Maximum Gradient Description

Keywords: Models, Transport Phenomena Based, Maximum Gradient

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Maximum Gradient Description:

In this model may be considered to be just a simplified multiple gradient models in which the dispersion terms are deleted and only one derivative are retained in the bulk flow term. In this model all dispersion is neglected and only the largest (one dimensional) component of the gradient of dependent variable is retained in each balance, for example in the maximum gradient representation of a chemical reactor or gas absorber only concentration gradients in the axial direction caused b the bulk flow are considered and all radial gradients dispersion and the like are ignored

Maximum gradient models are the models commonly treated in elementary text books for continuous process and are as follows:

Mass balance for ith species:

$$\frac{\partial C_i}{\partial t} + \frac{\partial v_z C_i}{\partial z} = Ri + m_i^{(t)} \qquad \ldots 9.1$$

Energy Balance:

$$\rho c_p \frac{\partial T}{\partial t} + v_z \frac{\partial T}{\partial z} = S_R + E_i^{(t)} \qquad \ldots 9.2$$

The maximum gradient model is often called the plug flow model. In this momentum balance is ignored since we normally assume the velocity is constant or some simple functions of z. in the energy balance the term SR represents the net energy released by the process during the chemical reaction indicated in the mass balance by R_i. The term mi$^{(t)}$ stands for the rate of molar transfer per unit volume of the ith species across the system boundaries of surface area S.

For an unsteady state tubular reaction with $v_r = v_Q = 0$ and symmetry in the θ direction

$$\frac{\partial C_i}{\partial t}+\frac{\partial v_z C_i}{\partial z}=\overline{D_L}\frac{\partial^2 C_i}{\partial z^2}+\overline{D_R}\frac{1}{r}\frac{\partial\left(r\frac{\partial C}{\partial r}\right)}{\partial r}+Rrxn \qquad \ldots 9.3$$

The concentration is a value at a point and is function of both r and z. The first step in the evolution of the maximum gradient balance is to multiple each term of the above equation by the elemental area 2πrdr, divide by the cross section area A and integrate each term from 0 to R.

$$\frac{1}{A}\int_0^R\frac{\partial C(r,z)}{\partial t}\,2\pi r dr+\frac{1}{A}\int_0^R\frac{\partial vz(r,z)C(r,z)}{\partial z}\,2\pi r dr$$
$$=\frac{\overline{D_L}}{A}\int_0^R\frac{\partial^2 C(r,z)}{\partial z^2}2\pi r dr+\frac{\overline{D_R}}{A}\int_0^R\frac{1}{r}\frac{\partial\left(r\frac{\partial C(r,z)}{\partial r}\right)}{\partial r}2\pi r dr+\frac{1}{A}\int_0^R Rrxn * 2\pi r dr$$

…9.4

Let us defined the average concentration and velocity across the tube cross section

$$\overline{C(z)}=\frac{1}{A}\int_0^R C(r,z)2\pi r dr$$

$$\overline{v_z(z)C(z)}=\frac{1}{A}\int_0^R v_z(r,z)(z)C(r,z)2\pi r dr$$

$$\overline{\frac{\partial C(z)}{\partial t}}=\frac{1}{A}\int_0^R\frac{\partial C(r,z)}{\partial t}2\pi r dr$$

$$\overline{\frac{\partial C(z)}{\partial z}}=\frac{1}{A}\int_0^R\frac{\partial C(r,z)}{\partial z}2\pi r dr$$

$$\overline{\frac{\partial v_z(z)C(z)}{\partial z}}=\frac{1}{A}\int_0^R\frac{\partial v_z(r,z)C(r,z)}{\partial z}2\pi r dr$$

$$\overline{\frac{\partial^2 C(z)}{\partial z^2}}=\frac{1}{A}\int_0^R 2\pi r\frac{\partial^2 C(r,z)}{\partial z^2}dr$$

$$\frac{\partial C(z)}{\partial t} + \frac{\partial v_z(z)C(z)}{\partial z} = \overline{D_L}\frac{\partial^2 C_i}{\partial z^2} + \overline{D_R}\left[\frac{\partial C(r,z)}{\partial r}2\pi r\right] + Rrxn \qquad \ldots 9.5$$

The middle term on the RHS is evaluated at the upper limit of R and at the tube centre

$$\overline{D_R}\left[\frac{\partial C(r,z)}{\partial r}2\pi R\right]$$

At the tube centre the flux will be 0

By symmetry

$$-\overline{D_R}\left|\frac{\partial C(r,z)}{\partial r}\right|(at\ r = R) = k\left[\overline{C(z)} - C_s(z)\right] \qquad \ldots 9.6$$

$$-\overline{D_R}\left|\frac{\partial C(r,z)}{\partial r}\right|(at\ r = R) = k\left[\overline{C(z)}\right] \qquad \ldots 9.7$$

CONVERSION IN TUBULAR CHEMICAL REACTORS

Consider the tubular chemical reactor for simplicity in analysis a first order reaction A-R will be assumed to be occurring

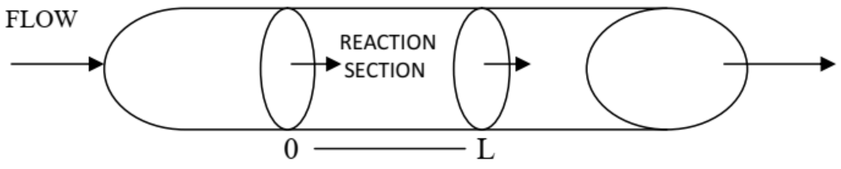

Fig. 9.1: Conversion in Tubular Reactor

The simplest type of model to use for predicting the conversion is the maximum gradient model. The physical assumptions are follows:

- There is flat velocity profile (turbulent flow)
- No radial dispersion (isothermal operation)
- No Axial dispersion
- With steady flow the time derivative or accumulation term is zero

$$v_z \frac{dC_A}{dz} = R_A = -kC_A \qquad \ldots 9.8$$

This is simple differential equation can be solved for the boundary condition that at z=0 the reactant concentration is the feed concentration.

$$C_A(0) = C_{A,0} \qquad \ldots 9.9$$

on integrating

$$\ln C_A = -k\frac{z}{v_z} + constt$$

$$C_A = (const)e^{-k\,^{z}/_{v_z}} \qquad \ldots 9.10$$

$$const = C_{A,0}$$

$$\frac{C_A}{C_{A,0}} = e^{-k\frac{z}{v_z}} \qquad \ldots 9.11$$

At the exit of the reactor the conversion is

$$(1-x_A) = C_A/C_{A,0} = e^{-kL/vz} = e^{-kt}$$

t = nominal holding time

$$= L/v_z$$

To assess the importance of axial dispersion the problem will be solved again with all the same assumptions expect that the axial dispersion term will be retained the general mass balance now reduces to

$$v_z \frac{dC_A}{dz} = \overline{D}_z \frac{\partial^2 C_z}{\partial z^2} - kC_A$$

The solution of equation is

$$\frac{C_A}{C_{A0}} = \frac{4a exp(\frac{1}{2} v_z\ L/\overline{D_z}\,)}{(1+a)^2 \exp\left[\left(\frac{a}{2}\right)\left(v_z \frac{L}{D_z}\right)\right] - (1-a)^2 \exp\left[-\left(\frac{a}{2}\right)\left(v_z \frac{L}{D_z}\right)\right]}$$

$$a = \left[1 + 4k \mp \frac{D_z}{v_z L}\right]^{1/2}$$

Macroscopic Description

Keywords: Models, Transport Phenomena Based, Macroscopic Description

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In this we ignore all the inside details of the subsystems, and a consequence no special gradients are involved in the mathematical statements. Only time remains as a differential independent variable in the general balances. The dependent variables such as concentration and temperature are not the functions of positions and here represents averages over the volume of the subsystems. For process with clearly defined boundaries, the macroscopic equations are as follows;

Mass Balance for α^{th} species:

$$\frac{d(m_{x,tot})}{dt} = -\Delta(\rho_\alpha \langle v \rangle S) + W_i^m + r_{\alpha,av} V_{tot} \qquad \dots 10.1$$

Momentum Balance:

$$\frac{d(\rho_{t,tot})}{dt} = -\Delta(\rho\langle v^2 \rangle S_i + \langle P \rangle S_i) + F_i^m + m_{tot} g_i + F_i \qquad \dots 10.2$$

Energy Balance:

$$\frac{dE_{tot}}{dt} = -\Delta\left[\left(\widehat{H} + \frac{1}{2}\frac{\langle v^3 \rangle}{\langle v \rangle} + \hat{\varphi}\right)(\rho\langle v \rangle S)\right] + q - W + Q^m + S_R \qquad \dots 10.3$$

MODEL OF FILLING OF AN EMPTY CYLINDER

Assume an insulated cylinder is completely evacuated and the filled with helium from a very large source at 1 atmosphere. Set up the governing relations between the amount of gas entering and its temperature in the cylinder.

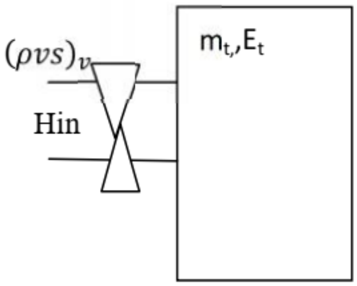

Fig. 10.1: Filing of a Gas Cylinder

We will make use of the energy and mass balances with the following simplifications;

$m_t = total\ mass$

E_t = total energy

Assumptions:

- No exit stream $(\rho V_S)_{OUT} = 0$
- No chemical reaction ($r_{xt} = 0, s_r = 0$)
- No potential energy change ($\Delta\Phi = 0$)
- No interphase mass transfer ($w^m = \beta^{(m)} = 0$)
- No work done since tank is rigid (w =0)
- No heat transfer (Q =0)

$$\frac{dM_t}{dt} = (\rho V_S)_{in} \qquad \ldots 10.4$$

$$\frac{dE_t}{dt} = [(\hat{U} + p\,\widehat{v} + \widehat{k})\rho vs] \qquad \ldots 10.5$$

Since no information is given to find the k.e. , we shall neglect this term, although the inlet nozzle may be of such a design that there is substantial k.e. in the inlet stream.

Let

$\hat{U} + p\,\widehat{v} = \widehat{h}$, enthalpy per hour of entering stream

$E_T = U_T$ no contributions kinetic and potential energy

If we assume $c_{v,t}$ is constant and take reference temp. T = 0,

$$c_{v,t}\frac{d(Tm_t)}{dt} = [\widehat{H}\mathrm{Pvs}] = (\ C_P\ \mathrm{T}\ \rho VS) \qquad \ldots 10.6$$

After differentiation of the left hand side of the above equation we have............

$$c_{v,t}\ [m_t\frac{dT_t}{dt} + T_t\frac{dm_t}{dt}] = c_{v,t}[\ c_{v,t}\ [n_t\frac{dT_t}{dt} + T_{t(pvs)in}\ ] \qquad \ldots 10.7$$

If the physical parameters are known then above equations can be solved simultaneously.

Alternate Classification of Transport Phenomena Models

Keywords: Models, Alternate Classifications

ALTERNATE CLASSIFICATION OF TRANSPORT PHENOMENA MODELS

There are many additional ways to classify mathematical models. For one purposes it is most satisfactory to first consider grouping the models into opposite points.

- **Deterministic vs. Probabilistic**
- Linear vs. Nonlinear
- Steady state vs. Unsteady state
- Lumped parameter vs. Distributed parameter

Deterministic vs. Probabilistic

Deterministic models are those in which each variable and parameter can be assigned a definite fixed number, or a series of fixed numbers, for any given set of conditions. The principle of uncertainty introduced.

Linear vs. Nonlinear

If the output, y, of a subsystem is completely determined by the input x ,

$$Y = Hx$$

The operation H represents any form of conversion of x into y. Suppose now two separate inputs are applied simultaneously to the subsystem so that;

$Y = H(X_1 + X_2) = H(X_1) + H(X_2) = Y_1 + Y_2$

A system is termed linear if its operator is linear, otherwise model is nonlinear.

- **Steady state vs. Non steady state models;**

Steady state means that the accumulation terms in the various balances of interest are zero. If the boundary conditions are time dependent the model is known as non steady state otherwise steady state.

- **Distributed vs. Lumped parameter model;**

In the case of lumped parameter model the system is considered to be homogenous, but in the case of distributed heterogeneous behaviour of system is to be considered.

Model of Distillation Column

The mass and energy balances are (x is the wt. Fraction of a component in the liquid and y is the wt. Fraction of a component in the vapour, l is the liquid flow rate and v is the vapour flow rate).

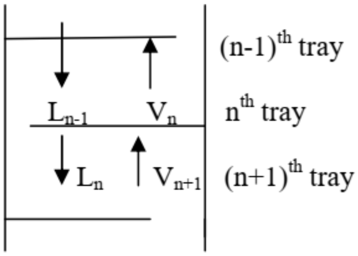

Fig. 11.1: Section of Discussion Column

Mass balance (of component α)

$$\frac{dm_{\alpha,n}}{dt} = L_{n-1}\, x_{\alpha,n-1} + V_{n+1}\, y_{\alpha,n+1} - L_n\, x_{\alpha,n} - V_n\, y_{\alpha n} \qquad \ldots 11.1$$

Mass (overall);

$$\frac{dm_{tot}}{dt} = L_{n-1} + V_{n+l} - L_n - V_n \qquad \ldots 11.2$$

Energy

$$\frac{dH_{tot}}{dt} = L_{n-1} h^L_{n-1} + V_{n+1}\, h^V_{n+1} - L_n\, h^L_n - V_n\, h^V_n + Q \qquad \ldots 11.3$$

In the above equations the mass transfer through the system boundary is written using the equations which are developed for microscopic description.

Steady state two phase flow:

Flow of superheated Freon-1 in horizontal pipes using the apparatus as shown in figure,

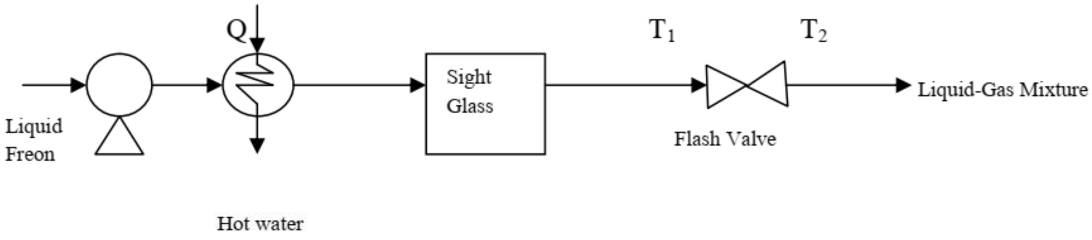

Fig. 11.2: Two Phase Flow in a Pipes

This is a steady state problem. [$\frac{dm_{td}}{dt} = \frac{dE_{td}}{dt} = 0$]

There is no interphase mass transfer.[$w^m = Q^m = 0$]

There is no reaction. [$r_{\alpha,avg.} = s_R = 0$]

There is no work done.[W=0]

The pipe is horizontal.[$\Delta\Phi = 0$]

The flow was turbulent.[$\frac{1}{2} \frac{<V^3>}{<V>}] \approx \frac{1}{2} V^2$

With this information the mass balance reduces to "in equals out "for the system defined from T_O to T_1 or T_1 *to* T_2.

$$\rho_0 V_0 S_0 = \rho_1 V_1 S_1 = \rho_2 V_2 S_2 = W$$

And energy balance equations becomes;

$$Q = W [(\widetilde{H_2} - \widetilde{H_1}) + \frac{1}{2}(V_2^2 - V_0^2)]$$

The term representing the change in i.e. proved to be very much less than the change of enthalpy and can be neglected. If the enthalpy of the vapour at;

$$\widetilde{H_2} = \Delta H_{vap2}\, w_2 + \widetilde{H_{L2}}$$

$$W_{V2} = \frac{\frac{Q}{W} - C_{P,L}(T_2 - T_O)}{\Delta H_{VAP2}}$$

$$W_{V2} = \frac{-C_{P,L}(T_2 - T_1)}{\Delta H_{VAP2}}$$

In above equations w indicates the wt. Fraction and the subscripts L and V indicate liquid and vapour respectively.

Population Balance Models

Keywords: Models, Population Balance

All the previous models discussed in last lectures have been based on the basic mass, momentum and energy balances. The equations that involve dispersion are most representative of a process when the mixing is on a relatively small scale. For mixing in stirred tanks (in turbulence), dispersion models are not effective. Certain categories of models which cannot successfully be treated within the framework of the models based on transport phenomena can be treated by the population balance concept.

The application of population -balance principles to the modelling of flow and mixing characteristics in vessels was formally organized by Danckwert's. He defined certain distribution functions for the residence time of the fluid elements in a process vessel.RTD functions give information about the fraction of the fluid that spends a certain time in a process vessel. RTD models do not give point- to – point variation of the dependent variables. Danckwert's description was based on macroscopic lumped-population-balance. Population balance models represents macro-mixing that are sufficient ti give adequate estimates of the behavior of the process.

Description of Flow Pattern's in Process Vessel's

There are two types of ideal flow patterns in our process vessels;

1. Plug flow pattern – Piston Flow
2. Bochmix Flow Pattern – Perfectly mixed

Plug flow occurs when the fluid velocity is uniform over the entire cross-section of the vessel.

Perfect mixing assumes that the vessel contents are completely homogenous down to a molecular scale.

Between these two extreme's lie flow patterns in actual process.

In channeling (known as by-passing) some elements of fluid slip on pass through the vessel considerably faster than others do. Channeling may be found in flow through purely packed vessels, through vessels of small length-to-diameter ratios or through heat exchanger's with proper baffling.

Stagnant packets (dead space) may occur in header's, at the base of pressure gauges, or in the odd-shaped corner's, represents regions with extremely pure contacting.

AGE DISTRIBUTION FUNCTIONS

The residence time of a fluid element is the time that elapses from the time the element enters the vessel to the time it leaves it. The age of a fluid element at a given instant of time is the time that elapses between the element's entrance into the vessel and the given instant , and is of course , less than or equal to the residence time. The age is equal to the residence time for those molecules that are just leaving the vessel.

INTERNAL AGE DISTRIBUTION OF A FLUID IN A CLOSED VESSEL

The functional notation I(t) will be used for the internal age distribution frequency of fluid elements in a vessel. I(t) have the unit- fraction of ages per unit time.

$$\int_0^\infty I(t)\,dt = 1 \qquad \ldots 12.1$$

The time t=0 refers to an arbitrary initial time and not the start of the flow of fluid into the vessel. In physical terms, eq. (12.1) states that all fluid has an age between 0 and ∞.

As a consequence of the above, the fraction of vessel contents younger than a specified age t is,

$$\int_0^t I(t')\,dt' = 1 \qquad \ldots 12.2$$

While the fraction older than t is ,

$$\int_t^\infty I(t')\,dt' = 1 - \int_0^t I(t')\,dt' \qquad \ldots 12.3$$

Age Distribution of the Exit Stream; The Residence Distribution of fluid in a closed vessel, E(t)

The function E(t) is the age distribution frequency of the fluid elements leaving the vessel and has the units of fraction of ages per unit time. The fraction of exit ages itself is E(t)Δt. The function is normalized to;

$$\int_0^{\infty} E(t)\,dt = 1 \qquad \text{…12.4}$$

The fraction of fluid in the exit stream younger than age t is

$$\int_0^{t} E(t')\,dt' = 1 \qquad \text{…12.5}$$

while the fraction of material older than t is

$$\int_t^{\infty} E(t')\,dt' = 1 - \int_0^{t} E(t')\,dt' = 1 \qquad \text{…12.6}$$

The mean RTD is found from the first moment

$$\bar{t} = \int_0^{\infty} tE(t)\,dt = \frac{V}{Q} \qquad \text{…12.7}$$

$$\frac{V}{Q} = \bar{t} = \boldsymbol{\tau}$$

In a similar fashion the mean age of fluid elements inside the vessel is,

$$\bar{t_1} = \int_0^{\infty} tI(t)\,dt \qquad \text{…12.8}$$

Intensity Function, Λ(t)

It is defined as fraction of fluid in the vessel of age t that will leave at time between t and t+Δt. The intensity function is useful in detecting the existence of dead space and by passing.

Relations between Age Distribution Functions:

The three age distribution frequency functions described above are related through the unsteady state macroscopic age population balance. The balance is made in the units of time. The input age distribution is zero. The general macroscopic population balances can be used to relate E(t) and I(t), but a simpler alternate method is used here.

Consider a constant volume vessel, V, with constant flow rate Q and call all fluid entering the vessel at t>0 new fluid. The existing contents at t=0 are the old fluid. At some time t, eq. 12.2 gives the function of new fluid.

$$\text{Amount of new fluid in vessel} = V\int_0^t I(t')\,dt'$$

Eq. 12.6 gives the fraction of out flowing fluid at any instant of time, that has an age greater than t; the amount of old fluid that has left the vessel during all times from 0 to t is

$$\text{Amount of old fluid gone from the vessel} = \int_0^t Q\,dt' \int_{t'}^{\infty} E(t'')\,dt''$$

Then by a simple balance, the old fluid left must have been replaced by the new fluid,

$$V\int_0^t I(t')\,dt' = \int_0^t Q\,dt' \int_{t'}^{\infty} E(t'')\,dt'' \qquad \text{…12.9}$$

Differentiation of both sides of eq. 12.9 with respect to time with the introduction of eq.12.7 gives,

$$\bar{t}I(t) = \int_t^{\infty} E(t')\,dt' = 1 - \int_0^t E(t')\,dt' \qquad \text{…12.10}$$

Differentiating once more,

$$E(t) = -\bar{t}\frac{dI(t)}{dt} \qquad \text{…12.11}$$

The intensity function can also be related to the E(t) and I(t) functions from

$$\left\{\begin{array}{l}\text{Amount of fluid}\\ \text{leaving between}\\ \text{t and t+}\Delta\text{t}\end{array}\right\} = \left\{\begin{array}{l}\text{Amount not leaving}\\ \text{before time t}\end{array}\right\} \left[\begin{array}{l}\text{Fraction of age t}\\ \text{that will leave}\\ \text{between times t, t+}\Delta\text{t}\end{array}\right]$$

$$QE(t)dt = [VI(t)][\Lambda(t)dt] \qquad \text{…12.12}$$

$$\Lambda(t) = \frac{1}{\bar{t}}\frac{E(t)}{I(t)} = -\frac{d[ln\bar{t}I(t)]}{dt} \qquad \text{…12.13}$$

Each of the age distribution functions can be expressed in dimensionless form.

$$\theta = \frac{t}{\bar{t}} \qquad \text{…12.14}$$

Thus, $E(\theta)d\theta = E(t)dt, I(\theta)d\theta = I(t)dt$

$$E(\theta) = \bar{t}E(t) \qquad \text{…12.15}$$

$$I(\theta) = \bar{t}I(t) \qquad \text{…12.16}$$

$$\Lambda(\theta) = \bar{t}\Lambda(t) \qquad \text{…12.17}$$

$$E(\theta) = -\frac{d\,I(\theta)}{d\theta}\,I(\theta) \qquad \text{…12.18}$$

$$\Lambda(\theta) = \frac{E(\theta)}{I(\theta)} = - -\frac{\ln(\theta)}{d\theta} \qquad \text{…12.19}$$