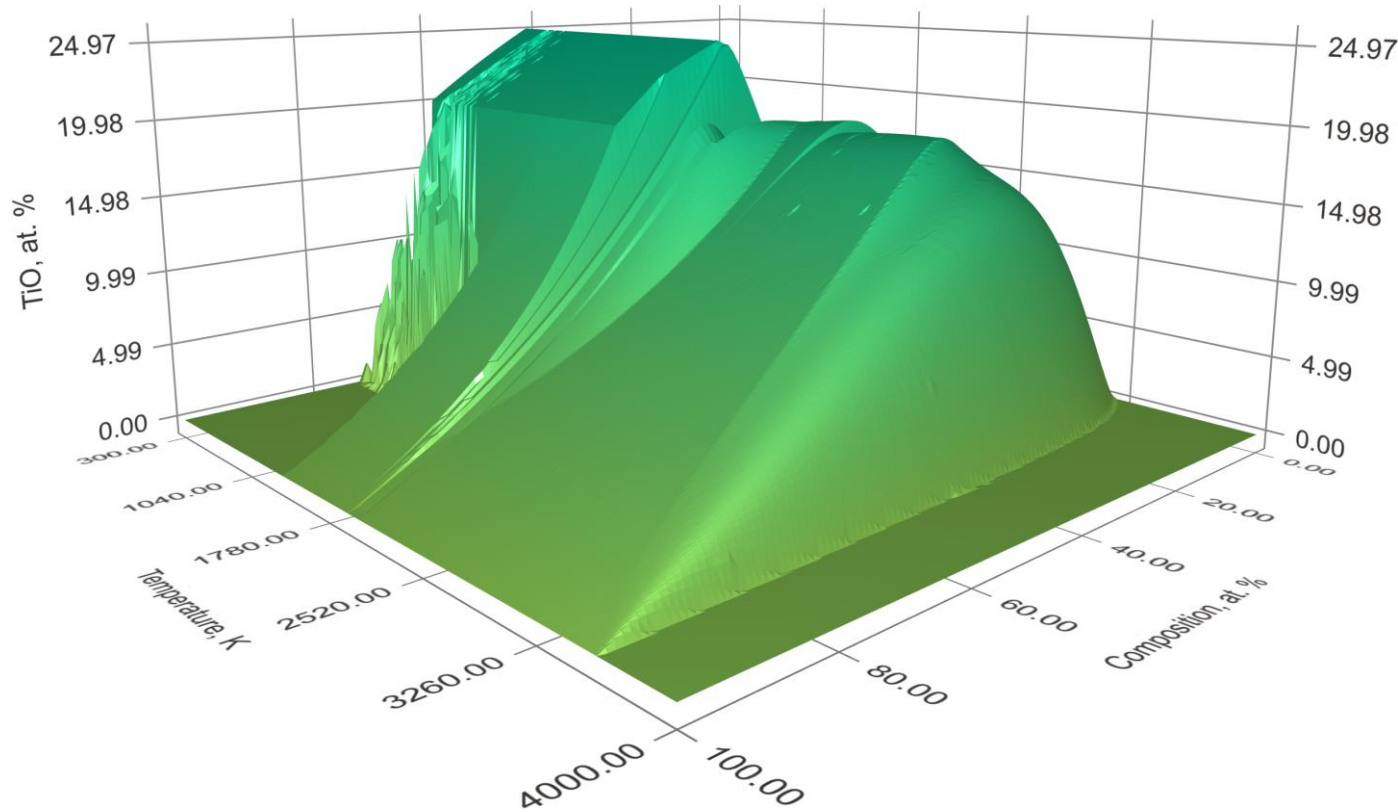




ATC - Adiabatic Temperature Calculator



ATC is a high quality, visual, open source tool for thermodynamic calculations and visualization of phase diagrams.

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ATC - Adiabatic Temperature Calculator

<https://github.com/alexonemore/atc>

The ATC program allows you to calculate the equilibrium composition and adiabatic temperature of the system consisting of the specified components.

To determine the equilibrium, the Gibbs energy of the system is minimized.

To determine the adiabatic temperature, a search is performed for the temperature at which the enthalpy of the equilibrium system is equal to the enthalpy of the initial system.

The program allows you to perform calculations in 4 modes:

1. For one point of initial values
2. Varying the initial temperature of the system in a given range
3. Varying the composition of the system in a given range
4. Varying both the initial temperature and the composition of the system simultaneously

The program uses two different databases of thermodynamic quantities:

1. The original database from Thermo program containing 3017 substances.
2. The database from the HSC program containing 9074 substances excluding ions and complex organics (28477 substances in total).

For example, you can plot the dependence of the adiabatic temperature of the mixture depending on the initial temperature or on the content of any component or group of components in it.

You can plot a graph in the form of a heat map or in 3D for a pseudo-binary phase diagram, while there will be a separate graph for each component.

Workmode	Target	
	Equilibrium	Adiabatic temperature
Single point		
Temperature range		
Composition range		
Temperature – composition range		



The problem of determining the **equilibrium composition** of the system at the temperature T is reduced to minimizing the following function

$$G = \sum_i^N n_i \left(G_i + RT \ln \left(\frac{n_i}{\sum_i^N n_i} \right) \right) + \sum_i^L n_i \left(G_i + RT \ln \left(\frac{n_i}{\sum_i^L n_i} \right) \right) + \sum_i^K n_i G_i$$

with J constraints

$$\sum_i^N a_{ji} n_i + \sum_i^L a_{ji} n_i + \sum_i^K a_{ji} n_i = b_j$$

where

b_j - amount of element j in the system,

J - number of elements in the system,

N - number of gases in the system,

L - number of liquids in the system,

K - number of individual condensed substances in the system,

n_i - amount of the substance i in the system,

G_i - Gibbs energy of the substance i in the system,

a_{ji} - amount of element j in the substance i .

To minimize the Gibbs energy function, the following methods are used:

- Augmented Lagrangian method
- Sequential Quadratic Programming



Liquid solution

You can choose whether to take into account the presence of liquid solutions.

If a *liquid solution* is selected - *one*, then the minimization of the Gibbs energy according to the above formula.

If selected - *no*, then according to the following formula:

$$G = \sum_i^N n_i \left(G_i + RT \ln \left(\frac{n_i}{\sum_i^N n_i} \right) \right) + \underbrace{\sum_i^L n_i G_i}_{\text{Liquids}} + \sum_i^K n_i G_i$$

Workmode

Single point

Target

Adiabatic temperature

Liquid solution

One

H initial by

As checked

Database

HSC

Minimization function

Gibbs energy

Extrapolation

Enable

Ranges

Composition

Temperature

Pressure

Start

0

300

0.1

Stop

100

1000

1

Step

10

10

0.1

Units

at. %

K

MPa

Liquids



ATC - Adiabatic Temperature Calculator

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Adiabatic temperature of the system with given initial temperature. In this case, a search is performed for the temperature at which the enthalpy of the equilibrium system is equal to the enthalpy of the initial given system in temperature diapason from 298.15 to 10000 K. The initial enthalpy of the system is calculated either in accordance with a given composition (as checked), or with a choice of substances having a lower Gibbs energy value with the same composition (by minimum Gibbs energy). This is set in the H field. For example, if the initial temperature of the system is 500 K and 1 mol of H₂O(l) is set, then "*as checked*" literally means 1 mol of liquid water at 500 K, and "*by minimum Gibbs energy*" means that H₂O(g) will be automatically selected instead of H₂O(l). As a result of the calculation, you will also get the composition of the equilibrium system at adiabatic temperature.

Workmode

Single point

Target

Adiabatic temperature

Liquid solution

One

H initial by

As checked

Database

HSC

Minimization function

Gibbs energy

Extrapolation

Enable

Ranges

Composition

Temperature

Pressure

Start

0

300

0.1

Stop

100

1000

1

Step

10

10

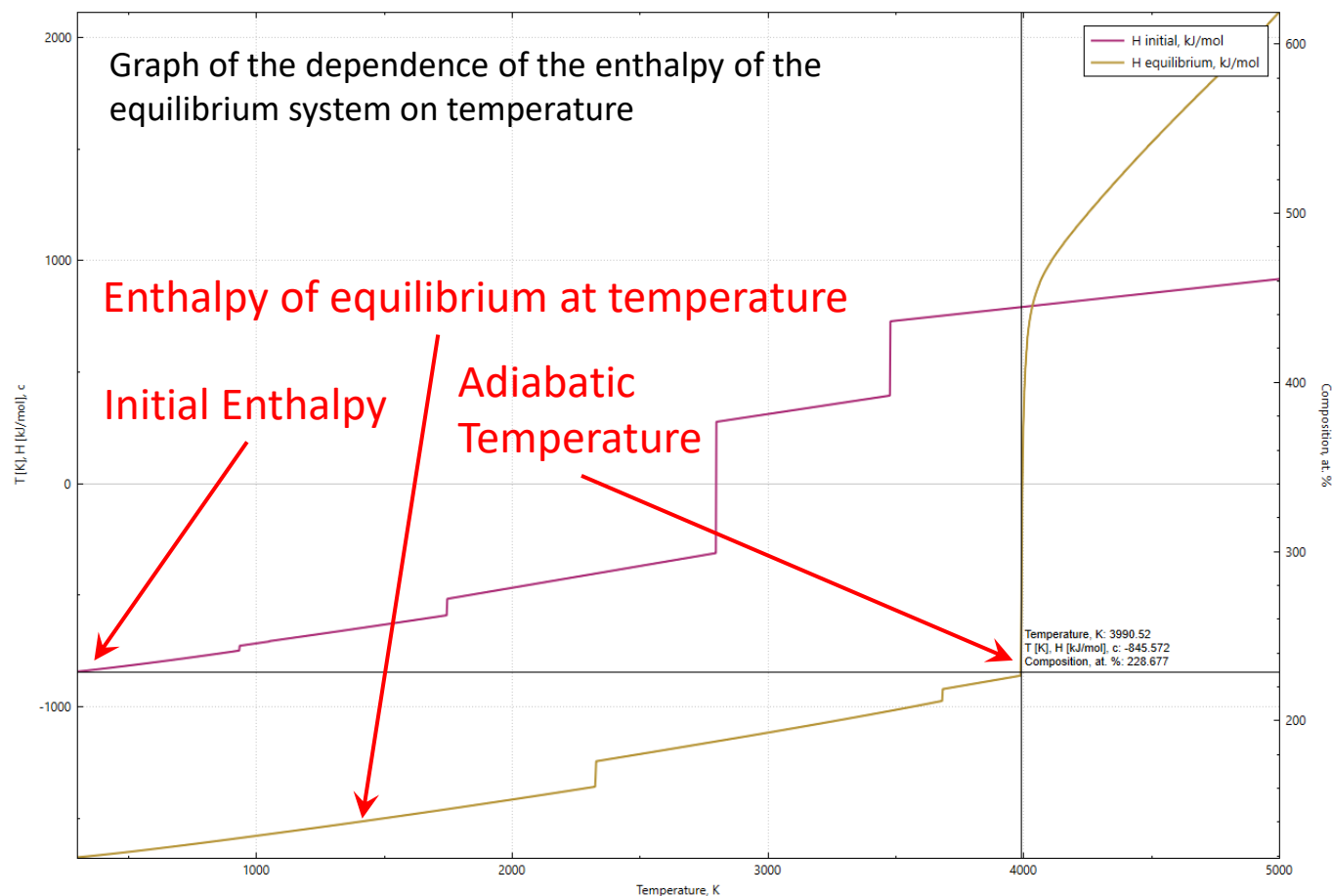
0.1

Units

at. %

K

MPa





When **extrapolation** is disabled, substances exist only within their ranges

Workmode
Single point

Target
Adiabatic temperature

Liquid solution
One

H initial by
As checked

Database
HSC

Minimization function
Gibbs energy

Extrapolation
Disable

Ranges Composition Temperature Pressure

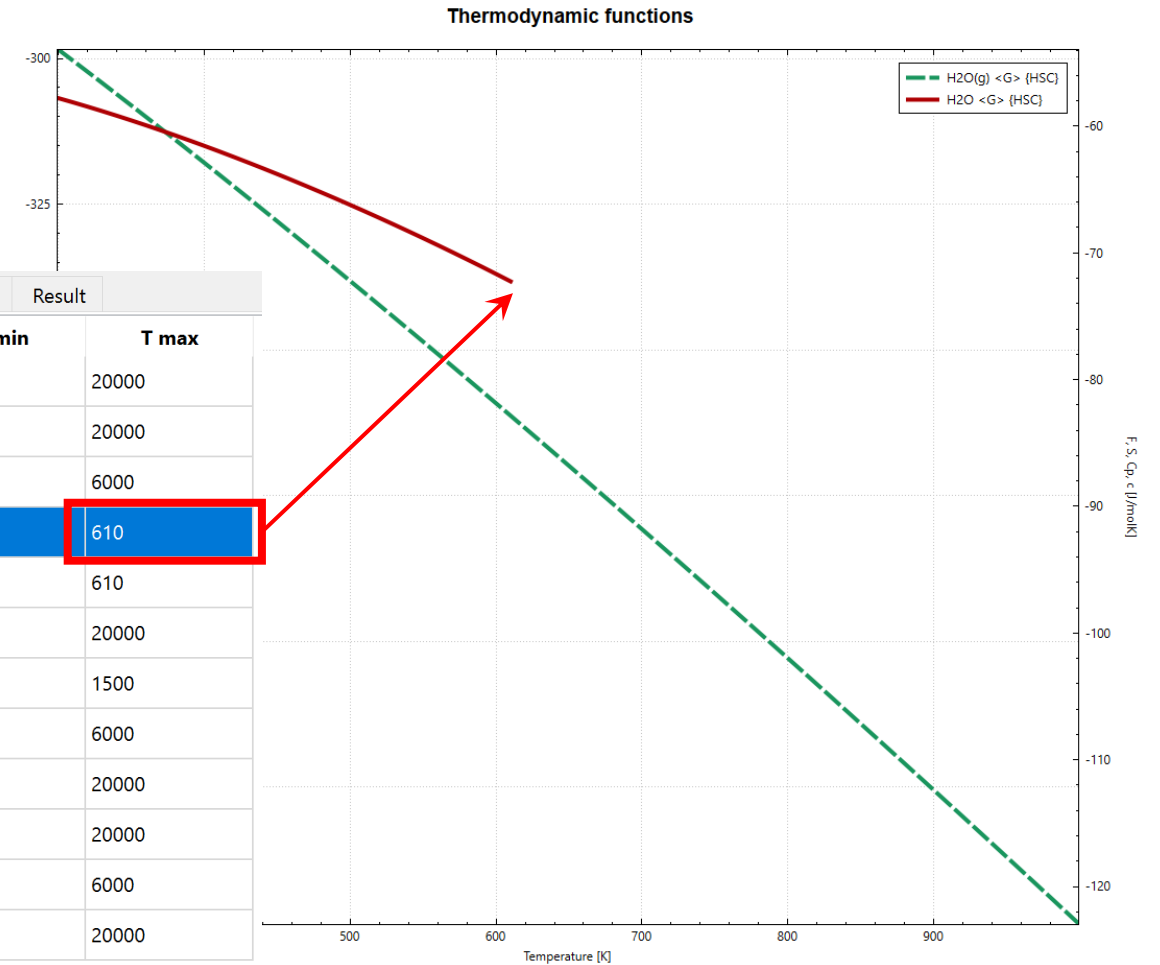
Start 0 300 0.1

Stop 100 1000 1

Step 10 10 0.1

Units at. % K MPa

Substances	Thermodynamic functions	Amounts	Result Table	Result
Formula	Name	Weight	T min	T max
H(g)	Hydrogen (Hydrogen; ...	1.00794	100	20000
H2(g)	Hydrogen (Hydrogen; ...	2.01588	50	20000
HO2(g)	Hydrogen superoxide; ...	33.0067	298.15	6000
H2O	Hydrogen oxide (Water)	18.0153	3.00001	610
H2O(l)	Hydrogen oxide (Water)	18.0153	273.151	610
H2O(g)	Hydrogen oxide (Water)	18.0153	298.15	20000
H2O2(l)	Hydrogen peroxide	34.0147	298.15	1500
H2O2(g)	Hydrogen peroxide	34.0147	25	6000
O(g)	Oxygen (Oxygen; atomic)	15.9994	50	20000
O2(g)	Oxygen	31.9988	100	20000
O3(g)	Ozone (Trioxxygen)	47.9982	50	6000
OH(g)	Hydroxyl radical	17.0073	298.15	20000





ATC - Adiabatic Temperature Calculator

<https://github.com/alexonemore/atc>

ATC program is equipped with two databases **Thermo** and **HSC**. Both are in sqlite3 format.

Thermo database. Thermodynamic data are taken from the old program [Thermo](#). Most of the data in this database are taken from [Glu]. Temperature dependencies in Thermo database presented by the Free Enthalpy Function FEF.

$$F^{\circ}(T) \left[\frac{J}{mol \cdot K} \right] = \varphi_1 + \varphi_2 \ln x + \varphi_3 x^{-2} + \varphi_4 x^{-1} + \varphi_5 x + \varphi_6 x^2 + \varphi_7 x^3$$

$$S^{\circ}(T) \left[\frac{J}{mol \cdot K} \right] = \varphi_1 + \varphi_2 (1 + \ln x) - \varphi_3 x^{-2} + 2\varphi_5 x + 3\varphi_6 x^2 + 4\varphi_7 x^3$$

$$H^{\circ}(T) \left[\frac{J}{mol} \right] = H^{\circ}(0) + 10 \cdot (\varphi_2 x - 2\varphi_3 x^{-1} - \varphi_4 + \varphi_5 x^2 + 2\varphi_6 x^3 + 3\varphi_7 x^4)$$

$$C_p(T) \left[\frac{J}{mol \cdot K} \right] = \varphi_2 + 2\varphi_3 x^{-2} + 2\varphi_5 x + 6\varphi_6 x^2 + 12\varphi_7 x^3$$

$$G^{\circ}(T) \left[\frac{kJ}{mol} \right] = H^{\circ}(0) - T \cdot F^{\circ}(T) \left[\frac{J}{mol \cdot K} \right] \cdot 10^{-3}$$

where $x = T[K] \cdot 10^{-4}$.



HSC database. HSC database are made by program [HSCtoSQL \(HSC to SQLite database converter\)](#). Temperature dependencies in HSC database presented by the Heat capacity function C_p . Thermodynamic functions can be calculated using the following formulas. At standard state.

$$C_p(T) = A + BT \cdot 10^{-3} + CT^{-2} \cdot 10^5 + DT^2 \cdot 10^{-6} + ET^{-3} \cdot 10^8 + FT^3 \cdot 10^{-9}$$

$$\frac{C_p(T)}{T} = A \cdot T^{-1} + 10^{-3} \cdot B + 10^5 \cdot C \cdot T^{-3} + 10^{-6} \cdot D \cdot T + 10^8 \cdot E \cdot T^{-4} + 10^{-9} \cdot F \cdot T^2$$

$$\int C_p(T) dT = A \cdot T + 2 \cdot 10^{-3} \cdot B \cdot T^2 - 10^5 \cdot C \cdot T^{-1} + \frac{1}{3} \cdot 10^{-6} \cdot D \cdot T^3 - 5 \cdot 10^7 \cdot E \cdot T^{-2} + 2.5 \cdot 10^{-10} \cdot F \cdot T^4$$

$$\int \frac{C_p(T)}{T} dT = A \cdot \ln T + 10^{-3} \cdot B \cdot T - 5 \cdot 10^4 \cdot C \cdot T^{-2} + 5 \cdot 10^{-7} \cdot D \cdot T^2 - \frac{1}{3} \cdot 10^8 \cdot E \cdot T^{-3} + \frac{1}{3} \cdot 10^{-9} \cdot F \cdot T^3$$

$$H^\circ(T) = H^\circ(298.15) + \int_{298.15}^{T_1} C_{p1}(T) dT + \Delta H_1 + \int_{T_1}^{T_2} C_{p2}(T) dT + \Delta H_2 + \dots$$

$$S^\circ(T) = S^\circ(298.15) + \int_{298.15}^{T_1} \frac{C_{p1}(T)}{T} dT + \frac{\Delta H_1}{T_1} + \int_{T_1}^{T_2} \frac{C_{p2}(T)}{T} dT + \frac{\Delta H_2}{T_2} + \dots$$

$$G^\circ(T) = H^\circ(T) - TS^\circ(T)$$

$$G^\circ(T) = H^\circ(0) - TF^\circ(T)$$



Workmode: Single point

The system consists of two parts: the main (green column) and variable (red column). You can set the composition separately for each of them in moles or grams, as well as for the sum values. You can exclude a substances from the calculation by unchecking the *Included* column. In the workmodes *Single point* and *Temperature range*, the calculation is for the total system (*Sum column*). Initial temperature takes from field *Temperature initial*.

Workmode

Single point

Target

Adiabatic temperature

H initial by

As checked

Minimization function

Gibbs energy

AT accuracy

1

Threads

12

Temperature initial

300

K

Pressure initial

0.1

MPa

Clear

Update

Calculate

Liquid solution

One

Database

HSC

Extrapolation

Disable

Show phases

☒ Gas
☒ Liquid
☒ Solid
☐ Aqueous
☐ Ions

Ranges

Composition

Temperature

Pressure

Start

0

300

0.1

Stop

100

1000

1

Step

10

10

0.1

Units

at. %

K

MPa

Substances	Thermodynamic functions	Amounts	Result Table	Result						
Formula	Weight	Main mol	Main gram	Variable mol	Variable gram	Sum mol	Sum gram	Sum at.%	Sum wt.%	Included
Sum		2	85.6749	2	74.8485	4	160.523	100	100	18 of 20
Al	26.9815	1	26.9815	1	26.9815	2	53.9631	50	33.6169	<input checked="" type="checkbox"/> +
Al(l)	26.9815									<input type="checkbox"/> -
Al(g)	26.9815									<input checked="" type="checkbox"/> +
Al2(g)	53.9631									<input checked="" type="checkbox"/> +
AlNi3	203.062									<input checked="" type="checkbox"/> +
Al3Ni	139.638									<input checked="" type="checkbox"/> +
Al3Ni2	198.331									<input checked="" type="checkbox"/> +
AlTi	74.8485									<input checked="" type="checkbox"/> +
Al3Ti	128.812									<input checked="" type="checkbox"/> +
Ni	58.6934	1	58.6934			1	58.6934	25	36.5637	<input checked="" type="checkbox"/> +
Ni(l)	58.6934									<input type="checkbox"/> -
Ni(g)	58.6934									<input checked="" type="checkbox"/> +
Ni2(g)	117.387									<input checked="" type="checkbox"/> +
NiAl	85.6749									<input checked="" type="checkbox"/> +
NiTi	106.56									<input checked="" type="checkbox"/> +
NiTi2	154.427									<input checked="" type="checkbox"/> +
Ni3Ti	223.947									<input checked="" type="checkbox"/> +
Ti	47.867			1	47.867	1	47.867	25	29.8193	<input checked="" type="checkbox"/> +
Ti(g)	47.867									<input checked="" type="checkbox"/> +
Ti2(g)	95.734									<input checked="" type="checkbox"/> +



Workmode: Temperature range

Same as in Single point workmode the composition of the system takes from *Sum columns*. The initial temperatures varies from *Start* to *Stop* by *Step*, the values takes from *Ranges Temperature* fields.

Workmode	Target	
	Equilibrium	Adiabatic temperature
Single point		
Temperature range	✓	✓
Composition range		
Temperature – composition range		

Substances	Thermodynamic functions	Amounts	Result Table	Result						
Formula	Weight	Main mol	Main gram	Variable mol	Variable gram	Sum mol	Sum gram	Sum at.%	Sum wt.%	Included
Sum		2	85.6749	2	74.8485	4	160.523	100	100	18 of 20
Al	26.9815	1	26.9815	1	26.9815	2	53.9631	50	33.6169	<input checked="" type="checkbox"/> +
Al(l)	26.9815									<input type="checkbox"/> -
Al(g)	26.9815									

Workmode

Temperature range

Target

Adiabatic temperature

Liquid solution

One

H initial by

As checked

Database

HSC

Minimization function

Gibbs energy

Extrapolation

Disable

Ranges

Composition

Temperature

Pressure

Start

0

300

0.1

Stop

100

1000

1

Step

10

10

0.1

Units

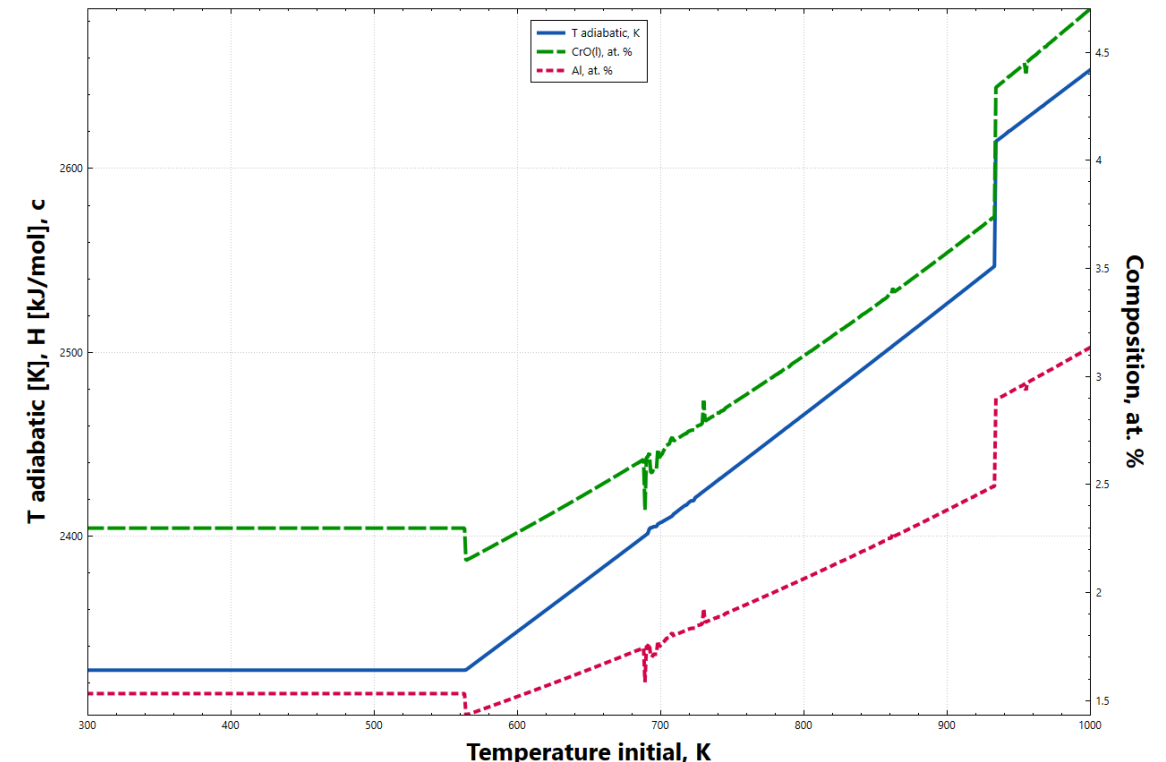
at. %

K

MPa

When you calculate in *Temperature range workmode*, you can plot graphs.

- If you calculate *Adiabatic temperature Target* you can plot the dependence of the adiabatic temperature on the initial temperature and the composition of the equilibrium system at the adiabatic temperature.
- If you calculate *Equilibrium Target* you can plot the dependence of the composition of the equilibrium system on the initial temperature.





Workmode	Target	
	Equilibrium	Adiabatic temperature
Single point		
Temperature range		
Composition range	✓	✓
Temperature – composition range		

Workmode: Composition range

In *Composition range workmode* you can vary the composition of the *Variable* part of the system, which is set in the red column. The values that are taken from the *Composition range* fields (*Start*, *Stop*, *Step*) set the *Sum* of the *Variable* part of the system. The initial temperature takes from the field *Temperature initial*. In *Composition range workmode*, you can plot the dependence of various parameters on the composition of the initial system.

You can get the initial composition of the system for each iteration by checking *Show Initial Composition in the Result Table* checkbox and then clicking *Update* button.

Workmode
Composition range

AT accuracy
1

Threads
12

target
Adiabatic temperature

Liquid solution
One

H initial by
As checked

Database
HSC

Minimization function
Gibbs energy

Extrapolation
Enable

Temperature initial
300 K

Pressure initial
0.1 MPa

Ranges
Composition
Start 0 Stop 100 Step 10 Units at. %

Temperature
300 1000 10 K

Pressure
0.1 MPa

Show phases
☒ Gas
☒ Liquid
☒ Solid
☐ Aqueous
☐ Ions

Clear
Update
Calculate

Result settings
☐ Show Initial Composition in the Result Table

Show Result in units
K at. %

Substances	Thermodynamic functions	Amounts	Result Table	Result						
Formula	Weight	Main mol	Main gram	Variable mol	Variable gram	Sum mol	Sum gram	Sum at.%	Sum wt.%	Included
Sum		1	26.9815	1	58.6934	2	85.6749	100	100	10 of 12
Al	26.9815	1	26.9815			1	26.9815	50	31.4929	<input checked="" type="checkbox"/> +
Al(l)	26.9815									<input type="checkbox"/> -
Al(g)	26.9815									<input checked="" type="checkbox"/> +
Al2(g)	53.9631									<input checked="" type="checkbox"/> +
AlNi3	203.062									<input checked="" type="checkbox"/> +
Al3Ni	139.638									<input checked="" type="checkbox"/> +
Al3Ni2	198.331									<input checked="" type="checkbox"/> +
Ni	58.6934			1	58.6934	1	58.6934	50	68.5071	<input checked="" type="checkbox"/> +
Ni(l)	58.6934									<input type="checkbox"/> -
Ni(g)	58.6934									<input checked="" type="checkbox"/> +
Ni2(g)	117.387									<input checked="" type="checkbox"/> +
NiAl	85.6749									<input checked="" type="checkbox"/> +



Workmode	Target	
	Equilibrium	Adiabatic temperature
Single point		
Temperature range		
Composition range		
Temperature – composition range	✓	✓

Workmode: Temperature - Composition range

Temperature - Composition range workmode is actually a mode of constructing pseudo-binary phase diagrams. In this workmode the initial temperature and the initial composition of the system change simultaneously. When you choose *Equilibrium Target* you get the composition of the equilibrium system at the initial temperatures as in conventional phase diagrams. When you choose *Adiabatic Temperature Target* you get the adiabatic temperature and equilibrium composition of the system at the adiabatic temperature. Unlike conventional phase diagrams, the ATC program displays the composition of each substance of the system separately on the *HeatMap* and on the *3DView*.

Workmode
Temperature-composition range

Target
Equilibrium

Liquid solution
One

H initial by
By minimum Gibbs energy

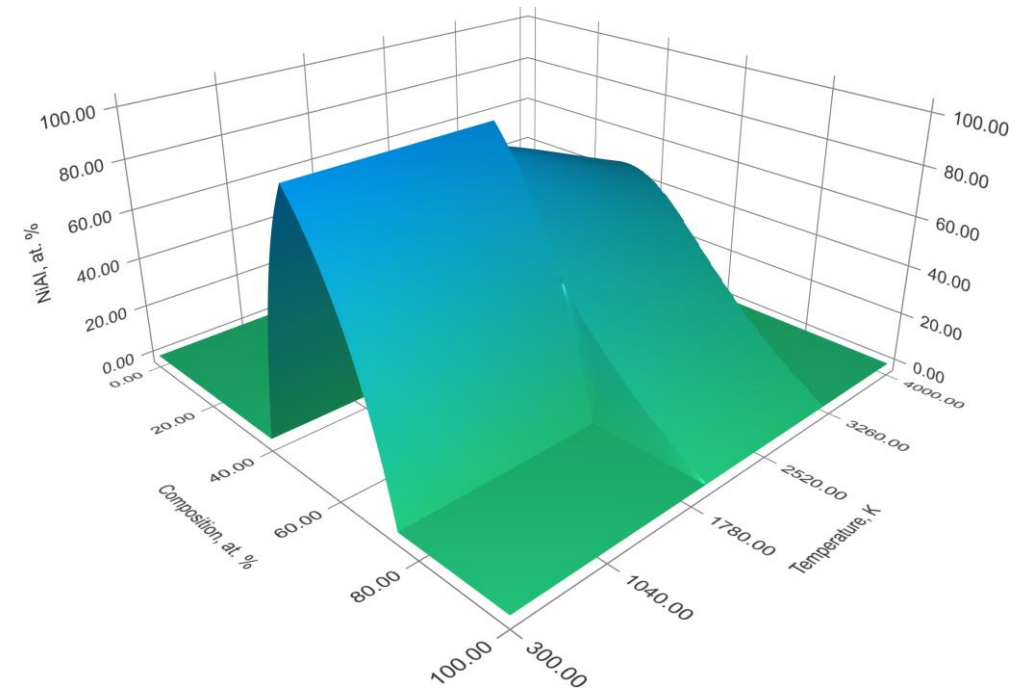
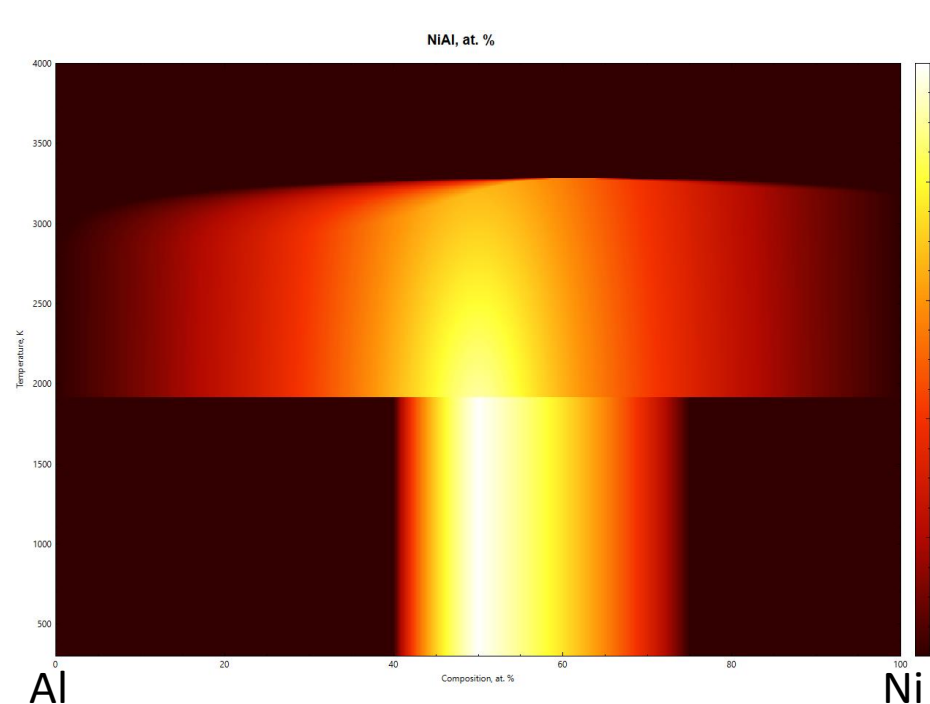
Database
HSC

Minimization function
Gibbs energy

Extrapolation
Enable

Ranges
Composition Temperature Pressure
Start 0 300 0.1
Stop 100 4000 1
Step 0.1 10 0.1
Units at. % K MPa

For example, composition of the NiAl in the Al-Ni system





ATC - Adiabatic Temperature Calculator

<https://github.com/alexonemore/atc>

Workmode	
Composition range	
Target	Liquid solution
Adiabatic temperature	One
H initial by	Database
As checked	HSC
Minimization function	Extrapolation
Gibbs energy	Enable

AT accuracy	Threads
1	12
Temperature initial	
300	K
Pressure initial	
0.1	MPa

In the *AT accuracy* field, you can specify the number of decimal places when calculating the adiabatic temperature.

In the *Threads* field, you can specify the number of processor threads used in the calculation. With long-term calculations, you can reduce the number of threads used to free up computer resources for other purposes or to reduce computer heating.

It is recommended to exclude from the calculation those substances that can be duplicated in any temperature range

[illegible]