Simulation of Diffusion

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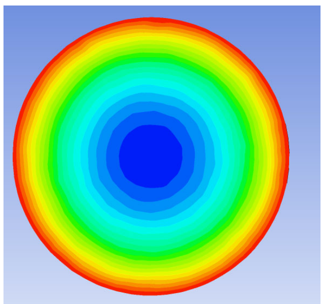
Steady-State Diffusion

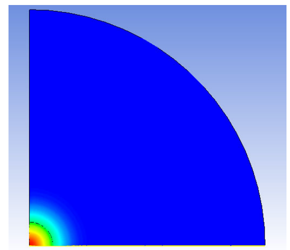
Solve for concentration of oxygen in a spherical metastatic liver lesion

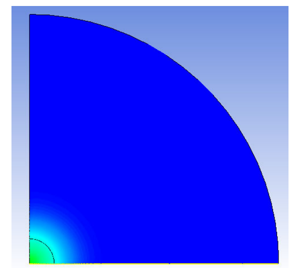


ANSYS tutorial:
https://confluence.cornell.edu/x/W0iJFg

Transient Diffusion

Solve for time variation of drug concentration in a spherical skull





ANSYS tutorial:
https://confluence.cornell.edu/x/Y0iJFg

Steady-State Diffusion: Problem Statement

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BME 2000 and ENGRD 2202
Biomedical Transport Phenomena
Solutions from Fall 2018
Material for class starting 2019-10-24

1. Consider the steady-state solution for radial diffusion (no convection) in a solute-solution that obeys Fick's law.

   (a) Please cross out terms in Truskey-Yuan-Katz (Second edition) Table 7.2 p. 350, Eq. 7.3.13c to determine the governing diffusion equation.
   No convection: $\mathbf{v} = 0$. Steady state: $\partial/\partial t = 0$. Radial diffusion: $C(r,\theta,\phi) = C(r)$ so $\partial/\partial\theta = 0$ and $\partial/\partial\phi = 0$. The result is

$$0 = D_{i,j}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_i}{\partial r}\right)\right) + R_i. \qquad (1186)$$

   i. What are the two boundary conditions?

$$C_i(r = R) = C_0 \qquad (1198)$$

$$C_i(r) < \infty \text{ for all } 0 \le r \le R. \qquad (1199)$$

Pre-Analysis

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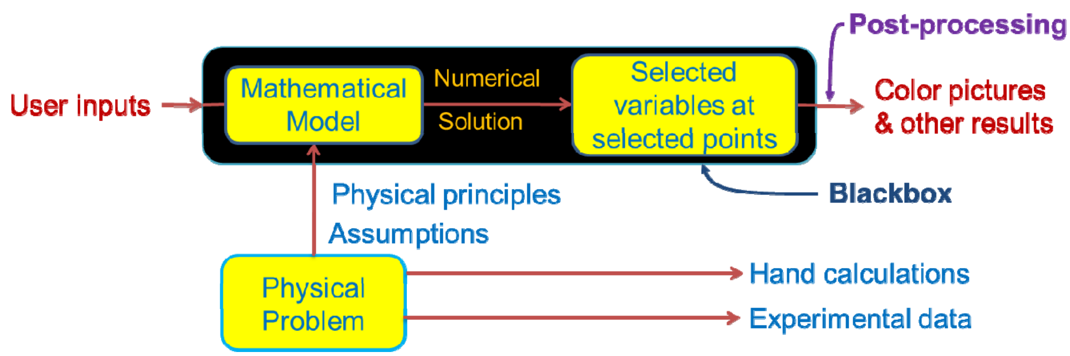

1. Mathematical model
2. Numerical solution procedure
3. Hand-calculations of expected results/trends

Governing Equation Comparison

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Steady-State Diffusion

$$0 = D_{i,j}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_i}{\partial r}\right)\right) + R_i.$$

Artery

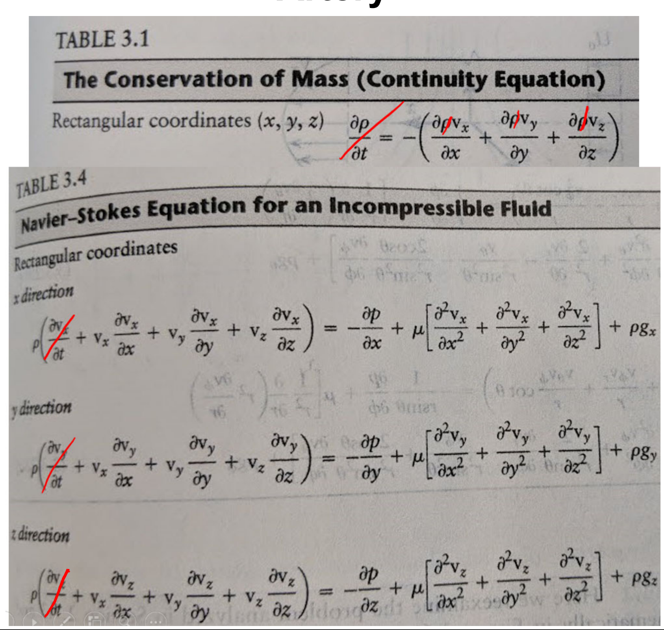

TABLE 3.1

The Conservation of Mass (Continuity Equation)

Rectangular coordinates (x, y, z) $\quad \frac{\partial \rho}{\partial t} = -\left(\frac{\partial \rho v_x}{\partial x} + \frac{\partial \rho v_y}{\partial y} + \frac{\partial \rho v_z}{\partial z}\right)$

TABLE 3.4

Navier-Stokes Equation for an Incompressible Fluid

Rectangular coordinates

x direction

$$\rho\left(\frac{\partial v_x}{\partial t} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right) = -\frac{\partial p}{\partial x} + \mu\left[\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right] + \rho g_x$$

y direction

$$\rho\left(\frac{\partial v_y}{\partial t} + v_x\frac{\partial v_y}{\partial x} + v_y\frac{\partial v_y}{\partial y} + v_z\frac{\partial v_y}{\partial z}\right) = -\frac{\partial p}{\partial y} + \mu\left[\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2}\right] + \rho g_y$$

z direction

$$\rho\left(\frac{\partial v_z}{\partial t} + v_x\frac{\partial v_z}{\partial x} + v_y\frac{\partial v_z}{\partial y} + v_z\frac{\partial v_z}{\partial z}\right) = -\frac{\partial p}{\partial z} + \mu\left[\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2}\right] + \rho g_z$$

Governing Equation in Different Coordinate Systems

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TABLE 7.2

Conservation Relations for Dilute Solutions

Rectangular	$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$
Cylindrical	$\frac{\partial C_i}{\partial t} + v_r \frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_i}{\partial \theta^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$
Spherical	$\frac{\partial C_i}{\partial t} + v_r \frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial C_i}{\partial \phi}$ $= D_{ij}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial C_i}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 C_i}{\partial \phi^2}\right) + R_i$

Heat Transfer Analogy

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TABLE 7.2

Conservation Relations for Dilute Solutions

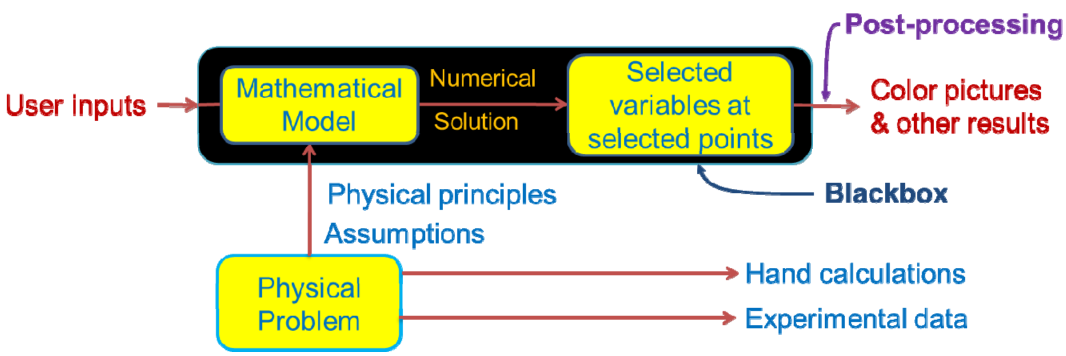
Rectangular	$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$

Heat Conduction in ANSYS with No Flow

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) + S \qquad \alpha = \frac{k}{\rho\, C_p}$$

Solve as heat transfer problem in ANSYS and interpret temperature T as concentration

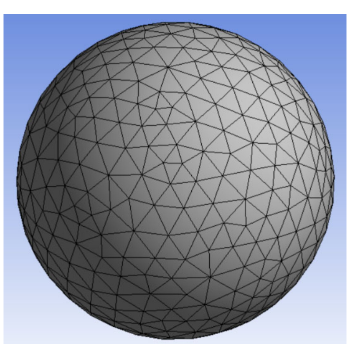
Pre-Analysis

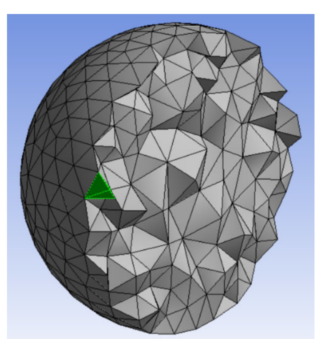


1. Mathematical model
2. Numerical solution procedure
3. Hand-calculations of expected results/trends

Finite Volume Method

- Divide the domain into multiple control volumes or “cells”
- Reduce the problem to determining temperature values at cell centers
- Use interpolation of cell center values to determine values at other locations within a cell





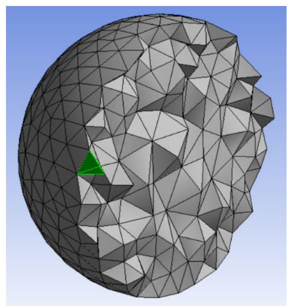
“Discretization”

How to Find Temperature at Cell Centers?

Mathematical Model (Boundary Value Problem) → System of algebraic equations in cell-center values → Invert → Cell-center values of T → Post processing → $T(x, y, z)$

Control volume balance for each cell

Each algebraic equation will relate a cell-center value to its neighbors



Discretization and Linearization: Overview

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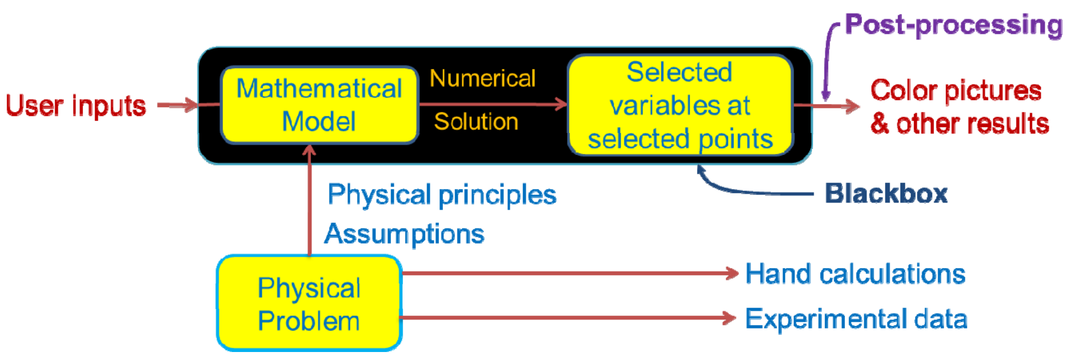
Differential form of governing equations + BCs → Integral form of governing equations + BCs → Discretization error → Algebraic equations relating cell-center values → Solve iteratively updating guess after each iteration → Stop iterations when heat imbalance is below tolerance

Pre-Analysis



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Hand Calculations of Expected Results/Trends

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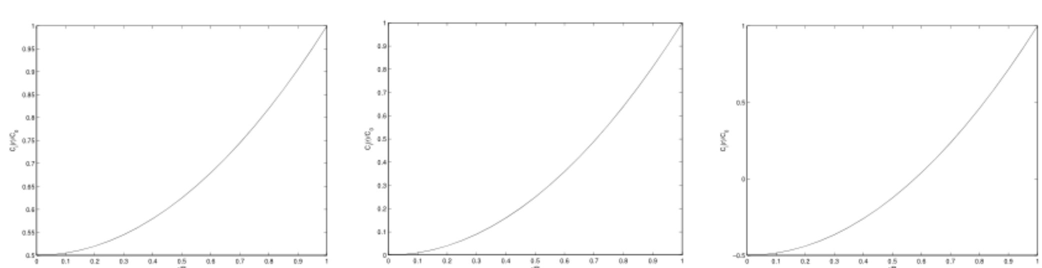
vi. Please define α by

$$\alpha = \frac{R^2}{6}\frac{|R_i|}{|D_{i,j}|}\frac{1}{|C_0|}. \tag{1208}$$

Please note that α is a pure number without units. Please plot $C_i(r)/C_0$ versus r/R for three values of α: $\alpha \in \{1/2, 1, 3/2\}$.
Note that

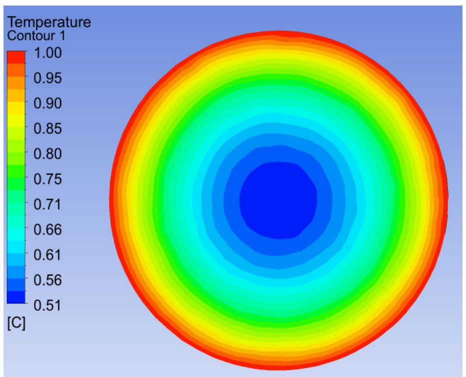
$$C_i(r)/C_0 \quad = \quad -\alpha\left(1-\left(\frac{r}{R}\right)^2\right)+1. \tag{1209}$$

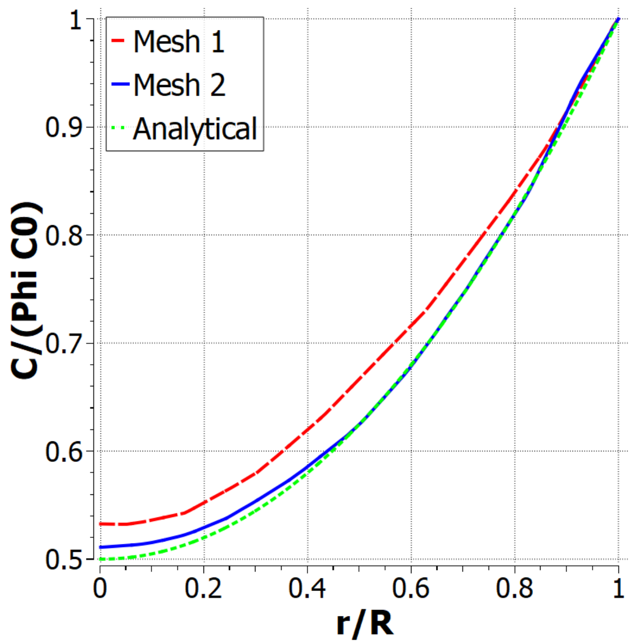


$\alpha = 1/2$ $\qquad$ $\alpha = 1$ $\qquad$ $\alpha = 3/2$

ANSYS Solution and Results

- List of ANSYS steps is attached

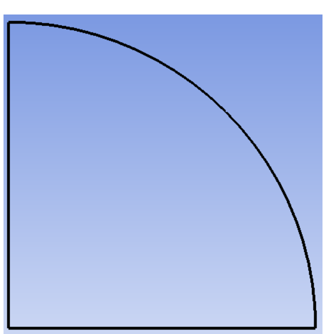




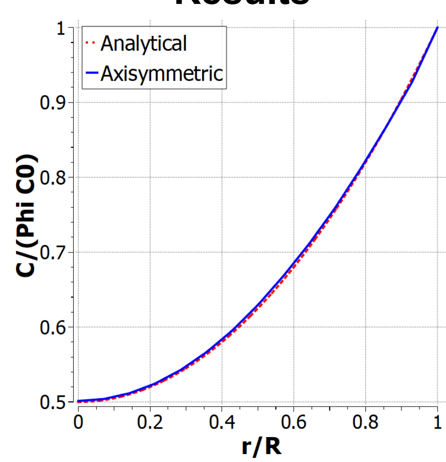
Steady-State Diffusion: Axisymmetric Solution

Cylindrical $\cancel{\frac{\partial C_i}{\partial t}} + \cancel{v_r \frac{\partial C_i}{\partial r}} + \cancel{\frac{v_\theta}{r} \frac{\partial C_i}{\partial \theta}} + \cancel{v_z \frac{\partial C_i}{\partial z}} = D_{ij}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right) + \cancel{\frac{1}{r^2}\frac{\partial^2 C_i}{\partial \theta^2}} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$

Domain and BCs



Results



Transient Diffusion: Problem Statement

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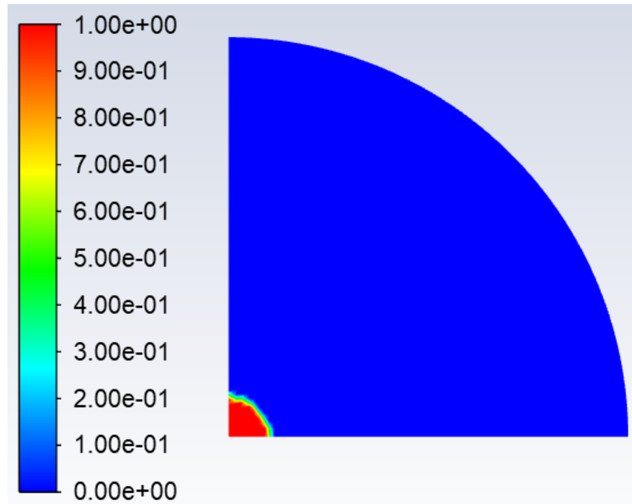
- Calculate how a drug will diffuse from some central deposit into surrounding tissue
- A finite sphere of radius *R* as the brain
- No-flux boundary condition at the edge of the brain:
  - $\frac{\partial C}{\partial r} = 0 \ \ at \ \ r = R$
- Initial condition: Set the initial concentration as
  - C_0 from $0 < r < r_0$
    Take $C_0 = 1$ and $r_0 = 0.1\,R$
  - 0 everywhere else

Initial Concentration



Transient Diffusion: Mathematical Model

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Governing equation using axisymmetric assumption:

Cylindrical $$\frac{\partial C_i}{\partial t} + v_r\frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_i}{\partial \theta^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

- In ANSYS, it's advantageous to non-dimensionalize time and r in the governing equation
  - $t^* = \frac{Dt}{R^2}$
  - $r^* = \frac{r}{R}$
- One can now solve the problem once in ANSYS and rescale the results for any values of *D* and *R*

Governing eq. in terms of t^* and r^*

$$\frac{\partial C}{\partial t} = 1\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right)\right) + \frac{\partial^2 C}{\partial z^2}$$

Transient Diffusion: Boundary and Initial Conditions

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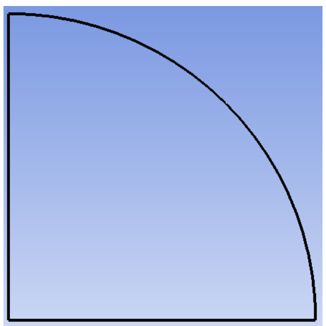
Domain and BCs



Initial condition at $t = 0$:

- C_0 from $0 < r < r_0$
  Take $C_0 = 1$ and $r_0 = 0.1\ R$
- 0 everywhere else

Pre-Analysis

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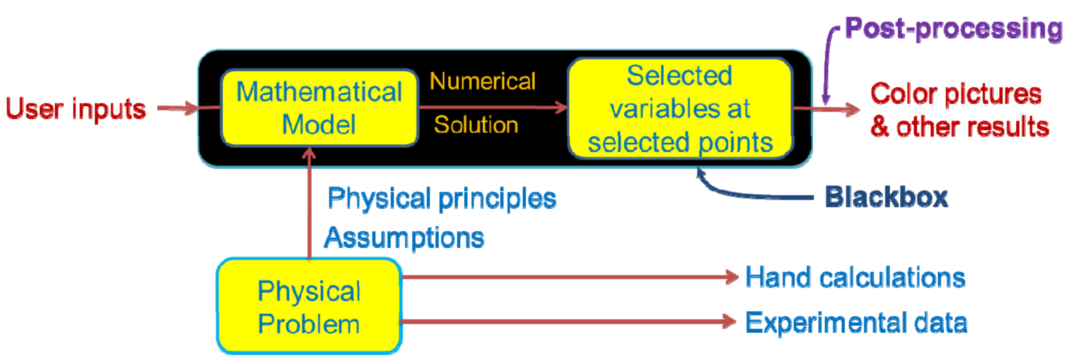

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Finite Volume Method

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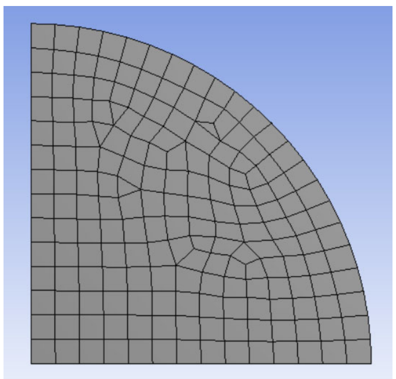

“Discretization”

How to Find Temperature at Cell Centers?

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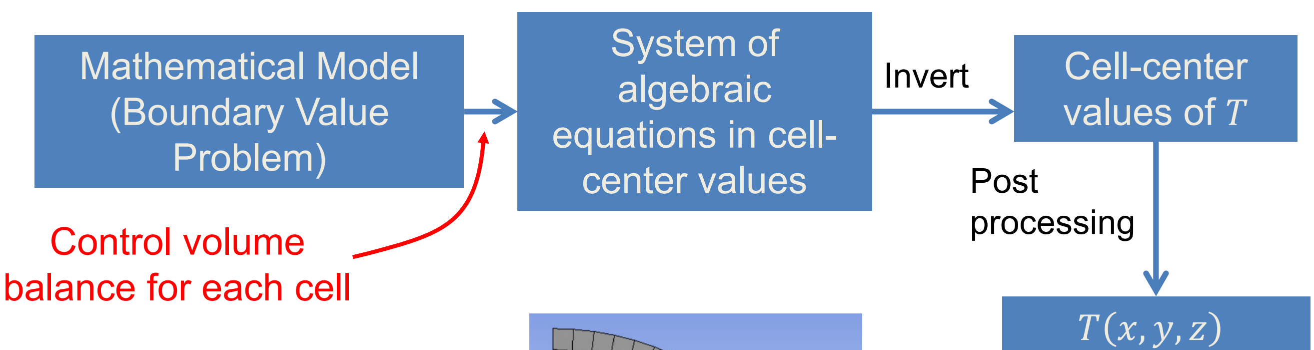
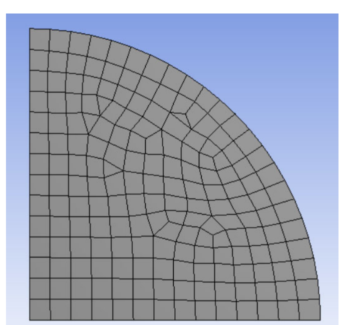


Each algebraic equation will relate a cell-center value to its neighbors



Discretization of Time Derivative

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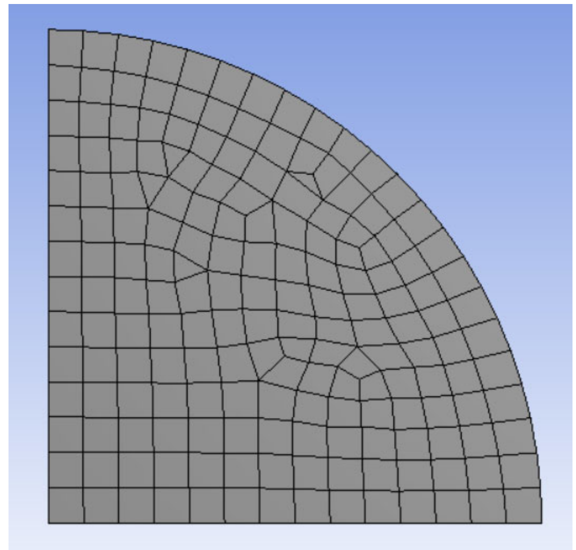
- Exact
  - $\frac{\partial C}{\partial t} = \frac{C(t+\Delta t)-C(t)}{\Delta t}$
- Numerical
  - $\frac{\partial C}{\partial t} \sim \frac{C(t+\Delta t)-C(t)}{\Delta t}$



Hand Calculations of Expected Results/Trends

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Analytical Solution

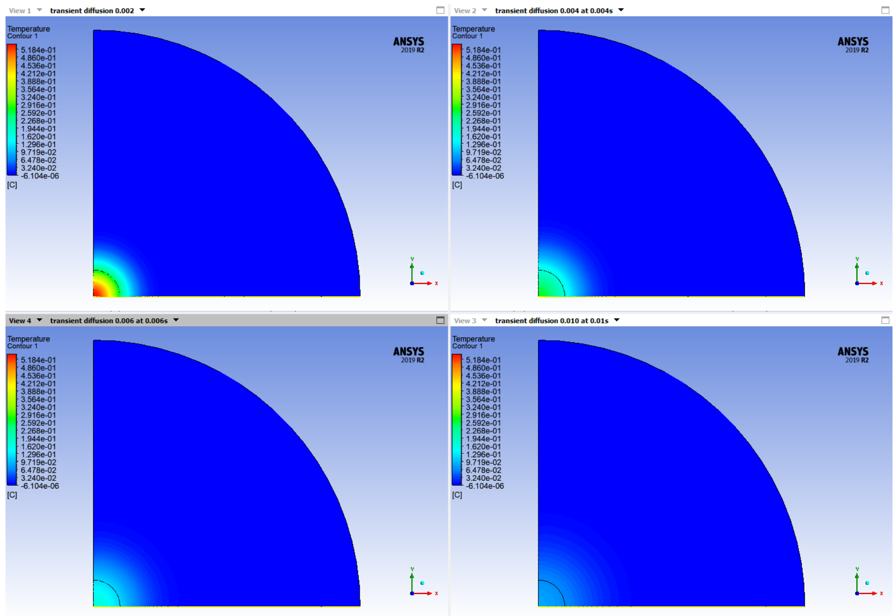
Use separation of variables

$$T(r,t) = C_0 + \sum_{n=1}^{\infty} C_n \frac{\sin(\lambda_n r)}{r} e^{-\alpha \lambda_n^2 t}$$

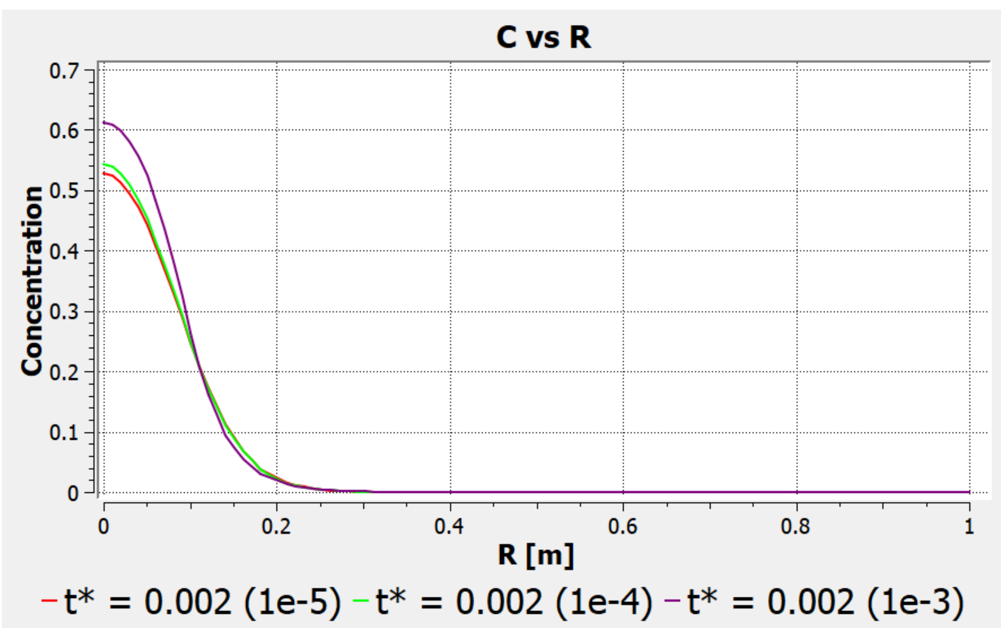
$$b\lambda_n \cot \lambda_n b = 1 \quad \rightarrow \quad \lambda_n \quad \text{for} \quad n = 0, 1, 2, 3, \ldots$$

ANSYS Solution and Results

- List of ANSYS steps for transient case is attached



Transient Case: Time-Step Sensitivity

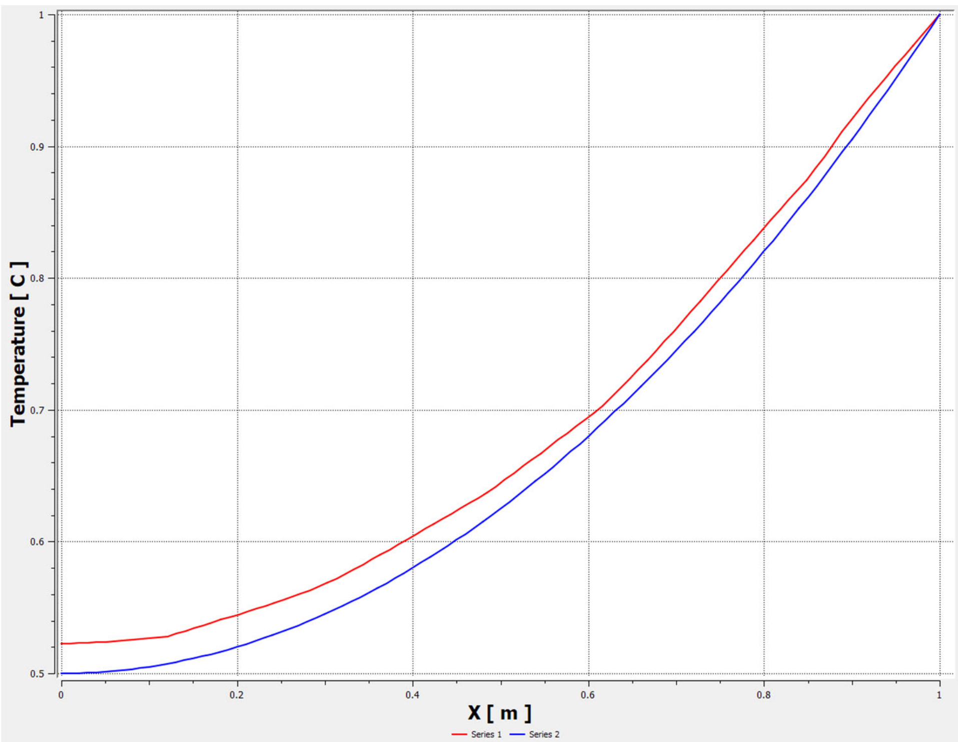


Diffusion: Outline of Steps in ANSYS

Steady State

1. Start Workbench 2019R2
2. Under Analysis Systems, double-click Fluid Flow (Fluent)
3. Rename it to "Diffusion (Steady)"
4. Double-click Geometry to launch SpaceClaim
5. Create a sphere at the origin with diameter of 2 meters
6. Exit SpaceClaim, then double-click on Mesh to launch the mesher
7. Add Body Sizing, Element Size = 0.1 meters. (Soft) MAKE SURE THE UNITS ARE CORRECT.
8. Named Selections: farfield, fluid_domain
9. Exit the mesher and make sure Mesh is updated in Workbench window
10. Save project now and often
11. Double-click on Setup to launch Fluent
12. Enable energy equation
13. Specify material properties:
    a Thermal conductivity, density, specific heat = 1 (to give non-dimensional problem)
    b Leave viscosity as default value
14. Specify the Cell Zone conditions
    a Enable Source Terms
    b Source Terms tab > Energy > Edit
        i. Number of Energy sources = 1
        ii. Down arrow next to gray box > Select Constant
        iii. Value = -3 W/m3 (for alpha = ½)
15. Domain > Mesh > Units > Temperature = C
16. Specify the boundary conditions:
    a Farfield: Wall: Temperature = 1°C
    b NOTE: For Axisymmetric case, you will need both an axis and a symmetry boundary condition
17. Controls > Equations > disable Flow
18. Add Surface Report
    a Report Definitions > New > Surface Integral > Area-weighted Average > Wall Fluxes > Total Surface Heat Flux > Surfaces: farfield
19. Monitors > Residual > Convergence Conditions > Add
    a Choose the report definition we just made
    b Use Iterations = 5
    c All Conditions are Met
20. Initialization > Standard Initialization
    a T = 1°C
21. Run Calculation > Number of Iterations: 20
22. Click on Calculate to have the solver calculate cell center temperatures
23. Close out of Fluent and then double-click on Results to launch CFD-Post

24. Post-process the results in CFD Post
    a Create a line (0,0,0) to (1,0,0)
    b Plot temperature along the line
    c Variable tab > Temperature > Units > C
    d Import csv of analytical results
    e Change axes titles under the respective axis tab
    f Change series names under the Line Display tab
    g Change font sizes under the Chart Display tab



25. Refine the mesh, re-run and check sensitivity of results to the mesh

Transient

Note: We will use Axisymmetric to reduce computational time.

1. Start Workbench 2019R2
2. Under Analysis Systems, double-click Fluid Flow (Fluent)
3. Rename it to "Diffusion (Transient)"
4. Set Analysis Type to 2D and then double-click Geometry to launch SpaceClaim
5. Sketch two concentric circles of diameter 2m and 200mm for use with the patch initialization
6. Use lines to cut circles into quadrants and delete all but the top-right quadrant
7. Exit SpaceClaim, then double-click on Mesh to launch the mesher
8. Add two Face Sizings, one to each face, Element Size = 1/10 of the radius of the face. (Soft) MAKE SURE THE UNITS ARE CORRECT.
1. Named Selections: outer_boundary, axis, symmetry, inner_region, outer_region
9. Exit the mesher and make sure Mesh is updated in Workbench window

10. Save project now and often
11. Double-click on Setup to launch Fluent
12. Change Steady to Transient, set 2D Planar to 2D Axisymmetric
13. Enable energy equation
14. Specify material properties:
    a. Thermal conductivity, density, specific heat = 1 (to give non-dimensional problem)
    b. Leave viscosity as default value
15. Domain > Mesh > Units > Temperature = C
16. Specify the boundary conditions:
    a. Outer-boundary: Wall: Heat Flux = 0
    b. NOTE: You will need to have both an axis and a symmetry boundary condition.
17. Controls > Equations > disable Flow
18. Add Volume Report
    a. Report Definitions > New > Volume Integral > Volume-weighted Average > Temperature > Static Temperature > Zones: inner_region
19. Initialization > Standard Initialization
    a. T = 0°C
    b. Patch > Apply T = 1°C to inner_region
20. Calculation Activities > Create > Solution Data Export
    a. File Type: CDAT for Ensight and CFD Post
    b. Cell Zones: both
    c. Quantities: Static Temperature
    d. Export Data Every 0.002 seconds, change Time Step to Flow Time
        i. Exporting only at the required non-dimensional times keeps the file size smaller
    e. Make sure "Write Case File Every Time" is selected
    f. Choose a File Name
        i. Note: Make sure to change the file name when you rerun the simulation with a different time-step or it will overwrite your previous results
    g. Append File Name with flow-time, only need 3 decimal places
21. Run Calculation
    a. Time step: 1e-5 seconds (suggested)
        i. Make sure that this value is visibly changing with each time step, but also make sure that it doesn't reach steady state too quickly (in this case, aim for at least 100 time steps)
    b. Number of Iterations: 1000
22. Click on Calculate to have the solver calculate cell center temperatures
23. Close out of Fluent
24. Add a separate Results cell and double-click to launch CFD-Post
25. Load results and choose "Load only the last results"
26. Post-process the results in CFD Post
    a. Create a line (0,0,0) to (1,0,0) with 100 samples
    b. Plot temperature along the line

c. Variable tab > Temperature > Units > C
d. Import csv of analytical results
e. Change axes titles under the respective axis tab
f. Change series names under the Line Display tab
g. Change font sizes under the Chart Display tab

27. Refine the mesh, re-run and check sensitivity of results to the mesh