

# LES and Atmospheric Chemistry/Aerosol Modeling ?

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# LES and Closure

- LES models assume that all scales above the filter scale (spatial) are fully resolved.
- In practice, the model spatial scale becomes the filter scale
- The sub-grid scale (SGS) or below filter scale (for turbulence) for example can be represented by Smagorinsky dissipation equation (this is all unresolved scales below filter length scale)
- $\mu_{sgs} = \rho (C_s \Delta)^2 |S|$     delta is the filter scale
- In 1-D the equation for any reactive tracer would be
- $$\frac{\partial \langle w C_i \rangle}{\partial z} = \langle w^2 \rangle \frac{\partial C_i}{\partial z} - \frac{\partial \langle w^2 C_i \rangle}{\partial z} + \frac{g}{\theta} \langle C_i \theta \rangle - \frac{1}{\rho} \langle C_i \frac{\partial P}{\partial z} \rangle + \langle w R_i \rangle$$
- Using the LES model for dynamics, we will be resolving these terms independently, which gives us an opportunity to fully represent the flow-chemistry interactions in a turbulent flow.

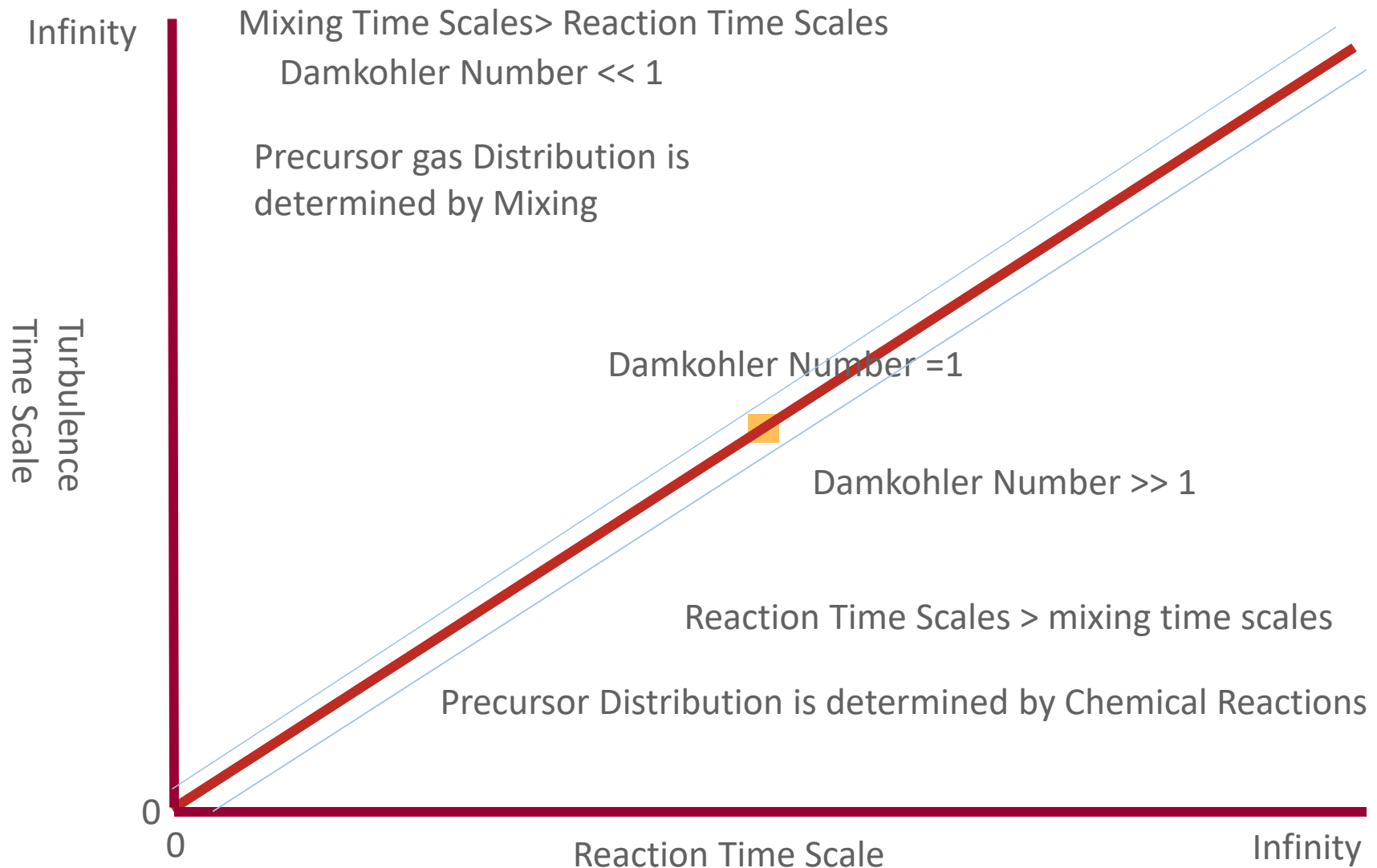


## LES, particles and reactive precursors

- We need to model the SGS for 'some' of the tracers, which ones are those?
- $\langle wC_i \rangle = \frac{2k}{\epsilon A} \langle w^2 \rangle \frac{\partial C_i}{\partial z}$  (?) (SGS scalar flux needed for closure)
- To determine which of the chemical precursors or may be even aerosols that are changing rapidly to include in a LES formulation can be assessed using two ratios, one is the Damkohler number and the second is the segregation ratio
- Damkohler number is simply the ratio of reaction time scale/turbulent time scale.
- Reaction Time Scale =  $\frac{1}{k \cdot \text{reactant}}$
- Turbulent Time Scale =  $\frac{ku^{**}}{z_0}$

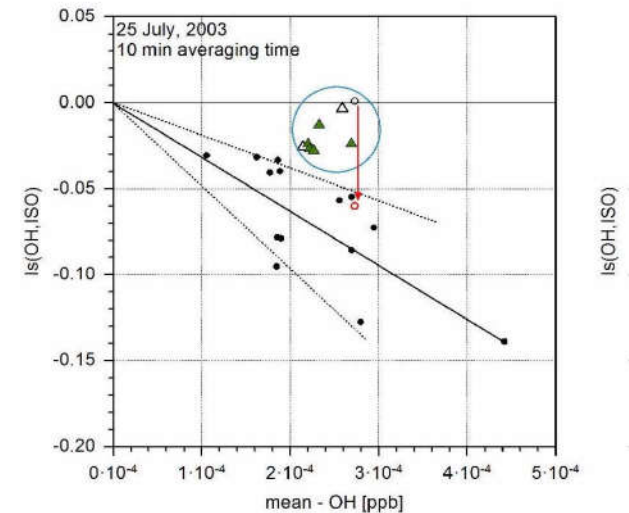
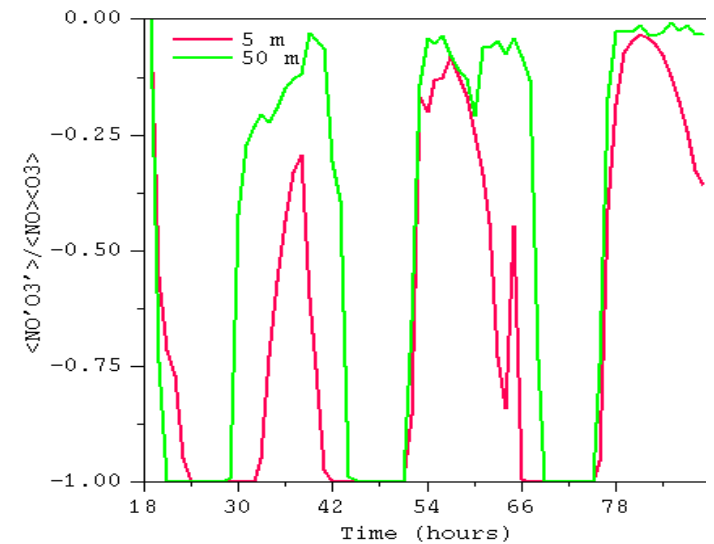


# Damkohler Number (Reaction Time/Mixing Time)



# LES, particles and reactive precursors

- If DN is much greater than one then the reaction time scales are bigger than turbulence time scales and we need not worry about turbulence at SGS scales as having any effect on the precursor chemistry or aerosol chemistry
- A second concept of interest would be segregation ratio. This is defined as the ratio of the covariance of a reactant (in terms of Reynold averaging this would be the 'primed' quantities) to their mean values. The segregation ratios vary between -1 and 0. Values closer to -1 signify complete segregation and closer to 0 signifies complete mixing  $\frac{\overline{C_i' C_j'}}{\overline{C_i} \overline{C_j}}$  (biomolecular reaction)
- To includes aerosol chemistry into the LES framework, we really have to determine which of the reactions are fast enough that we need to consider mixing at these scales that would give significantly different results.



Ding et al., 2003

