Modeling Local and Advective Diffusion of Fuel Vapors to Understand Aqueous Foams in Fighting Fires

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Abstract

The purpose of this project is to model the diffusion of fuel vapors through both aqueous film surfaces and aqueous foam surfaces. Aqueous foams are currently being employed to combat fuel pool fires. Once an aqueous foam is applied to a fuel pool fire, an aqueous film forms on the surface of the liquid hydrocarbon pool due to the liquid drainage of the foam. It is the film that is responsible for the suppression of the fuel vapors. Experiments by Leonard [1] and Williams [2] have shown that the film's suppression of fuel vapors is not constant over time. It has become clear that by some process, fuel vapors are able to diffuse through the film and foam layers. This presents a hazard because the fuel vapors above the foam layer can re-ignite the fuel pool fire. A model will be created that simulates local and advective diffusion of fuel vapors over time until a steady state is reached. The diffusion coefficient's space will be explored in an attempt to match this state to the observed steady state concentrations in [1] and [2]. This will allow us to calculate the diffusion coefficient of fuel vapors in both film and foam layers.

1 Background

To combat fuel pool fires, the United States Navy employs several types of fluorinated fire fighting foams. Once applied to a pool fire, a portion of the liquid in the foam drains over a short period of time, depositing a layer of film on top of the fuel pool. The fluorine surfactant in the foam is responsible for decreasing the surface tension of the foam solution, allowing the aqueous layer to "float" on the surface of the fuel pool. This layer of film on the surface of the fuel pool suppresses further evaporation of the fuel. However, several experiments have shown that this suppression of fuel vapors is not constant over time.

In the 1970's, Dr. Joseph Leonard et al at the Naval Research Laboratory (NRL) in Washington, D.C. began testing the suppression ability of the then new aqueous film forming foam (AFFF) [1]. To test AFFF, they took the film that the foam creates and placed a specified amount on a fuel pool. Then they measured the concentration of fuel vapors over a specified amount of time. Their results confirmed that the film created by AFFF was capable of initially suppressing the vapors of several fuel types [1]. What they did not expect to find was that after the initial suppression, the concentration of fuel vapors increased with time. In some cases, fuel vapor concentrations reached levels characteristic of when foam is absent. Recently, this phenomenon has gained interest.

Dr. Bradley Williams, also of NRL, is currently working on an experiment similar to Dr. Leonard's. His experiment involves placing an aqueous foam layer on the surface of a fuel pool rather than the film layer only. When measuring fuel vapor concentration levels over a period of time, Dr. Williams has also found that the concentration of fuel vapor increases with time after the initial suppression by the foam layer.

To motivate my project, I propose an all too realistic situation. In the case of an on-board fire involving fuel spills, an aqueous foam such as AFFF will be applied to the surface. All visually apparent flames will be put out by applying AFFF, but there may exist an ember or an unseen open flame in the vicinity of the foam layer. Suppose that in some area, away from the open flame, the foam surface is compromised. If the fuel vapor concentration above the still intact foam surface reaches a certain level, the unseen open flame may ignite a fire above the foam surface [3], which is known as "ghosting." The "ghost" flames could then travel towards the open fuel pool surface resulting in re-ignition.

Currently, the Navy is involved in "burnback" experiments which test the length of time it takes for an open flame in the vicinity of a foam covered fuel pool to induce "ghosting" and re-ignition [3]. The aqueous foams that the Navy employs have a short filming time as well as a short "burnback" time. This short "burnback" time is directly related to the rate at which fuel vapors are diffusing through the film and foam layers [3].

In addition to not having constant vapor suppression, these fluorinated film forming foams are environmentally unfriendly and carcinogenic. Research is currently being done in order to find a replacement, however a satisfactory

one has not yet been found. Comparison tests are necessary between the current product and any possible replacements in order to insure safety and effectiveness. In order to properly compare, the processes taking place in the current product must be understood. Thus, it is very important to design a model that can calculate the rate at which fuel vapors diffuse through the foam and film layers. This will help us to understand processes such as "ghosting", but also to find replacement products.

2 The Model Equations and Algorithms

The model domain for this project will be the same domain used in [1] and [2]. All calculations will be done in cylindrical coordinates. It will be assumed that the domain is axisymmetric, which will reduce the problem to a two dimensional case. The problem will be divided into two domains of the aqueous film or aqueous foam layer and the remainder of the container. From this point on, the film or foam domain will be denoted domain 1 and the remainder of the container will be domain 2. By splitting the model domain into two, we will be able to pass the top boundary values of domain 1 as a lower boundary condition for domain 2. The film or foam in domain 1 will be assumed to be a continuum.

In both Leonard's and Williams's experiments, air is pumped through a fritted glass disk, positioned two centimeters above the film or foam surface. Air then flows out of the top of the container and the fuel vapor content of that flow is analyzed. Because the air flow in [1] and [2] is slow, the foam layer will be assumed stationary. This leaves us with solving the species fraction equation (Eq. 1) for both domains and the momentum equations (Eq. 2 and 3) for domain 2.

$$\frac{\partial Y_{FV}}{\partial t} + \nabla \cdot (\mathbf{v} Y_{FV}) = -D \nabla \cdot (\nabla (Y_{FV})) \qquad \mathbf{v} = (u, w) \tag{1}$$

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

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial r} + w\frac{\partial w}{\partial z} = -\frac{1}{\rho}\frac{\partial P}{\partial z} + \frac{\mu}{\rho}\left(\frac{\partial^2 w}{\partial r^2} + \frac{1}{r}\frac{\partial w}{\partial r} + \frac{\partial^2 w}{\partial z^2}\right) \tag{3}$$

Y_{FV} denotes the species fraction of fuel vapors [4]. The variable u represents the radial velocity and the variable w represents the axial velocity [5]. Also, D represents the diffusion coefficient. In domain 2, the diffusion coefficient (D_2) of fuel vapors in air is known. In domain 1, the diffusion coefficient (D_1) is not known. We will be optimizing over D_1 to find a diffusion coefficient corresponding to the steady state data from [1] and [2]. Because the mixing of fuel vapors with air, foam, and film results in a small change in density, density will be assumed constant in both domains. This means that $\nabla \cdot (\mathbf{v}) = 0$ from the continuity equation. Thus, we can use the relation $\nabla \cdot (\mathbf{v} Y_{FV}) = \mathbf{v} \nabla Y_{FV} + Y_{FV} \nabla \cdot (\mathbf{v})$ and simplify it to $\nabla \cdot (\mathbf{v} Y_{FV}) = \mathbf{v} \nabla Y_{FV}$ by applying $\nabla \cdot (\mathbf{v}) = 0$. Thus, equation 1 can be rewritten in cylindrical coordinates as

$$\frac{\partial Y_{FV}}{\partial t} + u\frac{\partial Y_{FV}}{\partial r} + w\frac{\partial Y_{FV}}{\partial z} = -D\left(\frac{\partial^2 Y_{FV}}{\partial r^2} + \frac{1}{r}\frac{\partial Y_{FV}}{\partial r} + \frac{\partial^2 Y_{FV}}{\partial z^2}\right) \quad (4)$$

To solve equation 4, we will employ an upwind difference algorithm outlined in [6]. After applying the upwind differencing, we will solve for $Y_{FV} \equiv Y$ at the next timestep according to equation 5.

$$Y_{i,j}^{n+1} = Y_{i,j}^{n} - \Delta t\left[u_{i,j}^{n}\frac{Y_{i,j}^{n} - Y_{i-1,j}^{n}}{\Delta r} + w_{i,j}^{n}\frac{Y_{i,j}^{n} - Y_{i,j-1}^{n}}{\Delta z} + D\left(\frac{Y_{i+1,j}^{n} - 2Y_{i,j}^{n} + Y_{i-1,j}^{n}}{\Delta r^2} + \frac{1}{i\Delta r}\frac{Y_{i+1,j}^{n} - Y_{i-1,j}^{n}}{2\Delta r} + \frac{Y_{i,j+1}^{n} - 2Y_{i,j}^{n} + Y_{i,j-1}^{n}}{\Delta z^2}\right)\right] \quad (5)$$

To solve the momentum equations, the substitution $u = \frac{-1}{r}\frac{\partial \psi}{\partial z}$ and $w = \frac{1}{r}\frac{\partial \psi}{\partial r}$ will be made into equations 2 and 3, where ψ represents the stream function [7]. Then the relation $\nabla^2\psi = -\Omega$ will be applied, where Ω represents vorticity [7]. This will leave us with

$$\nabla^2\psi = -\Omega \quad (6)$$

$$\frac{\partial \Omega}{\partial t} + u\frac{\partial \Omega}{\partial r} + w\frac{\partial \Omega}{\partial z} = \frac{u\Omega}{r} + \eta\left[\frac{1}{r}\frac{\partial \Omega}{\partial r} - \frac{\Omega}{r^2} + \frac{\partial^2 \Omega}{\partial r^2} + \frac{\partial^2 \Omega}{\partial z^2}\right] \quad (7)$$

(8)

Note that by making the substitution $u = \frac{-1}{r}\frac{\partial \psi}{\partial z}$ and $w = \frac{1}{r}\frac{\partial \psi}{\partial r}$ and by applying $\nabla^2\psi = -\Omega$, the momentum equations transform into two equations that do not involve pressure [7].

To solve equations 6 and 7, an algorithm presented in [6] will be used. To begin, the vorticity will be calculated from the velocity fields. Then vorticity at the next time step will be found by using an upwind differencing scheme on equation 7. This will result in an equation similar to equation 5. Then the stream function ψ will be solved for by using an explicit point-successive over-relaxation method on the Poisson equation of $\nabla^2\psi = -\Omega$. Once ψ is found, u and w will be calculated from ψ and the algorithm will be repeated until the final time is reached. For both the species fraction algorithm and this algorithm, the methods used are consistent and the stability depends on the relation $4\alpha_r + |c_r| + |c_z| < 1$, where $\alpha_r = \frac{D\Delta t}{\Delta r^2}$, $c_r = \frac{u\Delta t}{\Delta r}$, and $c_z = \frac{w\Delta t}{\Delta z}$. This stability restraint is that of the upwind differencing scheme [6].

The boundary conditions for domain 1 will only concern the species fraction equation. Along the fuel pool boundary, the fraction will be set to the saturation fraction. Along the walls and top layer, a natural boundary condition will be set. In domain 2, the boundary against the film layer will be set to the values of domain 1's top boundary. Along the remainder of domain 2's

boundaries, a natural boundary condition will be set. As for the stream function and vorticity equation, boundary conditions that equate to no slip conditions will be set on all boundaries except where air is entering and exiting the domain. Where air is entering the system a velocity will be set. Where air is exiting the system a natural boundary condition will be used. The initial condition for the species fraction equation will be the saturation fraction found in experiments before the foam or film is applied. The initial condition for the stream function and vorticity equation will be one that equates to no movement.

3 Verification and Application

In order to verify the model, domain 1 will be removed, leaving only domain 2. This will allow us to model the diffusion of fuel vapors into the air from a fuel pool. There exists experimental data for this type of setup and the diffusion coefficient for fuel vapors in air is known. This experimental data will serve as input for the model, allowing the model to match a diffusion coefficient D_2 to the data. The diffusion coefficient D_2 found by the model will be compared to the known diffusion coefficient. If the two coefficients match, the model will be verified. In addition, we will also be comparing the numerical solution of the air flow with the analytical solution for stagnation flow, which will further verify the model.

After verification, domain 1 will be restored, D_2 will be set to the known coefficient constant, and the steady state data from [1] will be applied to the model. This will find the diffusion coefficient D_1 for fuel vapors in an aqueous film. After this, the process will be repeated by applying the steady data from [2] to our model, which in turn will calculate the diffusion coefficient D_1 for fuel vapors in foam. After finding both of these diffusion coefficients, a parametric study will be performed to test the effect the thickness of the foam layer has on suppression. The effectiveness of a foam layer with a film layer will also be tested against the effectiveness of a foam layer alone. It is important to note that the type of fuel is not being specified within the model. The only way the fuel type is specified is through the input data. This will allow the user to find the diffusion coefficient for the vapors of any fuel in films or foams.

4 Platform, Deliverables, and Timeline

This model will be written in Fortran90 and will be compiled using an Intel Fortran compiler. Upon compiling, simulations will be run on a MacBook Pro containing a 2.4 GHz Intel Core 2 Duo processor and 3 GB of memory. After the project is completed, a software package that is capable of finding diffusion coefficients for a fuel type in a film or foam will be delivered. The experimental concentration data that served as an input to the model will also be delivered.

The time line for this project is as follows. In October and November, the upwind differencing algorithm will be programmed as well as the stream function and vorticity algorithms. The analytical solution for stagnation flow

will also be found during this time. During December, January, and February, the optimization routine will be coded and the code will be verified. From March to April, the model will be applied to the data from [1] and [2]. The results will be organized and the final report written during the month of May.

5 References

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