# SOLVING TRANSPORT MODELS VIA AREA-AVERAGING APPROACH IN IRREGULAR DOMAINS OF RECTANGULAR GEOMETRY

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## Introduction

Microscopic equations describing transport processes (e.g., diffusion, momentum, conduction, & electrostatics) exist in multidimensional domains and they display different levels of complexities depending on the geometry for which they are applied. For example, the 3D electrostatic potential equation have been applied to several geometries in hydrogel structures to describe the effect of the electrostatic field on the transport of macromolecules found in electrophoresis and electro-osmosis.

Research has shown the role of diverging channels, compared to regular channels, when used in the electrophoretic separation of macromolecules such as DNA fragments & proteins (Pascal, Medidhi et al. 2019). In general, and potentially, parallel channels in nanocomposite gels offer a better separation than diverging channels (Simhadri *et al*, Gohosal *et al*). Further research is needed to understand the reason behind this result. This poster focuses on Laplace type equations, namely: 2D electrostatic potential equation, as applied to a diverging rectangular domain to present upscaled solutions.

## Model Formulation

A typical diverging pore (found in nanocomposite gels) is sketched in Figure 1. This is a representation of a diverging pore associated with the morphology of hydrogels with nanoparticle fillers. These pores are of varying sizes and thus when considering a *predictive model* to analyze these systems, scaling is a necessary step in achieving a useful result for the design of the pore.

In this poster, using area averaging technique, we were able to scale up the microscopic equation to the entire pore to describe transport along the axial variable.

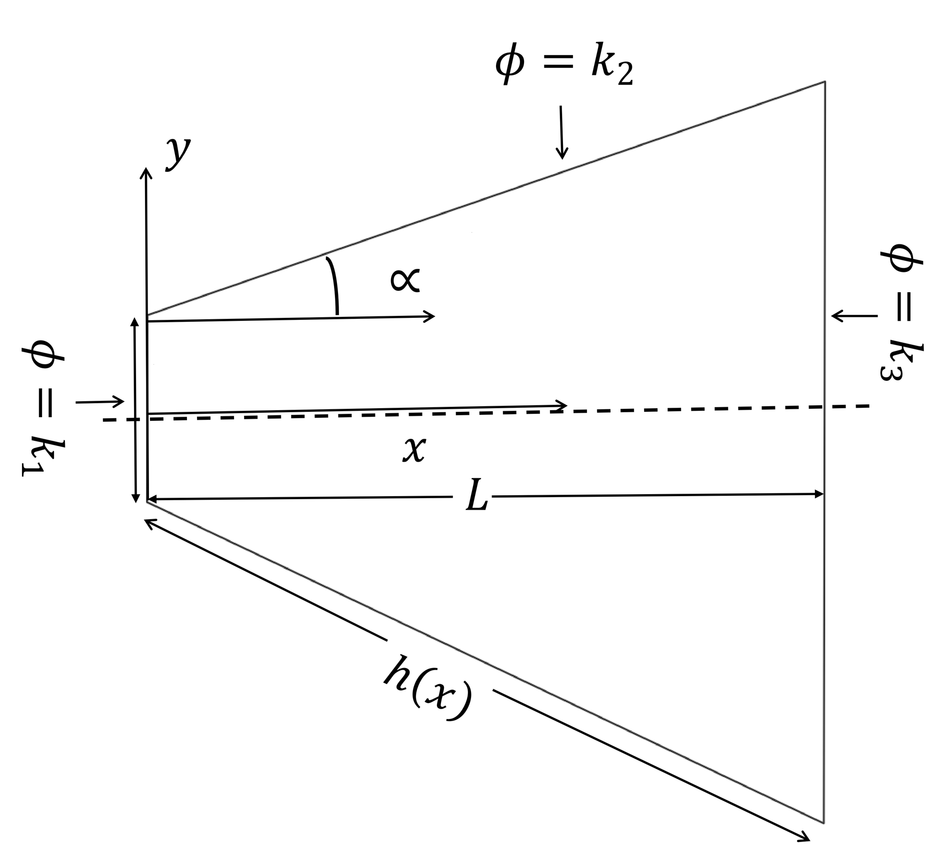


Fig 1: Geometry of channel analyzed: Diverging rectangle

## General Observations about the Formulation

### A-Assumptions

The conservation equation is based on the conservation of charges (i.e., the Coulomb Equation) under steady-state conditions. Further the two key dimensions of interest are the perpendicular coordinate ("y") to the axial coordinate ("x") as the depth of the pore is assumed symmetrical (see Figure 1). Thus, the model become the Laplace equation in 2D. See Equation (1) with BC indicated in Figure 1.

### B-General Strategy to Up-Scale the Laplace Equation

The general strategy used for upscaling the electrostatic potential is presented in figure 2. A step by step implementation of this algorithm was used to upscale equation (1).

1. Determine the governing equations
2. Describe boundary conditions

3. Apply Area-Average formula to Governing equation

4. Re-write governing equation in terms of average and deviation

5. Subtract final expression of the averaged governing equation from the re-written governing equation (i.e., step (3) – step (4))

6. Apply simplifying assumptions to equation from step (5) and effectively reduce the terms in the equation

7. Derive deviation equation and substitute deviation variables to Boundary conditions

8. Determine closure equation for the proposed solution and solve the deviation variable

9. Substitute the deviation variable into the area average expression to determine the area average of the governing equation

10. Solve the area average governing equation according to the boundary conditions

Fig 2: Algorithm for implementing area averaging

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## The Electrostatic problem and Solution Approach

The microscopic electrostatic model equation of the Laplace type in a 2D space is given by equation (1)

$$\text{Step 1: } \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = 0 \qquad (1)$$

$$\text{Step 2: } x = 0, \phi = k_1; \;\; x = L, \phi = k_3$$

Using the definition of area averaging (Equation 2), the equations is scaled up(Equation 3).

$$F(x,y,z) = \langle F(x,y,z)\rangle + \tilde{F}(x,y,z) \qquad (2)$$

$$\text{Step 3: } \frac{\partial^2}{\partial x^2} < \phi > + \frac{1}{h(x)} \frac{\partial \phi}{\partial y}\Big|_0^{h(x)} = 0 \qquad (3)$$

With

$$h(x) = x.\tan(\alpha) + \frac{H}{2}$$

Following the systematic algorithm (see Figure 2) of area averaging, the general 'decomposition" for equation is:

$$\text{Step 4: } \phi = \langle\phi\rangle + \tilde{\phi} \qquad (4)$$

Where $\langle\phi\rangle$ is the average electrostatic potential along the channel (a function of x) and $\tilde{\phi}$ is the deviation of electrostatic potential (function x and y). Now a "closure approach" is needed. Using the Payne *et al*. approach and with the following B.C.

$$x = 0, \phi = k_1; \;\; x = L, \phi = k_3 \qquad (5)$$

Solving the equation (1), using the definition in equation (3) we obtain:

1. The deviation part of the potential is computed using the boundary condition:

$$y = 0, \tilde{\phi} = 0; y = h(x), \tilde{\phi} = k_2 \qquad (6)$$

$$\text{Step 8: } \tilde{\phi} = \left(3\left(\frac{y}{h(x)}\right) - 1\right)\left(\frac{k_2 - \langle\phi\rangle}{2}\right) \qquad (7)$$

To solve the deviation term completely, a solution to the average electrostatic potential needs to be obtained.

2. The average electrostatic potential is derived by substituting equation (7) into equation (3), while noting:

$$\frac{\partial\tilde{\phi}}{\partial y} = \frac{\partial\phi}{\partial y} \qquad (7)$$

The resulting function is the differentiated with respect to y from 0 to h(x). The resulting function, as a function of the length, of the channel is given by:

$$\text{Step 10: } \langle\phi\rangle = A\cosh\left(\frac{x\sqrt{3}}{h(x)}\right) + B\sinh\left(\frac{x\sqrt{3}}{h(x)}\right) + K_2 \qquad (8)$$

Where: $A = k_1 - k_2, \;\; B = \dfrac{(k_3-k_2) - \left((k_1-k_2)\cosh\left(\frac{L\sqrt{3}}{h(x)}\right)\right)}{\sinh\left(\frac{L\sqrt{3}}{h(x)}\right)}$ (9)

## Results and Discussion

The graphical solution to the electrostatic potential problem is presented below. K2 is potential applied in the negative orthogonal direction (negative y direction). The plot presented represents the summation of the deviation term and the average term. See Equation (4)

The combined effect of the deviation term and the average term is presented in Figure 3. The illustration shows that there exists some variation in the at the entrance and at the exit of the domain. This entrance effect is observed, from both ends, to be approximated to about 60% of the whole domain. The region in which the solution electrostatic potential is constant with respect to x-axis, is significant for upscaling purposes of the species continuity equation.

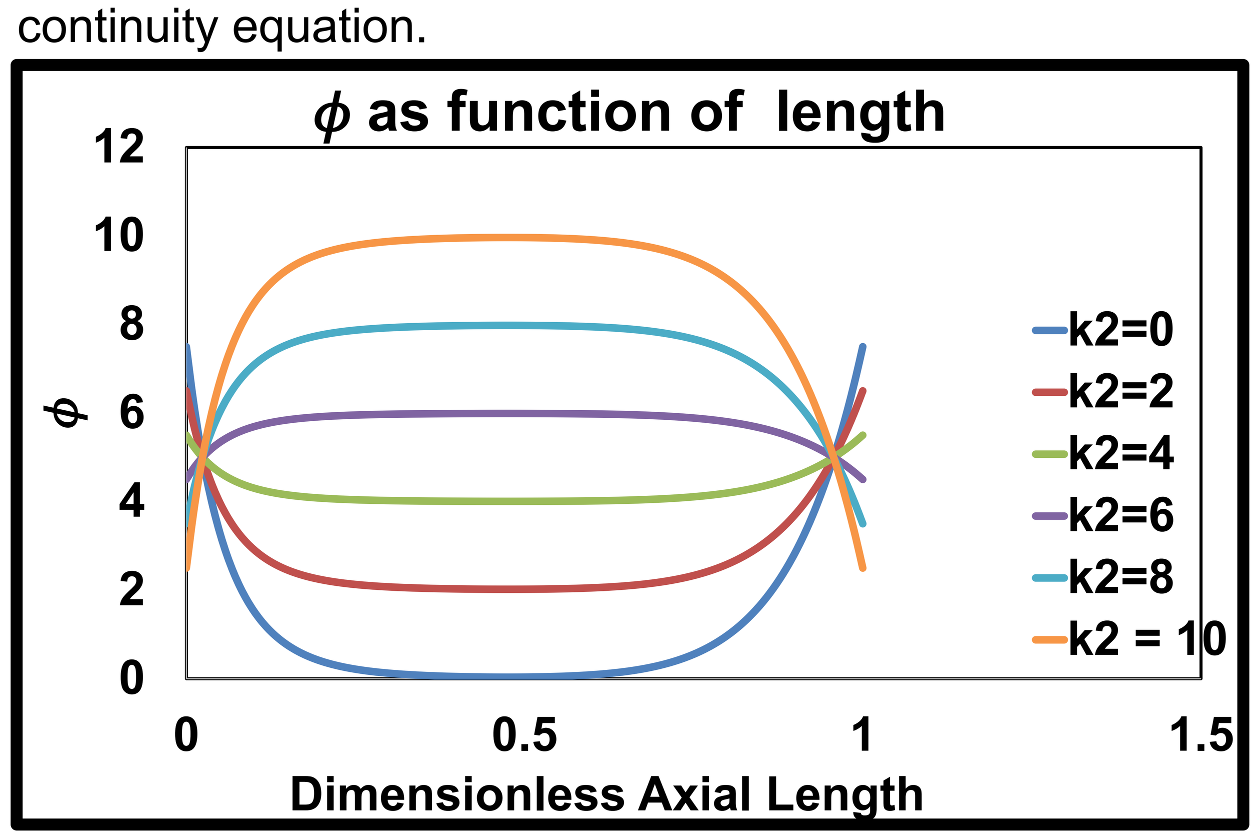


Fig 3: Electrostatic potential distribution in a diverging rectangular domain with varying K2.

The results from the analysis points to electrostatic potential being constant in about 60% region of the domain. This result is significant because it will allow us to be able to further simplify our analysis of the species mass analysis of the system.

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