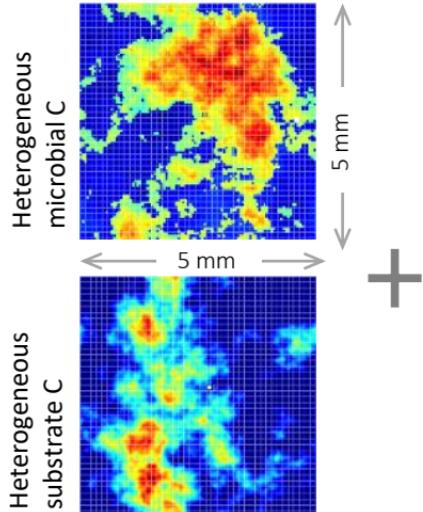
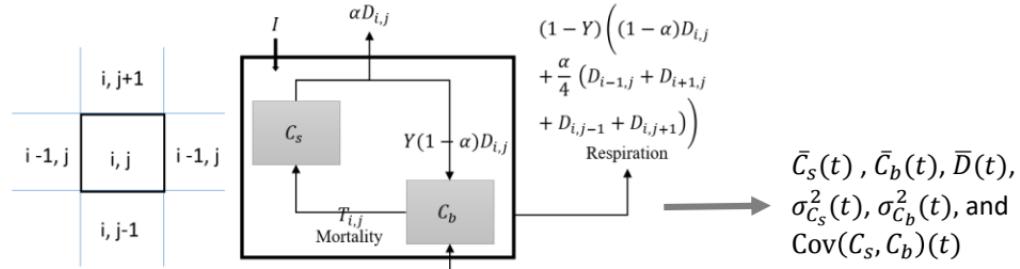


Numerical spatial averaging



Microscale model



$$D = k_L C_s$$

$$D = k_M C_s C_b$$

$$D = \frac{k_{MM} C_s C_b}{K_{MM} + C_s}$$

$$D = \frac{k_{IMM} C_s C_b}{K_{IMM} + C_b}$$

Linear  
Multiplicative  
MM  
Inv. MM

$$\frac{\alpha}{4} (D_{i-1,j} + D_{i+1,j} + D_{i,j-1} + D_{i,j+1})$$

Analytical upscaling

Microscale model

$$D = k_L C_s$$

$$D = k_M C_s C_b$$

$$D = \frac{k_{MM} C_s C_b}{K_{MM} + C_s}$$

$$D = \frac{k_{IMM} C_s C_b}{K_{IMM} + C_b}$$

Scale transition theory

Macroscale model

$$\bar{D} = \bar{k}_L \bar{C}_s + SOT$$

$$\bar{D} = \bar{k}_M \bar{C}_s \bar{C}_b + SOT$$

$$\bar{D} = \frac{\bar{k}_{MM} \bar{C}_s \bar{C}_b}{\bar{K}_{MM} + \bar{C}_s} + SOT$$

$$\bar{D} = \frac{\bar{k}_{IMM} \bar{C}_s \bar{C}_b}{\bar{K}_{IMM} + \bar{C}_b} + SOT$$

Numerical results are explained using results from analytical upscaling