Modeling Local and Advective Diffusion of Fuel Vapors: Final Report

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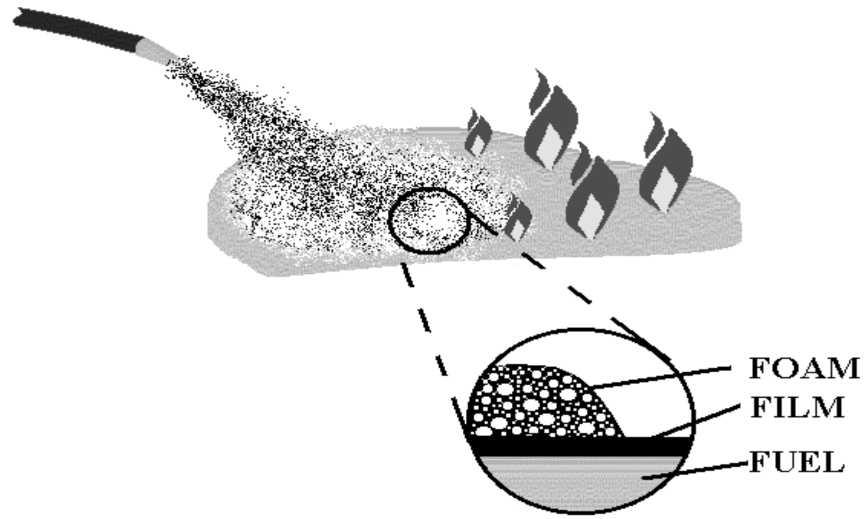
Outline

- Background of the issue
- Purpose of project
- Governing equations
- Validation
  - Simplified domain
  - Experimental domain
  - Secant method
- Application to data
  - Boundary conditions
  - Film layer

Background

- Fuel pool fire
  - Two dimensional fire
  - Class B fire
- Class B aqueous foams
  - Film forming foams
  - Non-film forming foams
- Current product environmentally unfriendly
- New product development
  - Understanding of old product required

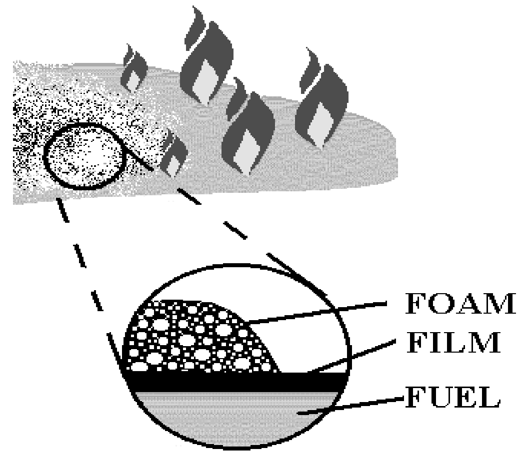


Background

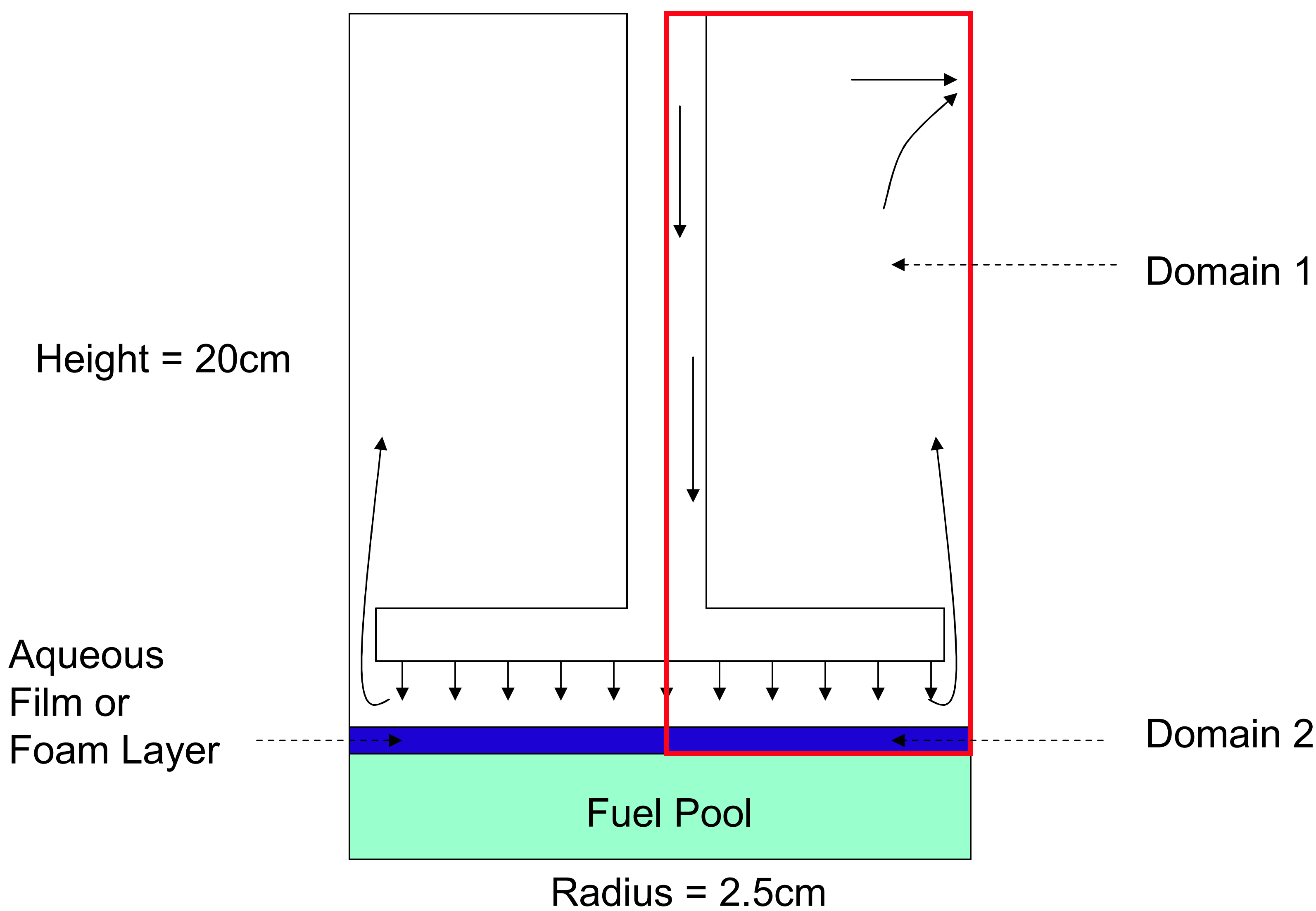
- Purpose of the film/foam
  - Suppress fuel evaporation
  - Suppression not constant over time
- Current suppression theories
  - Fuel vapors dissolve and diffuse
    - Rate governed by D_F
  - Fuel emulsifies

Background

- Purpose of project
  - Consider only fuel vapors in film/foam layer and air
  - Model past experiments of Leonard and Williams
  - Assume dissolving and diffusing transport
  - Match numerical results to experimental data by changing D_F
  - Categorize transport mechanisms by analyzing D_F and resulting concentrations



Experiment to be Modeled



Experiment to be Modeled

- Modeling effort involved solving for
  - Axial and Radial velocities in Domain 1
  - Concentration of fuel vapors in Domain 1 & 2
- Deliverables
  - Software package that
    - models experiments of Leonard and Williams by assuming the dissolve and diffusive mechanism
    - is capable of finding D_F for a film or foam
    - input data

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

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

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

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

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

Solution Algorithms

- Upwind differencing

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

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

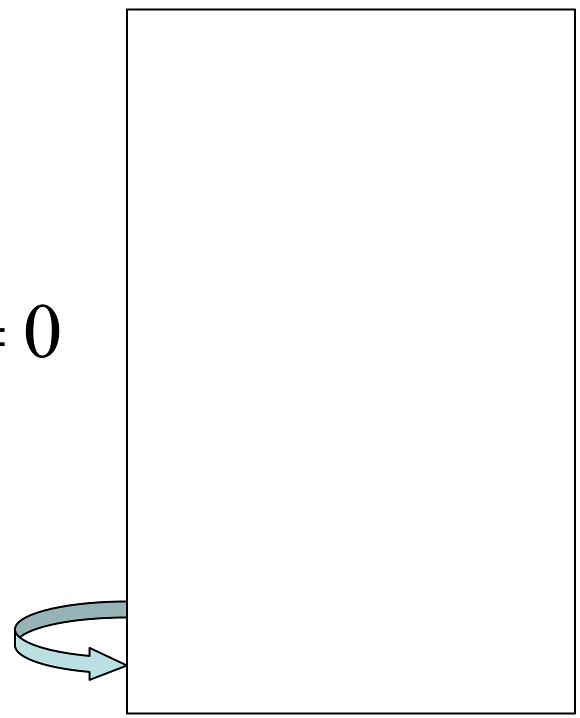
- Successive over relaxation

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

Simplified Domain B.C.

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

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



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

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

Validation and Testing

- Simplified domain
  - Species fraction solver
    - Pure advection $$\frac{\partial Y}{\partial t} + c\frac{\partial Y}{\partial z} = 0$$
    - Pure diffusion $$\frac{\partial Y}{\partial t} = D\frac{\partial^2 Y}{\partial z^2}$$
  - Comparison of species fraction and vorticity solvers
  - Comparison of stream function solver to Matlab's finite element solver

Validation and Testing

- Experimental Domain
  - Specified flux at fuel pool surface
    - Implies specified amount of fuel evaporation
    - Test if at steady state same evaporation at outlet is achieved
  - Compared to experimental data
    - Uncovered n-heptane pool
    - Specified nitrogen flow rate
    - Matched data within experimental uncertainty region

Validation and Testing

- Secant Method for finding D_F
  - Compare uncovered and covered pool ratios between experimental and numerical results
  - Removes some experimental uncertainty

$$D_{n+1} = D_n - \left(R_{\exp} - R_n\right)\left[\frac{D_n - D_{n-1}}{(R_{\exp} - R_n) - (R_{\exp} - R_{n-1})}\right]$$

- Initial guesses
  - Chapman-Enskog Kinetic Theory (foam)
  - Wilke-Chang eq. for Liquid-Liquid Diffusion (film)

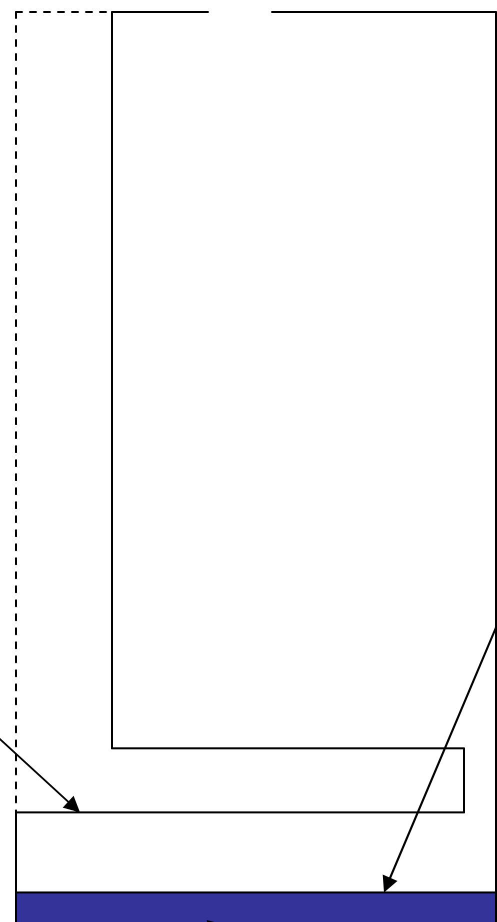
Validation and Testing

- Secant Method for finding D_F
  - Test Case: 3cm high foam layer with specified nitrogen flow
    - Uncovered steady state total flow known
    - Set $D_F = 0.01 cm^2 s^{-1}$ to find steady state total flow for covered case
    - Removed known D_F value and set $R_{\exp}$ as the ratio as the above total flow values
    - Asked code to find D_F that results in $R_{\exp}$
    - Found correct value of $D_F = 0.01 cm^2 s^{-1}$

Boundary Conditions

$$\rho Y w + \rho D_A \frac{\partial Y}{\partial z} = 0$$

No flux BC



Air Domain:

Henry's Law: Vapor pressure of a gas is proportional to the amount of gas dissolved in the liquid

$$\frac{P_v}{P_A} Y_F$$

Film Domain:

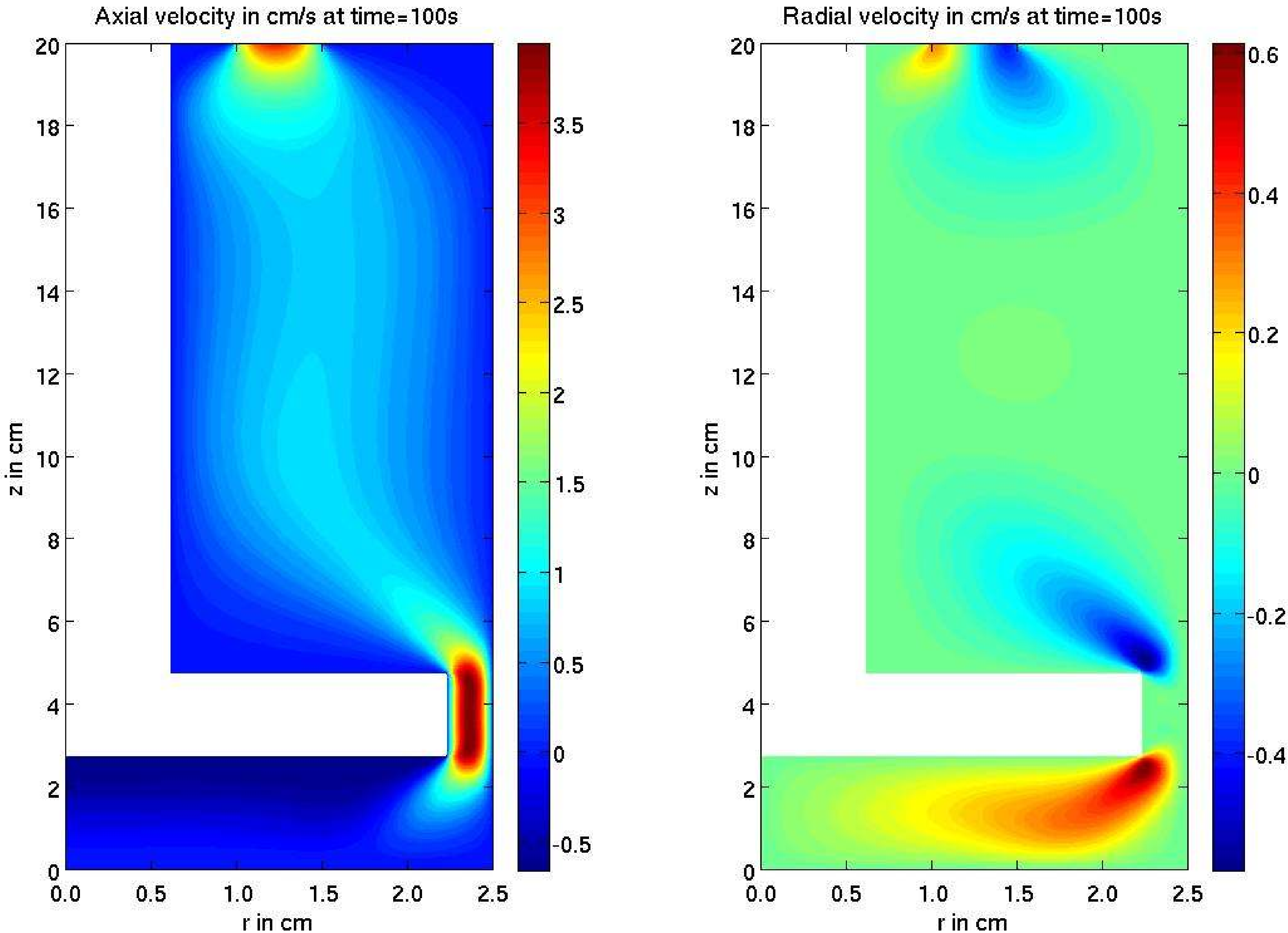
Matching fluxes

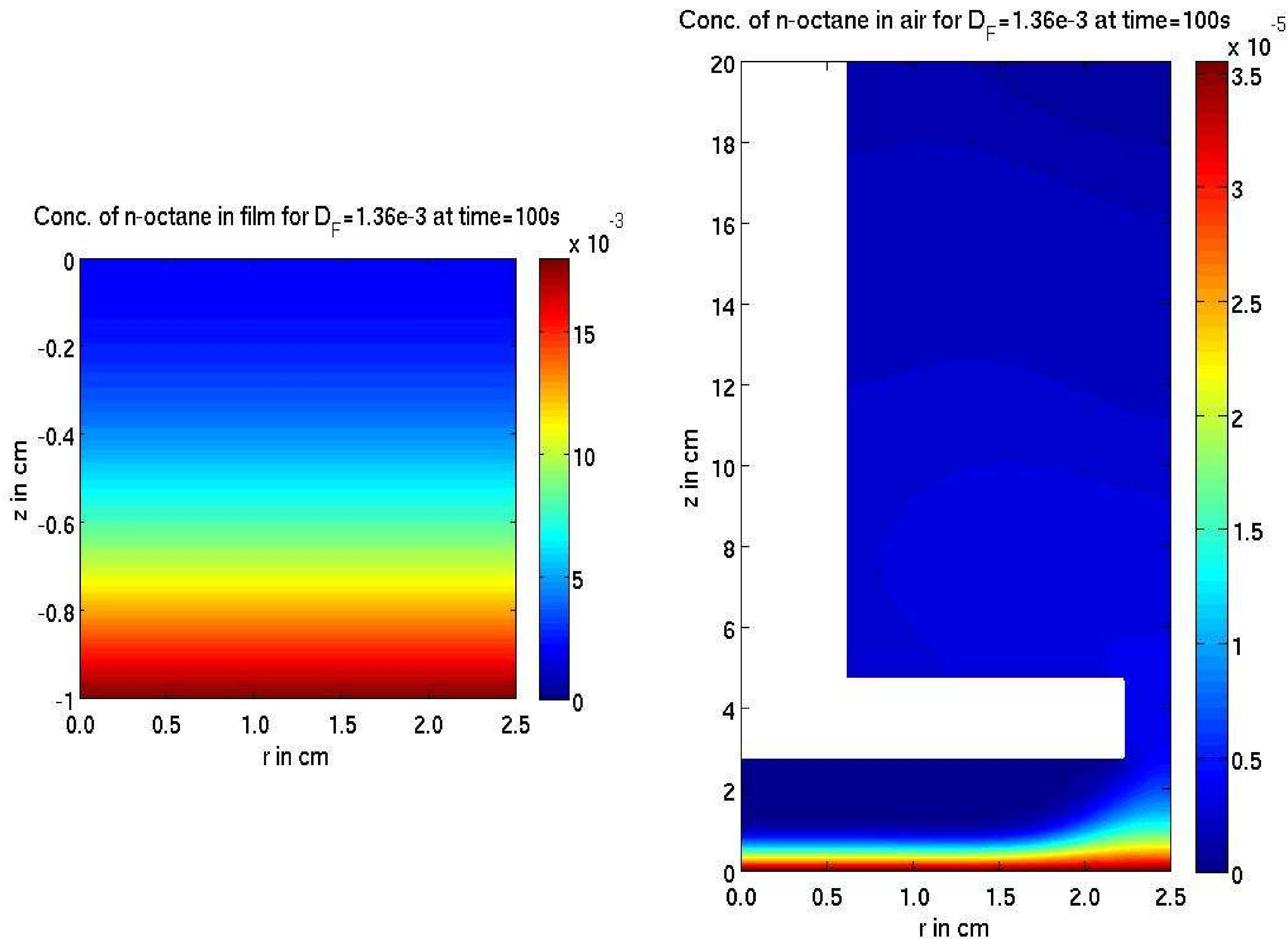
$$\rho_A D_A \frac{\partial Y_A}{\partial z} = \rho_F D_F \frac{\partial Y_F}{\partial z}$$

Mole Fraction resulting from solubility of fuel in water

Results: Case 1

- n-octane pool covered by 1cm of film
  - At 100s, concentration measured to be 0.15% of uncovered value
  - Flow rate of nitrogen was 630 cc per min
  - Mole fraction used for the bottom boundary condition is 0.018
  - $D_A = 0.06\, cm^2 s^{-1}$
  - $D_F = 1.36 \cdot 10^{-3}\, cm^2 s^{-1}$


Axial velocity in cm/s at time=100s
z in cm
r in cm
0.0
0.5
1.0
1.5
2.0
2.5
0
2
4
6
8
10
12
14
16
18
20
-0.5
0
0.5
1
1.5
2
2.5
3
3.5
Radial velocity in cm/s at time=100s
z in cm
r in cm
0.0
0.5
1.0
1.5
2.0
2.5
0
2
4
6
8
10
12
14
16
18
20
-0.4
-0.2
0
0.2
0.4
0.6

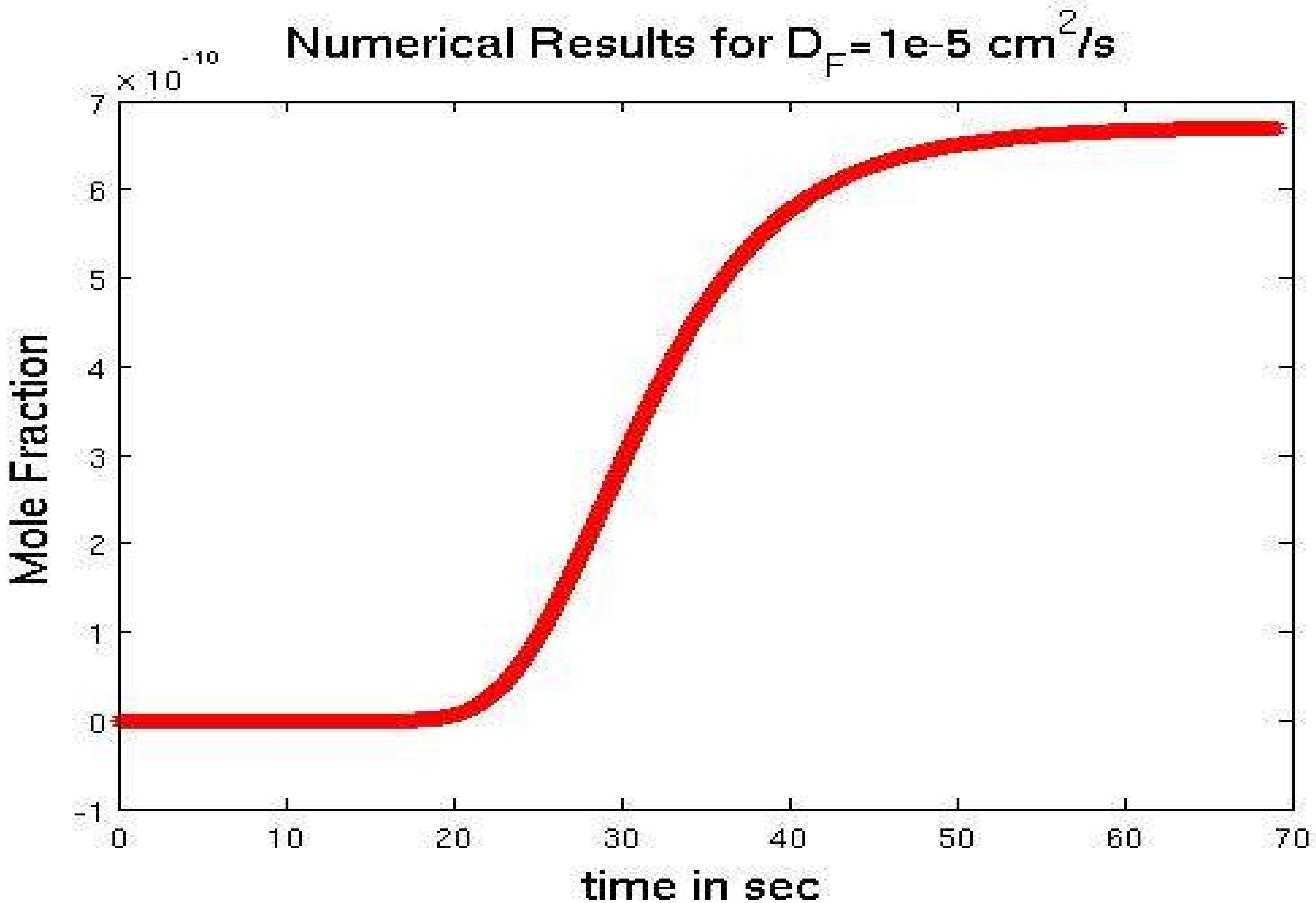


Conc. of n-octane in film for D_F=1.36e-3 at time=100s
x 10^{-3}
15
10
5
0
z in cm
0
-0.2
-0.4
-0.6
-0.8
-1
0.0
0.5
1.0
1.5
2.0
2.5
r in cm
Conc. of n-octane in air for D_F=1.36e-3 at time=100s
x 10^{-5}
3.5
3
2.5
2
1.5
1
0.5
0
z in cm
20
18
16
14
12
10
8
6
4
2
0
0.0
0.5
1.0
1.5
2.0
2.5
r in cm

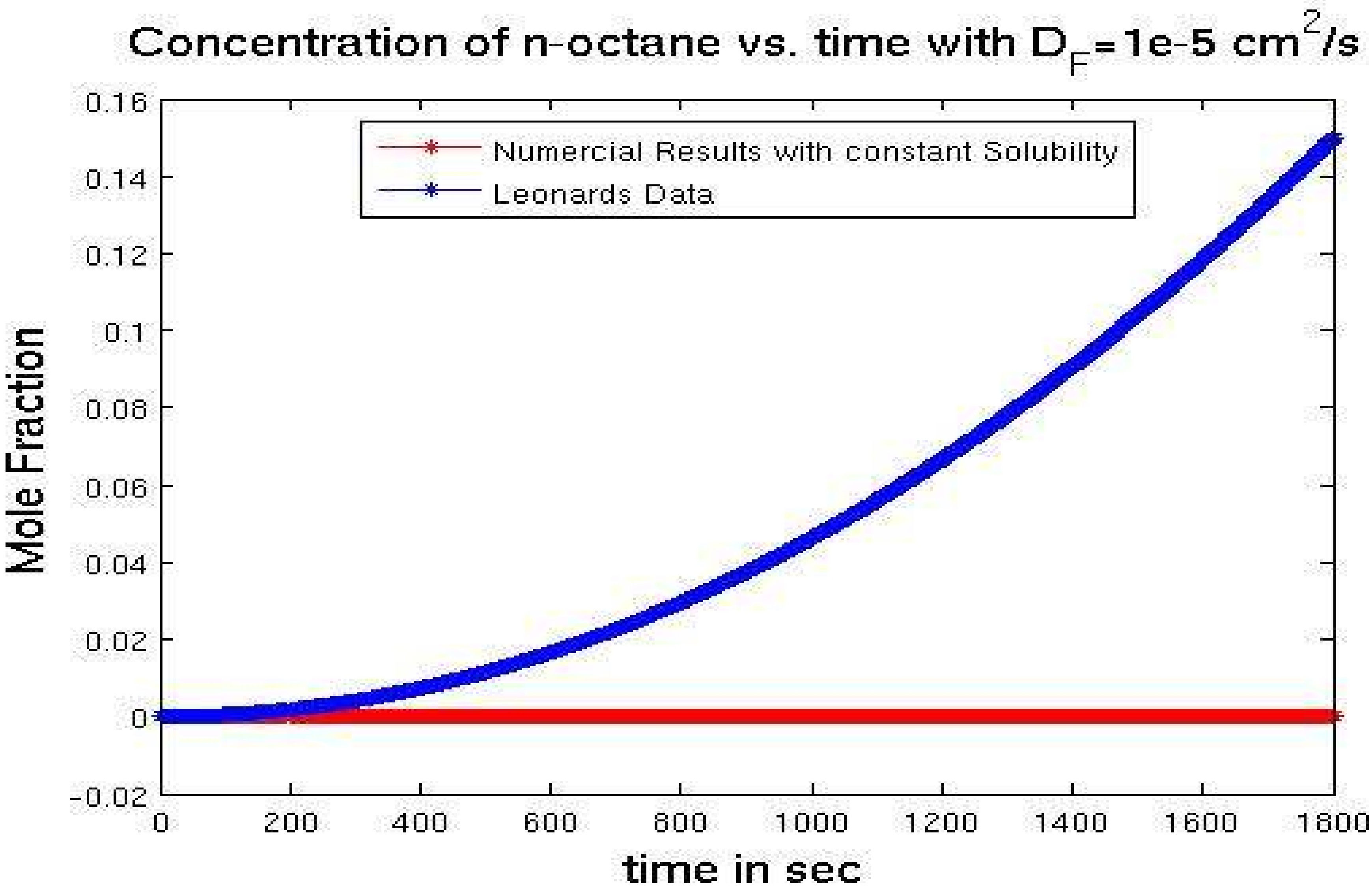
Results: Case 2 (Leonard's Data)

- n-octane pool covered by $2.35 \cdot 10^{-3}$ cm of film
  - At 1500s, concentration was measured to be 15% of uncovered value
  - Flow rate of nitrogen was 630 cc per min
  - Mole fraction resulting from solubility of n-octane in water is $3 \cdot 10^{-7}$
  - $D_A = 0.06\, cm^2 s^{-1}$
  - $D_F = 1 \cdot 10^{-5} cm^2 s^{-1}$

Results: Case 2 (Leonard's Data)



Results: Case 2 (Leonard's Data)



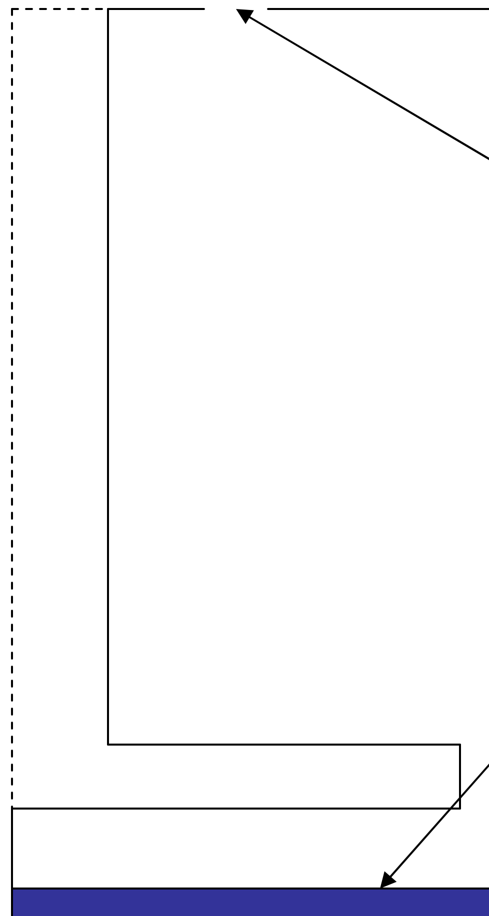
Results: Case 2 (Leonard's Data)

Uncovered Case:

$$Y = 2.35 \cdot 10^{-3}$$

Solubility:

$$Y_{Sol} = 3 \cdot 10^{-7}$$



$$Y = 3.525 \cdot 10^{-4}$$

$$Y_{Sur} > \frac{3.525 \cdot 10^{-4}}{0.018}$$

$$Y_{Sol} > Y_{Sur} > \frac{3.525 \cdot 10^{-4}}{0.018}$$

Conclusions

- Model correctly predicts uncovered case
- Current theories
  - Dissolve and diffuse
  - Emulsification
- Model suggest dissolving and diffusing is insufficient
  - High solubility necessary
- Possible time dependence of
  - Solubility of fuel in the film layer
  - Diffusion coefficient

Conclusions

- Delivered software package capable of
  - modeling experiments of Leonard and Williams
  - is capable of optimizing over D_F
  - input data
- Future Work
  - Find solubility and D_F necessary to replicate Leonard's film data
    - Solubility experiments
    - Rerun foam layer experiments

References

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Questions?