Partial Differential Equation Models

1. PDE models in chemical engineering
2. Finite difference approximations
3. PDE solution by finite difference
4. In-class exercise

Partial Differential Equation Models

PDE Models in Chemical Engineering

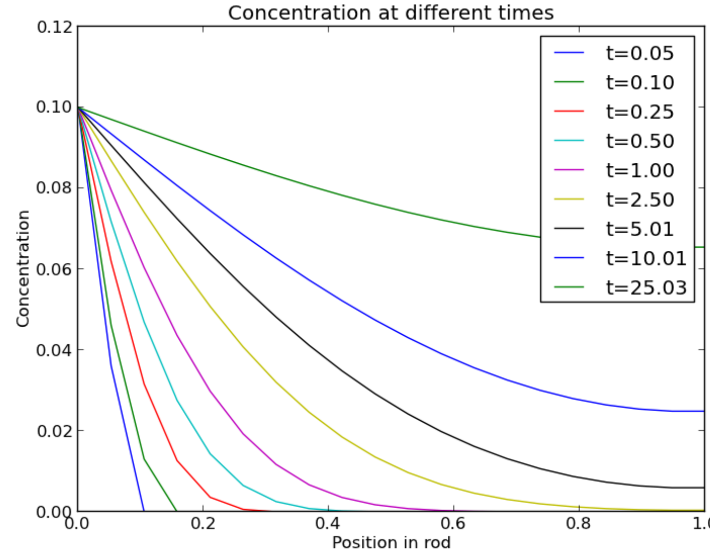
Partial Differential Equation Models

- ODE models have a single independent variable (a spatial coordinate or time)
- Partial differential equation (PDE) models have 2 or more independent variables (spatial coordinates and/or time)
- PDE models are very common in chemical engineering applications
- Solution methods developed for ODE models are not directly applicable to PDE models
- Here we will just introduce very basic concepts of PDE models and their solution

PDEs in Chemical Engineering

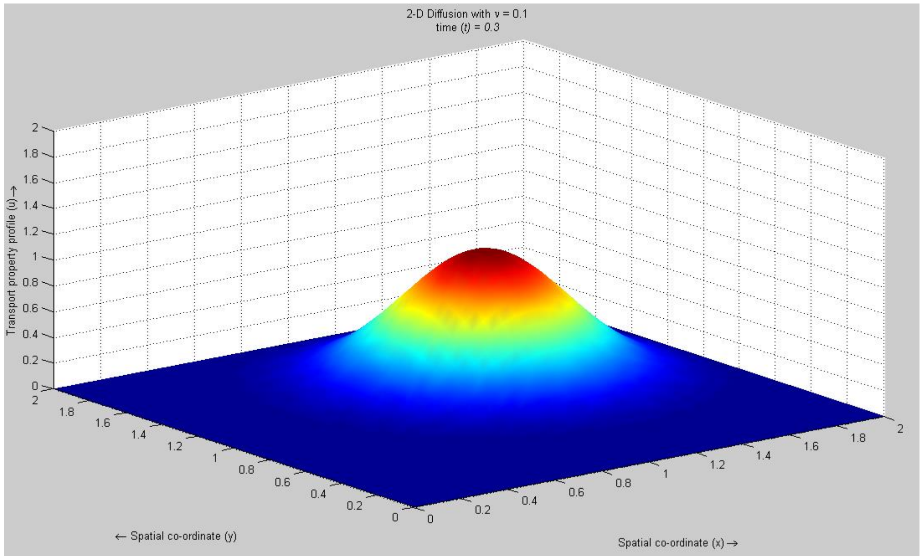
- 1-dimensional (1D) diffusion

$$\frac{\partial y(x,t)}{\partial t} = D\frac{\partial^2 y}{\partial x^2}$$



- 2D diffusion

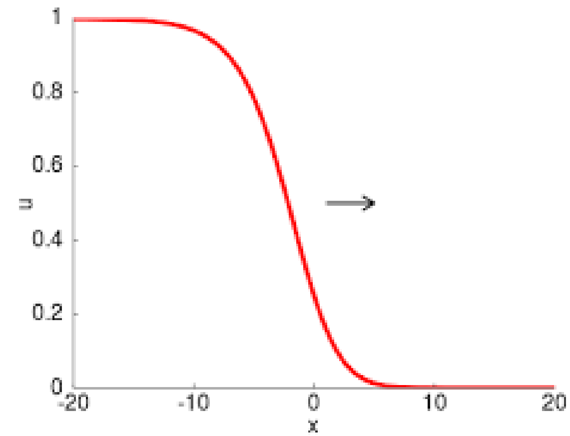
$$\frac{\partial y(x,z,t)}{\partial t} = D_x\frac{\partial^2 y}{\partial x^2} + D_z\frac{\partial^2 y}{\partial z^2}$$



PDEs in Chemical Engineering

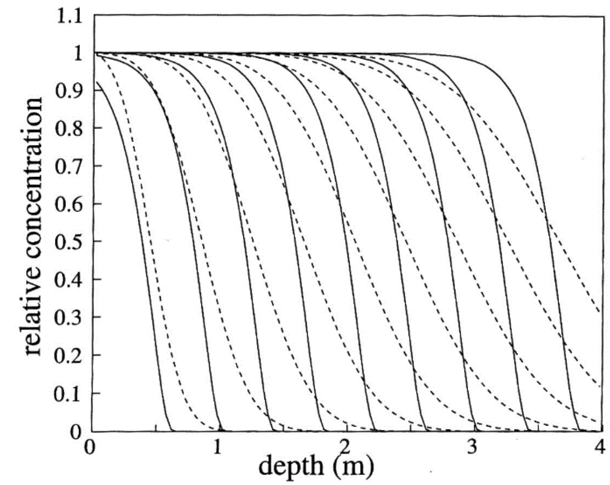
- 1D convection

$$\frac{\partial y(x,t)}{\partial t} = u\frac{\partial y}{\partial x}$$



- 1D convection-diffusion

$$\frac{\partial y(x,t)}{\partial t} = u\frac{\partial y}{\partial x} + D\frac{\partial^2 y}{\partial x^2}$$



- Steady-state 2D convection-diffusion

$$0 = u_x\frac{\partial y}{\partial x} + u_z\frac{\partial y}{\partial z} + D_x\frac{\partial^2 y}{\partial x^2} + D_z\frac{\partial^2 y}{\partial z^2}$$

Boundary Conditions

- First-order ODE systems

$$\frac{d\mathbf{y}(t)}{dt} = \mathbf{f}(t, \mathbf{y}) \qquad \frac{d\mathbf{y}(z)}{dz} = \mathbf{f}(z, \mathbf{y})$$

  » Initial value problems (IVPs) require an initial condition for each variable: $y_i(0)$

  » Boundary value problems (BVPs) require a boundary condition for each variable: $y_i(z_i)$

- PDE systems

  » Need an initial condition for each time dependent variable

  » Need boundary condition(s) for each spatially dependent variable

Example PDE Boundary Conditions

- 1D convection

$$\frac{\partial y(x,t)}{\partial t} = u\frac{\partial y}{\partial x}$$

  » Initial condition: $y(x,0) = y_0(x)$

  » Boundary condition: $y(L,t) = y_L(t)$

- 1D convection diffusion

$$\frac{\partial y(x,t)}{\partial t} = u\frac{\partial y}{\partial x} + D\frac{\partial^2 y}{\partial x^2}$$

  » Additional "no flux" boundary condition:

$$\frac{\partial y(0,t)}{\partial x} = 0$$

Partial Differential Equation Models

Finite Difference Approximations

Finite Difference Approximations

- The objective is to approximate derivatives of a function using only functional values

- Definition of the derivative

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- First-order derivatives: $x_{j+1} = x_j + h$

Forward $$\frac{df(x_j)}{dx} = \frac{f(x_{j+1}) - f(x_j)}{h}$$

Backward $$\frac{df(x_j)}{dx} = \frac{f(x_j) - f(x_{j-1})}{h}$$

Central $$\frac{df(x_j)}{dx} = \frac{f(x_{j+1}) - f(x_{j-1})}{2h}$$

First-Order Derivative Example

- Function: $y = 10e^{-2x}$
- Use central difference approximation to approximate derivative at x = 1 (exact answer is -2.7067)

$$\frac{df(x_j)}{dx} = \frac{f(x_{j+1}) - f(x_{j-1})}{2h} \quad \Rightarrow \quad \frac{df(1)}{dx} = \frac{f(1+h) - f(1-h)}{2h}$$

- h = 1

$$\frac{df(1)}{dx} = \frac{f(1+h) - f(1-h)}{2h} = \frac{f(2) - f(0)}{2} = \text{-4.9084}$$

- h = 0.1

$$\frac{df(1)}{dx} = \frac{f(1+h) - f(1-h)}{2h} = \frac{f(1.1) - f(0.9)}{0.2} = \text{-2.7248}$$

- h = 0.01

$$\frac{df(1)}{dx} = \frac{f(1+h) - f(1-h)}{2h} = \frac{f(1.01) - f(0.99)}{0.02} = \text{-2.7069}$$

Second-Order Finite Differences

- Forward difference: $$\frac{df(x_j)}{dx} = \frac{f(x_{j+1}) - f(x_j)}{h}$$

$$\frac{d^2 f(x_j)}{dx^2} = \frac{\dfrac{df(x_{j+1})}{dx} - \dfrac{df(x_j)}{dx}}{h}$$

$$= \frac{\dfrac{f(x_{j+2}) - f(x_{j+1})}{h} - \dfrac{f(x_{j+1}) - f(x_j)}{h}}{h}$$

$$= \frac{f(x_{j+2}) - 2f(x_{j+1}) + f(x_j)}{h^2}$$

- Backward difference: $$\frac{d^2 f(x_j)}{dx^2} = \frac{f(x_j) - 2f(x_{j-1}) + f(x_{j-2})}{h^2}$$

- Central difference: $$\frac{d^2 f(x_j)}{dx^2} = \frac{f(x_{j+1}) - 2f(x_j) + f(x_{j-1})}{h^2}$$

Second-Order Derivative Example

- Function: $y = 10e^{-2x}$
- Use central difference approximation to approximate derivative at x = 1 (exact answer is 5.4134)

$$\frac{d^2 f(x_j)}{dx^2} = \frac{f(x_{j+1}) - 2f(x_j) + f(x_{j-1})}{h^2} \quad \Rightarrow \quad \frac{d^2 f(1)}{dx^2} = \frac{f(1+h) - 2f(1) + f(1-h)}{h^2}$$

- h = 1

$$\frac{d^2 f(1)}{dx^2} = \frac{f(1+h) - 2f(1) + f(1-h)}{h^2} = \frac{f(2) - 2f(1) + f(0)}{1^2} = 7.4765$$

- h = 0.1

$$\frac{d^2 f(1)}{dx^2} = \frac{f(1+h) - 2f(1) + f(1-h)}{h^2} = \frac{f(1.1) - 2f(1) + f(0.9)}{0.1^2} = 5.4315$$

- h = 0.01

$$\frac{d^2 f(1)}{dx^2} = \frac{f(1+h) - 2f(1) + f(1-h)}{h^2} = \frac{f(1.01) - 2f(1) + f(0.99)}{0.01^2} = 5.4136$$

Simplified Notation

- More convenient to express the formulas in terms of $y = f(x)$
- First-order central difference

$$\frac{df(x_j)}{dx} = \frac{f(x_{j+1}) - f(x_{j-1})}{2h} \quad \Rightarrow \quad \frac{dy_j}{dx} = \frac{y_{j+1} - y_{j-1}}{2h}$$

- Second-order central difference

$$\frac{d^2 f(x_j)}{dx^2} = \frac{f(x_{j+1}) - 2f(x_j) + f(x_{j-1})}{h^2} \quad \Rightarrow \quad \frac{d^2 y_j}{dx^2} = \frac{y_{j+1} - 2y_j + y_{j-1}}{h^2}$$

Partial Differential Equation Models

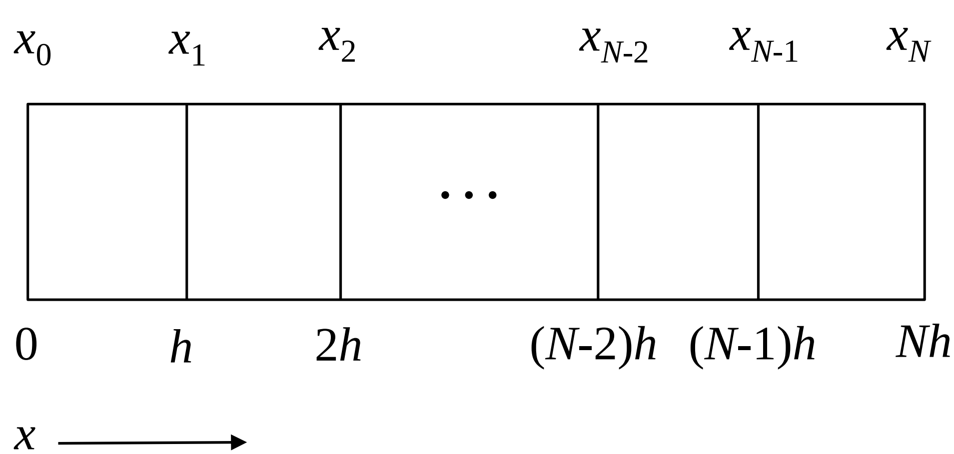
PDE Solution by Finite Differences

Finite Difference Method

- Consider a single PDE with time and one spatial coordinate as independent variables

$$\frac{dy}{dt} = f\left[x, y, \frac{dy}{dx}, \frac{d^2y}{dx^2}\right]$$

- The goal is to approximate the PDE as a set of time-dependent ODEs
- Then the ODE system can be integrated to yield an approximate solution for the PDE
- First the spatial domain is discretized into N node points



Finite Difference Method

- Then the PDE is approximated at each node point with an ODE

$$\frac{dy_j}{dt} = f\left[x_j, y_j, \frac{dy_j}{dx}, \frac{d^2 y_j}{dx^2}\right]$$

- The spatial derivatives are approximated by finite difference; e.g. central differences

$$\frac{dy_j}{dt} = f\left(x_j, y_{j-1}, y_j, y_{j+1}\right)$$

- Different formulas may be needed near the domain boundaries to implement the boundary conditions

Finite Difference Method

- The ODE system is integrated from the initial conditions to yield $y_j(t)$
- If h is "small", then $y_j(t)$ will be a good approximation of $y(x_j,t)$
- Can plot $y_j(t)$ versus t to visualize how y at a given location changes with time
- Can plot $y_j(t)$ versus j to visualize how y at a given time changes with location

1D Convection-Diffusion Equation

$$\frac{\partial y(x,t)}{\partial t} = u\frac{\partial y}{\partial x} + D\frac{\partial^2 y}{\partial x^2} \quad y(0,t) = 0 \quad \frac{\partial y(1,t)}{\partial x} = 0 \quad y(x,0) = 1$$

- Discretize equation

$$\frac{\partial y_j(t)}{\partial t} = u\frac{\partial y_j}{\partial x} + D\frac{\partial^2 y_j}{\partial x^2} \quad y_0(t) = 0 \quad \frac{\partial y_N(t)}{\partial x} = 0 \quad y_j(0) = 1$$

- Approximate spatial derivatives at point *j*

$$\frac{\partial y_j(t)}{\partial t} = u\frac{\partial y_j}{\partial x} + D\frac{\partial^2 y_j}{\partial x^2} = u\frac{y_{j+1} - y_{j-1}}{2h} + D\frac{y_{j+1} - 2y_j + y_{j-1}}{h^2}$$

UMASS.

1D Convection-Diffusion Equation

- Do not need an equation at $j = 0$ due to the boundary condition $y_0(t) = 0$
- Need a different formula at $j = N$ because y_{N+1} is not defined
- Apply backward difference and the boundary condition at $j = N$

$$\frac{\partial y_N(t)}{\partial t} = u\frac{\partial y_N}{\partial x} + D\frac{\partial^2 y_N}{\partial x^2} = D\frac{\partial^2 y_N}{\partial x^2} = D\frac{y_N - 2y_{N-1} + y_{N-2}}{h^2}$$

Summary of Equations

$$y_0(t) = 0$$

$$\frac{\partial y_j(t)}{\partial t} = u\,\frac{y_{j+1} - y_{j-1}}{2h} + D\,\frac{y_{j+1} - 2y_j + y_{j-1}}{h^2}$$

$$\frac{\partial y_N(t)}{\partial t} = D\,\frac{y_N - 2y_{N-1} + y_{N-2}}{h^2}$$

$$y_j(0) = 1$$

pde_example_odes

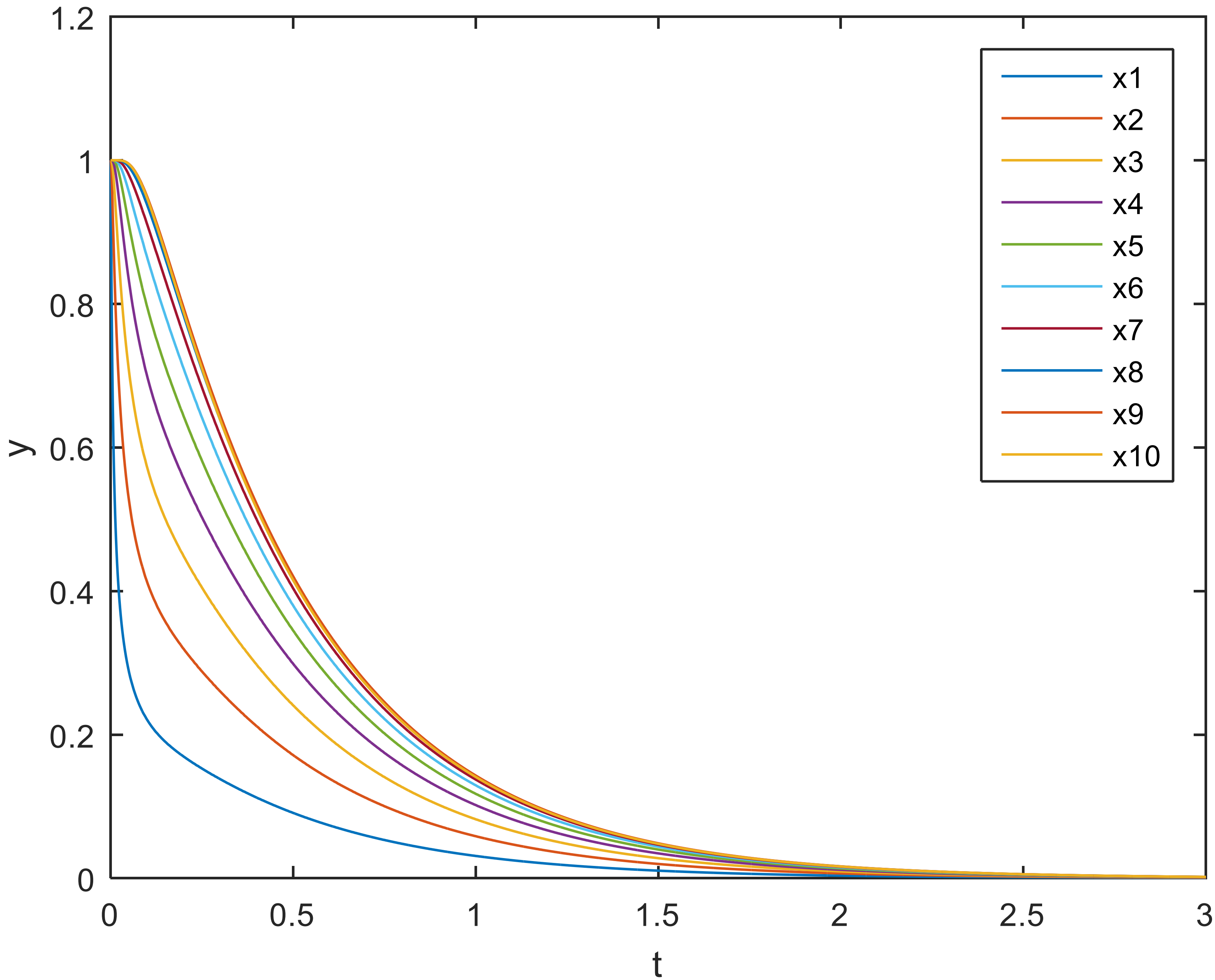
```
function f = pde_example_odes(t,y)
u = 1;
D = 1;
N = 10;
h = 1/N;
y0 = 0;
for i=1:N
    if i==1
        f(i) = u*(y(i+1)-y0)/(2*h)+D*(y(i+1)-2*y(i)+y0)/h^2;
    elseif i==N
        f(i) = D*(y(i)-2*y(i-1)+y(i-2))/h^2;
    else
        f(i) = u*(y(i+1)-y(i-1))/(2*h)+D*(y(i+1)-2*y(i)+y(i-1))/h^2;
    end
end
f = f';
```

Generate and Plot Results

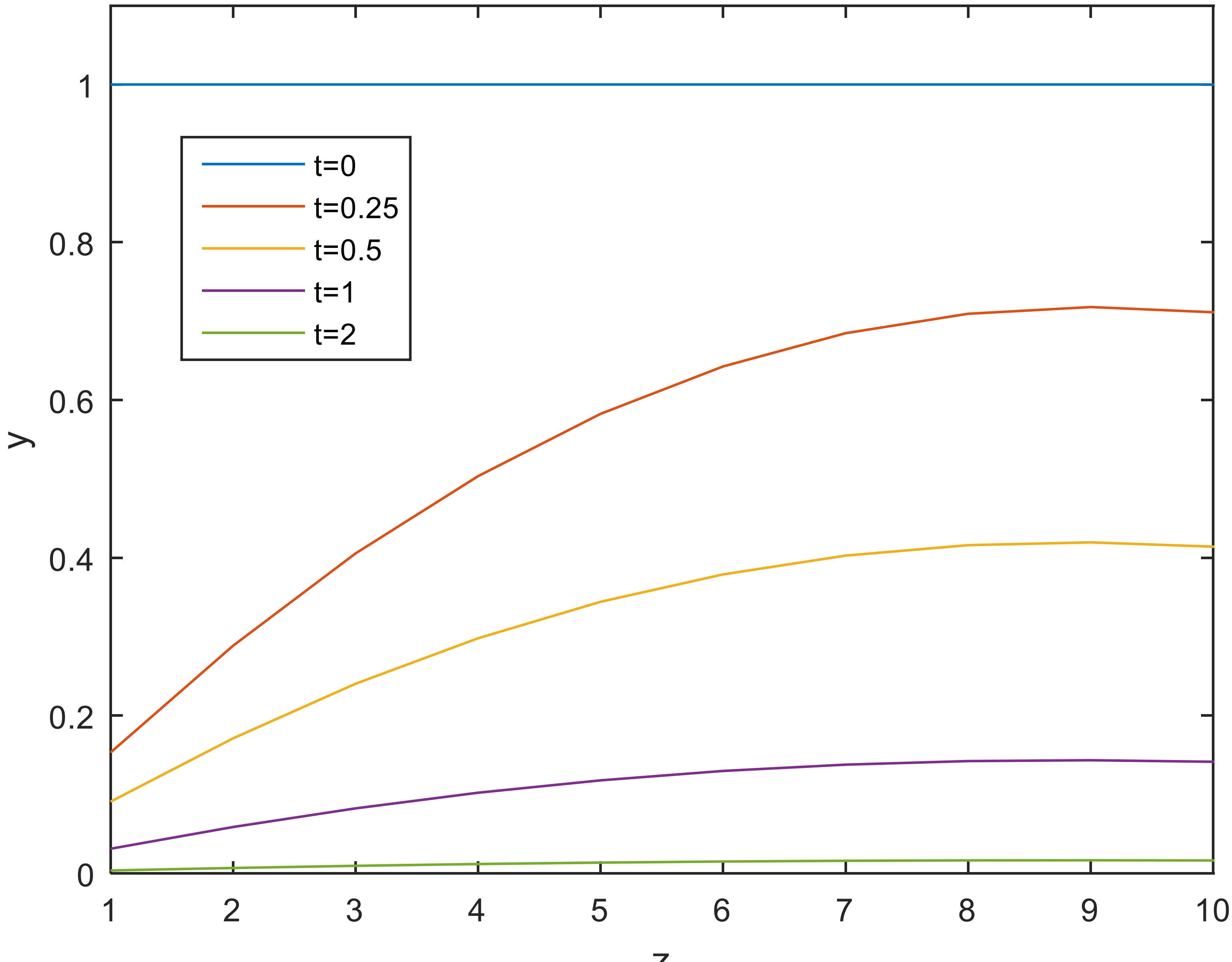
```
>> N = 10;
>> yo = ones(1,N);
>> [t,x]=ode45('pde_example_odes',[0 3],yo,[]);
>> figure
>> plot(t,x)
>> ylabel('y')
>> xlabel('t')
>> legend('x1','x2','x3','x4','x5','x6','x7','x8','x9','x10')
```

```
>> t([1 126 244 478 950])'
ans =   0    0.2493    0.5009    0.9989    2.0006
>> plot(j,x(1,:))
>> hold
Current plot released
>> plot(j,x(126,:))
>> plot(j,x(244,:))
>> plot(j,x(478,:))
>> plot(j,x(950,:))
>> ylabel('y')
>> xlabel('z')
>> legend('t=0','t=0.25','t=0.5','t=1','t=2')
```

Simulation Results (u=1, D=1, N=10)



Simulation Results (u=1, D=1, N=10)



Partial Differential Equation Models

In-class Exercise