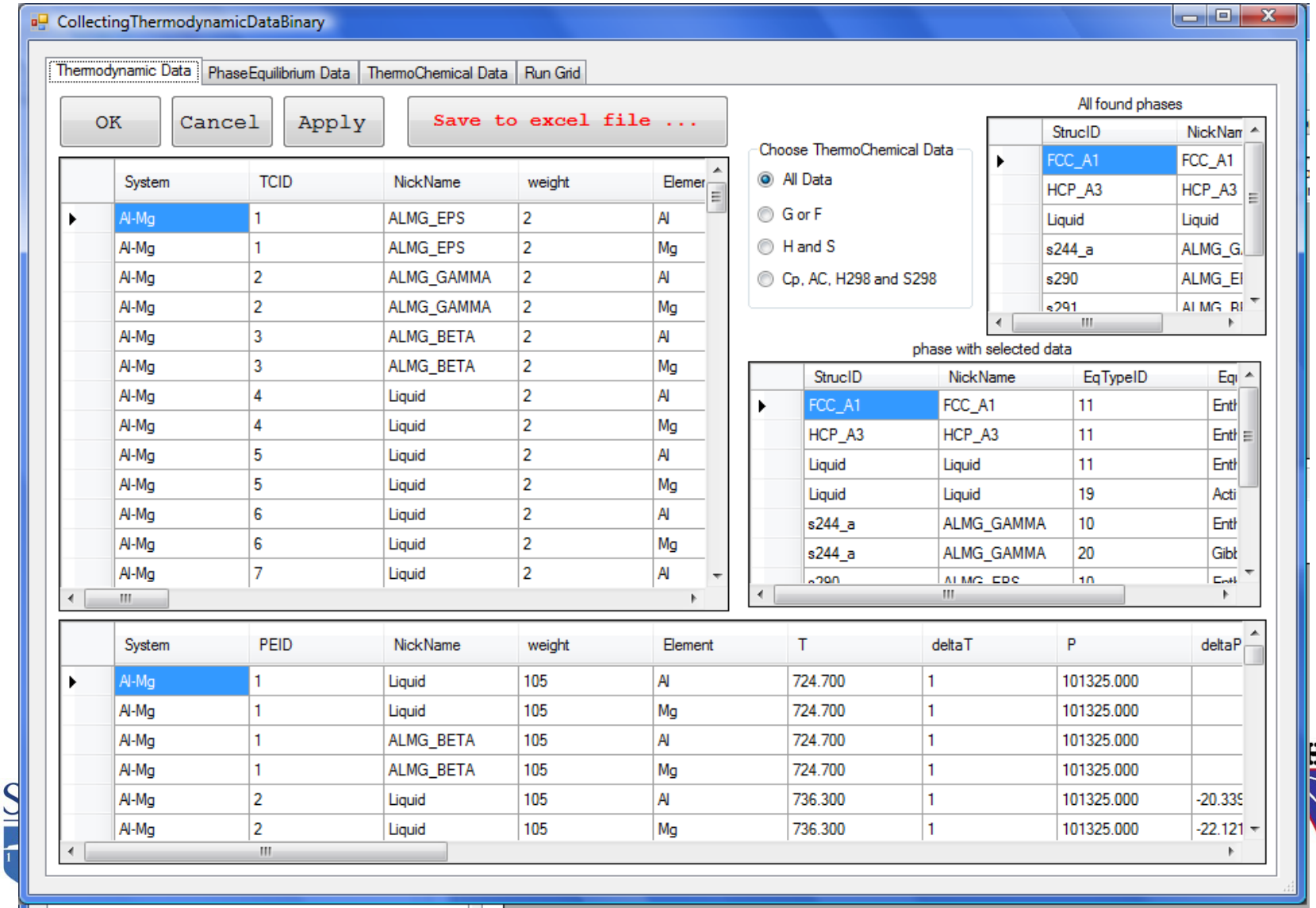
ESPEI: Starting Window



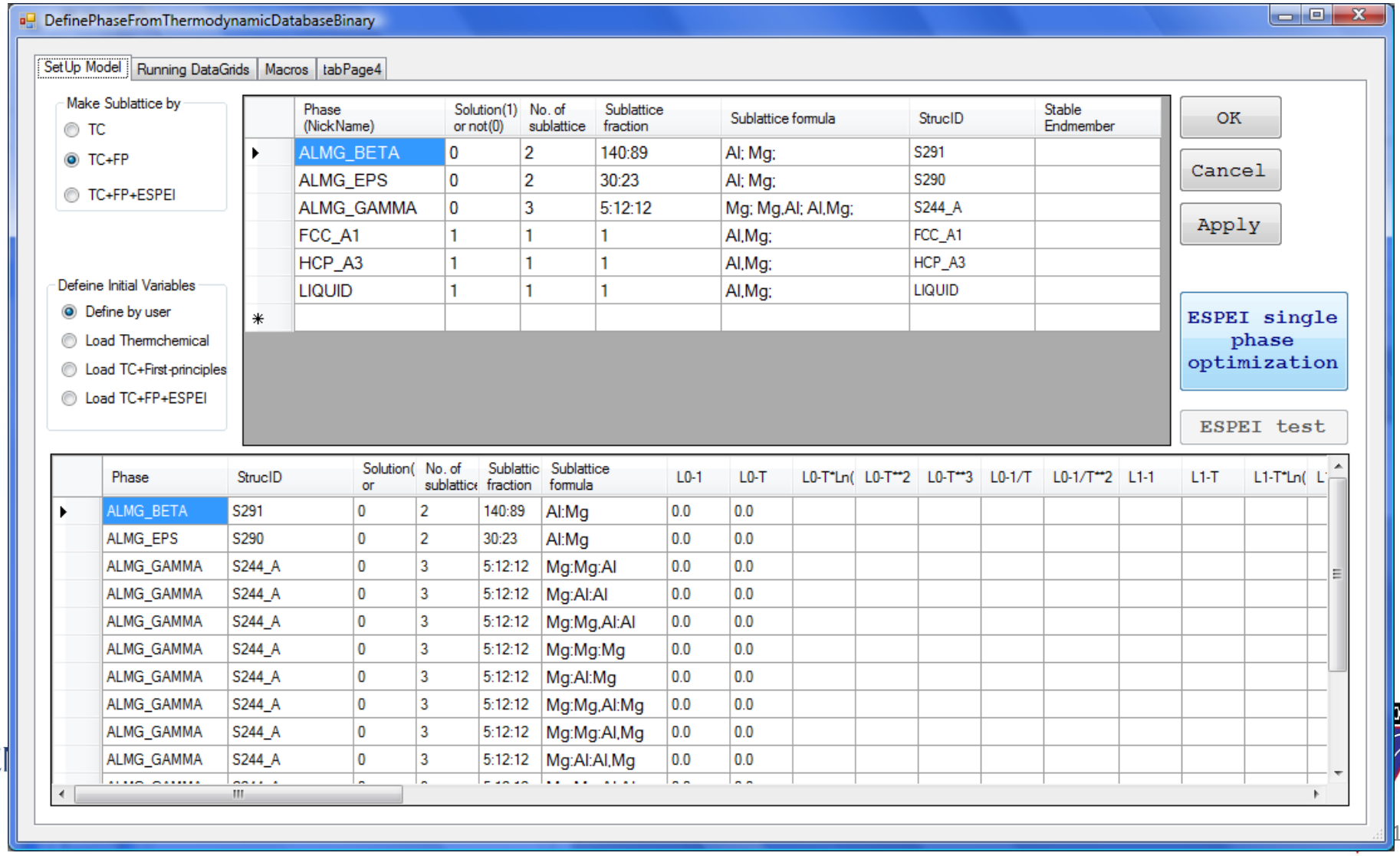
Al-Mg: Collect Thermodynamic Data



Al-Mg: Collected thermodynamic data



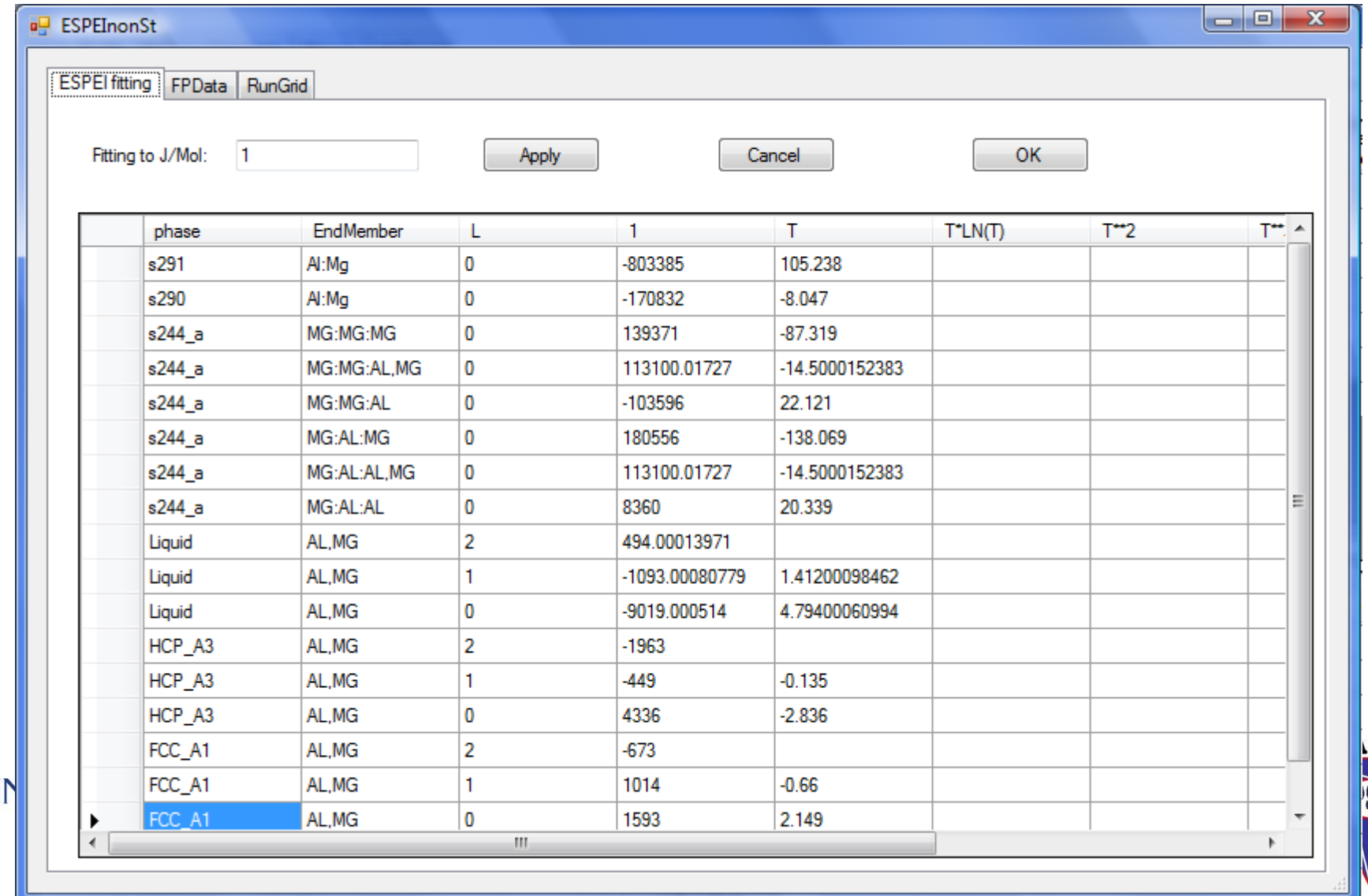
Al-Mg: ESPEI single phase optimization model and model parameters



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	

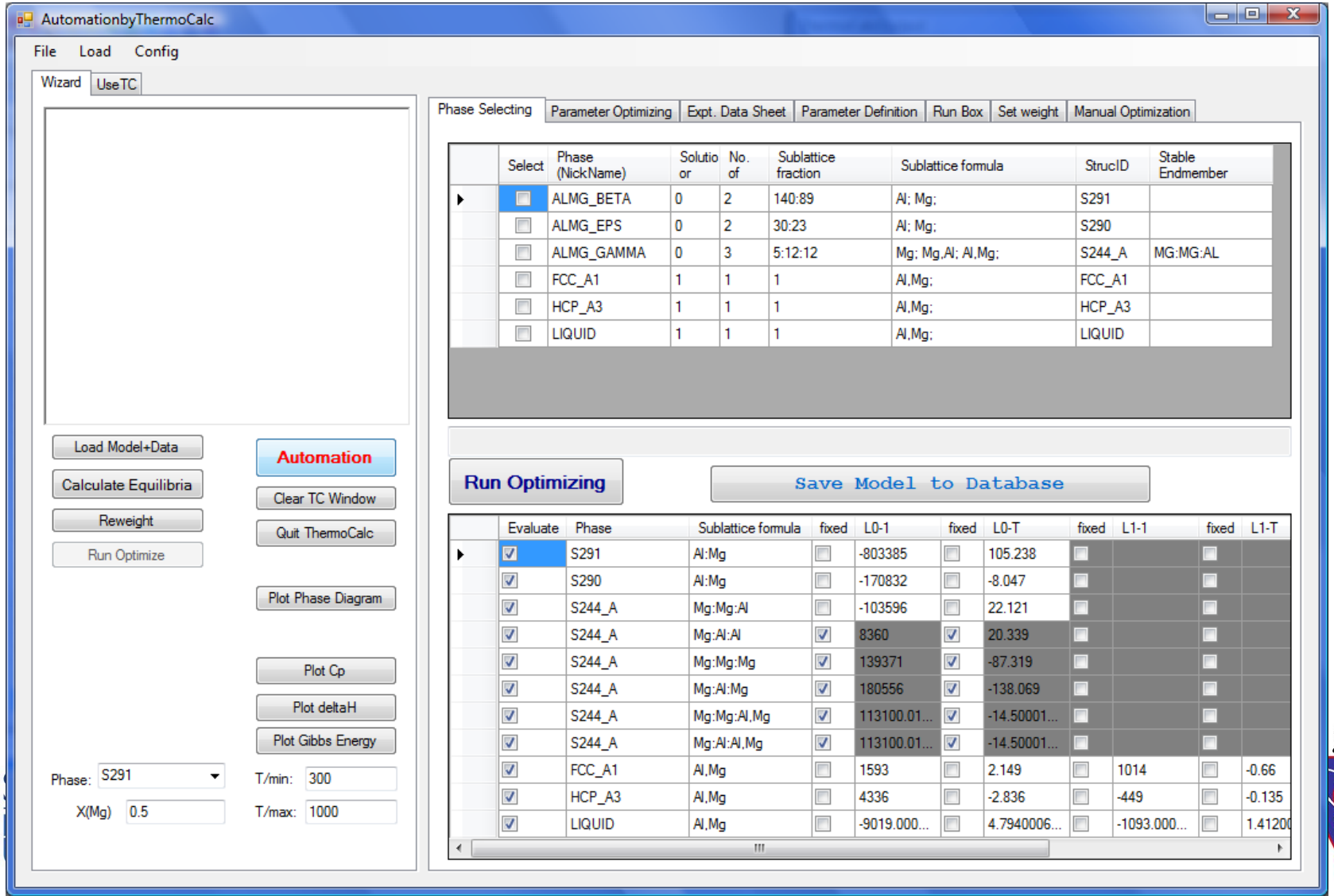
Phase	StrucID	Solution(or	No. of sublattic	Sublattic fraction	Sublattice formula	L0-1	L0-T	L0-T*Ln(	L0-T**2	L0-T**3	L0-1/T	L0-1/T**2	L1-1	L1-T	L1-T*Ln(
ALMG_BETA	S291	0	2	140:89	Al:Mg	0.0	0.0								
ALMG_EPS	S290	0	2	30:23	Al:Mg	0.0	0.0								
ALMG_GAMMA	S244_A	0	3	5:12:12	Mg:Mg:Al	0.0	0.0								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

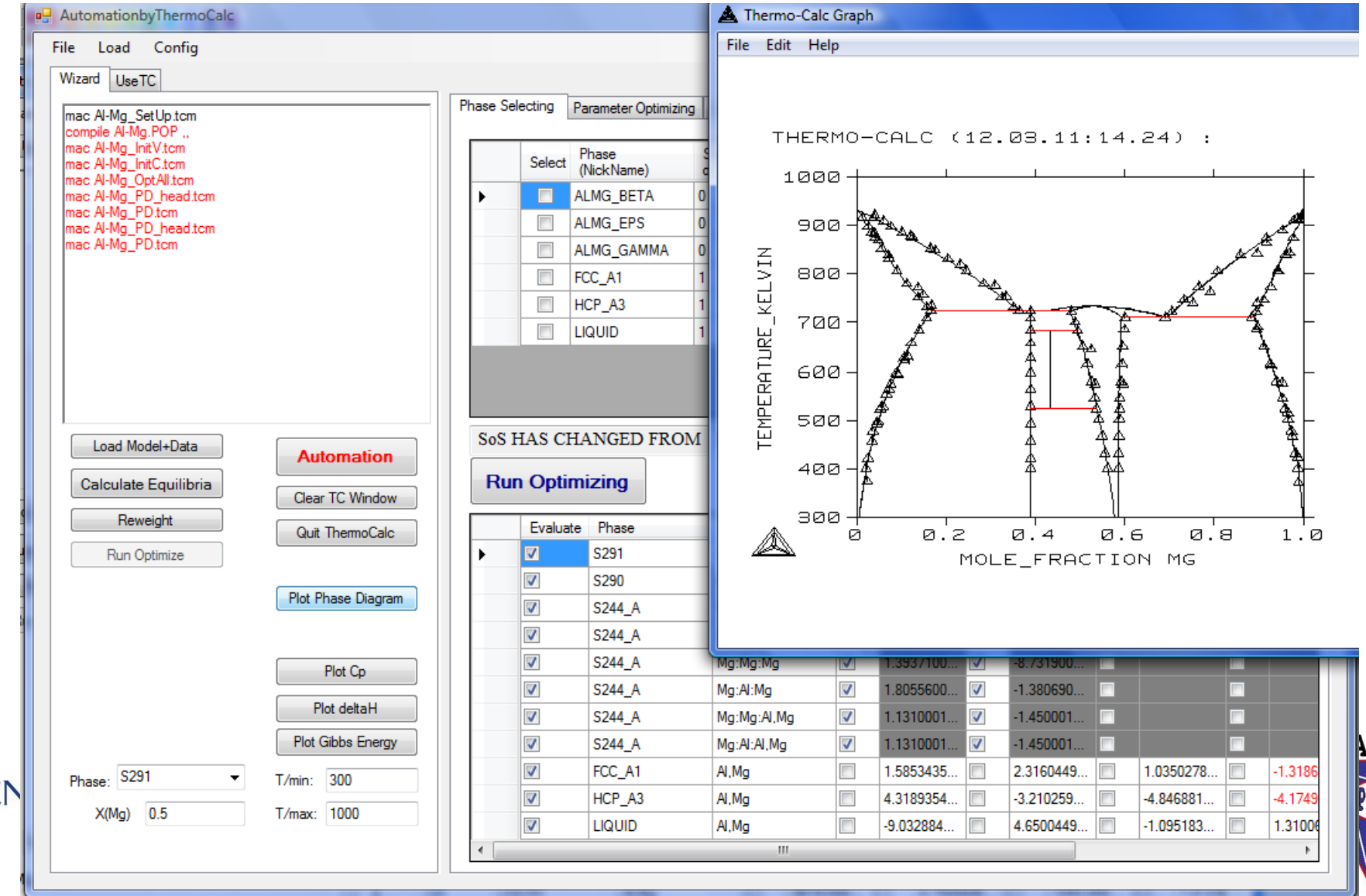


phase	EndMember	L	1	T	T*LN(T)	T**2	T**
s291	Al:Mg	0	-803385	105.238			
s290	Al:Mg	0	-170832	-8.047			
s244_a	MG:MG:MG	0	139371	-87.319			
s244_a	MG:MG:AL,MG	0	113100.01727	-14.5000152383			
s244_a	MG:MG:AL	0	-103596	22.121			
s244_a	MG:AL:MG	0	180556	-138.069			
s244_a	MG:AL:AL,MG	0	113100.01727	-14.5000152383			
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			

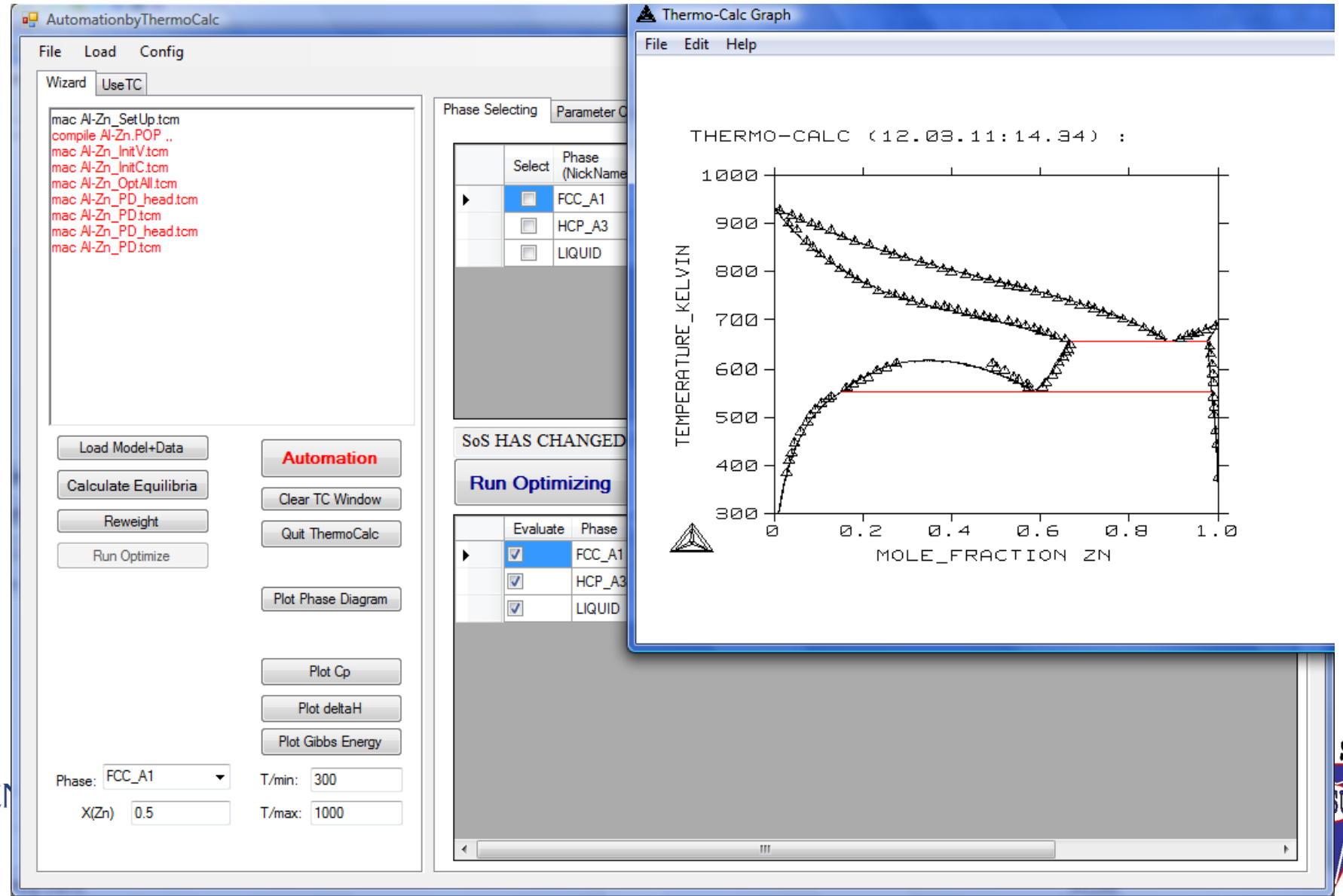
Al-Mg: Automation window



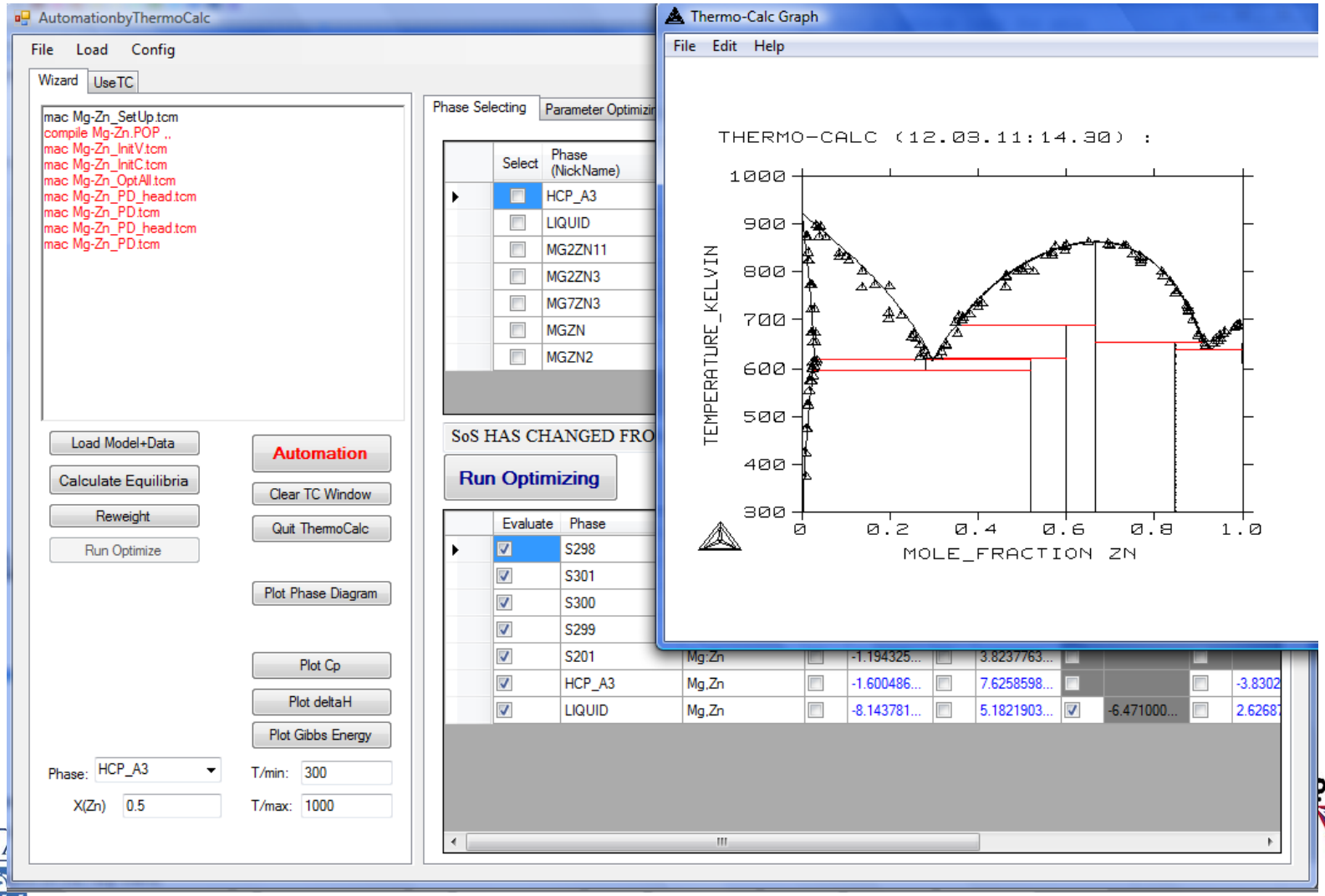
Al-Mg: Results of automation



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
Parameter C
Select
Phase (NickName
FCC_A1
HCP_A3
LIQUID
SoS HAS CHANGED
Run Optimizing
Evaluate
Phase
FCC_A1
HCP_A3
LIQUID
Thermo-Calc Graph
File
Edit
Help
THERMO-CALC (12.03.11:14.34) :
TEMPERATURE_KELVIN
1000
900
800
700
600
500
400
300
0
0.2
0.4
0.6
0.8
1.0
MOLE_FRACTION ZN

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
Calculate Equilibria
Reweight
Run Optimize
Automation
Clear TC Window
Quit ThermoCalc
Plot Phase Diagram
Plot Cp
Plot deltaH
Plot Gibbs Energy
Phase: HCP_A3
T/min: 300
X(Zn) 0.5
T/max: 1000
Phase Selecting
Parameter Optimizir
Select
Phase (NickName)
HCP_A3
LIQUID
MG2ZN11
MG2ZN3
MG7ZN3
MGZN
MGZN2
SoS HAS CHANGED FRO
Run Optimizing
Evaluate
Phase
S298
S301
S300
S299
S201
HCP_A3
LIQUID
Thermo-Calc Graph
File Edit Help
THERMO-CALC (12.03.11:14.30) :
TEMPERATURE_KELVIN
MOLE_FRACTION ZN
1000
900
800
700
600
500
400
300
0
0.2
0.4
0.6
0.8
1.0