

the macroscopic equations, we need a control volume, say 10 times larger than the “point box”, *i.e.* about 0.1 μm . Bear in mind however that this control volume must in turn be much smaller than the computational domain, giving another factor of 10–100 at least, resulting the “internal” lengthscale of 1–10 μm . Thus, the continuum equation cannot be expected to be reliable below 1–10 μm .

In addition, when modelling fluid motions in a microchannel of diameter of 10 μm (10^{-5} m) using CFD codes, if the mesh in the *Y* direction has 100 cells (in the control volume), each cell thus has a scale of 10^{-7} m, which would be smaller than the “internal” lengthscale as discussed earlier. Furthermore, the no-slip boundary condition at the wall commonly fails at a scale of 10^{-7} m.^{104,105}

What about meso devices? The flow in meso COBCs is laminar, often in the Stokes (or creeping) flow regime, in order to accommodate the required residence time. There have been debates on why there is no diffusion velocity in the macroscopic Navier–Stokes equations,^{106,107} as diffusion is an irreversible flow, while convection is regarded as a reversible event. From a CFD viewpoint, modelling of diffusion velocity is often done with the extended Navier–Stokes equations, where more than one mass conservation equation is solved together with other terms (*e.g.* chemical reactions, density differences) that could create a concentration gradient to act as the driving force.

The relativity of convection and diffusion was captured by a dimensionless number called the Peclet number ($Pe = Lu/D$),^{108,109} where *L* is a characteristic length scale (or reactor system). When the Peclet number is greater than one, the influence of convection exceeds that of diffusion in balancing the overall mass transfer or mass flux, as in macro COBCs. When the Peclet number is less than one, diffusion plays a more significant role in mass transfer than convection, like in micro channels. It is however difficult to quantify the relative contributions of convection and diffusion in meso COBCs. Figure 3.10

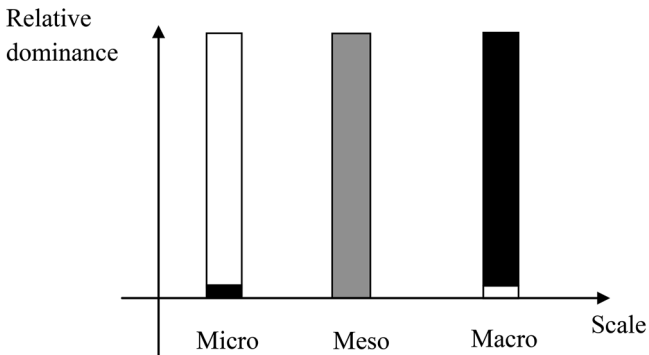


Figure 3.10 Illustration of degree of significance *vs.* scale (Filled rectangles denote convection, empty rectangles denote diffusion, grey colour refers to unknown).