Mass transfer

In engineering, the mass transfer coefficient is a diffusion rate constant that relates the mass transfer rate, mass transfer area, and concentration change as driving force

This can be used to quantify the mass transfer between phases, immiscible and partially miscible fluid mixtures (or between a fluid and a porous solid). Quantifying mass transfer allows for design and manufacture of separation process equipment that can meet specified requirements, estimate what will happen in real life situations (chemical spill), etc.

Mass transfer coefficients can be estimated from many different theoretical equations, correlations, and analogies that are functions of material properties, intensive properties and flow regime (laminar or turbulent flow). Selection of the most applicable model is dependent on the materials and the system, or environment, being studied.

A methodology for the determination of mass transfer resistances of fast reactions in three-phase mechanically agitated slurry reactors under the reaction conditions is presented. The mass transfer resistances affect significantly the overall mass transfer rate, the design equation and consequently the scale up of the reactor. There is not established methodology to separate the mass transfer resistances under reaction conditions by changing catalyst loading and manipulating the process variables, pressure and agitation speed. This allows to avoid the use of different catalyst particles and give the chance to calculate the mass transfer resistances without caring about the type of catalyst. We calculate each mass transfer resistance under conditions which do not allow to neglect any of the resistances. It is shown that the level off of mass transfer rate which is developed in the plot of mass transfer rate against agitation speed plots is not enough to determine the limiting regime.

Introduction

Gas-liquid-solid three phase reactors are of great importance in pharmaceutical and fine chemical industry. The mechanically agitated slurry reactors are the most common type of three phase reactors which are used within these industries. During the three-phase reactions a number of mass transfer processes need to take place before the surface catalytic reaction:

(a) gas-liquid mass transfer,

(b) liquid-solid mass transfer, and

(c) the combined internal pore diffusion and the surface chemical reaction. Each of the mass transfer processes and the intrinsic reaction rate affect the overall process rate indifferent extent. The design of three phase reactors requires the determination of the mass transfer coefficients and the reaction rate constant. The determination of mass transfer coefficients becomes even more important when the reaction rate constant and external mass transfer is of comparable magnitude. This happens in the case of fast chemical reactions. In fast chemical reactions, even if intense mixing conditions take place, the external mass transfer processes are not faster than the surface chemical reaction. Many researchers have used several methods to separate the effect of each of the mass transfer coefficients. Currently, there is not any established methodology for the separation of each of the mass transfer coefficients and the reaction rate constant (a) under the reaction conditions, (b) without changing the size of the catalyst, (c) under conditions which do not allow to neglect any of the rate, and (d) without needing to use low substrate concentration. Many researchers have studied the hydrogenations of unsaturated organic compounds by varying the hydrogen partial pressure but they have not manipulated the overall mass transfer resistance against the square root of hydrogen concentration in gas-liquid interface

The change of mass transfer resistance with time has been examined for membrane-based carbon dioxide absorption in water. A commercial polypropylene hollow fiber membrane module was used with gas flow through the lumen side and liquid cross-flow on the shell side. Experiments were carried out for a prolonged period of time to evaluate absorption performance. Absorption flux decreased significantly with time due to a developing resistance to mass transfer. However, the initial flux value was restored after membrane drying, indicating that the additional resistance was reversible. A theoretical model was developed to analyze and predict flux deterioration with time in terms of partial resistances in series. The resistance against pure gas mass transfer was considered to be the sum of the liquid phase resistance and the resistance of the membrane; the latter arises from membrane pore filling by gas or liquid or both. A shell side mass transfer correlation was used for the prediction of the liquid phase resistance. The experimental absorption flux decline with time was attributed to gradual partial pore filling by liquid, and it was used to estimate the magnitude of the membrane resistance and its temporal variation.

Model predictions, in good agreement with experimental results, permitted the estimation of liquid penetration into the membrane matrix. Although this was relatively low (~ 3%), the resulting resistance of the liquid-filled pores accounted for over 98% of the membrane resistance and for 20–50% of the total resistance to absorption.

Mass Transport in biological systems

Understanding fluxes

- The requirements for diffusion are: a vacant lattice position within which to move (a vacancy) and sufficient energy to overcome the restraints of bonding in the current position (vibration energy).

Diffusion is defined as the movement of molecules from a highly concentrated area to a lowly or zero concentration area with regard to that substance through a semi permeable membrane. Osmosis on the other hand is the reverse, i.e. from low to high.

Using different fluxes to achieve separation

- **Ultracentrifugation –** uses pressure through gravity forces and achieves separation by size
- **Electrophoresis –** uses potential gradients through an electric field and achieves separation on the basis of charge per mass
- **Isoelectric focusing –** uses chemical potential. gradient through PH (Hydrogen ions) and achieves separation on the basis of charge per mass
- **Membranes –** uses chemical potential gradients across another material and achieves separation on the basis of solubility and hydrodynamic radius

Mechanism of diffusion: Temperature influences manifest in the diffusion coefficient hence, diffusion coefficient increases with temperature as is summarized in following five points below

1. As temperature increases, the concentrated vacancies or sites within which to diffuse also increases. This affects the gradient and down field.

2. As temperature increases, the concentration of atoms/ molecules of appropriate energy to diffuse also increases. This affects the gradient and down field.
3. As temperature increases, the thermal excitation of atoms/ molecules on the lattice also increases. This affects the medium through which atoms diffuse.
4. Viscosity is also affected by temperature which can affect diffusivity.
5. The activation energy for diffusion integrates all of these contributing energy effects

Most real diffusion in the solid state is non-steady state.

Understanding diffusion

1. Diffusion is a molecular phenomenon
2. The process $\mathbf{D_{ij}}$ involves diffusivity D of the solute i in the solvent j.
3. Molecules are always solvated. This means they form tight associations with a few solvent molecules that change their effective molecular weight.
4. Solvated molecules have a solvo-dynamic (in water hydro-dynamic) radius which is different than the radius predicted from its structure.
5. Solvent molecules are themselves diffusing
6. $\mathbf{D_{ij}}$ assumes the dilute solution limit wherein solute-to-solute interactions are non-existent

All of this is also true for diffusion in gases.

Let me introduce the next and last audio lecture, lecture twelve…

So, we will be talking more about packed bed reactors, their applications and different types of packed bed reactors… so let's get to it

Packed bed reactors

What are packed bed reactors? In chemical processing, a packed bed is a hollow tube, pipe, or other vessel that is filled with a packing material. The packing can be randomly filled with small objects like Raschig rings or else it can be a specifically designed structured packing. Packed beds may also contain catalyst particles or adsorbents such as zeolite pellets, granular activated carbon, etc.

The purpose of a packed bed is typically to improve contact between two phases in a chemical or similar process. Packed beds can be used in a chemical reactor, a distillation process, or a scrubber, but packed beds have also been used to store heat in chemical plants. In this case, hot gases are allowed to escape through a vessel that is packed with a refractory material until the packing is hot. Air or other cool gas is then fed back to the plant through the hot bed, thereby pre-heating the air or gas feed.

Applications

Packed column

In industry, a packed column is a type of packed bed used to perform separation processes, such as absorption, stripping, and distillation. A packed column is a pressure vessel that has a packed section.

Columns used in certain types of chromatography consisting of a tube filled with packing material can also be called packed columns and their structure has similarities to packed beds.

Column structure: random and stacked packed columns

The column can be filled with random dumped packing (creating a random packed column) or with structured packing sections, which are arranged or stacked (creating a stacked packed column). In the column, liquids tend to wet the surface of the packing and the vapors pass across this wetted surface, where mass transfer takes place. Packing material can be used instead of trays to improve separation in distillation columns. Packing offers the advantage of a lower pressure drop across the column (when compared to plates or trays), which is beneficial while operating under vacuum. Differently shaped packing materials have different surface areas and void space between the packing. Both of these factors affect packing performance.

Liquid and vapor distribution (vapor to liquid ratio)

Another factor in performance, in addition to the packing shape and surface area, is the liquid and vapor distribution that enters the packed bed. The number of theoretical stages required to make a given separation is calculated using a specific vapor to liquid ratio. If the liquid and vapor are not evenly distributed across the superficial tower area as it enters the packed bed, the liquid to vapor ratio will not be correct and the required separation will not be achieved. The packing will appear to not be working properly. The height equivalent to a theoretical plate (HETP) will be greater than expected. The problem is not the packing itself but the mal-distribution of the fluids entering the packed bed. These columns can contain liquid distributors and redistributors which help to distribute the liquid evenly over a section of packing, increasing the efficiency of the mass transfer. The design of the liquid distributors used to introduce the feed and reflux to a packed bed is critical to making the packing perform at maximum efficiency.

Packed column vapor-equilibrium curve

Packed columns have a continuous vapor-equilibrium curve, unlike conventional tray distillation in which every tray represents a separate point of vapor-liquid equilibrium. However, when modeling packed columns, it is useful to compute a number of theoretical plates to denote the separation efficiency of the packed column with respect to more traditional trays. In design, the number of necessary theoretical equilibrium stages is first determined and then the packing height equivalent to a theoretical equilibrium stage, known as the height equivalent to a theoretical plate (HETP), is also determined. The total packing height required is the number theoretical stages multiplied by the HETP.