# UNIT -2

## Reactor Design for Single Reactions

**CLASSIFICATION OF REACTORS**

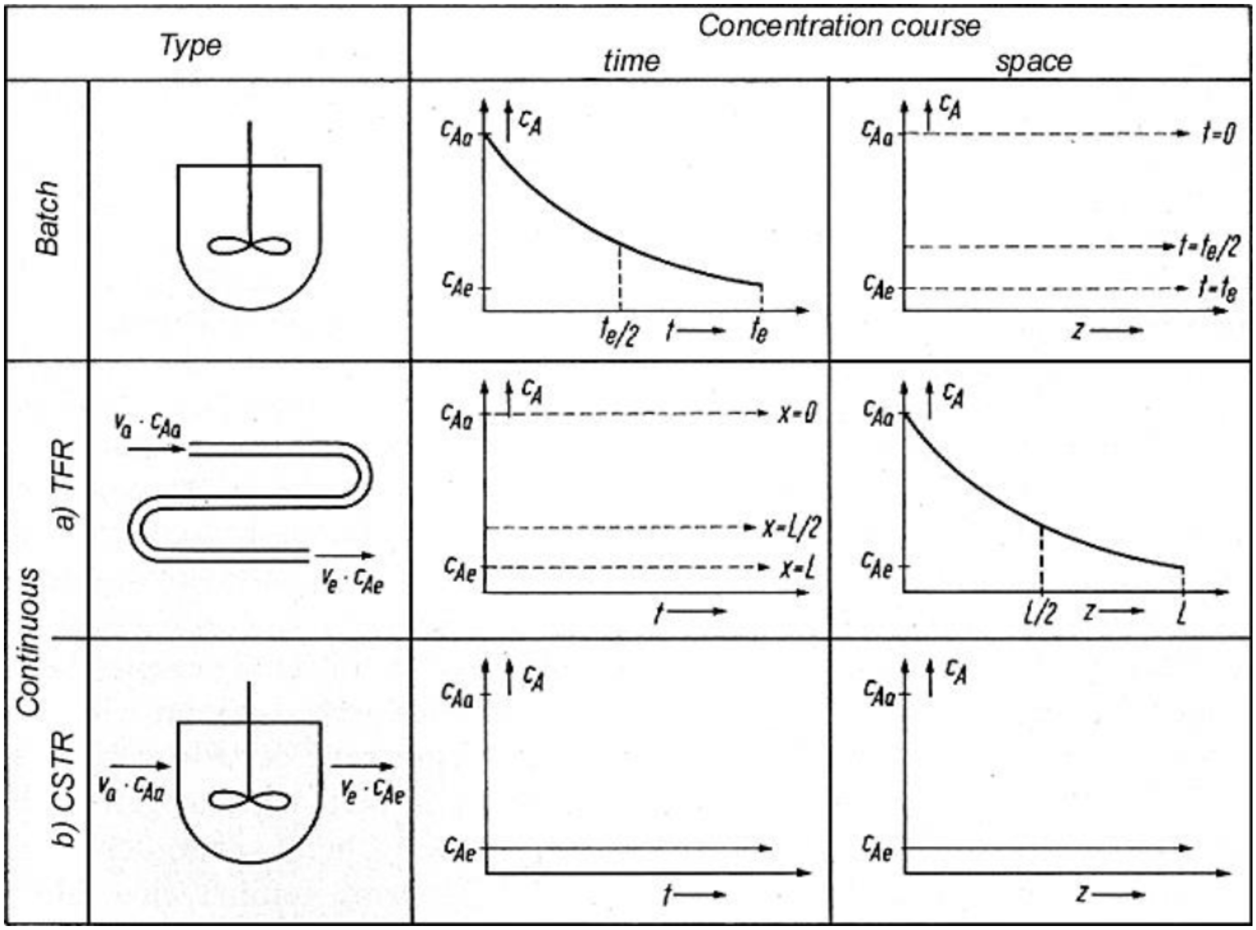
Reactors are classified based on

1. Method of operation: Batch or Continuous reactor

2. Phases: Homogeneous or Heterogeneous reactor

**REACTOR TYPES**

Equipment in which homogeneous reactions are effected can be one of three general types : the batch , the steady –state flow and the un-steady-state flow or semibatch reactor. The batch reactor is simple, needs little supporting equipment and is therefore ideal for small scale experimental studies on reaction kinetics. Industrially it is used when relatively small amounts of material are to be treated. The steady state flow reactor is ideal for industrial purposes when large quantities of material are to be processed and when the rate of the reaction is fairly high to extremely high. Extremely good product quality control can be obtained. This is a reactor which is widely used in the oil industry. The semibatch reactor is a flexible system but is more difficult to analyze than the other reactor types. It offers good control of reaction speed because the reaction proceeds as reactants are added. Such reactors are used in a variety of applications from the calorimetric titrations in the laboratory to the large open hearth furnaces for steel production.




**Reactor Design**

The starting point for all design is the material balance expressed for any reactant

***Material balance***

Rate of reactant flow into element of volume =rate of reactant flow out of element of volume + rate of reactant loss due to chemical reaction within the element of volume + rate of accumulation of reactant in element of volume.

In nonisothermal operations energy balance must be used in conjunction with material balances

***Energy balance***

Rate of heat flow into element of volume =rate of heat flow out of element of volume + rate of disappearance of heat by reaction within the element of volume + rate of accumulation of heat in element of volume.

**Factors to be considered for design of reactor**

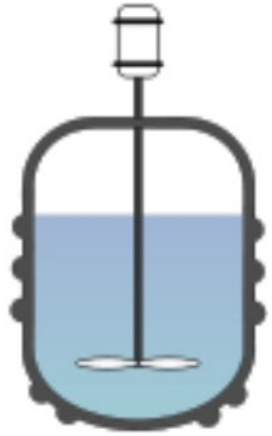
The different factors required for reactor design are (i) Size of reactor (ii) Type of reactor (iii) Time or duration of reaction (iv) Temperature & Composition of reacting material in the reactor (v) Heat removal or added and (vi) Flow pattern of fluid in the reactor.

**Ideal Reactors**

Ideal reactors (BR, PFR, and MFR) are relatively easy to treat. In addition, one or other usually represents the best way of contacting the reactants – no matter what the operation. For these reason, we often try to design real reactors so that their flows approach these ideals.

**Ideal Batch Reactor**

A batch reactor (BR) is one in which reactants are initially charged into a container, are well mixed, and are left to react for a certain period. The resultant mixture is then discharged. This is an unsteady state operation where composition changes with time; however at any instant the composition throughout the reactor is uniform. The advantages of a batch reactor are (i) small instrumentation cost and (ii) flexibility of operation. A batch reactor has the disadvantages of (i) high labour (ii) poor quality control of the product and (iii) considerable shutdown time has taken to empty, clean out and refill.



Making a material balance for component A..Noting that no fluid enters or leaves the reaction mixture

Input = output + disappearance +accumulation (1)

Input = 0

Output = 0

Disappearance of A by reaction moles/time = $( -r_A)V$

Accumulation of A by reaction moles/time = $dN_A/dt$

By replacing these two terms

$( -r_A)V = N_{AO}\, dX_A/dt$

Rearranging and integrating gives

$t= N_{AO} \int dX_A/ ( -r_A)V$

$t= C_{AO} \int dX_A/ ( -r_A) = - \int dC_A/ ( -r_A)$ FOR $\epsilon_A =0$

**Space time and space velocity**

Space velocity: It is the reciprocal of space time and applied in the analysis of continuous flow reactors such as plug flow reactor and CSTR. It is defined as the number of rector volumes of a feed at specified conditions which can be treated in unit time. A space velocity of 10 h –1 means that ten reactor volumes of the feed at specified conditions are treated in a reactor per hour.

Space time and space velocity are the proper performance measures of flow reactors.

Space time

$\tau$ = 1/s = time required to process one reactor volume of feed measured at specified conditions (time)

Space velocity

s= 1/$\tau$ = number of reactor volumes of feed at specified conditions which can be treated in unit time ($time^{-1}$)

$\tau = VC_{AO}/F_{AO} = 1/s$

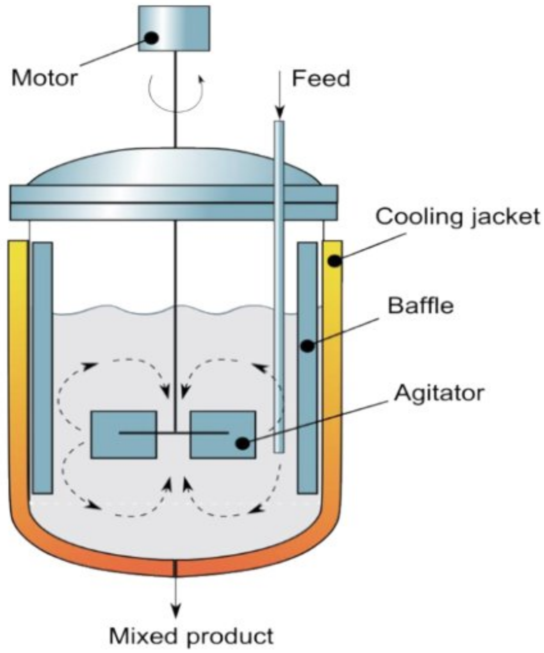
**Holding time**: It is the mean residence time of flowing material in the reactor. It is given by the expression t = CAo + d XA)/] / [(-rA) (1+ $_{A}X_{A}$)

For constant density systems (all liquids and constant density gases) t = $\tau$ Where 'V' is the volume of the reactor and 'v' is the volumetric flow rate of reacting fluid

For constant density systems, the performance equation for Batch reactor and Plug flow reactor are identical.

## Steady state mixed flow reactor or Continuous stirred tank reactor (CSTR)

Mixed flow reactor (MFR) is also called as back mix reactor or continuous stirred rank reactor (CSTR) or constant flow stirred tank reactor (CFSTR). In this reactor, the contents are well stirred and uniform throughout. The exit stream from the reactor has the same composition as the fluid within the reactor.




Since the composition is uniform throughout , the accounting can be made about the reactor as a whole.

Input = output + disappearance +accumulation (2)

Accumulation = 0

Input of A.moles /time = $F_{AO}$

Output of A.moles /time = $F_A = F_{AO}(1-X_A)$

Disappearance of A by reaction moles/time = $(-r_A)V$

Introducing all these terms in eqn 2

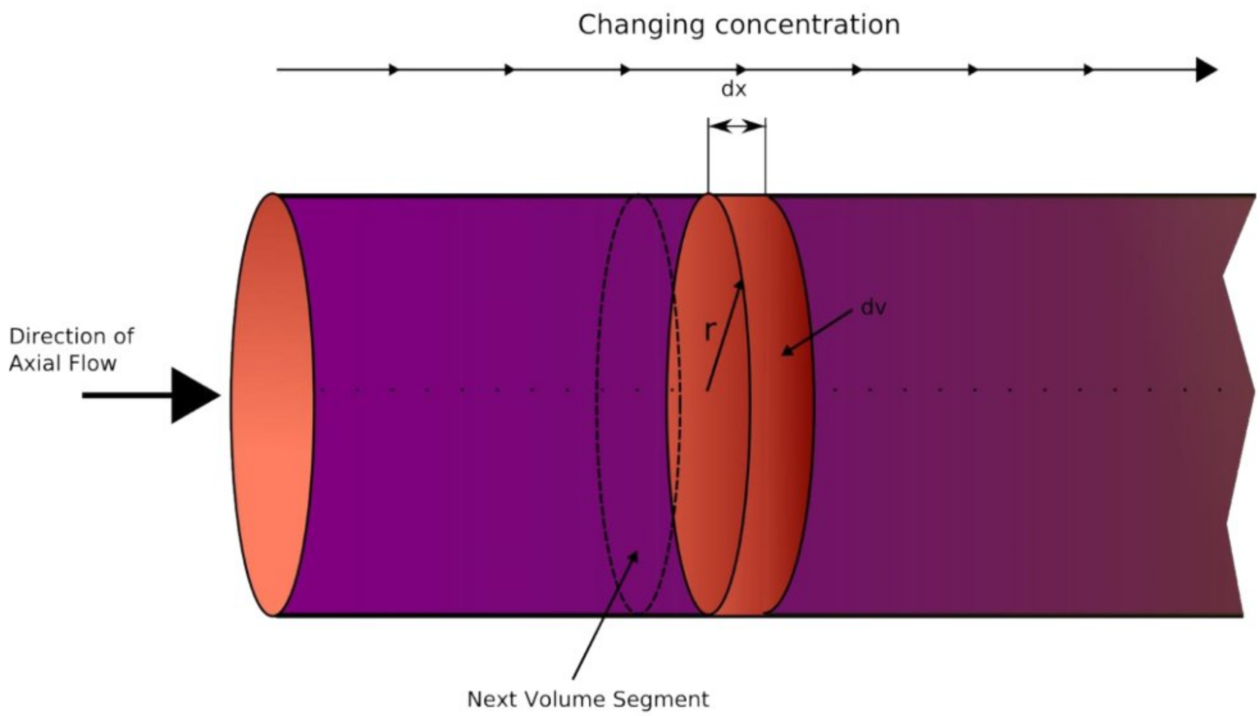
$F_{AO} X_A = (-r_A)V$

Which on rearrangement becomes

$V/ F_{AO} = \tau / C_{AO} = X_A / ( -r_A)$

**Steady state Plug flow reactor or Tubular reactor**

Plug flow reactor (PFR) is also referred as slug flow, piston flow, ideal tubular, and unmixed flow reactor. It specifically refers to the pattern of flow as plug flow. It is characterized by the fact that the flow of fluid through the reactor is orderly no element of fluid overtaking or mixing with any other element ahead or behind. Actually, there may be lateral mixing of fluid in a PFR; however, there must be no mixing or diffusion along the flow path. The necessary and sufficient condition for plug flow is the residence time in the reactor to be the same for all elements of fluid




Input = output + disappearance +accumulation (3)

Accumulation = 0

Input of A.moles /time = $F_{AO}$

Output of A.moles /time = $F_A + d\,F_A$

Disappearance of A by reaction moles/time = $( -r_A)dV$

Introducing all these terms in eqn 3

$F_A = F_A + d\,F_A + ( -r_A)dV$

Noting that

$d\,F_A = d\,[F_A ( 1-X_A) ] = - F_{AO}\, dX_A$

we obtain on replacement

$F_{AO}\, dX_A = ( -r_A)dV$

Grouping the terms accordingly and integrating

$V/ F_{AO} = \tau / C_{AO} = \int dX_A / ( -r_A)$

# Plug flow and mixed flow reactor design

## Mixed flow reactor design

Applying mass balance performance equation for mixed flow reactor

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{\Delta X_A}{-r_A} = \frac{X_A}{-r_A}$$

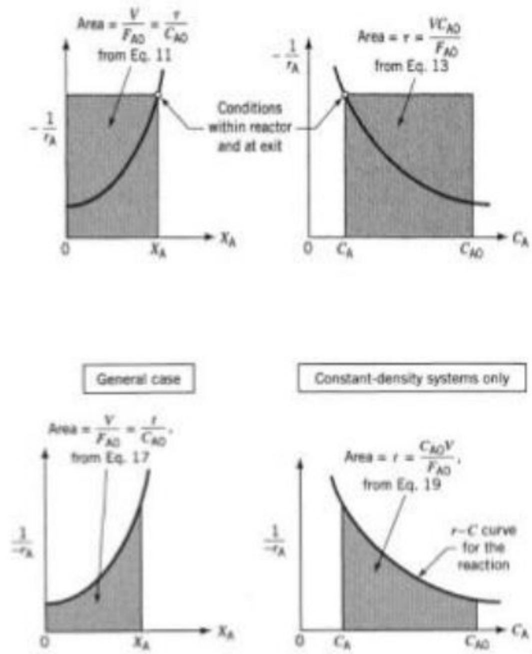
$$\tau = \frac{1}{s} = \frac{V}{v_0} = \frac{VC_{A0}}{F_{A0}} = \frac{C_{A0}X_A}{-r_A}$$

## Plug flow reactor design

Performance equation for plug flow reactor

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\tau = \frac{V}{v_0} = \frac{VC_{A0}}{F_{A0}} = C_{A0}\int_0^{X_{Af}} \frac{dX_A}{-r_A}$$




ideal reactors are based on simple models of flow patterns and mixing in the reaction vessel. In an ideal batch reactor, the concentration and temperature fields are assumed to be spatially uniform. In practice, the condition can be approximately realized by vigorous agitation or stirring. In the absence of stirring, beautiful spatial patterns, caused by an interaction between diffusion and reactions, may develop in some systems . All the elements of the fluid spend the same amount of time in the reactor, and hence have the same residence time. From the viewpoint of thermodynamics, a batch reactor represents a closed system. The steady states of the batch reactor correspond to states of reaction equilibria. Batch reactors are often used in the pharmaceutical industry, where small volumes of high-value products are made. The ideal continuous stirred tank reactor (CSTR) like in an ideal batch reactor, the concentration and temperature fields in an ideal CSTR are spatially uniform. As there are no spatial gradients, the species concentrations in the exit stream are identical to the corresponding values in the reactor. On the other hand, the species concentrations in the inlet stream are in general different from those in the reactor. Unlike the batch reactor, the CSTR is an open system as it can exchange heat and mass with the surroundings. Hence it operates away from equilibrium, and steady states are usually not states of reaction equilibria. On account of the assumption of perfect mixing, the sequence in which fluid elements leave the reactor is uncorrelated with the sequence in which they enter. As shown later, this leads to a distribution of residence times for the fluid leaving the reactor. These reactors are widely used for polymerization reactions such as the polymerization of styrene, production of explosives, synthetic rubber, etc. Compared to tubular reactors, CSTRs are easier to clean and permit better control of the temperature. (c) The plug flow reactor (PFR) The PFR is an idealization of a tubular reactor. The velocity, temperature, and concentration fields are assumed to be uniform across the cross section of the reactor. In practice, this situation can be approximately realized for the case of turbulent flow through a tube with a large ratio of the length to the diameter. The latter condition ensures that axial mixing has a negligible effect on the conversion. In a PFR, there is perfect mixing in the radial or transverse direction. Further, there is no mixing or diffusion in the axial direction. Like a CSTR, the PFR also represents an open system, and hence steady states are not states of reaction equilibrium. Owing to the assumption of plug flow, all the fluid elements have the same residence time. The velocity of the fluid is often treated as a constant, but this assumption must be relaxed when the density of the fluid changes significantly along the length of the tube. The steady state equations for a PFR are similar in form to the dynamic equations for an ideal batch reactor. In many cases, the results for the latter can be translated into results for a PFR operating at a steady state. Tubular reactors are used for many gas phase and liquid phase reactions, such as the oxidation of NO and the synthesis of NH3. These reactors are often modelled as PFRs, but more detailed models involving complications such as radial gradients, may be required in some cases.

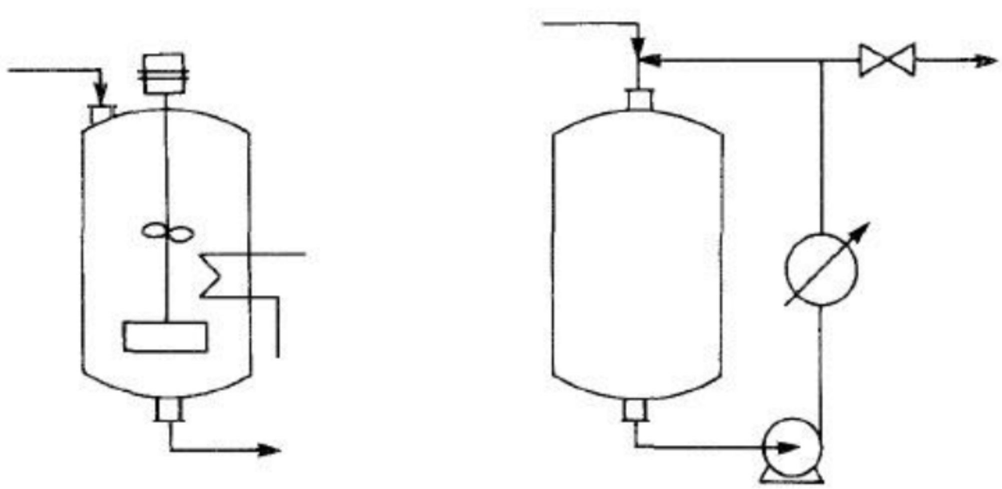
**Steady state reactor**

Reactors those in which the properties of the system do not change with time is said to be a steady state reactor. Example: Continuous stirred Tank reactor, plug flow reactor. Total mass inflow = Total mass outflow

**Unsteady state reactor**

Reactors are those in which the properties of the system changes with time and rate of reaction decreases with time expect for zero order reaction are said to be unsteady state reactor. Example: Batch reactor, Semi-batch reactor. There is accumulation in these reactors. Accumulation = input - output + generation - consumption.

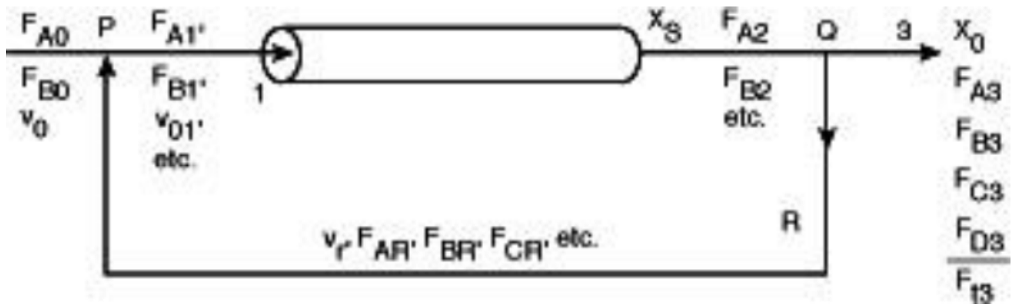
**<u>Semi batch reactor</u>**



(a) (b)

It is an unsteady state reactor. Reactors which are partially batch and partially continuous are referred to as semi-batch reactor. The semi batch reactors offers good control of reaction speed, because the reaction proceeds as reactants are added. Types: (i) volume changes but composition is unchanged (ii) composition changes but volume is constant.

**<u>Recycle reactor</u>**




In some reaction system, it is advantageous to divide the product stream and a part returned to reactor as recycle to increase the conversion rate. These reactors are called recycle reactors. The recycling provides a means for obtaining various degree of backmixing. Recycle ratio 'R' can be defined as the ratio of the volume fluid returned to the reactor entrance to the volume of fluid leaving the system or reactor. Significance: Recycle ratio can be made to vary from zero to infinity. Reflection suggests that as the recycle ratio is raised, the behavior shifts from plug flow (R = 0) to ). mixed flow (R =).), the recycle reactorWhen the recycle ratio 'R' becomes or tends to infinity (R= behaves like a CSTR. When material is to be processed to some fixed final conversion in a recycle reactor, there must be a particular recycle ratio 'R' that minimizes the reactor volume or space time. That recycle ratio is said to be optimum and the operation is said to be optimum recycle operation.

The actual conversion at inlet is given by: $$X_{A1} = \frac{1 - C_{A1}/C_{A0}}{1 + \varepsilon_A C_{A1}/C_{A0}}$$

The concentration at inlet to the reactor is given by

$$C_{A1} = \frac{F_{A1}}{v_1} = \frac{F_{A0} + F_{A3}}{v_0 + \boldsymbol{R} v_f} = \frac{F_{A0} + \boldsymbol{R} F_{A0}(1 - X_{Af})}{v_0 + \boldsymbol{R} v_0 (1 + \varepsilon_A X_{Af})} = C_{A0}\left(\frac{1 + \boldsymbol{R} - \boldsymbol{R} X_{Af}}{1 + \boldsymbol{R} + \boldsymbol{R}\varepsilon_A X_{Af}}\right)$$

So finally we get the following results: $$X_{A1} = \left(\frac{\boldsymbol{R}}{\boldsymbol{R}+1}\right) X_{Af}$$

The final equation for any expansion factor value is:

$$\frac{V}{F_{A0}} = (\boldsymbol{R} + 1)\int_{\left(\frac{\boldsymbol{R}}{\boldsymbol{R}+1}\right) X_{Af}}^{X_{Af}} \frac{dX_A}{-r_A} \quad \ldots \text{any } \varepsilon_A$$

Also in terms of concentration,

$$\tau = \frac{C_{A0} V}{F_{A0}} = -(\boldsymbol{R} + 1)\int_{\frac{C_{A0} + \boldsymbol{R} C_{Af}}{\boldsymbol{R} + 1}}^{C_{Af}} \frac{dC_A}{-r_A} \quad \ldots \varepsilon_A = 0$$