The Concept of Block-Effective Macrodispersion for Numerical Modeling of Contaminant Transport

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Background

- Upscaling of permeability has been a major area of research;
- Important results available for effective conductivity for various models of spatial variability, various flow regimes and space dimensionalities;
- Theories are also available for upscaling to the numerical grid-block scale (length scale of the homogenized domain is comparable to the scale of heterogeneity);
- Much less work has been done on the transport side, specifically:
- how to assign dispersion coefficients to numerical grid blocks?

Goal of this presentation:

- Propose an approach toward a rational design of numerical analysis of transport which accounts for the various length scales affecting transport including: scales of heterogeneity, pore-scale dispersivity, dimensions of the solute plume, numerical grid block dimensions and travel distances, as well as space dimensionality;
- On a more fundamental level: bridge between stochastic concepts and numerical applications;

A common stochastic approach for modeling transport: The Concept of Macrodispersivity

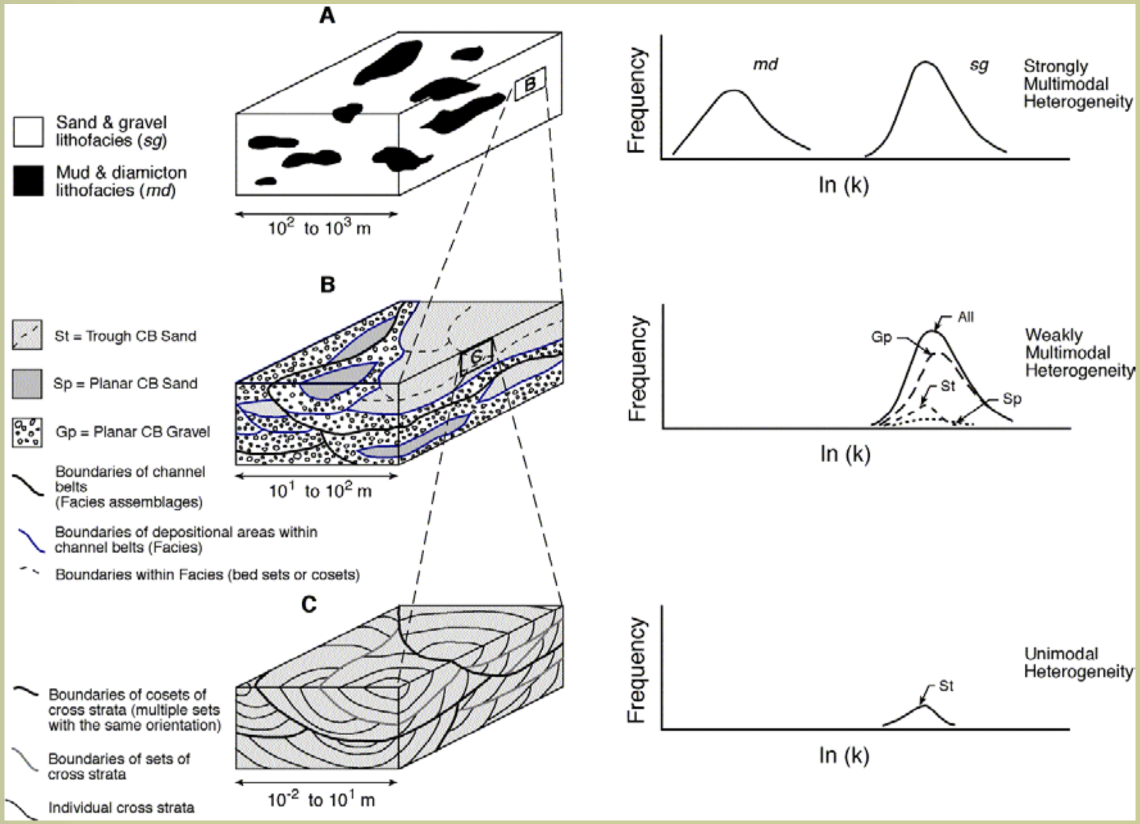
$$\frac{\partial C}{\partial t} + \mathbf{U} \cdot \nabla C = \nabla \cdot \left[\left(\mathbf{D} + \mathbf{D}_d \right) \nabla C \right]$$

Mean velocity

Macrodispersion tensor

Local pore-scale dispersion tensor

Transport in complex geological structure can be analyzed: multi-scale, hierarchical heterogeneity

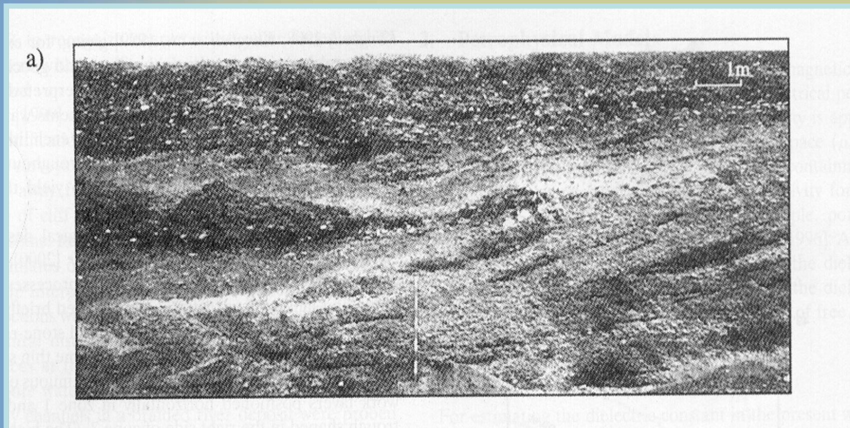


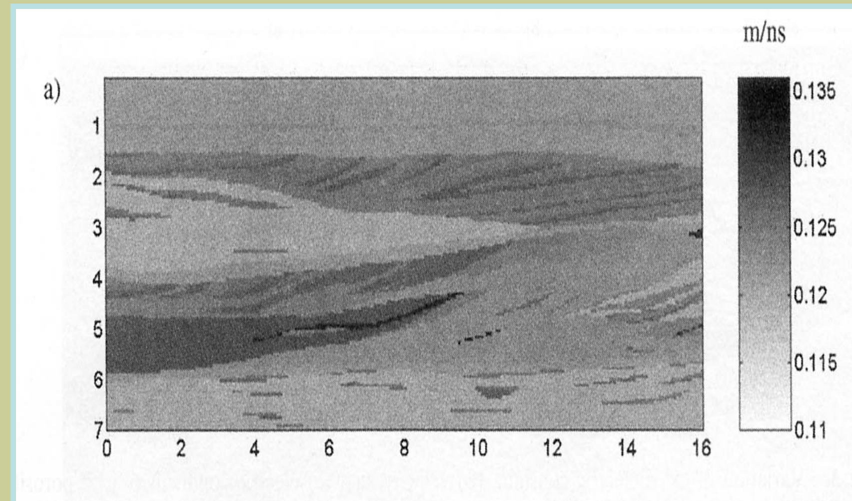
Hierarchical organization of lithofacies and corresponding permeability Modes (Ritzi et al., Water Resources Research, 40(3), 2004)

Important considerations:

- Concept is limited to modeling plumes that are large with respect to the scales of heterogeneity (ergodic*), because:
- When plume is ergodic, all variability is local, and its effects can be modeled deterministically through dispersion coefficients;
- This concept is not useful in numerical applications, where we usually deal with non-ergodic plumes, and in that case:
- It is important to capture the large scale spatial variability directly on the grid;
- *(Dagan, G., JFM, 1991)

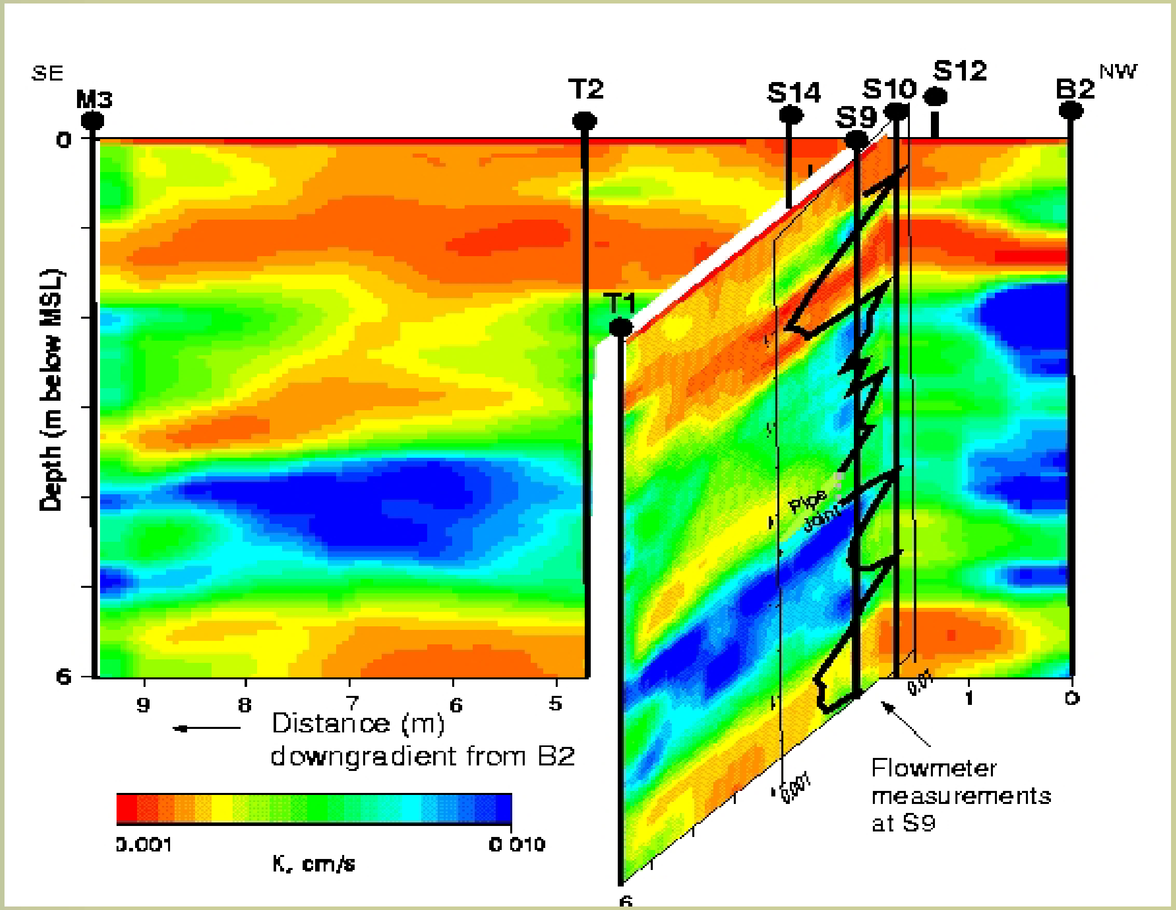
Large scale variability of the hydraulic properties
can be identified using GPR





Kowalsky, M., et al, *Water Resources Research*, 37(6), 2001

Subsurface imaging using GPR at the Oyster site in Virginia:



Hubbard et al., *Water Resources Research*, 37(10), 2001

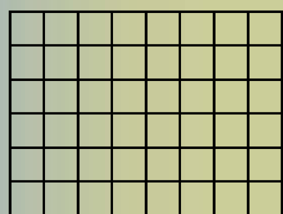
Detailed Site Characterization and Fine Grid Simulation

$$\frac{\partial C}{\partial t} + (\mathbf{U} + \mathbf{u}') \cdot \nabla C = \nabla \cdot \left[(\cancel{\mathbf{D}} + \mathbf{D}_d) \nabla C \right]$$

$\boxed{\text{Heterogeneous velocity field}}$

MONTE CARLO SIMULATIONS

Detailed, high resolution
Spatial distributions



$$\Delta \approx I_Y / 4$$

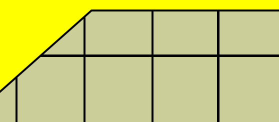
High computational cost

Block-scale dispersion tensor

$$\frac{\partial C}{\partial t} + (\mathbf{U} + \overline{\mathbf{u}}') \cdot \nabla C = \nabla \cdot \left[(\mathbf{D}_b + \mathbf{D}_d) \nabla C \right]$$

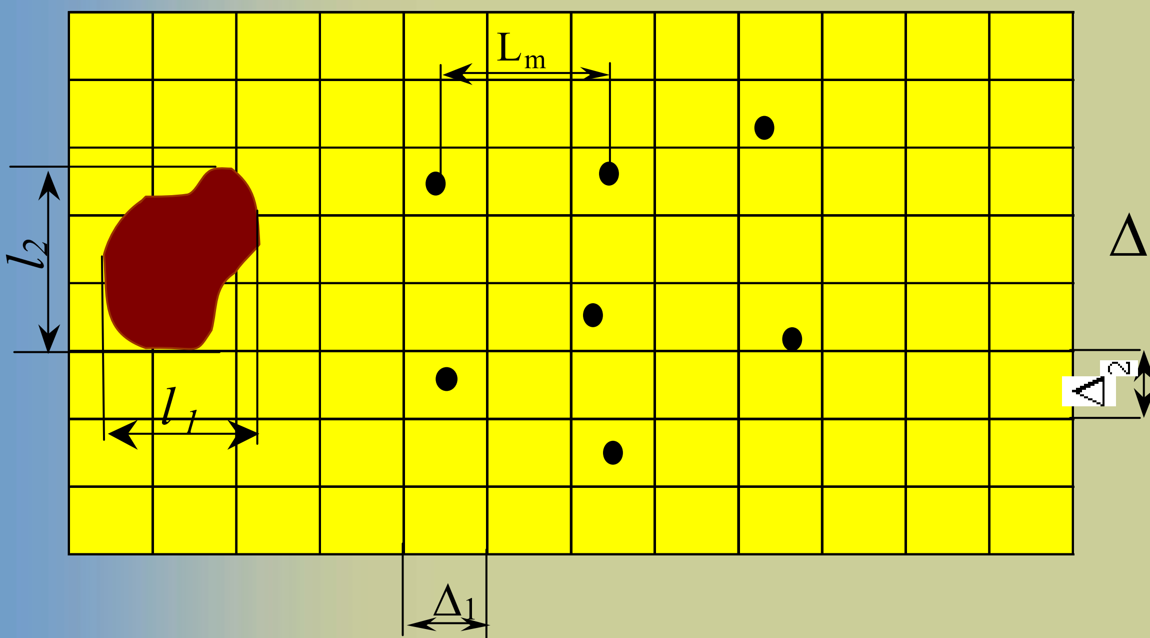
Reproduced over the grid

$$\mathbf{D}_b \rightarrow \boxed{f(\tilde{\mathbf{u}}')}$$



Measures should be taken to compensate for the wiped-out variability

Length-scales



l_1, l_2 : plume dimensions

L_m : spacing between measurements

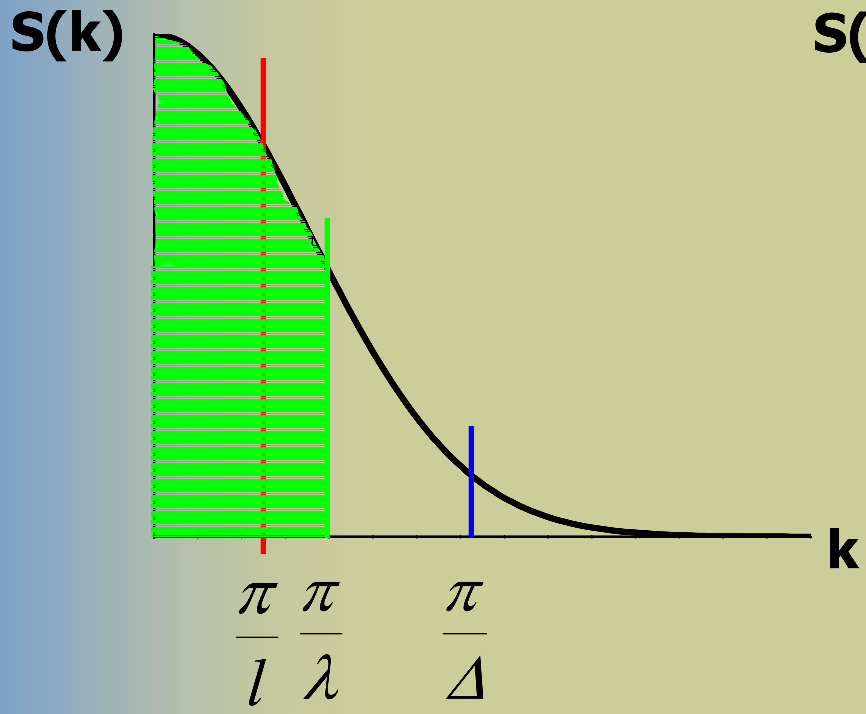
Δ_1, Δ_2 : grid dimensions

2λ : smallest length scale reproducible on the grid

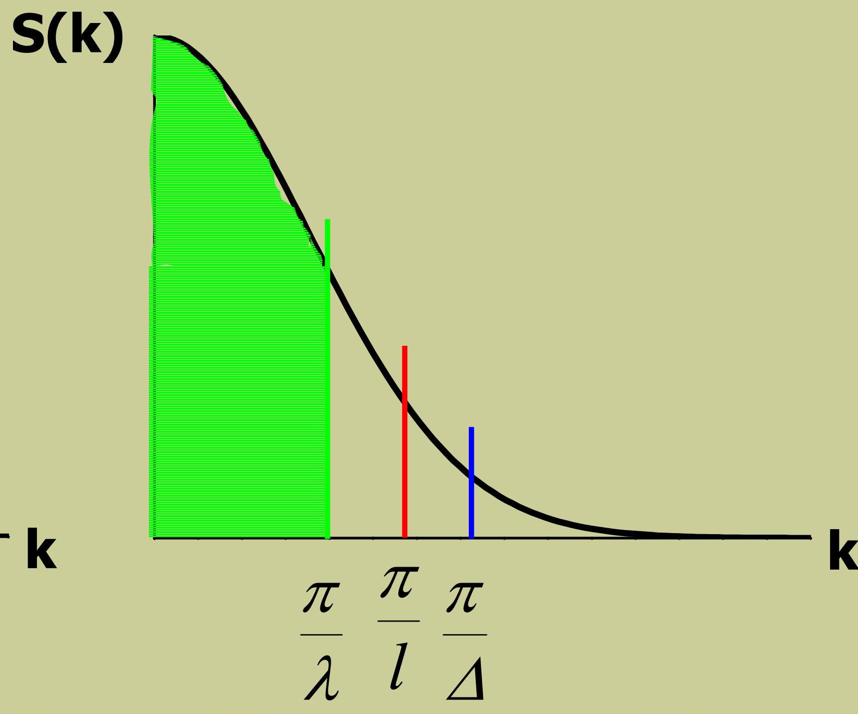
Practical limitation $\lambda > \Delta$

Nyquist Theorem: relates between the sampling scale and the identifiable scales

LARGE PLUME



SMALL PLUME



Block-scale macrodispersion

$$Y = \ln K; \quad Y = m_Y + \overline{Y}' + \widetilde{Y}'$$

Wiped-out variability

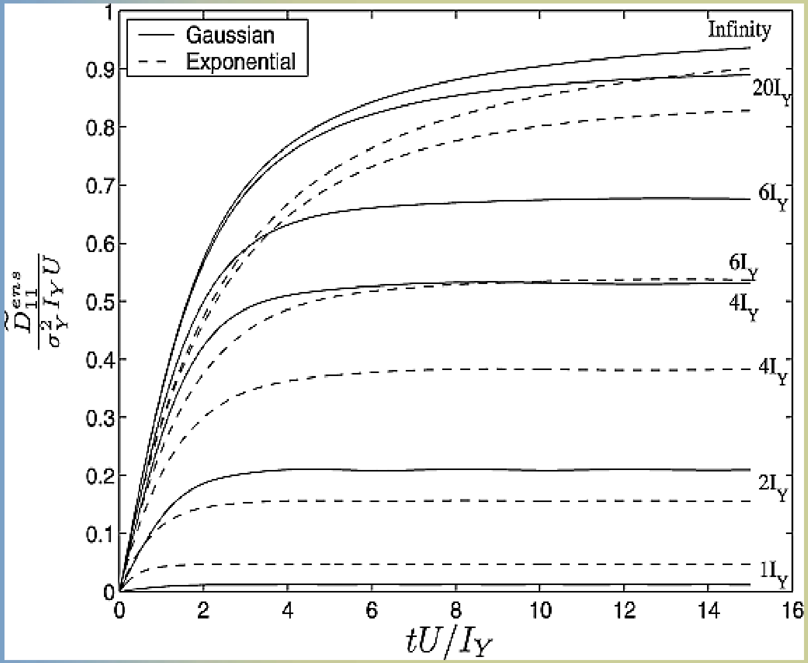
Variability reproduced directly on the grid

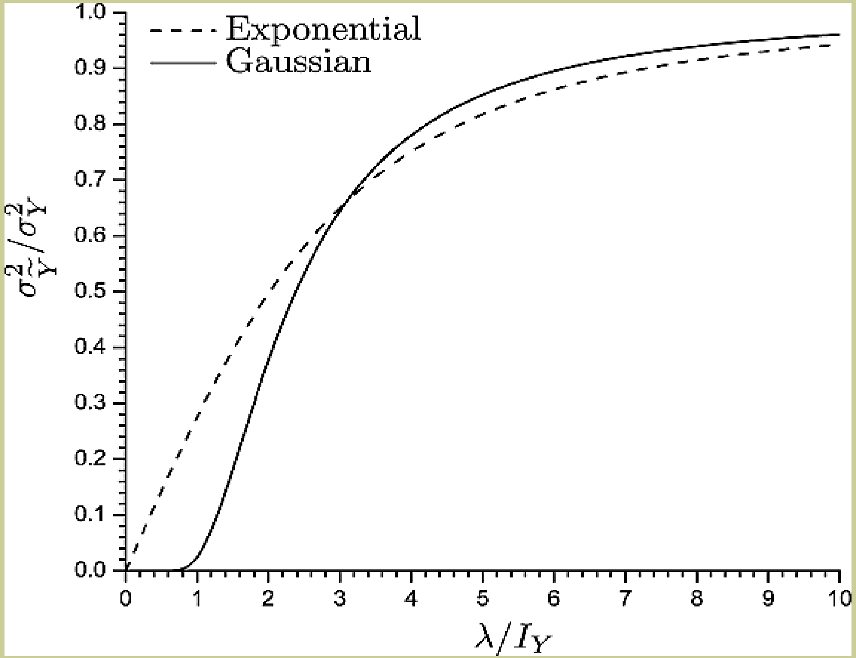
$$D_{ij}(t) = \overline{D}_{ij}(t) + \widetilde{D}_{b,ij}(t)$$

$$\widetilde{D}_{b,ij}(t) = \frac{U^2}{(2\pi)^{m/2}} \int_0^t \left[\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-ik_1 U t'} \left(\delta_{1i} - \frac{k_1 k_i}{k^2} \right) \left(\delta_{1j} - \frac{k_1 k_j}{k^2} \right) F(\mathbf{k})\, \hat{C}_Y(\mathbf{k})\, d\mathbf{k} \right] dt'$$

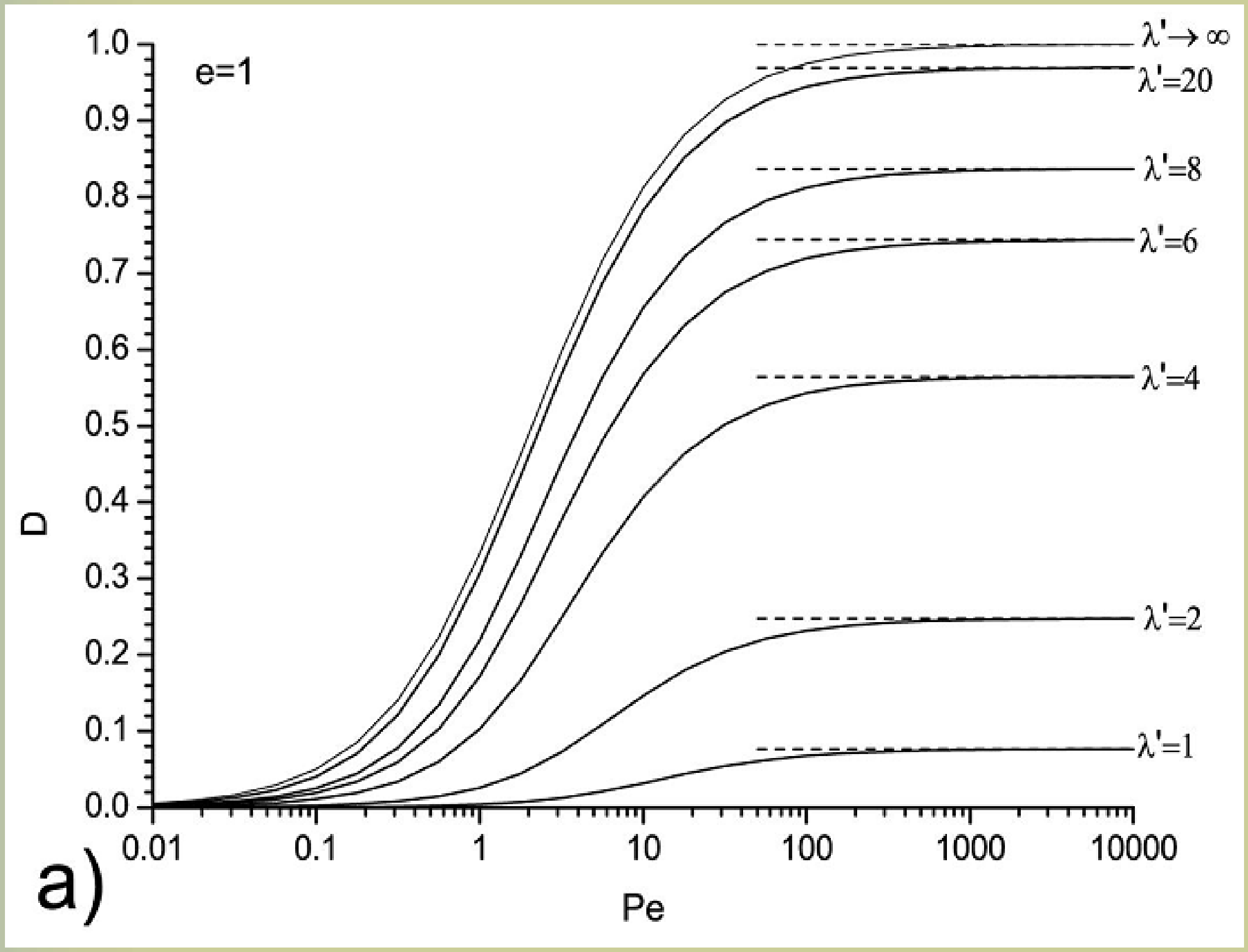
HIGH PASS FILTER $F(\mathbf{k}) = \begin{cases} 0 & \text{for } |k_i| \le \pi / \lambda_i \;, i = 1, \ldots m \\ 1 & \text{otherwise} \end{cases}$

longitudinal block-scale macrodispersion

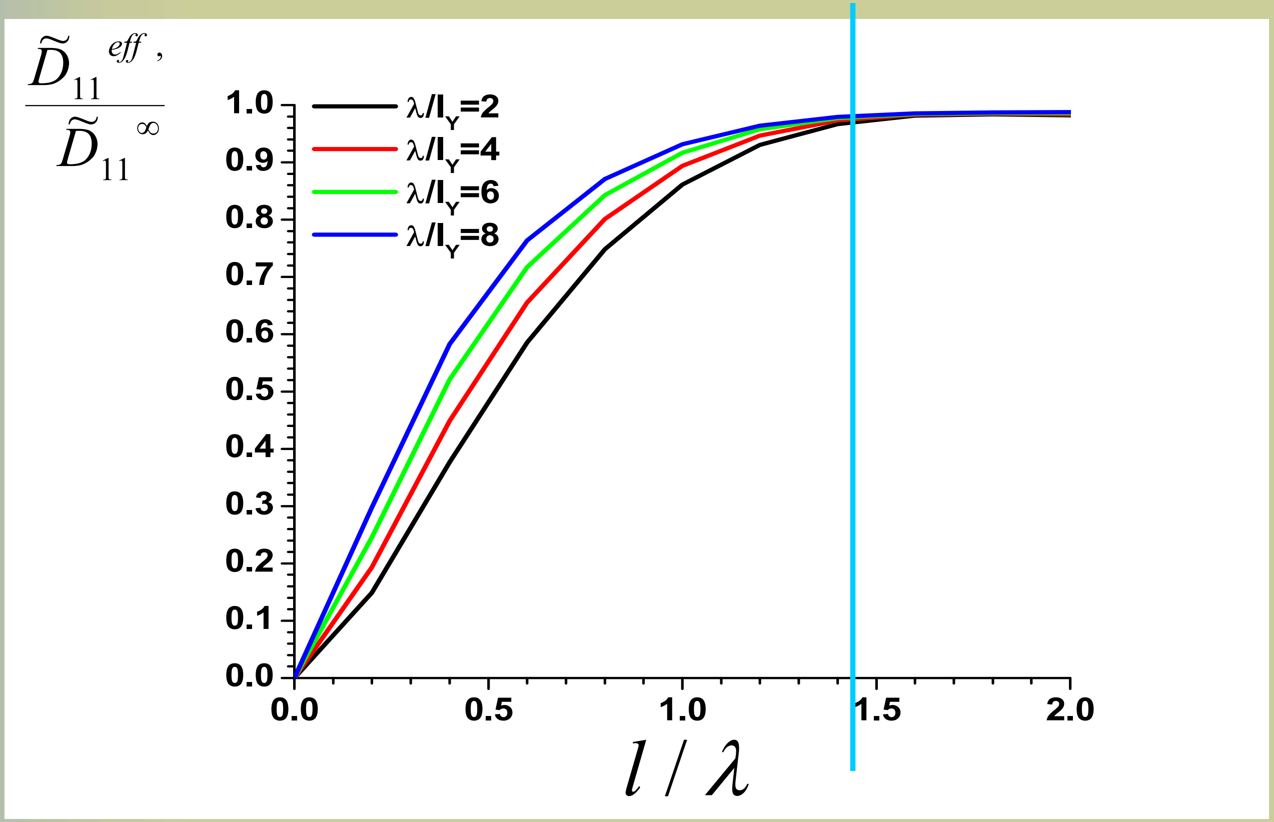




Longitudinal macrodispersion is a function of $Pe=Ul_Y/D_d$.
The λ' values denote the dimensions of the homogenized regions.



Small plume case



The block-scale macrodispersion reaches the ergodic limit for $l / \lambda \approx 1.5$

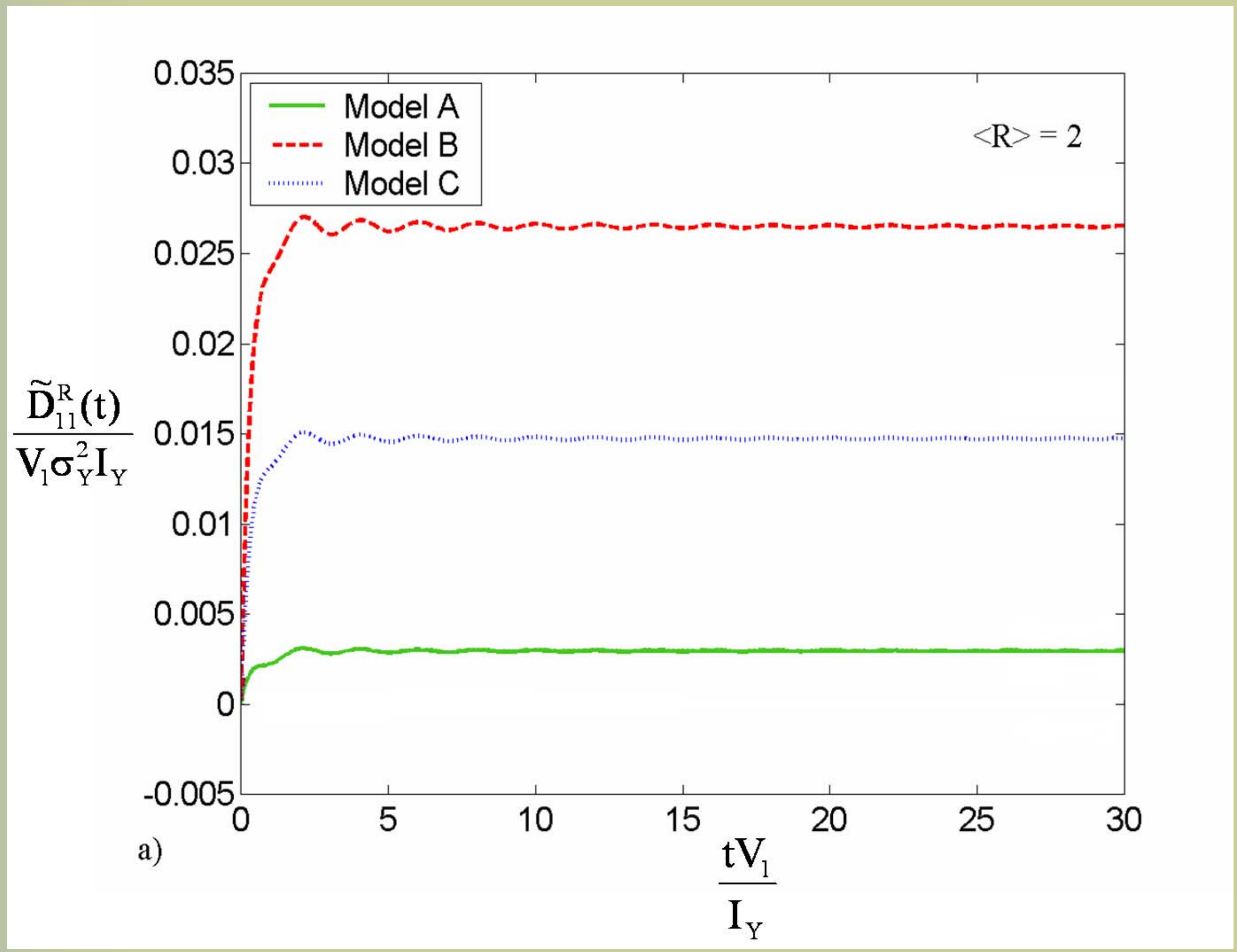
At this ratio, the plume becomes ergodic (=deterministic), and no-longer a function of the plume scale.

First-order Instantaneous Sorption

$$\ln\left[K_d(\mathbf{x})\right] = aY(\mathbf{x}) + W(\mathbf{x})$$

- Negative correlation between the hydraulic conductivity and the distribution coefficient is often applicable. Positive correlation is also plausible. We will consider the extremes:
- (A) perfect positive correlation;
- (B) perfect negative correlation and
- (C) no correlation.

Longitudinal Macrodispersion with Spatially variable distribution coefficient (for λ=1)



Summary

- A theory is presented for modeling the effects of sub-grid scale variability on solute mixing, using block-scale macrodispersion coefficients;
- The goal is to allow flexibility in numerical grid design without discounting the effects of the sub-grid (unmodeled) variability, while at the same time:
- Avoiding unnecessary high grid density;
- The approach incorporates several concepts:
  - Rational treatment of the relationships between the various length scales involved;
  - **Nyquist's Theorem** is used to separate between the length scales affecting mixing and those which affect advection. The outcome is a Space Random Function;
  - **Ergodicity**: The block-scale macrodispersion coefficients are defined in the ergodic limit (about 50% larger than the scale of the homogenized blocks), which allows to treat them as deterministic;

References:

- Rubin, Y., Applied Stochastic Hydrogeology, Oxford University Press, 2003;
- Rubin, Y., A. Bellin, and A. Lawrence, Water Resources Research, 39(9), 2003;
- Bellin, A., A. Lawrence and Y. Rubin, Stochastic Env. Research and Risk Analysis (SERRA), 18, 31-38, 2004.