Mole balance

|  |  |  |  |
| --- | --- | --- | --- |
|  | BSTR | CSTR | PFR |
| M.B. |  |  |  |
| R |  constant V nonconstant V |  |  |
| t/ |  |  |  |
| V |  |  |  |

Gas phase reaction constant volume:

Liquid phase reaction constant volume:

 net number of moles consumed or produced at over number of moles total feed

Rxn with phase change

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Species |  |  |  |  |
| A |  |  |  |  |
| B |  |  |  |  |
| C | 0 or  |  |  |  |
| D | 0 or  |  |  |  |

After condensation,

b.c.

a.c.

**Elementary step -** a single, irreversible microscopic process, the reaction rate reflects stoichiometry.

Molecularity = number of molecules in irreversible step

 A is the frequency of attempts per molecule.

 is the probability of single attempt by a molecule to overcome the barrier resulting in success.

**PSSH, pseudo-steady state hypothesis, the rate of change in the radicals = 0.**

**Quasiequilibrated** , the number of ith mechanistic step required to complete the overall equation

|  |  |
| --- | --- |
|  |  |

If  ****

**Startup of CSTR**

If If

**Semibatch example - selectivity**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Reactive distillation** Mole balance on A:  | Stoichiometric table

|  |  |  |  |
| --- | --- | --- | --- |
| Species |  |  |  |
| A |  |  |  |
| B |  |  |  |
| C | 0 |  |  |
| D | 0 |  |  |

 |

|  |  |
| --- | --- |
|  |  |