Understanding Classical Diffusion Theory in a Cleanroom Airflow Field

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Note: The following is the theory section to a field study supported the theory presented below. The client for whom the study was performed and bore the cost thereof has declined to have the experimental data published.

The mass transfer mechanism of gaseous species diffusion in a cleanroom environment seems to be largely misunderstood. The classical definition of mass transfer by diffusion refers to movement of a molecular species relative to another. Both experiments and theory have shown that diffusion can result from pressure gradients (pressure diffusion), temperature gradients (thermal diffusion), external force fields (forced diffusion) and concentration gradients [Reid et al]. Diffusion mass transfer by means other than a concentration gradients are usually second order effects. For this reason, diffusion due to a concentration gradient, or ordinary diffusion, is often the only molecular mass transfer mechanism considered in this investigation.

With the exception of some specially controlled environments, diffusion is a composite of several mechanisms --specifically ordinary diffusion and flow turbulence. The question addressed in this study is if, and under what conditions, does ordinary diffusion play a significant role in the mass transfer of a gaseous contaminate in a cleanroom environment.

Ordinary diffusion is described by Fick's Law as

$$J = -D\frac{\partial C}{\partial X}$$

where J is the molar flux, D is the diffusion coefficient and C is the concentration of the species of interest. For many binary gas systems, the concentration can be defined in terms of partial pressures by applying the Ideal Gas law. This has led to a common misunderstanding that gaseous contaminate propagation, such as in a cleanroom, is only a function of partial pressure differences. What is not necessarily obvious is that the partial pressure terms are a function of the turbulence in the flow field. That is, the bulk air and/or micro- turbulence directly affects the concentration gradients, and thus the rate of ordinary diffusion.

The governing equations for CFD are algaebraic approximations of the Navier-Stokes equations that describe viscous, incompressible fluid flow. These equations form a set of differential equations, the generic form of which is called the Convection-Diffusion (sometimes called the Advection-Diffusion) equation. It is of the form

$$\frac{\partial}{\partial t}(r \cdot j) + div(r \cdot \vec{u} \cdot j) - div(\Gamma \cdot grad\, j_{l}) = R_l$$

transient + advection - diffusion = source where φ represents predictable quantities such as velocity, temperature or concentration [Flovent Manual]. A molecular species that is both advected and diffused follows the Advection-Diffusion equation of the form

$$\frac{\partial(C)}{\partial t}+\frac{\partial(uC)}{\partial x}+\frac{\partial(vC)}{\partial y}+\frac{\partial(wC)}{\partial z}-\frac{\partial}{\partial x}\left(D_{eff}\,\frac{\partial c}{\partial x}\right)-\frac{\partial}{\partial y}\left(D_{eff}\,\frac{\partial c}{\partial y}\right)-\frac{\partial}{\partial z}\left(D_{eff}\,\frac{\partial c}{\partial z}\right)=0$$

with C defined as the concentration gradient (kg species/cubic meter fluid), and

$$D_{eff} = D + D_t$$

where D is the ordinary diffusion coefficient of the contaminate species in the fluid medium. D_t is the turbulent diffusion coefficient, defined as

$$D_t = \frac{m_t}{Sc_t \cdot r}$$

where Sc_t is the turbulent Schmidt number and μ_t is the turbulent viscosity. Since μ_t is a direct function of the representative flow field velocity, determining which diffusion coefficient dominates will be a function of the cleanroom's average velocity.

Computational Fluid Dynamics methodologies have been scrutinized for their ability to accurately predict turbulent diffusion [Baker et al]. Accurately modeling a flow field in terms of laminar/turbulent behavior has been the subject of much development in recent years. Care must be taken in choosing the most appropriate turbulence mathematical form. This need arises from the necessary discretization of the solution domain – that is, the turbulent length scale is usually much, much smaller than a practical grid cell size. If turbulent diffusion is the dominant mechanism for molecular species mass transfer (usually the case), the mathematical turbulence model selection is vital for correctly modeling the motion of a gaseous contaminate.

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