



# PHASE EQUILIBRIA WITH ELEMENTS OF CHEMICAL THERMODYNAMICS

## Basic definitions

**Phenomenological thermodynamics** is a branch of science dealing with macroscopic properties and phenomena without going into molecular (atomic) translation.

**The system** is a part of nature (space), whose properties or phenomena occurring in it are examined.

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International interdisciplinary PhD Studies in Materials Science with English as the language of instruction

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**The surroundings** is the part of nature (space) out of the system.

**The phase** is a part of the system with clear boundaries (separated from the rest by clear boundaries), in which one equation of state applies (applies).

Within the phase, macroscopic physical and chemical properties may change continuously, and at the phase boundaries, at least some of the physical and chemical macroscopic properties change discontinuously.



The phases due to their physical and chemical properties can be:

- a) homogeneous
- b) non-homogeneous

**The homogeneous phase** is one whose macroscopic physical and chemical properties are identical at its different locations.

**Non-homogeneous phase** is such that the macroscopic physical and chemical properties are different in the different places.

**Division of systems or phases due to the number of components:**

- a) one component systems (phase)
- b) multicomponent systems (phase)



## **Division of systems due to the number of phases:**

a) one phase (homogeneous) systems (one or multi-component)

b) multi-phase (heterogeneous) systems (one or multi-component)





## **Equilibrium due to some process**

One can say that the system is in equilibrium due to any process when this process does not go and it can not go.

Equilibrium in relation to some process, it is a state in which this process does not take place and can not take place.

The system or phase is in a state of equilibrium in relation to certain processes, if it is in a state in which neither of these processes takes place nor can occur.

If in given circumstances no process takes place and can not occur, then we say, that the phase or system is in a state of equilibrium.



## **State parameters.**

The quantities whose knowledge is necessary and sufficient to determine the state of the phase are called state parameters.

We say that the state of the system is determined when the state parameters of all phases of the system are known.

Demarcation (cover, boundary)

- a) diathermic
- b) adiabatic



**The adiabatic demarcation (cover, boundary, separation) of the system from the environment is one that, despite the changes outside the system, does not change the volume of the system.**

This means that no mechanical work has been done on the system or via the system.

**Diathermy (diathermic) demarcation** is characterized by the following property:

if phase 1 is in equilibrium with phase 2 and with phase 3, then phase 2 is in equilibrium with phase 3.



If the system is surrounded by an adiabatic boundary (demarcation, cover), then whatever changes (processes) it experiences, we will call, by definition, transformations (transition) or adiabatic processes.

By definition, the adiabatic cover (delimitation) of the system shows that with any non-adiabatic shields, changes outside the system cause, as a rule, changes in the system state, and thus the state of the system depends on the state outside the system.

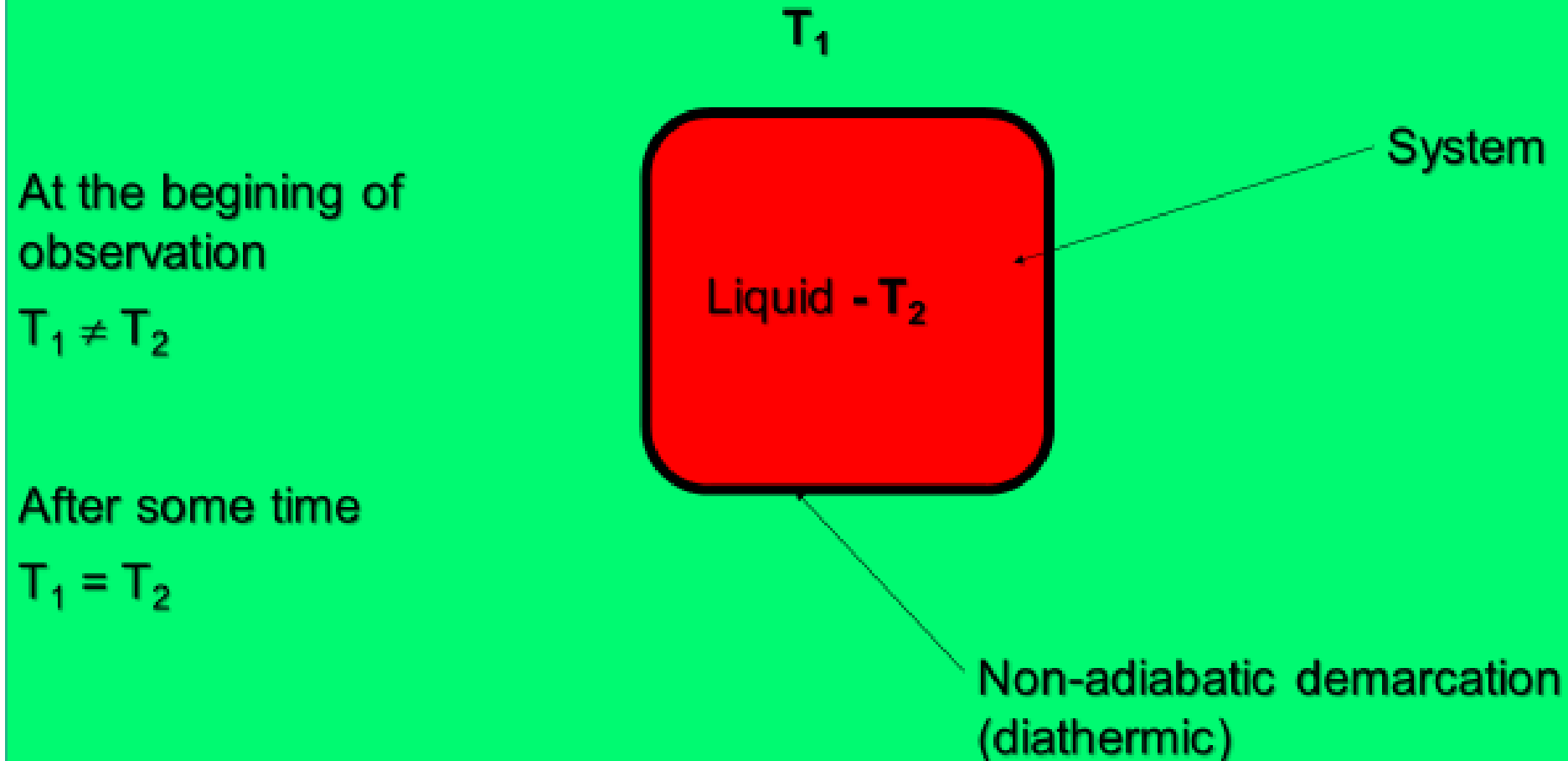
It follows that if two phases of the boundary system (separated) are from each other a adiabatic border (cover, demarcation), then the equilibrium in the first phase is completely independent of the equilibrium in the second phase.



# Examples

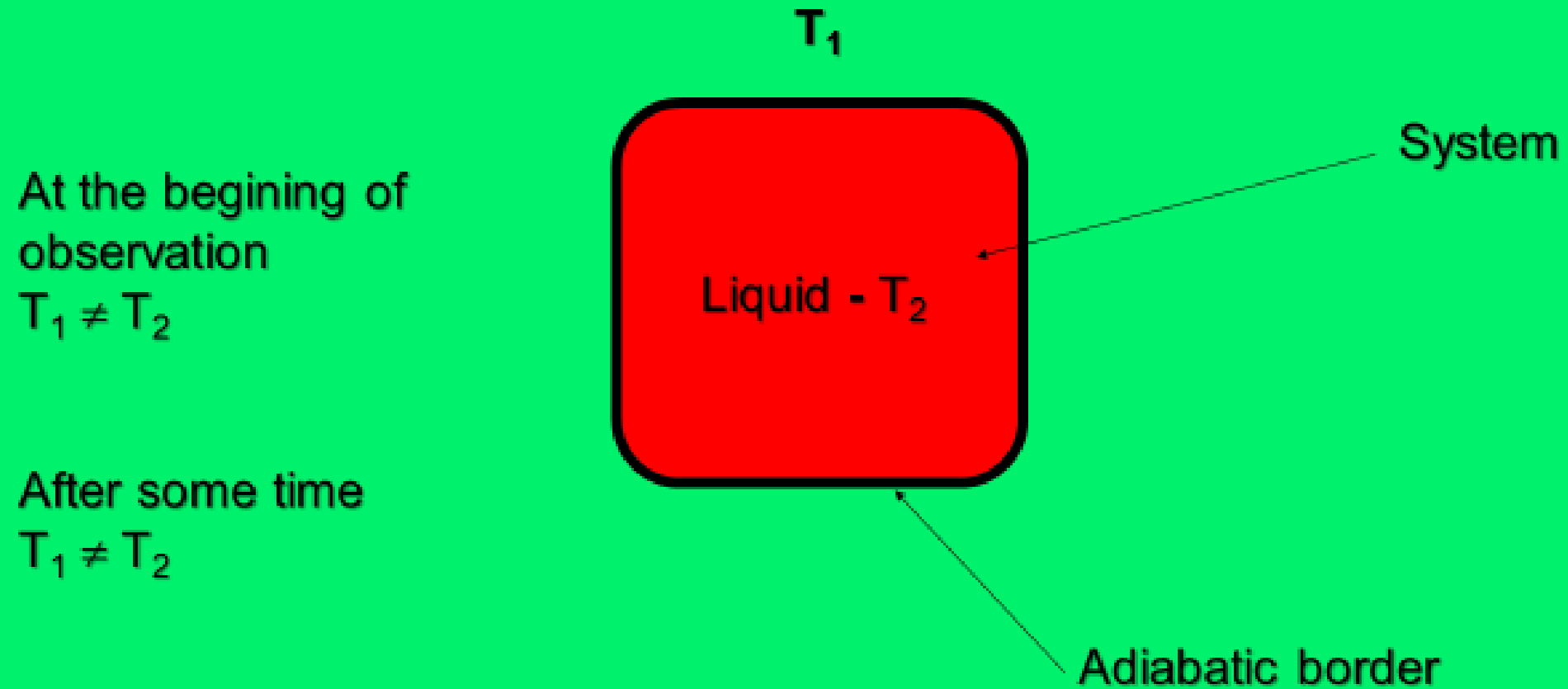


Surroundings (air, liquid) of temperature =  $T_1$





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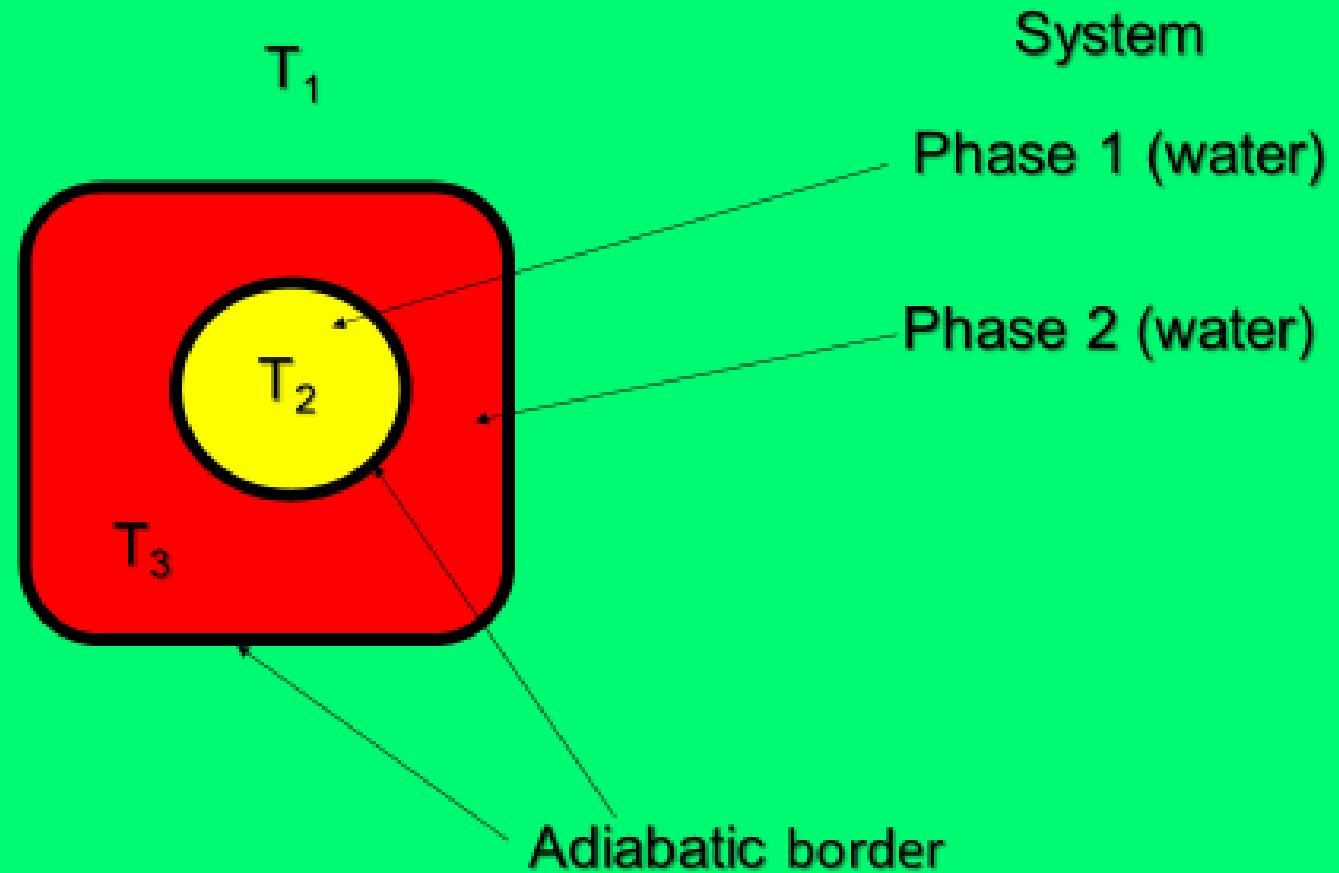




Surroundings (air, liquid) of temperature =  $T_1$

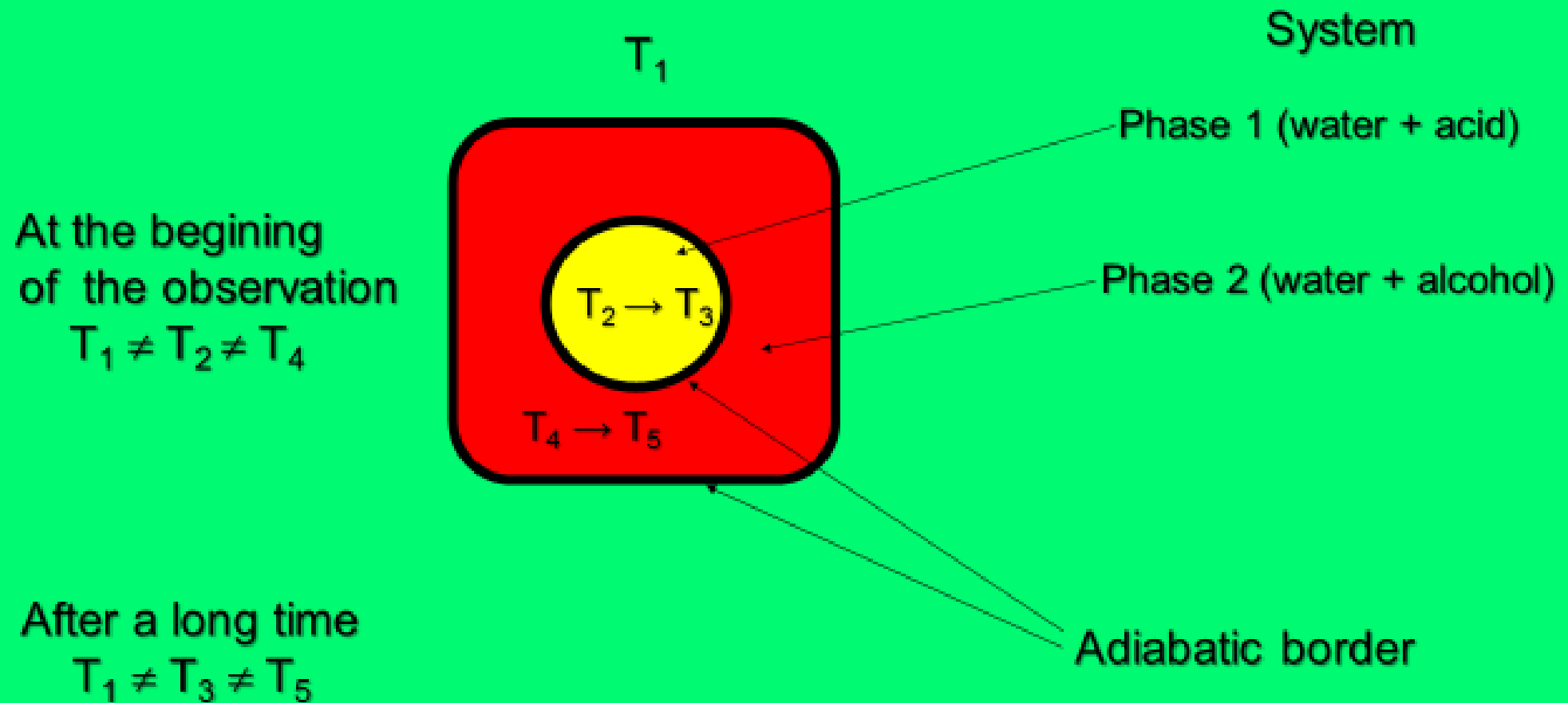
At the beginning  
of the observation  
 $T_1 \neq T_2 \neq T_3$

After a long time  
 $T_1 \neq T_2 \neq T_3$



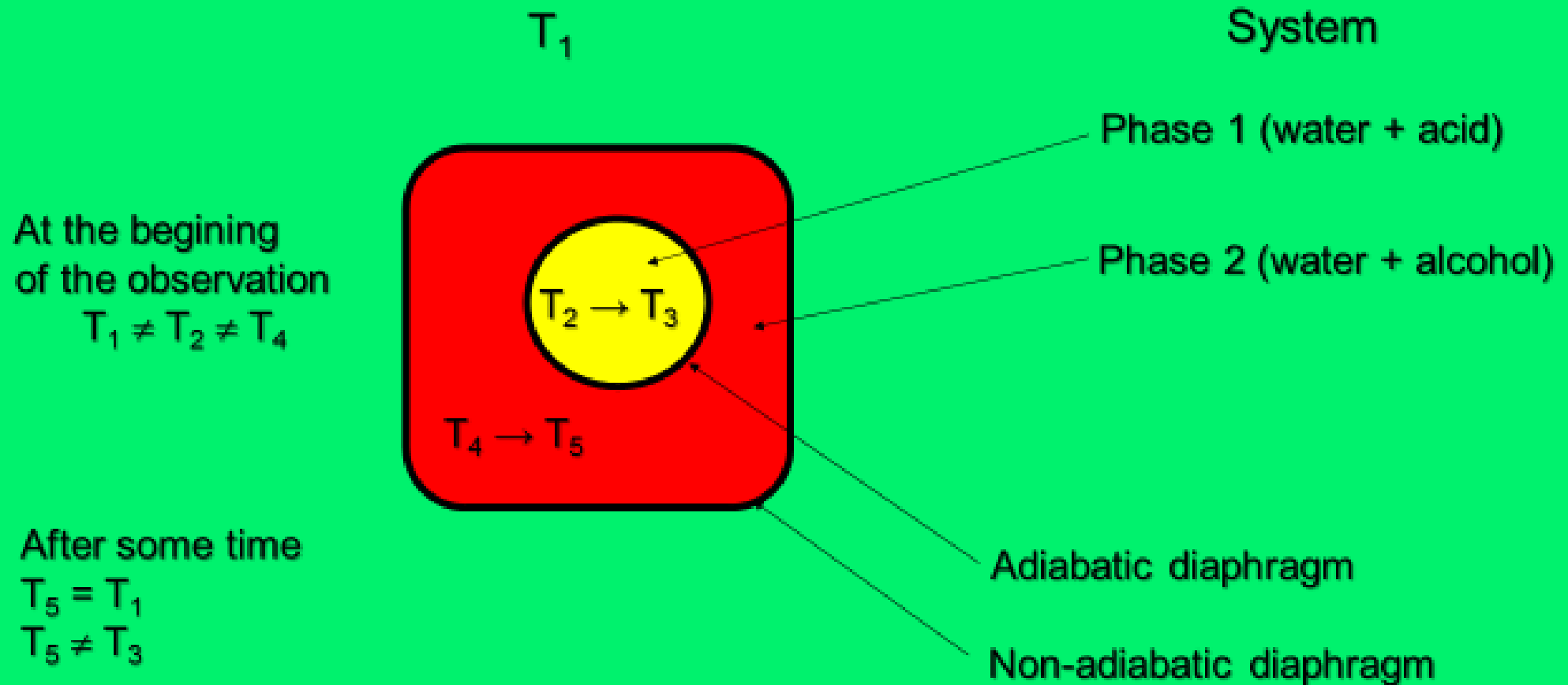


Surroundings (air, liquid) of temperature =  $T_1$





## Surroundings of temperature $T_1$ (air, liquid, solid)





In the case of non-adiabatic phase separation, the equilibrium state of one phase can not be adjacent to any equilibrium state of the second phase. It follows that the equilibrium states of the two phases are dependent on each other, and the nature of this relationship results from the nature of the boundary between the phases.

Therefore, for each non-adiabatic phase boundary, the state parameters of both phases denoted  $X_1, X_2, X_3 \dots$  and  $Y_1, Y_2, Y_3 \dots$  have to meet a certain condition of the following form:

$$F(X_1, X_2, X_3, \dots, Y_1, Y_2, Y_3, \dots) = 0$$

This condition results from the nature of a given boundary and is characteristic for it.



In a system with non-adiabatic boundaries, the system state parameters must meet in equilibrium a series of equations of the above type.

Thus, the number of independent parameters will be equal to the difference between the number of all state parameters and the number of these equations.

Independent state parameters are called independent variables of the system, because their set defines the state of the system in equilibrium.

Thus, each equilibrium state of the system can be presented as a point in the  $n$ -dimensional space, i.e. in the space of  $n$  independent variables ( $n$  independent state parameters).



Consider three phases (1, 2, 3) in a given system, which are separated by the diathermic border.

Based on the definition of diathermic boundary if it is known that: phase 1 is in equilibrium with phase 2 and phase 1 is in equilibrium with phase 3 then always the phase 2 is in equilibrium with the phase 3.

Mathematically it means that the following equations must be met:

$$F_1(X_1, X_2, X_3, \dots, Y_1, Y_2, Y_3, \dots) = 0 \quad \textit{phase 1 in equilibrium with phase 2}$$

$$F_1(X_1, X_2, X_3, \dots, Y_1, Y_2, Y_3, \dots) = 0 \quad \textit{phase 1 in equilibrium with phase 2}$$

then also the following equation must be met:

$$F_3(Y_1, Y_2, Y_3, \dots, Z_1, Z_2, Z_3, \dots) = 0 \quad \textit{phase 1 in equilibrium with phase 3}$$



It is known from mathematics that such relations are possible only if the above 3 equations are equivalent to the following equations:

$$F_1(X_1, X_2, X_3, \dots) = F_2(Y_1, Y_2, Y_3, \dots) = F_3(Z_1, Z_2, Z_3, \dots) = t$$

where:  $T$  is the value of  $F_1, F_2, F_3$  functions, the same for all phases, which are diathermic separated and in the equilibrium.

From the definitione each of the equation;

$$F_1(X_1, X_2, X_3, \dots) = T; \quad F_2(Y_1, Y_2, Y_3, \dots) = T; \quad F_3(Z_1, Z_2, Z_3, \dots) = T$$

the state equation is called and  $T$  is the temperature of phase.





If in a given system, independent variables are:

for the phase 1;  $X_1, X_2, X_3$

for the phase 2;  $Y_1, Y_2, Y_3$

for the phase 3;  $Z_1, Z_2, Z_3$

and these phases are diathermic separated and in equilibrium, then one can eliminate for each phase, one variable using the state equation and replace it with the common variable  $T$ . Then in the system analyzed the independent variables are as follows:

$T, X_2, X_3, \dots,$        $T, Y_2, Y_3, \dots,$        $T, Z_2, Z_3$



## Quasi-static processes

Processes in which the temperature and external forces are infinitesimally different from the temperature and system's own power, we define as the quasi-static processes.

Transformations in which only the condition of equality of forces will be fulfilled are called mechanically quasi-static processes.

The quasi-static processes are particularly useful in theoretical considerations, and their significance is:

- 1) the value of work results from their own forces and is therefore bound with the phase state of
- 2) the ambient temperature is equal to the temperature of the system.

In the case of the quasi-static process, the work is denoted as  $DW$  to distinguish from the elementary work, designated  $W_{el}$ .



# Elementary work

The elementary work is expressed as follows:

$$W_{el} = L_1 dL_1 + L_2 dL_2 + L_3 dL_3 + \dots$$

Where:  $L_1, L_2, L_3, \dots$  forces resulting from the state of the system.

The expression for work in the quasi-static process has a specific mathematical character and depends on the state of the phase.

In the case of nonquasi-static process (transformation), the expression for work is not mathematical and can take any value.



# Volume elementary work

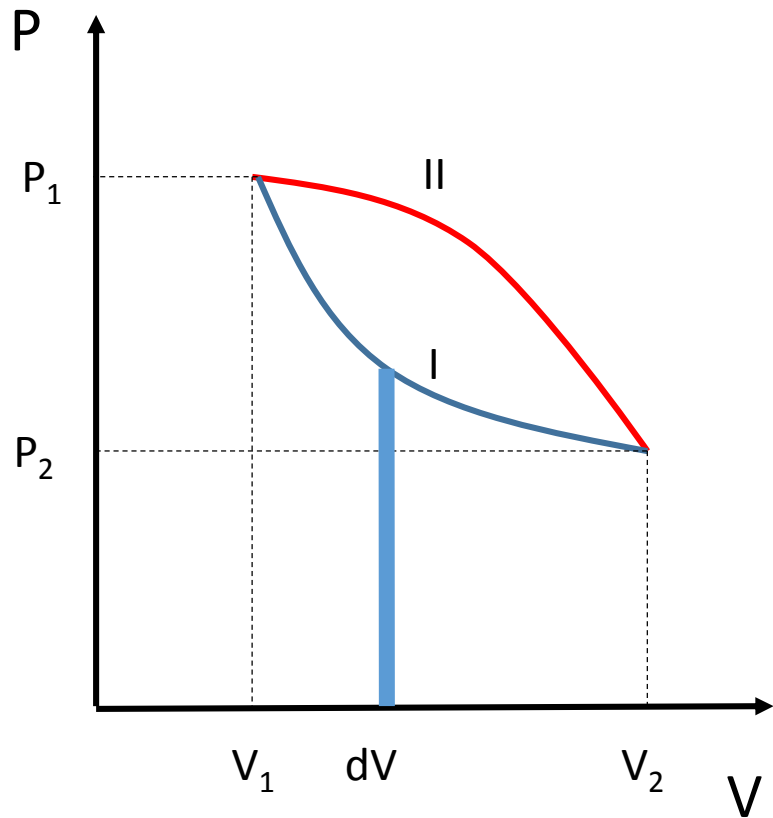
Elemental volume work is associated with a change in the volume of the medium (fluid, gas, solid) and is given by:

$$W_{el} = -pdV$$

Where: **p** is the pressure acting on the fluid during the change in volume by **dV**.

In the case of elementary quasi-static work, the volume work is equal to:

$$DW = -pdV$$



$$W_{el} = PdV$$

$$W_{el(I)} = \int_1^2 PdV$$

$$W_{el(II)} = \int_1^2 PdV$$

$$\int_1^2 PdV \neq \int_1^2 PdV$$

I II

# CONCLUSIONS

1. The work done (taken) when passing the system from state I to state II is generally dependent on the pathway on which this transformation took place.
2. When calculating the value of the volume work, we need to know the path it has taken (equation describing relation between the volume and pressure)
3. After summing up elementary works (after integration) you can not compare the work to a certain amount that is a difference in the initial and final state, and thus to the difference in value being a function of the state in these states.
4. Mathematically, this means that elementary work is not a total differential.





## **Mechanical work $W$ and heat $Q$ are not state functions.**

The types of work we encounter in thermodynamics:

Volume work:

$$\mathbf{DW} = -pdV$$

Work of surface forces, which is given by dependence:

$$\mathbf{DW}_s = \sigma dA$$

where:  $\sigma$  is surface tension, and  $dA$  is the elementary change of the liquid surface.

Mechanical work:

$$\mathbf{DW}_M = FdL$$

where:  $F$  is strength and  $dL$  is the way or the electric work:

$$\mathbf{DW}_e = Edq$$

where:  $E$  is the potential difference and  $dq$  is the charge.





# The first law of thermodynamics

## 1. Joule's experience.

Assumptions:

- a) The same initial state of the water (medium)
- b) Water in an adiabatic cover

Lessons from experience:

1. The same amount of work carried out always causes an identical change in the state of the phase, i.e. a change in density, temperature or volume
2. The amount of work required to produce an identical change in the phase state is proportional to the mass of the phase



Each phase of system in equilibrium is described by a state function  $U_j$  of the state parameters  $X_1, X_2, X_3 ..$

$$U_j = U(X_1, X_2, X_3 ..) - \text{a state function}$$

The state function  $U$  of the system with  $j$  phases:

$$U = \sum U_j, \quad j=1, 2, \dots$$

Difference between the states 2 and 1, in every adiabatic transition, is given as follows:

$$U_2 - U_1 = \Delta U = W, \quad \Delta U - W = 0,$$

**W** - the work done on or by the system

$$\Delta U - W = 0$$



The first law of thermodynamics postulates the existence of a state function **U**, which is a function of independent state parameters.

If the independent parameters are denoted by  $X_1, X_2, X_3, \dots$  then we can write the state function in the following form:

$$U = U(X_1, X_2, X_3, \dots)$$



The state function is a function whose complete difference is given by the formula:

$$dU = \frac{\delta U}{\delta X_1} dX_1 + \frac{\delta U}{\delta X_2} dX_2 + \dots$$

mixed derivatives are equal and do not dependent on the order of differentiation

$$dU = \alpha(x_1, x_2, \dots) dx_1 + \beta(x_1, x_2, \dots) dx_2 + \varphi(x_1, x_2, \dots) dx_3$$

$$\frac{\delta \alpha}{\delta x_2} = \frac{\delta \beta}{\delta x_1},$$

$$\frac{\delta \alpha}{\delta x_3} = \frac{\delta \varphi}{\delta x_1},$$

$$\frac{\delta \beta}{\delta x_3} = \frac{\delta \varphi}{\delta x_2}$$

the change of the U state function when transitioning from state A to state B is equal to:

$$\int_A^B dU = U_B - U_A$$



where:  $U_A$  and  $U_B$  are values of  $U$  function in a state A and B it means in the initial state (before the process) and in the final (after process).

## The physical meaning of the function $U$ ?

By definition, the elementary change in the  $U$  function in the adiabatic process is equal to:

$$dU = W_{el} \text{ (adiabatyczna)} \quad \text{lub} \quad dU = DW \text{ (adiabatyczna i kwazystyczna)}$$

It follows that:

- 1) the  $U$  function is quantitatively equal to work done in adiabatic transformation
- 2) this work was done at the expense of mechanical energy, hence
- 3)  $U$  value is measured in the same units and arises at the expense of mechanical energy, therefore,
- 4) the  $U$  function is different from mechanical energy and another form of energy, and we call it

**INTERNAL ENERGY.**



# The mathematical formulation of the first law of thermodynamics.

The first principle of thermodynamics can be written in the form of the following equations:

$dU = W_{el} + Q_{el}$  - in the case of elemental transformation  
or

$dU = DW + dQ$  - in the case of quasistatic transformation

The above mathematical formulations of the first law of thermodynamics are convenient for deriving practical conclusions from them.





# **Physical meaning of the equations of the first law of thermodynamics cited above:**

- 1. The first law of thermodynamics is a step towards the general principle of energy conservation, which also takes into account other types of energy,**
- 2. Under the concept of work one should understand – all possible types of work**



## Change in internal energy

The internal energy of the system can be changed by adding energy to it or by taking energy from the system.

If the energy is supplied to the system, it has a sign (+) and otherwise it has a minus sign (-).

According to this convention, volumetric work must be given by the equation:

$$W_{el} = - PdV$$

because, when  $dV$  is positive (system expands) work is done by the system it means that the system loses energy and when  $dV$  is negative, then the work is done on the system (compression) which means that the system gains energy.

To indicate that elementary work can consist of various works and to distinguish volumetric work from them, the expression for work is written in the following equation:

$$W_{el} = -PdV + \overline{W}_{el}$$

Considering the above, the first law of thermodynamics can be written for elemental transformation as:

$$dU = -PdV + Q_{el} + \overline{W}_{el}$$

and for the quasi-static transformation as:

$$dU = -PdV + DQ + D\overline{W}$$



# ENTHALPY

If the pressure  $P$  is the system's own pressure, the equation of the first law of thermodynamics can be written in a slightly different form taking into account the influence of own pressure and own volume.

By adding to both sides of the equation for the change of internal energy the expression  $d(PV)$ , the following relationships are obtained:

$$dU + d(PV) = -PdV + Q_{el} + \overline{W}_{el} + d(PV) \quad \text{p.el.}$$

$$dU + d(PV) = -PdV + DQ + \overline{DW} + d(PV) \quad \text{p.qs.}$$

and because

$$d(PV) = PdV + VdP$$

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the above equations one can write as follows:

$$d(U + PV) = VdP + Q_{el} + \overline{W}_{el} \quad \text{p.el.}$$

$$d(U + PV) = VdP + DQ + \overline{DW} \quad \text{p.qs.}$$

the expression in brackets :

$$H = U + PV$$

is new state function and it is named enthalpy.

Because **U** is the state function and **P** and **V** are state parameters, the enthalpy is also the state function.



The first principle of thermodynamics you can also write in the form of the enthalpy and it is as follows:

$$dH = VdP + Q_{el} + \overline{W}_{el} \quad el$$

$$dH = Vdp + DQ + D\overline{W} \quad qs$$

In the case of systems, in which we deal only with volumetric work, the first law of thermodynamics takes the form of the following equations:

$$dU = Q_{el} - PdV$$

$$dH = Q_{el} + VdP$$





**Isochoric processes** are those that run in a constant volume, i.e. for which:

$$\mathbf{V = const} \quad \text{and thus} \quad \mathbf{dV = 0}$$

But because:

$$dU = Q_{el} - PdV \quad \Rightarrow \quad dU = (Q_{el})_V$$

that is, the change of internal energy in the isochoric transformation is equal to the heat supplied to the system or separated by the system.





Let us consider a system consisting of only one uniform phase, whose state is function of temperature  $T$  and volume  $V$ . Then internal energy is a function of these state parameters and is expressed by the general formula:

$$dU = U (T, V)$$

and its complete differential is given by the equation:

$$dU = \left( \frac{\delta U}{\delta V} \right)_T dV + \left( \frac{\delta U}{\delta T} \right)_V dT$$

and for  $V = \text{const}$

$$dU = \left( \frac{\delta U}{\delta T} \right)_V dT$$



but because:

$$dU = (Q_{el})_V$$

then:

$$dU = \left(\frac{\delta U}{\delta T}\right)_V dT = (Q_{el})_V$$

that is, the heat delivered to the phase in the isochoric process is equal to the change in its internal energy. Because the internal energy **U** is a function of the parameters **V** and **T**, when the **V** is constant, the change in the internal energy of the system must cause a change in the temperature **T**.



So the change  $U$  caused by the heat  $Q_{el}$  (supplied or given up) is manifested in this case by a change in temperature by  $dT$ .

Dividing the last equation by  $dT$  we get a new dependence of the form:

$$\left(\frac{\delta U}{\delta T}\right)_V = \frac{(Q_{el})_V}{dT}$$

The right side of the equation gives information about the amount of heat to be delivered to the system (phase) to cause the change of temperature  $T$  of 1 degree.

If the system consists of 1 gram of phase, then the ratio  $(Q_{el})_V / dT$  is called the specific heat and we designate it as  $c_V$ .

If the system consists of 1 mole of atoms, we call it the thermal capacity or molar specific heat at a constant volume and it is denoted as  $C_V$ .



Relation between mentioned two kind of specific heats is as follows:

$$\left(\frac{\delta U}{\delta T}\right)_V = \left(\frac{Q_{el}}{dT}\right)_V = C_V = M c_V$$

where:  **$C_V$**  – the molar specific heat in [J/gramatom],  
 **$c_V$**  – the specific heat in [J/gram] and  **$M$**  – the atomic mass in  
[gram/mole]



## Conclusion

If the relations between the internal energy of any phase  $U$  and temperature  $T$  and molar volume  $V$  is known one can always calculate the heat capacity by constant volume by differentiation the internal energy with respect to the temperature  $T$ .

## Hess's law

Consider a system consisting of a series of phases in which isochoric transformation takes place. Then, in accordance with the first law of thermodynamics, we know that:

$$dU = (Q_{el})_V$$

That is, the change in internal energy = the heat of the isochoric transformation



The total change in internal energy as a function of state depends only on the state parameters, i.e. on the difference in its final (2) and initial (1) value. We can therefore write:

$$U_2 - U_1 = \int_1^2 dU = \int_1^2 \sum Q_{el} = Q_V$$

$Q_V$  – the transition thermal (heat) effect

$$U_2 - U_1 = Q_V$$

The thermal (heat) effect of the isochoric transition from state 1 to 2 is equal to the difference in internal energy in the final state (2) and the initial state (1). This difference does not depend on the path of isochoric transformation, but only on the initial and final state of transformation.



The consequence of the above law is that the heat of obtaining products from substrates in the isochoric process does not depend on intermediate reactions or their order.

In the case of an isobaric transformation, Hess's law sounds similar but it concerns enthalpy:

$$H_2 - H_1 = Q_p$$

The equation above says, that the thermal effect of the isobaric process from the initial state (1) to the final state (2) is equal to the enthalpy difference in both states. This difference does not depend on the transformation path but only on the initial and final state.

For chemical reactions, the thermal effect of receiving products from substrates does not depend on the intermediate reactions or their order.





$$H = U + PV$$

$$dH = Q_{el} + VdP \quad \text{for } p=const$$

$$dH = (Q_{el})_p \rightarrow dH = \left(\frac{Q_{el}}{dT}\right)_p dT$$

$$H = H(T, p) \rightarrow dH = \left(\frac{dH}{dT}\right)_p dT + \left(\frac{dH}{dp}\right)_T dp \quad \text{for } p=const$$

$$dH = \left(\frac{dH}{dT}\right)_p dT \rightarrow \left(\frac{dH}{dT}\right)_p = \left(\frac{Q_{el}}{dT}\right)_p = C_p \rightarrow dH = C_p dT$$

$$H_2 - H_1 = \int_1^2 C_p dT$$



# THE SECOND LAW OF THERMODYNAMICS

If state A is the state before the process and B is the state after the process, equality occurs for the reversible process:

$$(S_u + S_{ot})_B = (S_u + S_{ot})_A$$

And for the irreversible process:

$$(S_u + S_{ot})_B > (S_u + S_{ot})_A$$

$$dS \geq \frac{Q_{el}}{T}$$

Where:  $dS$  is a complete differential of entropy,  $T$  is the temperature and  $Q_{el}$  is the heat of transformation.



$$dS \geq \frac{Q_{el}}{T} \quad dS - \frac{dU - W_{el}}{T} \geq 0$$

$$TdS - (dU + W_{el}) \geq 0 \quad \text{or} \quad dU - TdS \geq W_{el}$$

$$d(U - TS) = W_{el}$$

$$F = U - TS \quad \text{- free energy, Helmholtz free energy}$$

$$F + PV = U - TS + PV \quad d(F + PV) = d(U - TS + PV)$$

$$F + PV = G = U - TS + PV = U + PV - TS$$

$$G = H - TS \quad \text{- free enthalpy, Gibbs free energy, Gibbs energy}$$



$$***G = U - TS + PV***$$

$$***G = H - TS***$$

$$***dG = dH - TdS***$$

$$***G_2 - G_1 = \int_1^2 C_p dT - T \int_1^2 \frac{C_p}{T} dT***$$

$$***C_p = a + bT + cT \ln T + dT^2***$$

*where: a, b, c, d – parameters obtained from measurements of  $C_p$*



# CALCULATION OF ENTHALPY, ENTROPY AND GIBBS FREE ENERGY

**Calculation of the enthalpy change of a substance.**

$$dH = \int C_p dT$$

$$C_p = a + bT + c/T^2 + dT^2$$

$$\Delta H = H_2 - H_1 = \int_1^2 C_p dT$$

**Calculation of the enthalpy at the temperature  $T_2$ :**

$$H_2 = \int_1^2 C_p dT + H_1$$

**$H_1$  must be known.**



When  $p = p^0 = 1 \text{ atm}$  oraz  $T_1 = T^0 = 298.16 \text{ K}$  (standard conditions), the enthalpy  $H_1$  is called the standard enthalpy and is designated by  $H_{T^0}^0$ .

$$H_2 = \int_1^2 C_p dT + H_{T^0}^0$$

$$H_2 = \int_1^2 \left( a + bT + \frac{c}{T^2} + dT^2 \right) dT + H_{T^0}^0$$

$$H_2 = a(T - T^0) + b \frac{T^2 - T^{02}}{2} + c \frac{T - T^0}{T \cdot T^0} + d \frac{T^3 - T^{03}}{3} + H_{T^0}^0$$

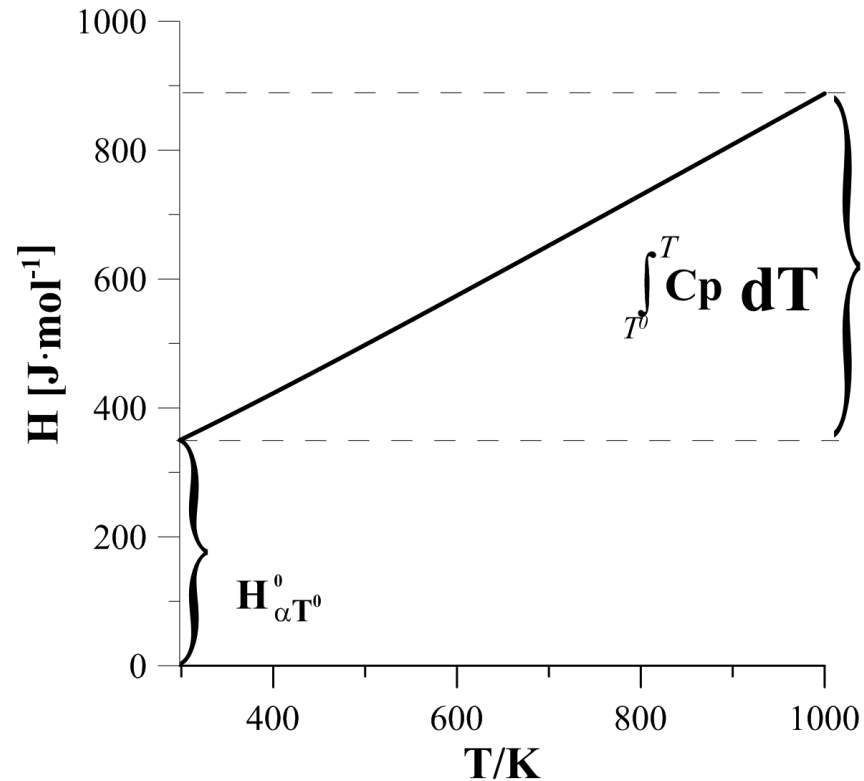
$h_1^0$	$h_2^0$	$h_3^0$	$h_4^0$

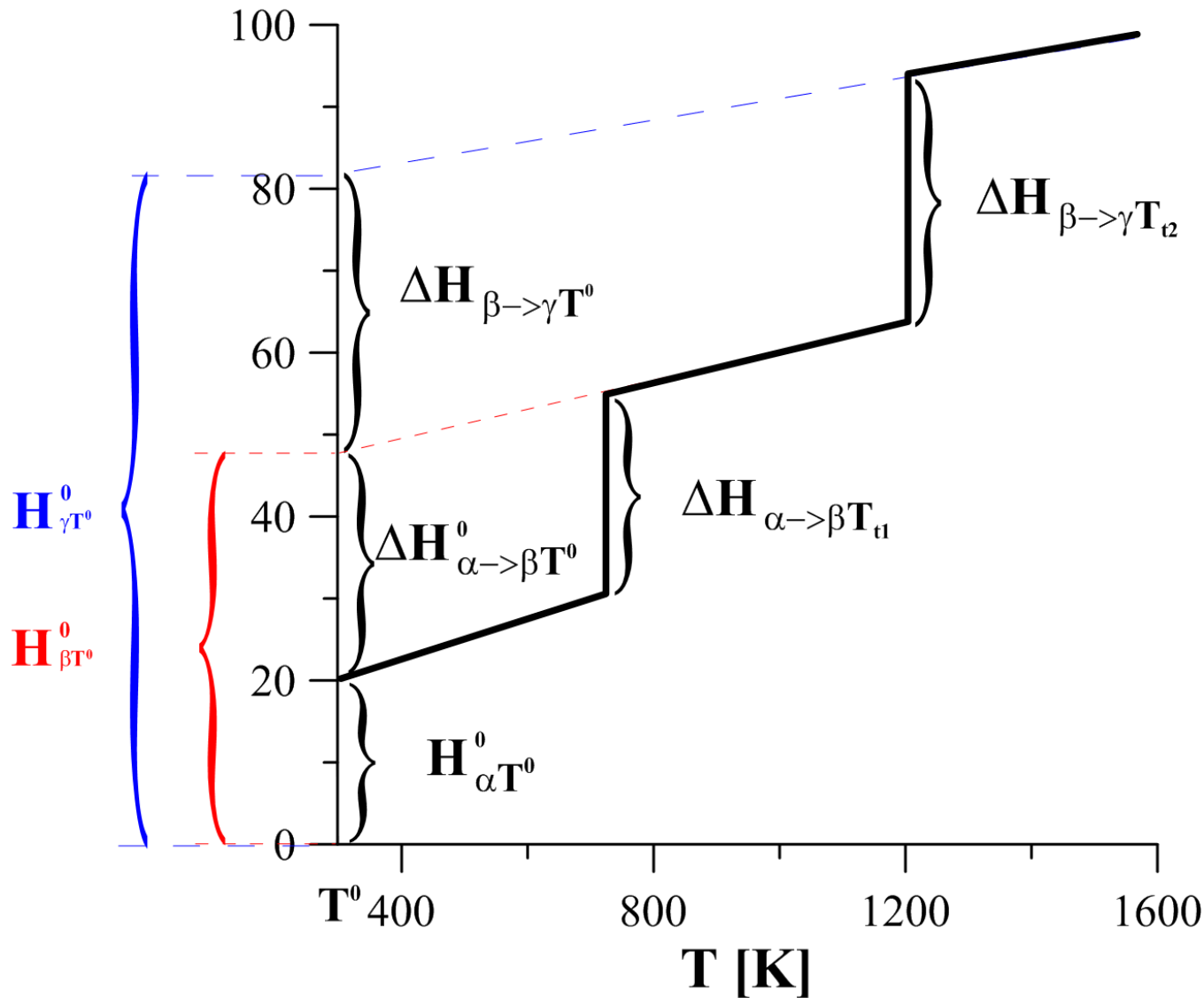




$$H_{\alpha T} = a_{\alpha} \cdot h_1^0 + b_{\alpha} \cdot h_2^0 + c_{\alpha} \cdot h_3^0 + d_{\alpha} \cdot h_4^0 + H_{\alpha T^0}^0$$

**$a$ ,  $b$ ,  $c$ ,  $d$**  – parameters of Kelley's equation for  $C_p$ ,  **$H_{\alpha T}$**  – the enthalpy at temperature  **$T$**  and  **$H_{\alpha T^0}^0$**  - the standard enthalpy of  $\alpha$  phase.





$H_{\alpha T^0}^0$  - the standard enthalpy of  $\alpha$  phase

$H_{\beta T^0}^0$  - the standard enthalpy of  $\beta$  phase

$H_{\gamma T^0}^0$  - the standard enthalpy of  $\gamma$  phase

$\Delta H_{\alpha \rightarrow \beta}$  - the transition enthalpy of  $\alpha$  to  $\beta$  phase

$\Delta H_{\beta \rightarrow \gamma}$  - the transition enthalpy of  $\beta$  to  $\gamma$  phase



$$S_2 = \int_1^2 \frac{C_p}{T} dT + S_{T^0}^0$$

$$S_2 = \int_1^2 \left( \frac{a}{T} + b + \frac{c}{T^3} + dT \right) dT + S_{T^0}^0$$

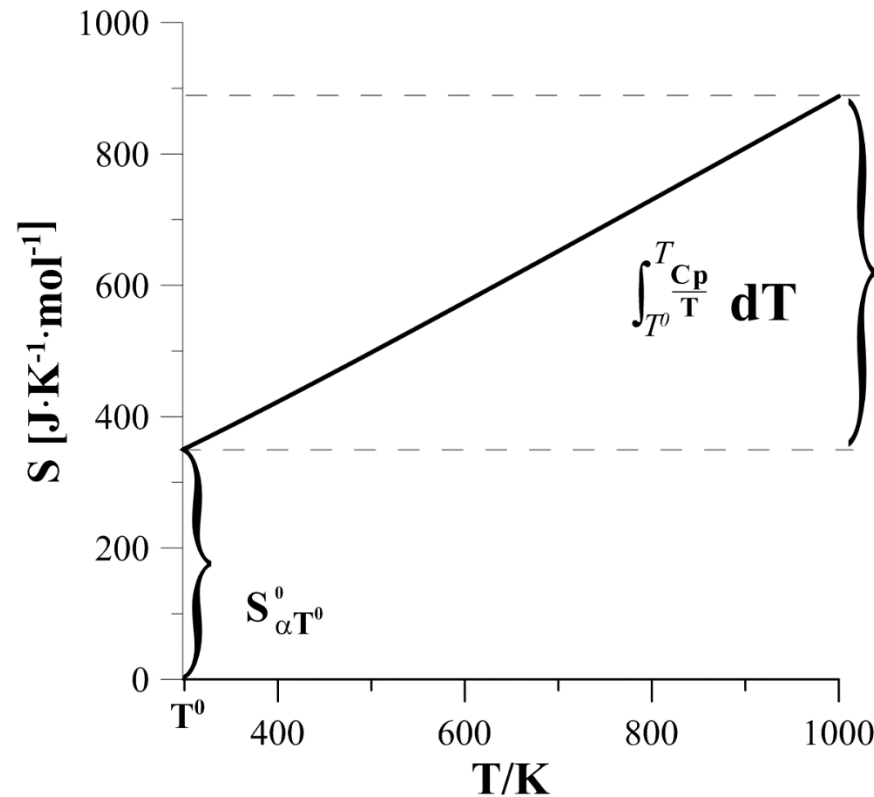
$$S_2 = a \ln \left( \frac{T}{T^0} \right) + b(T - T^0) + c \frac{T^2 - T^{02}}{2T^2 \cdot T^{02}} + d \frac{T^2 - T^{02}}{2} + S_{T^0}^0$$

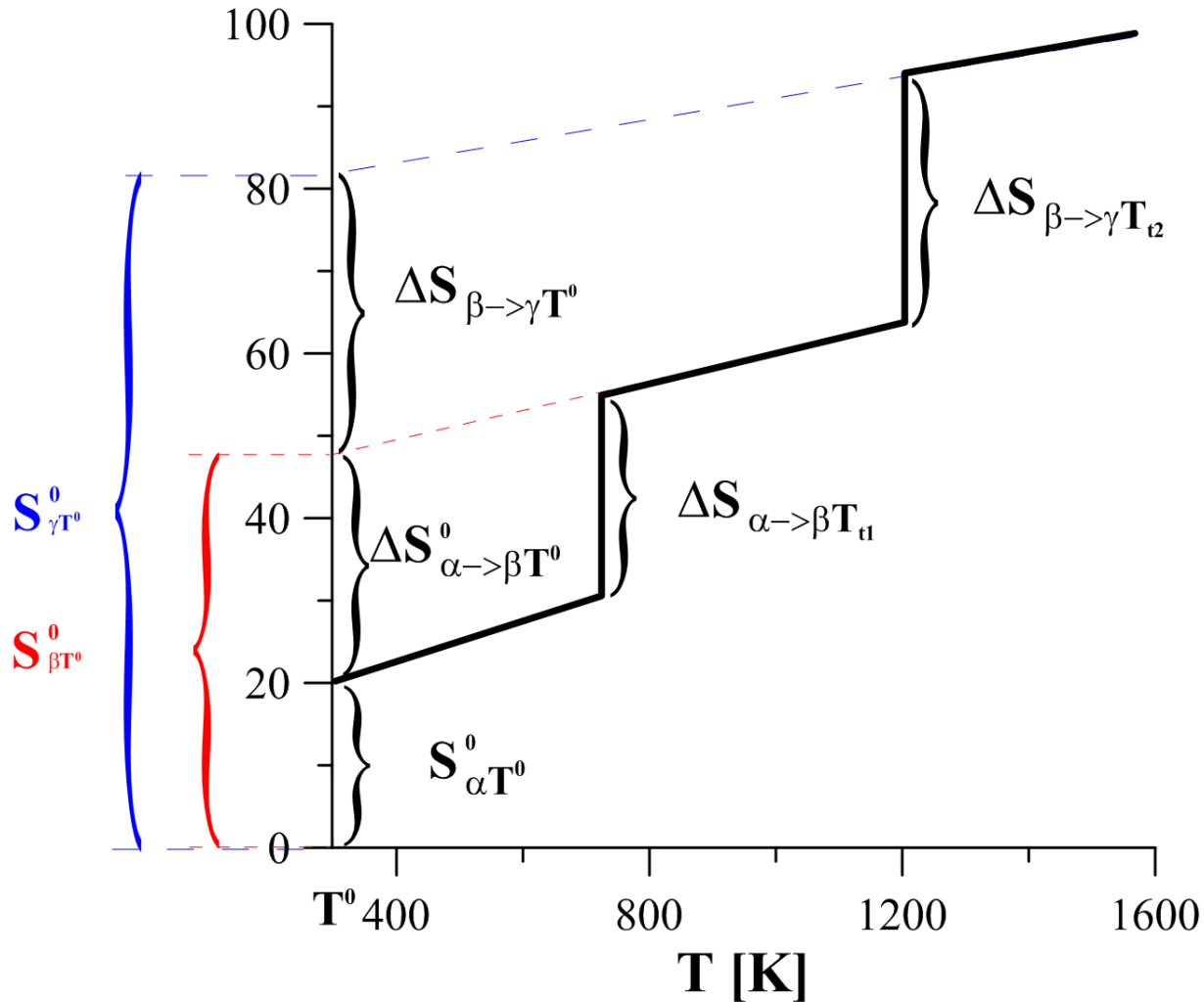
$S_1^0$	$S_2^0$	$S_3^0$	$S_4^0$



$$S_{\alpha T} = a_{\alpha} \cdot s_1^0 + b_{\alpha} \cdot s_2^0 + c_{\alpha} \cdot s_3^0 + d_{\alpha} \cdot s_4^0 + S_{\alpha T^0}^0$$

**$a, b, c, d$**  – parameters of Kelley's equation for  $C_p$ ,  $S_{\alpha T}$  – the entropy at temperature  $T$  and  $S_{\alpha T^0}^0$  - the standard entropy of  $\alpha$  phase.





$S_{\alpha T^0}^0$  - the standard entropy of  $\alpha$  phase

$S_{\beta T^0}^0$  - the standard entropy of  $\beta$  phase

$S_{\gamma T^0}^0$  - the standard entropy of  $\gamma$  phase

$\Delta S_{\alpha \rightarrow \beta}$  - the transition entropy of  $\alpha$  to  $\beta$  phase

$\Delta S_{\beta \rightarrow \gamma}$  - the transition entropy of  $\beta$  to  $\gamma$  phase



## Exercise 1

Calculate the change in the enthalpy and entropy of solid and liquid zinc in the temperature range from  $T^0 = 298.16$  K to  $T = 1000$  K, step = 100 K based on following data:

MPT=692.655K    BPT= 1180K

s - 4.956    2.99E-3    .199E+5    0.    298.14     $H_{\alpha T^0}^0 = 0.$      $S_{\alpha T^0}^0 = 9.95$

l - 7.5    3\*0.    692.655     $\Delta H_{s \rightarrow l} = 1750.$

g - 4.968    3\*0.    1180.     $\Delta H_{l \rightarrow g} = 27569.$