General Population Balance

Keywords: Models, General Population Balance

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Consider a distribution of entities, $\Psi(x, y, z, \xi_{1,}\xi_2, \dots \dots \dots, \xi_m, t)$, where x, y, z represents ordinary special coordinates, t is the time, and ξ_i represents the ith property of the entity. For example ξ_1 could be the area of a fluid element, or the activity or area of catalyst particle in a reactor.

$$\Psi \Delta x \Delta y \Delta z \Delta \xi_1 \dots \dots \dots \dots \Delta \xi_m \qquad \dots 14.1$$

is the fraction of entities in the geometric volume elements $\Delta V = \Delta x \Delta y \Delta z$, with property values in the range of $\Delta \xi_1, \Delta \xi_2, \dots \dots \dots \dots \Delta \xi_m$. Since all the entities must be in some region and have some property value,

$$\int \Psi(x, y, z, \xi_{1,}\xi_2, \dots \dots \dots, \xi_m, t) dx, dy, dz, d\xi_1, \dots . d\xi_m = 1 \qquad \dots 14.2$$

The net generation term will consist of birth and death functions;

$$B = \frac{birth\ of\ entities}{(unit\ time)(unit\ geometric\ volume)(unit\ property\ change)} \qquad \dots 14.3$$

$$D = \frac{death\ of\ entities}{(unit\ time)(unit\ geometric\ volume)(unit\ property\ change)} \qquad \dots 14.4$$

There are z+m independent variables that can be thought of as a z+m dimensional space. For an arbitrary small volume element in this space, R, the balance is,

Accumulation = Net Generation

$$\frac{d}{dt}\int \Psi dR = \int (B - D) dR \qquad \dots 14.5$$

where $dR = dxdydzd\xi_1 \dots \dots . d\xi_m$

For one dimension,

$$\frac{d}{dt}\int_{\alpha(t)}^{b(t)} f(x,t)dx = \int_{\alpha(t)}^{b(t)} \frac{\partial f(x,t)}{\partial t}dx + f[b(t),t\}\frac{db(t)}{dt} - f[\alpha(t),t]\frac{d\alpha(t)}{dt}$$

$$= \int_{\alpha(t)}^{b(t)} \left\{\frac{\partial f(x,y)}{\partial t} + \frac{d}{dx}\left[\frac{dx}{dt} f(x,t)\right]\right\} dx \qquad \ldots 14.6$$

$$\int \frac{\partial \Psi}{\partial t} + \frac{\partial(v_x\Psi)}{\partial x} + \frac{\partial(v_y\Psi)}{\partial y} + \frac{\partial(v_z\Psi)}{\partial z} + \sum_{i=1}^{m} \frac{\partial}{\partial \xi_i}\{(v_i\theta) + D - B\}dR = 0 \qquad \ldots 14.7$$

$$\frac{\partial \Psi}{\partial t} + \frac{\partial(v_x\Psi)}{\partial x} + \frac{\partial(v_y\Psi)}{\partial y} + \frac{\partial(v_z\Psi)}{\partial z} + \sum_{i=1}^{m} \frac{\partial}{\partial \xi_i}\{(v_i\theta) + D - B\} = 0 \qquad \ldots 14.8$$

Eq.(14.8) is the general microscopic population balance in x,y,z coordinates.
In many cases the described spatial dependence of Ψis not known and the average values of the properties are required. Then a very useful balance can be obtained from eq. 14.8 by integrating it over. The geometric volume V in vector notation is,

$$\int \left[\frac{\partial \Psi}{\partial t} + \nabla.(\vec{v}\Psi) + \sum_{i=1}^{m} \frac{\partial}{\partial \xi_i}\{(v_i\theta) + D - B\}\right] dxdydz = 0 \qquad \ldots 14.9$$

The geometrically averaged distribution function of interest is

$$\overline{\Psi} = \frac{1}{V}\int \Psi\, dV \qquad \ldots 14.10$$

$$\int \frac{\partial \Psi}{\partial t} dV = \frac{d}{dt}\int \Psi\, dV - \int \nabla.(v_s\Psi)dV = \frac{d}{dt} \qquad \ldots 14.11$$

The second line was obtained by the use of Gaussian divergence theorem. The term v_s stands for the velocity of any part of the surface S, containing the volume V and n is a vector normal to the surface pointing outward. Combing the result we get,

$$\int \left(\frac{\partial \Psi}{\partial t} + \nabla.v\Psi\right) dv = \frac{d}{dt}\int \Psi dv + \int n.(v - v_s)\Psi \qquad \ldots 14.12$$

Finally, the surface integral in eq.(14.12) can be broken up into two parts;

a) The integral over the inlet and outlet pipe surfaces, S_1 and S_2.
b) The integral over the remainder if the surface,S^1 =S- S_1- S_2

$$\int_S n.(v - v_s)\Psi ds = \int_{s_1+s_2} n.(v - v_s)\Psi ds + \int_{s_1} n.(v - v_s)\Psi ds = -\int_{s_1} v_1\Psi_1 ds_1 + \int_{s_2} v_2\Psi_2\, ds_2 + 0 \quad \ldots 14.13$$

where the minus sign appears in the first term because n was directed outwards and the flow at S_1 is inward.

Putting all of these terms back into Eq. 14.9 as using the definition of Ψ gives the final microscopic balance.

$$\frac{1}{V}\frac{\partial}{\partial t}(V\Psi) + \sum_{i=1}^{m}\frac{\partial(v_i\overline{\Psi})}{\partial \xi_i} + \overline{D} - \overline{B} = \frac{1}{V}[Q_{in}\Psi_{in} - Q_{out}\Psi_{out}] \quad \ldots 14.14$$

Source: http://nptel.ac.in/courses/103107096/14