Boundary Condition notes

-Bill Green, Fall 2015

Typically we need to specify boundary conditions at every boundary in our system, both the edges of the domain, and also where there is a discontinuity in the equations (e.g. you might you different equations inside a catalyst particle than outside it. The discontinuity might just be in parameters (e.g. the rate coefficient and the diffusivity change between inside and outside the catalyst). There are also typically discontinuities when there are phase changes, e.g. at the surface of a puddle.

Sometimes there are symmetries that tell you a boundary condition, e.g. $dC/dr = 0$ at $r=0$ if a problem has cylindrical or spherical symmetry (otherwise there would be a cusp in $C(r)$, which is usually unphysical). Sometimes one knows the value of a variable on a boundary so Dirichlet boundary condition. Often one assumes that nothing changes after a certain point, i.e. all the derivatives are zero, so von Neumann boundary conditions may be used.

When the state variable is a conserved scalar, then one knows that the flux of that scalar approaching the boundary must equal the flux leaving from the other side. This gives conditions like this for concentrations C (where D is the diffusivity and v is the flow into the boundary).

$-D\, dC/dx + v\, C$ on left side of boundary $=$ $-D\, dC/dx + v\, C$ on right hand side

Where the velocity v is positive if it is moving in the +x direction.

If the flow velocity is zero or negligible in one of the regions, one of the terms will disappear. Note that dC/dx can jump at an interface, e.g. if D is modeled as being discontinuous across the boundary, usually dC/dx will be discontinuous to match, so that the flux will be continuous.

A good example is the energy balance between a solid impermeable particle and the fluid that surrounds it. The heat transfer coefficient between the bulk of the fluid and the particle is known for many geometries and flow conditions (recall Nusselt numbers), so the energy flux coming in to the particle is:

$h(T_{bulk} - T_{surface})$

This must equal the energy flux at the surface of the particle, looking from the inside. For example for a spherical particle its magnitude is:

$k\ *dT/dr$

Where is the thermal conductivity of the solid. Putting these together, the boundary condition is

$h(T_{bulk} - T_{surface}) + Kappa*dT/dr = 0$

Note that often you would know (e.g. could easily measure) T_{bulk} but would need to compute the unknown $T_{surface}$ and dT/dr.

Another version of this flux conservation principle is the "Danckwerts" boundary conditions for flow into a packed-bed catalytic reactor:

$$F*y\_feed = -\rho \; AD*dy/dz + F*y$$

Where y is the mass fraction of the species of interest, ρ is the density, A is the cross-sectional area, and F is the mass flow rate (which is conserved across the boundary). Note that this is approximating that the mass fraction gradient is very small outside the reactor so we omitted the $-\rho$ A D*dy_feed/dz term from the left hand side, this approximation may not be very accurate.

For an example of using the Danckwerts condition: if y is a product absent from the feed, y_feed might be zero but y inside the reactor will be non-zero, so

$$0 = -\rho \; A D \; dy/dz + F*y$$

The analogous flux-balance equations for a multi-dimensional problem, where the boundary is perpendicular to the z-axis:

$$Vz*y\_feed = -D*dy/dz + Vz*y$$

Note that the velocity in the z direction Vz usually jumps as the flow enters the reactor because the packed bed reduces the free cross-sectional area, and because the temperature increase changes the density.

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