**Theory:**

**Reactor Models:**

The first thing is to choose a suitable reactor model. In fluid dynamic behavior point of view, there are two main continuous reactors:

1. PFR Reactor: in this case, we prefer to use the PFR Reactor, because of its higher productivity.
2. CSTR Reactor:

The second thing that must be considered is *interphase limitation*. If we plot concentration of reactant versus its position in bulk gas from catalyst surface, it will be shown as:

A blackboard with writing on it

Description automatically generated

In pseudo homogeneous model, the concentration of reactant at catalyst surface is exactly same as the concentration of reactant in gas bulk (Single set of governing equations). However, in the heterogeneous model, the concentration of reactant at catalyst surface is considerably lower than the concentration of reactant in gas bulk. In this model, a new set of equations for surface will be defined.

There’s a dimensionless number called “Damköhler Number” to describe the dominancy of fluid dynamics regime to reaction regime.

The other thing to be considered is the presence of intra phase (External) limitation! If we plot concentration of reactant versus its position in bulk gas from catalyst surface, it will be shown as:

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In pseudo homogeneous model, the concentration of reactant at catalyst surface is exactly same as the concentration of reactant in gas bulk (Single set of governing equations). However, in the heterogeneous model, the concentration of reactant at catalyst surface is considerably lower than the concentration of reactant in gas bulk. In this model, a new set of equations for surface will be defined.

For the external limitation, there’s a dimensionless number called “Thiele Module” that defined as below:

Also, we define the efficiency factor of Thiele Modulus, in order to correct the reaction rate as:

For the case , we have to follow pseudo homogeneous condition. In most cases, .

The main goal of this practical session is to develop a simple kinetics model for Methanol reactor. The schematic of this reactor is shown in the following figure:

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There are two main reactions occurring in the reactor:

Problem requests:

1. **Derive material balance and energy balance for pseudo homogeneous model!**
2. **Evaluate the hotspot temperature and its location. (in z axis)**
3. **Compute the overall productivity.**

*Derive material balance and energy balance for pseudo homogeneous model!*

Assume that there’s no diffusion limitation. We consider a single tube among the tubes of the reactor as a sample to simplify the modeling.

The general material balance will be written as:

We took a portion of the selected single tube:

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The reaction rate unit is typically equals to . The first thing that we have to do is to transfer the unit:

Using Taylor’s expansion, we can rewrite the material balance:

The equation above is a first order ODE that needs an initial condition.

Next step is to write an energy balance through the reactor. The general form is written as:

It is better to convert unit as mass based. Hence, the notation will be changed to .

In this case, we can define q as , which U represents the overall H.T coefficient, Sv represents surface/volume ratio, and represents temperature gradient ().

The dependency of pressure on z-axis position has been described by *Ergun’s equation*.

With approximation “d” to “”, we can rewrite the equations in the discrete mode:

The concentration, temperature, and reaction rate versus z-axis position for Methanol are shown in the figures below:

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