Modeling Local and Advective Diffusion of Fuel Vapors: Progress Report

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Outline

- Background
- Equations and Domain
- Current Model
  - Species Fraction Algorithm
    - Results
    - Testing
  - Vorticity and Stream Function Algorithm
- Timeline
- Future Work

Background

- Fuel Pool Fires
- Filming Foam
  - Issues with current surfactants
- Foam Layer and Ghosting
  - Diffusion of Fuel Vapors
  - Degradation of Film Layer
- Project Goal
  - Effective Diffusion Constant and Flux

Earlier Timeline

- October – November
  - Code Species Fraction and Stream Function/ Vorticity Algorithms
  - Stagnation flow solution from Leonard
- December – February
  - Verify code against Fuel Vapor in Air data
- March – April
  - Apply code to Film and Foam data
- May
  - Prepare report and final presentation

Governing Equations

$$u:\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial r}+w\frac{\partial u}{\partial z}=-\frac{1}{\rho}\frac{\partial P}{\partial r}+\frac{\mu}{\rho}\left(\frac{\partial^2 u}{\partial r^2}+\frac{1}{r}\frac{\partial u}{\partial r}+\frac{\partial^2 u}{\partial z^2}\right) \quad (1)$$

$$w:\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial r}+w\frac{\partial w}{\partial z}=-\frac{1}{\rho}\frac{\partial P}{\partial z}+\frac{\mu}{\rho}\left(\frac{\partial^2 w}{\partial r^2}+\frac{1}{r}\frac{\partial w}{\partial r}+\frac{\partial^2 w}{\partial z^2}\right) \quad (2)$$

$$Y:\frac{\partial Y}{\partial t}+u\frac{\partial Y}{\partial r}+w\frac{\partial Y}{\partial z}=D\left(\frac{\partial^2 Y}{\partial r^2}+\frac{1}{r}\frac{\partial Y}{\partial r}+\frac{\partial^2 Y}{\partial z^2}\right) \quad (3)$$

Transformed Governing Equations

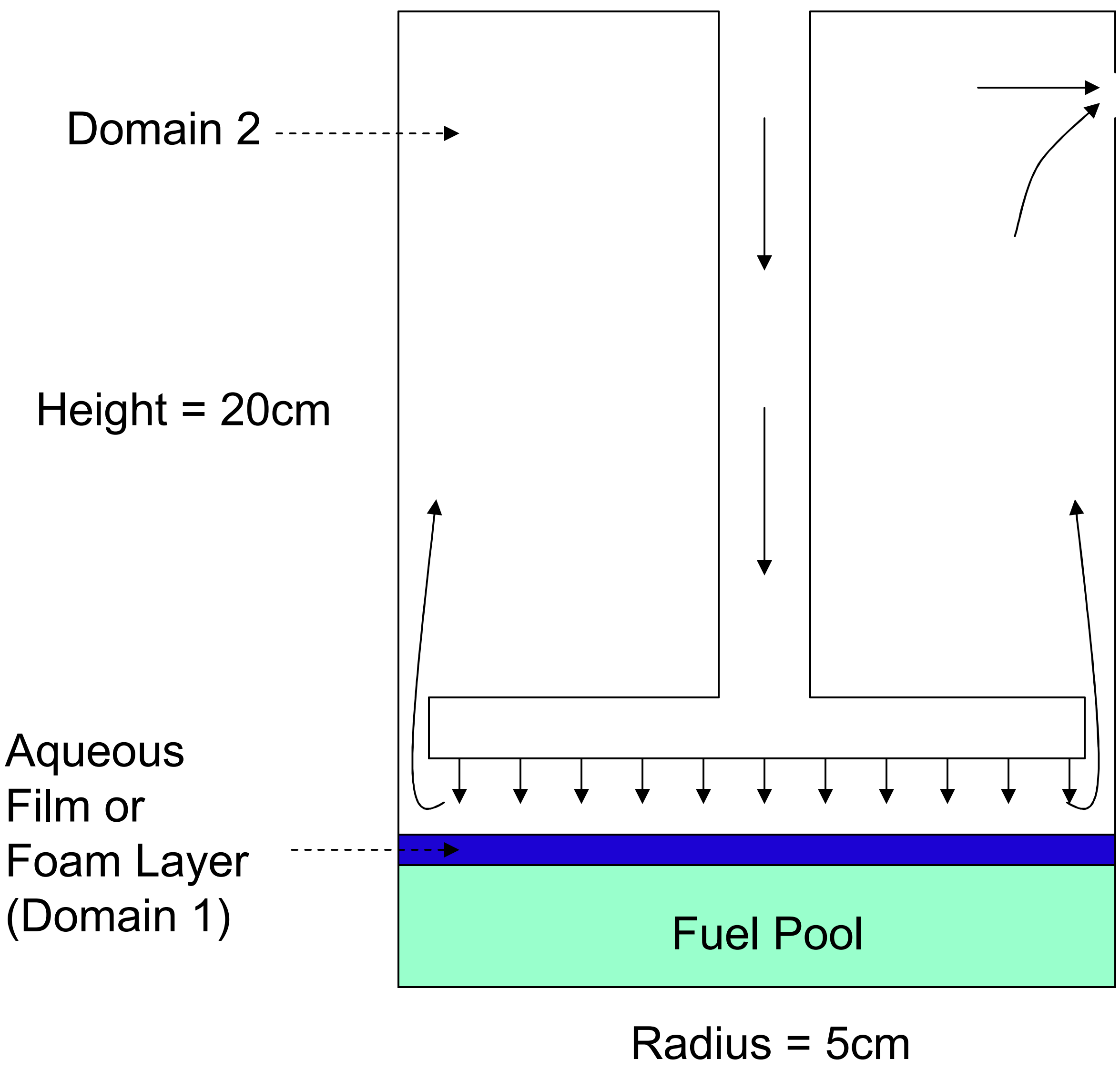
$$u = \frac{-1}{r}\frac{\partial \psi}{\partial z}, w = \frac{1}{r}\frac{\partial \psi}{\partial r}$$

$$\psi : -\Omega = \frac{-1}{r^2}\frac{\partial \psi}{\partial r} + \frac{1}{r}\frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r}\frac{\partial^2 \psi}{\partial z^2} \qquad (4)$$

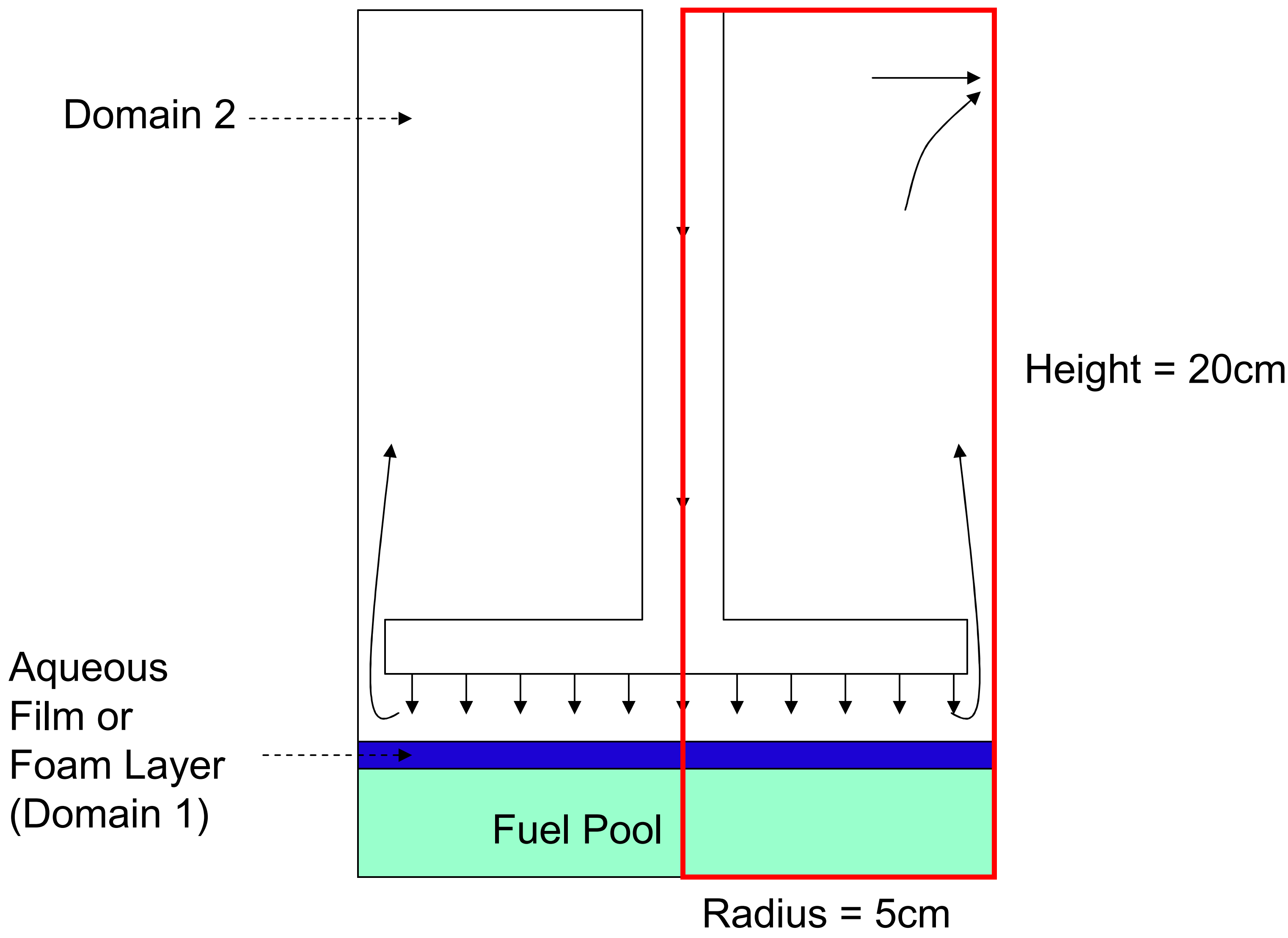
$$\Omega : \frac{\partial \Omega}{\partial t} + u\frac{\partial \Omega}{\partial r} + w\frac{\partial \Omega}{\partial z} = \frac{\Omega u}{r} + \eta\left[\frac{1}{r}\frac{\partial \Omega}{\partial r} - \frac{\Omega}{r^2} + \frac{\partial^2 \Omega}{\partial r^2} + \frac{\partial^2 \Omega}{\partial z^2}\right] \qquad (5)$$

$$Y : \frac{\partial Y}{\partial t} + u\frac{\partial Y}{\partial r} + w\frac{\partial Y}{\partial z} = D\left(\frac{\partial^2 Y}{\partial r^2} + \frac{1}{r}\frac{\partial Y}{\partial r} + \frac{\partial^2 Y}{\partial z^2}\right) \qquad (3)$$

The Experimental Domain



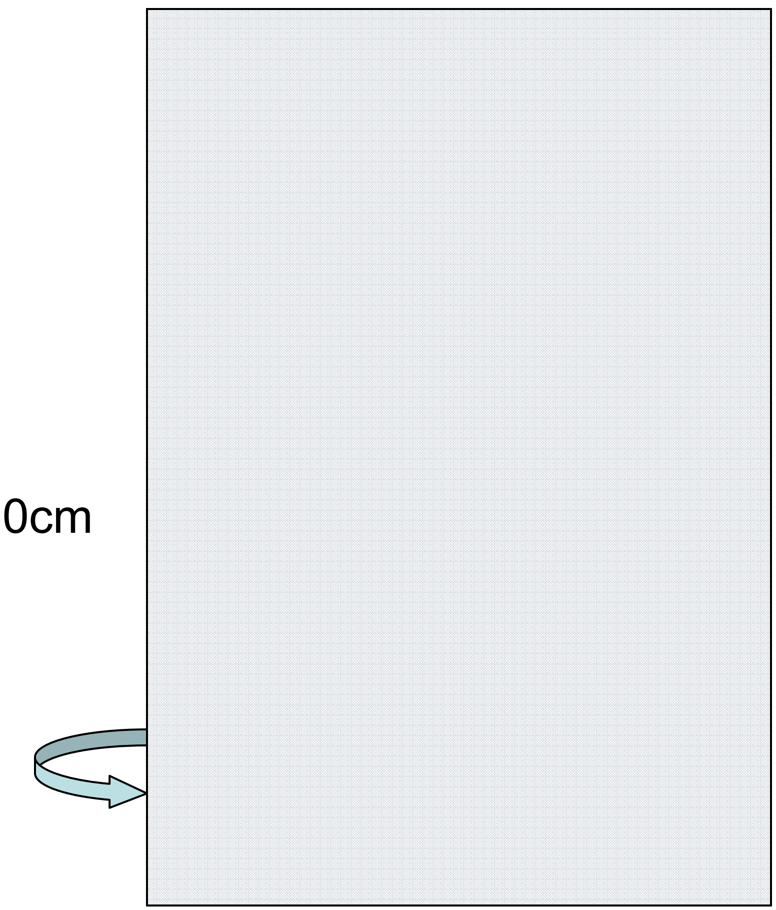
The Experimental Domain



Current Simplified Domain

Axis-Symmetric

Cylinder



Height = 20cm

Radius = 5cm

Species Fraction Algorithm

- Upwind Differencing Scheme
  - Backward Differencing on the convective terms
  - Centered Differencing on the diffusive terms
- $$\frac{\partial Y}{\partial t} + U\frac{\partial Y}{\partial r} = D\left(\frac{\partial^2 Y}{\partial r^2} + \frac{1}{r}\frac{\partial Y}{\partial r}\right)$$

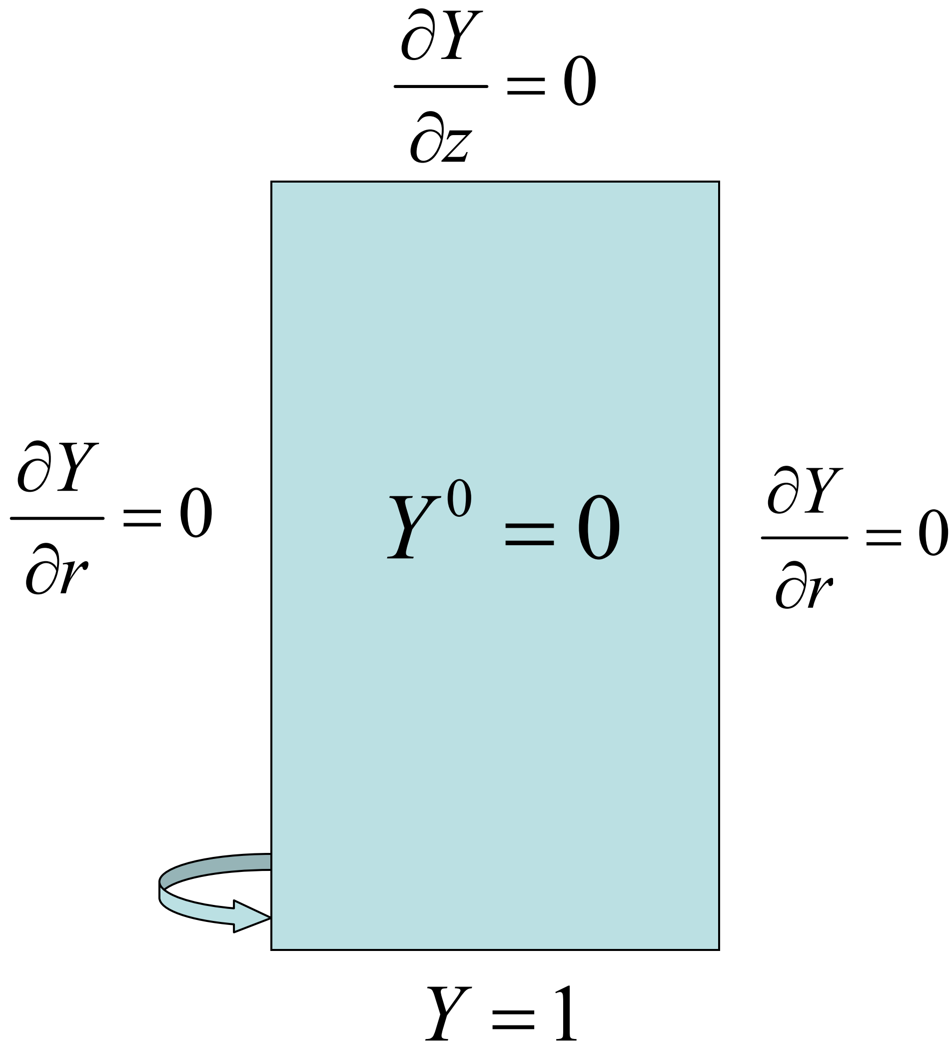
$$\Rightarrow \frac{Y_i^{n+1} - Y_i^n}{\Delta t} + U\frac{Y_i^n - Y_{i-1}^n}{\Delta r} = D\left(\frac{Y_{i+1}^n - 2Y_i^n + Y_{i-1}^n}{\Delta r^2} + \frac{1}{(i-1)\Delta r}\frac{Y_{i+1}^n - Y_{i-1}^n}{2\Delta r}\right)$$

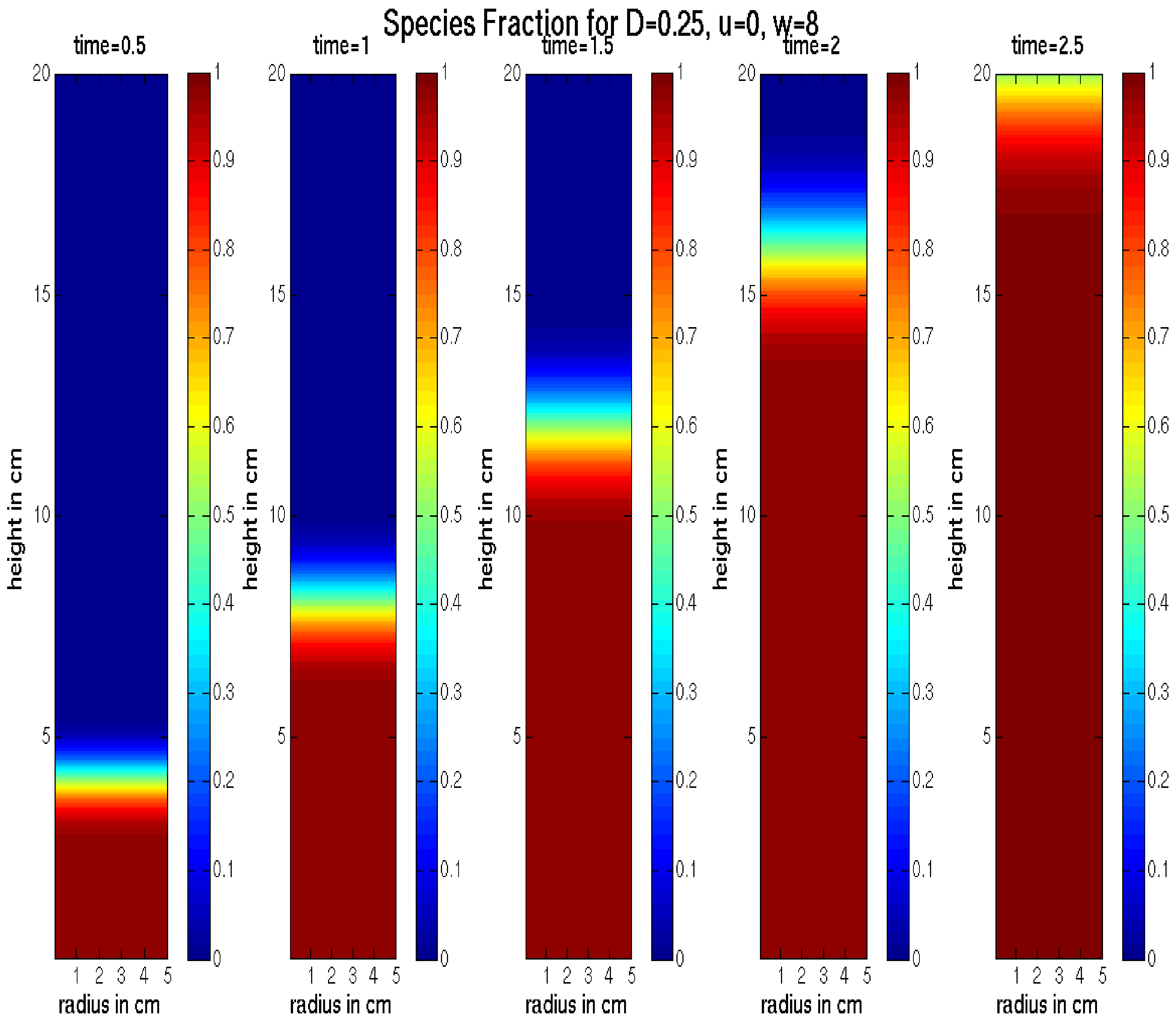
- Constant flow $u = 0, w = c\frac{cm}{s}$
  - slip conditions
- Diffusion of O_2 into N_2

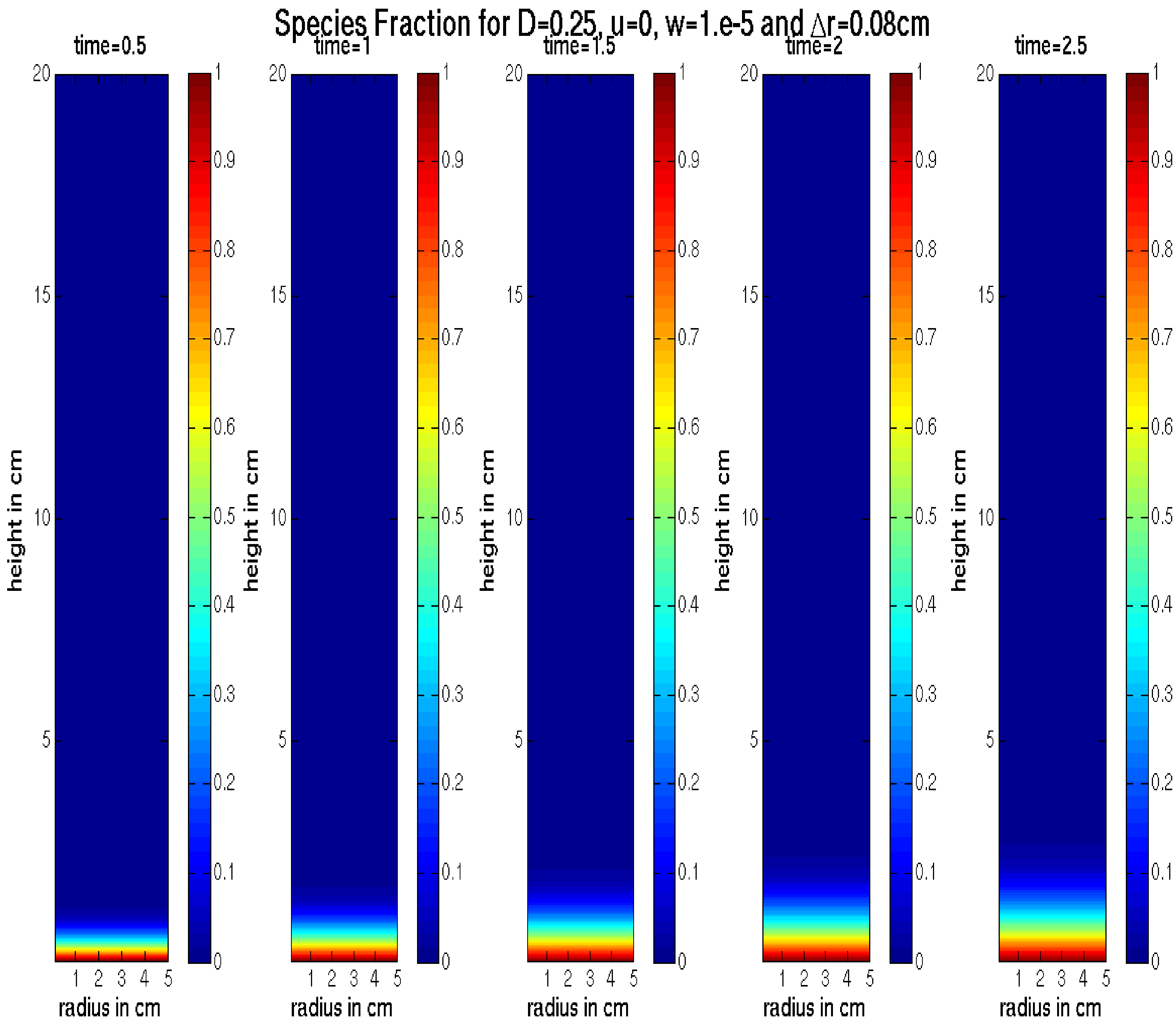
$$D = 0.25\frac{cm^2}{s}$$

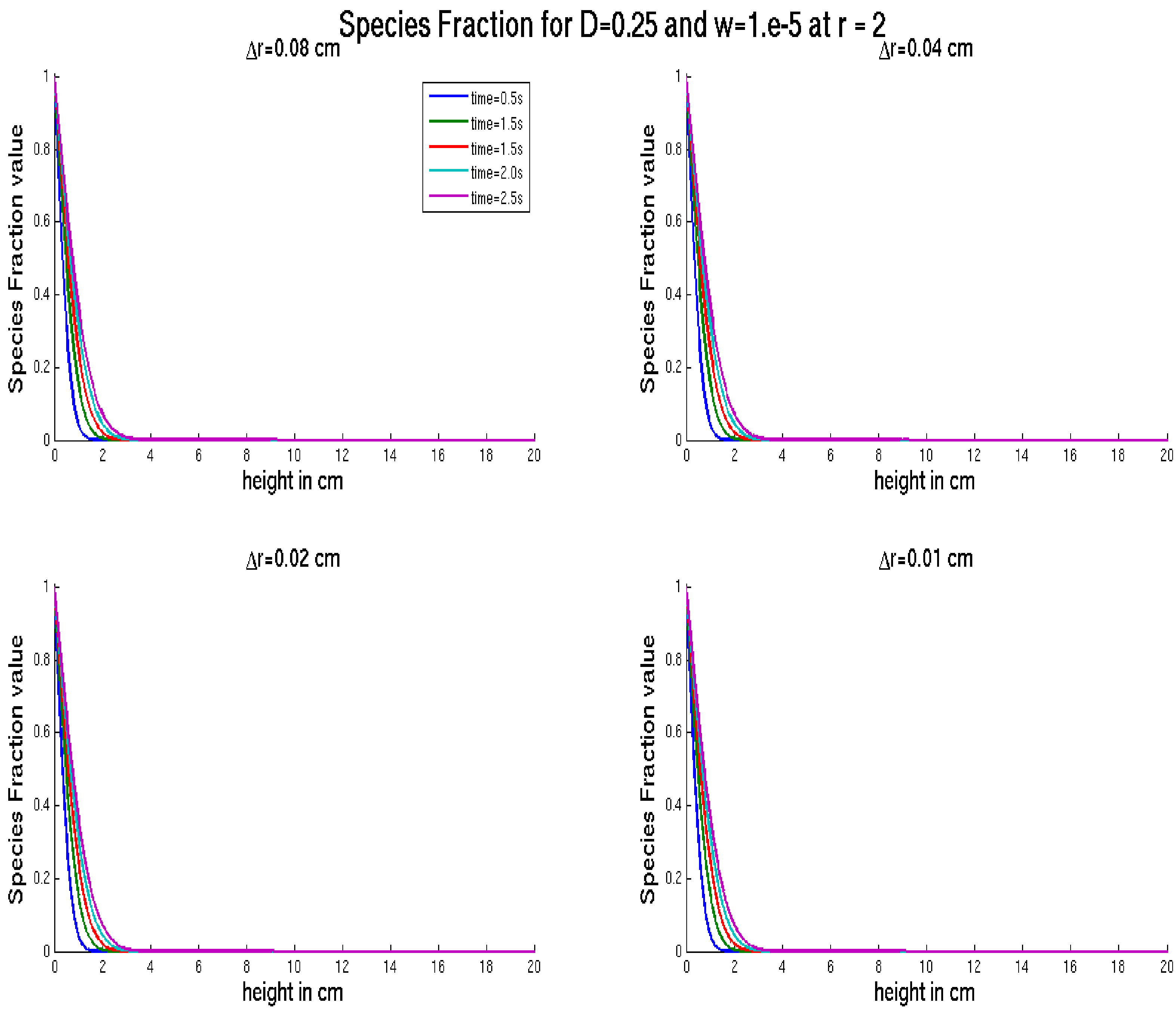
Species Fraction Model

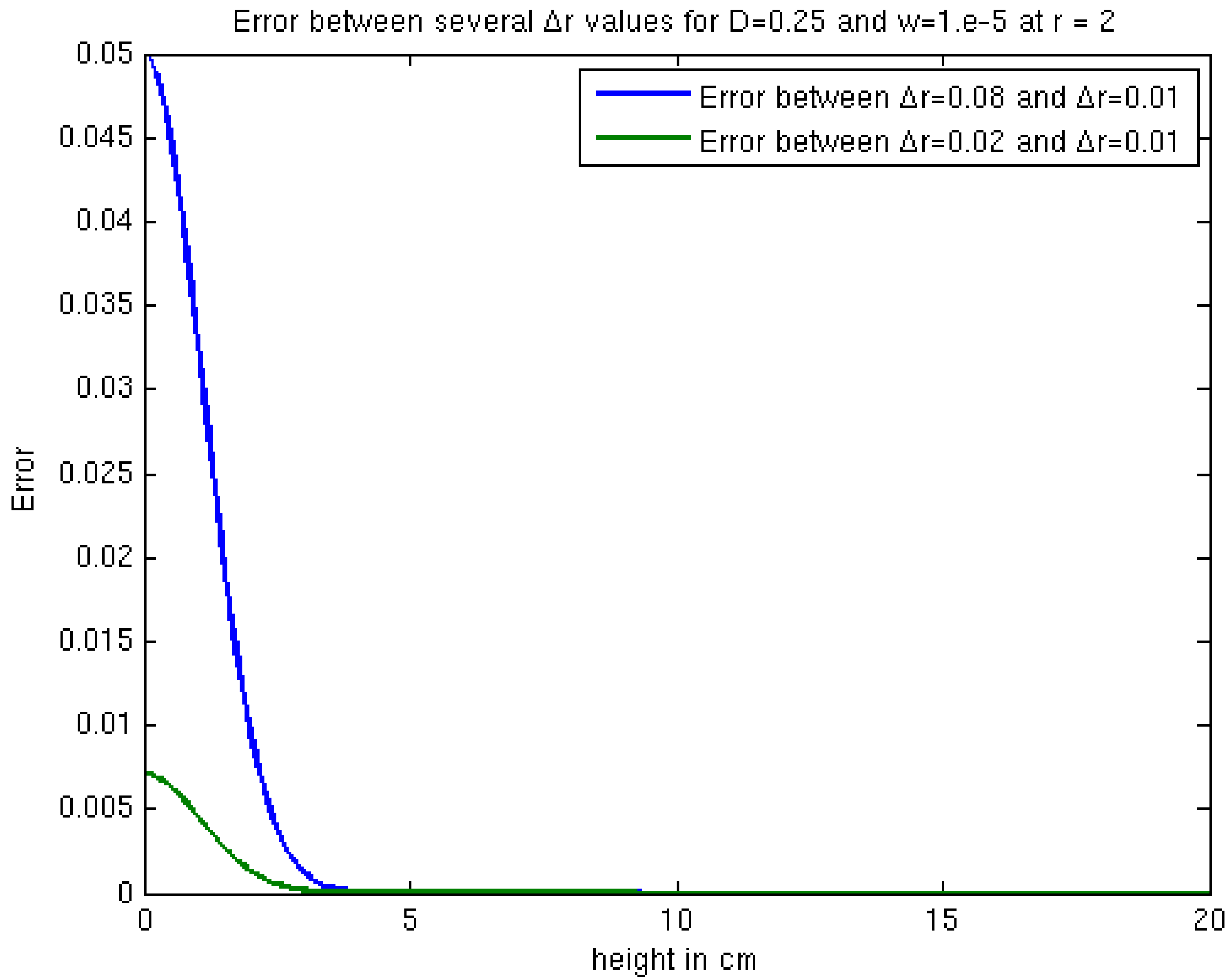
- Boundary conditions
- Initial conditions

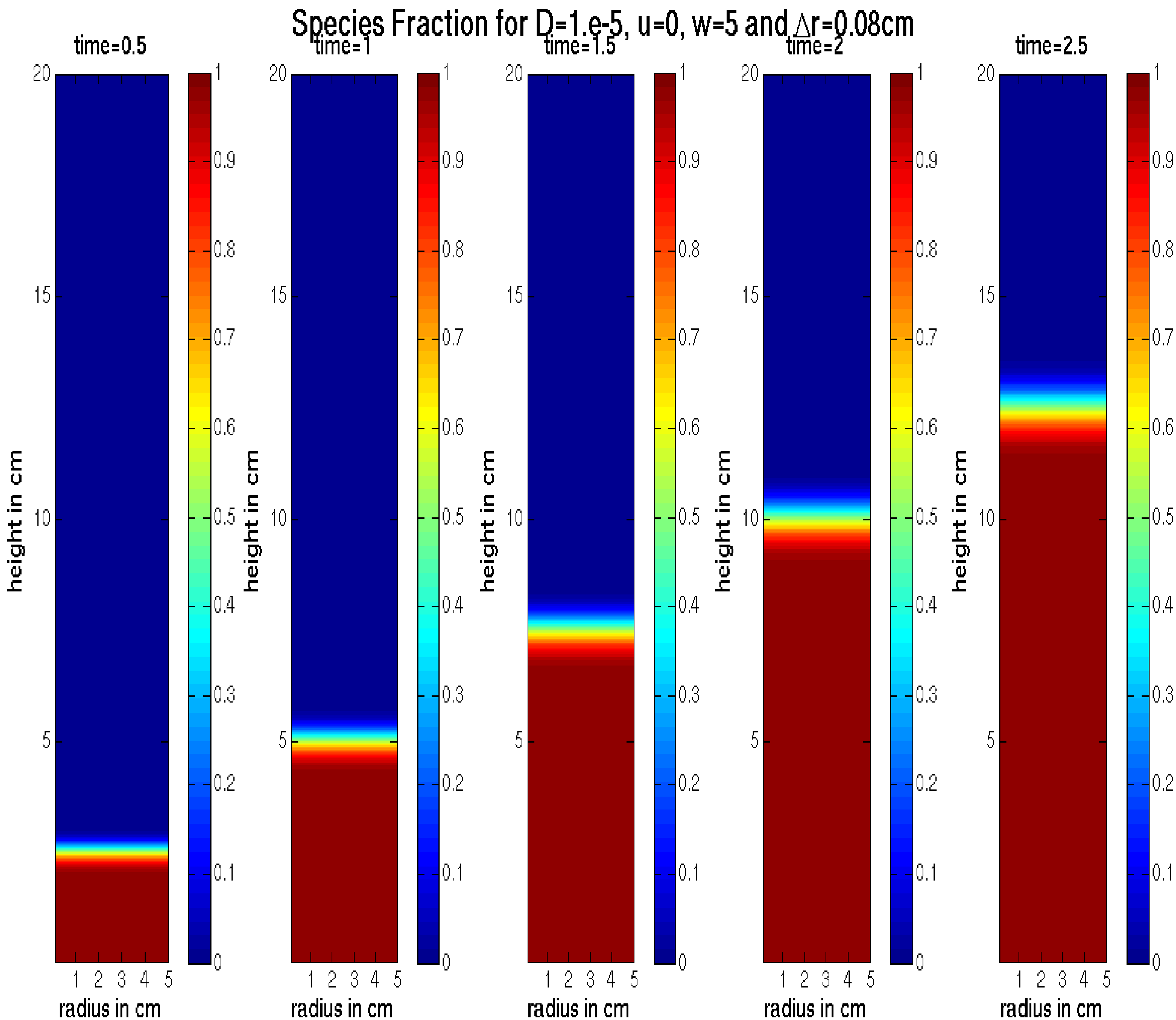


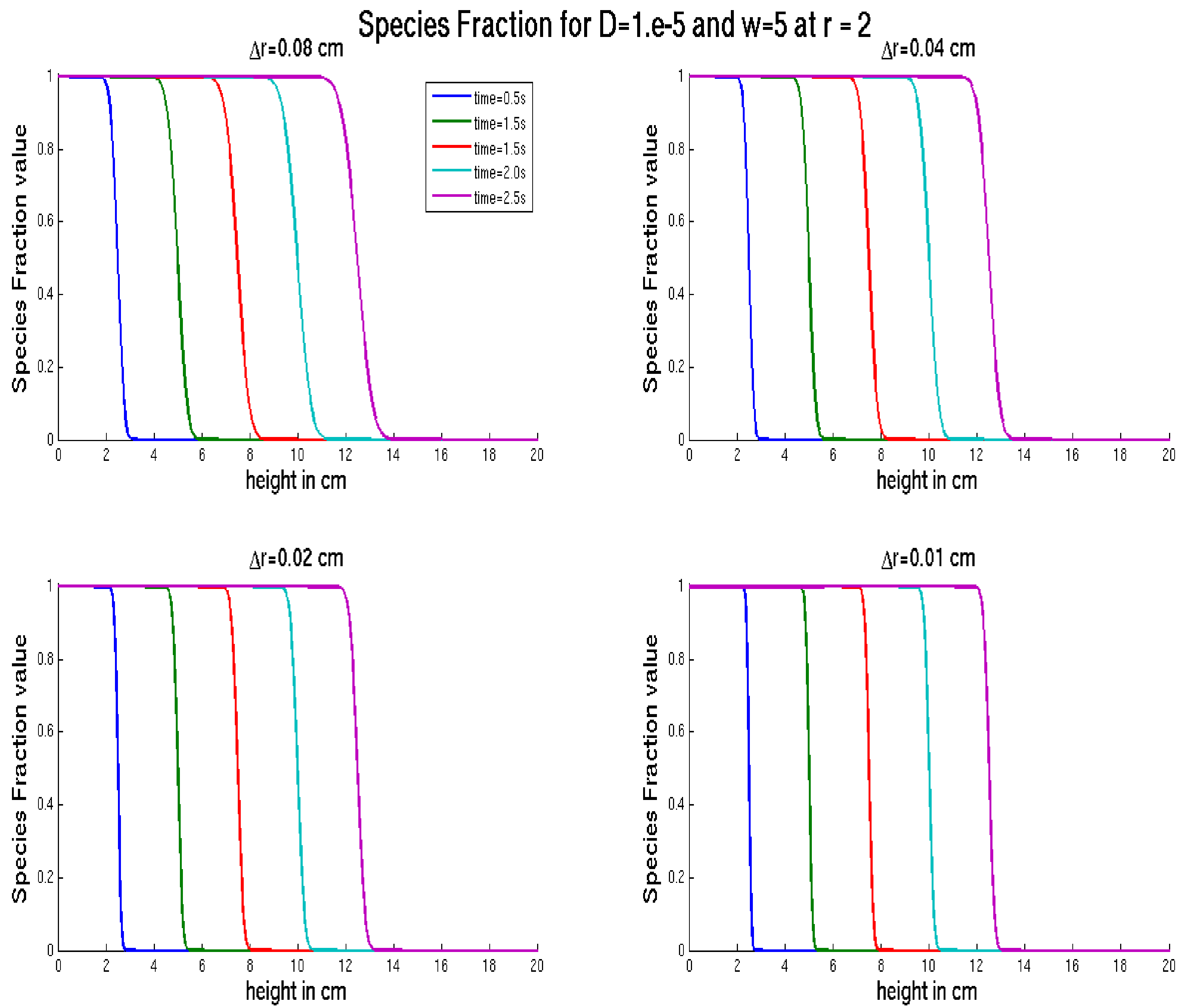

Species Fraction for D=0.25, u=0, w=8
time=0.5
time=1
time=1.5
time=2
time=2.5
height in cm
radius in cm
20
15
10
5
1 2 3 4 5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

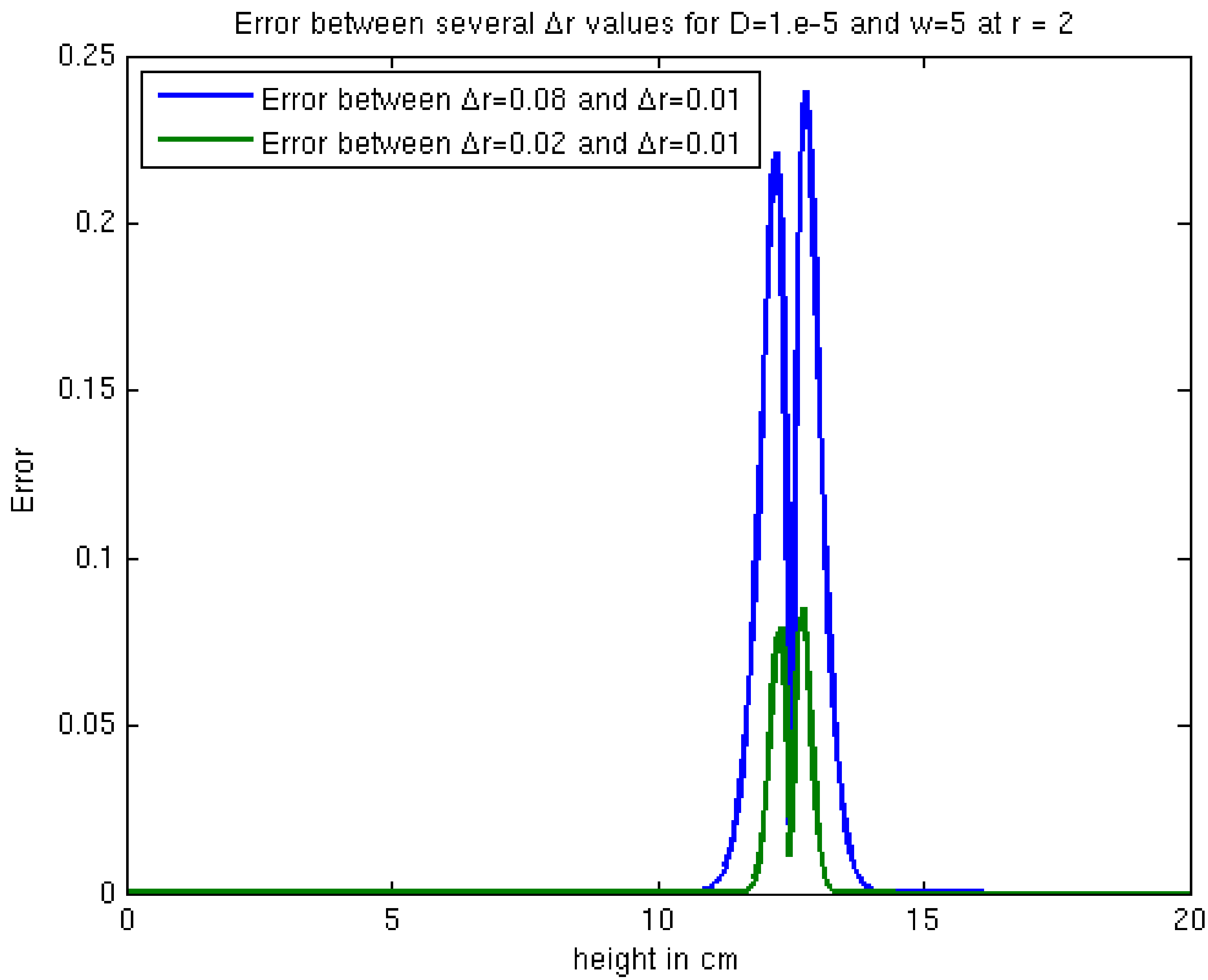

Species Fraction for D=0.25, u=0, w=1.e-5 and Δr=0.08cm
time=0.5
time=1
time=1.5
time=2
time=2.5
height in cm
radius in cm
20
15
10
5
1 2 3 4 5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Species Fraction for D=0.25 and w=1.e-5 at r = 2
Δr=0.08 cm
Δr=0.04 cm
Δr=0.02 cm
Δr=0.01 cm
time=0.5s
time=1.5s
time=1.5s
time=2.0s
time=2.5s
Species Fraction value
height in cm


Error between several Δr values for D=0.25 and w=1.e-5 at r = 2
Error between Δr=0.08 and Δr=0.01
Error between Δr=0.02 and Δr=0.01
Error
height in cm
0.05
0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
5
10
15
20


Species Fraction for D=1.e-5, u=0, w=5 and ∆r=0.08cm
time=0.5
time=1
time=1.5
time=2
time=2.5
height in cm
radius in cm
20
15
10
5
1 2 3 4 5
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1


Species Fraction for D=1.e-5 and w=5 at r = 2
Δr=0.08 cm
Δr=0.04 cm
Δr=0.02 cm
Δr=0.01 cm
time=0.5s
time=1.5s
time=1.5s
time=2.0s
time=2.5s
Species Fraction value
height in cm
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10
12
14
16
18
20


Error between several Δr values for D=1.e-5 and w=5 at r = 2
Error between Δr=0.08 and Δr=0.01
Error between Δr=0.02 and Δr=0.01
Error
height in cm
0
0.05
0.1
0.15
0.2
0.25
0
5
10
15
20

Vorticity Algorithm

- Solve $\Omega^n = \frac{\partial u^n}{\partial z} - \frac{\partial w^n}{\partial r}$
  - interior and exterior points
- Upwind Differencing Scheme

$$\frac{\partial \Omega}{\partial t} + u\frac{\partial \Omega}{\partial r} + w\frac{\partial \Omega}{\partial z} = \frac{\Omega u}{r} + \eta\left[\frac{1}{r}\frac{\partial \Omega}{\partial r} - \frac{\Omega}{r^2} + \frac{\partial^2 \Omega}{\partial r^2} + \frac{\partial^2 \Omega}{\partial z^2}\right] \quad (5)$$

- With Ω^{n+1} , solve

$$-\Omega^{n+1} = \frac{-1}{r^2}\frac{\partial \psi^{n+1}}{\partial r} + \frac{1}{r}\frac{\partial^2 \psi^{n+1}}{\partial r^2} + \frac{1}{r}\frac{\partial^2 \psi^{n+1}}{\partial z^2} \quad (4)$$

Stream Function Algorithm

- $$-\Omega = \frac{-1}{r^2}\frac{\partial \psi}{\partial r} + \frac{1}{r}\frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r}\frac{\partial^2 \psi}{\partial r^2} \qquad (4)$$
$$\Rightarrow e\psi(j,i) + h\Omega(j,i) + a\psi(j,i+1) + \ldots$$
$$b\psi(j,i-1) + c\psi(j+1,i) + d\psi(j-1,i) = 0 = res$$

- Successive Over Relaxation (SOR)

$$\psi(j,i) = \psi(j,i) - \omega\frac{res}{e}$$

Stream Function Algorithm

- SOR with Chebyshev Acceleration
  - Determining the relaxation parameter ω

$$\omega^0 = 1 \qquad \omega^1 = \frac{1}{1 - 0.5q^2}$$

$$\omega^k = \frac{1}{1 - 0.25q^2\omega^{k-1}}$$

where $$q = \frac{\cos\left(\frac{\pi}{m}\right) + \left(\frac{\Delta r}{\Delta z}\right)^2 \cos\left(\frac{\pi}{n}\right)}{1 + \left(\frac{\Delta r}{\Delta z}\right)^2}$$

Vorticity and Stream Function Boundary Conditions

$$\frac{\partial u}{\partial z} = \frac{\partial w}{\partial z} = 0$$

$$\frac{\partial u}{\partial r} = \frac{\partial w}{\partial r} = 0$$

$$u = w = 0\,\frac{cm}{s}$$

$$u = 0, w = c\,\frac{cm}{s}$$

Vorticity and Stream Function Boundary Conditions

$$\frac{\partial \psi}{\partial z} = \frac{\partial \Omega}{\partial z} = 0$$

$$\frac{\partial \psi}{\partial r} = \frac{\partial \Omega}{\partial r} = 0$$

$$\psi = 0$$

$$\frac{\partial \Omega}{\partial r} = 0$$

$$\psi = \frac{c}{2}(r^2 - R^2), \Omega = 0$$

Timeline

- October – November
  - Code Species Fraction Algorithm ☑
  - Code Stream Function/ Vorticity Algorithms ☑
  - Testing Species Fraction Code ☑
- December – February
  - Validation
    - Stagnation flow solution from Leonard
    - Species Fraction Test Cases
    - Diffusion of Fuel Vapors in air
- March – April
  - Apply code to Film and Foam data
- May
  - Prepare report and final presentation

Future Work

- Debug Stream Function/Vorticity Code
  – Test Cases
- Validation
  – Stagnation flow Solution
  – Species Fraction Test Cases
  – Diffusion of Fuel Vapors in air
- Introduce Pipe and Fritted Ceramic Disk
- Create the Film/Foam Layer Domain

References

1. Ananth, R, and Farley, J.P. *Suppression Dynamics of a Co-Flow Diffusion Flame with High Expansion Aqueous Foam.* Journal of Fire Sciences. 2010
2. Bird, R.B., Stewart, W.E., and Lightfoot, E.N. *Transport Phenomena*. 1960
3. Leonard, J.T., and Burnett, J.C. *Suppression of Fuel Evaporation by Aqueous Films of Flourochemical Surfactant Solutions.* NRL Report 7247. 1974

References

4. Panton, R.L. *Incompressible Flow.* 1984
5. Pozrikidis, C. *Introduction to Theoretical and Computational Fluid Dynamics. 1997*
6. Press, W.H., Teukolsky, S.A.,Vetterling, W.T., Flannery, B.P. *Numerical Recipes in Fortran.* 1992
7. Williams, B.A, Sheinson, R.S., and Taylor, J.C. *Regimes of Fire Spread Across an AFFF – Covered Liquid Pool*. NRL Report. 2010

Questions?