CAFE: A COMPUTER TOOL FOR ACCURATE SIMULATION OF THE REGULATORY POOL FIRE ENVIRONMENT FOR TYPE B PACKAGES

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ABSTRACT

The Container Analysis Fire Environment computer code (CAFE) is intended to provide Type B package designers with an enhanced engulfing fire boundary condition when combined with the PATRAN/P-Thermal commercial code. Historically an engulfing fire boundary condition has been modeled as σT^4 where σ is the Stefan-Boltzman constant, and T is the fire temperature. The CAFE code includes the necessary chemistry, thermal radiation, and fluid mechanics to model an engulfing fire. Effects included are the local cooling of gases that form a protective boundary layer that reduces the incoming radiant heat flux to values lower than expected from a simple σT^4 model. In addition, the effect of object shape on mixing that may increase the local fire temperature is included. Both high and low temperature regions that depend upon the local availability of oxygen are also calculated. Thus the competing effects that can both increase and decrease the local values of radiant heat flux are included in a manner that is not predictable a-priori. The CAFE package consists of a group of computer subroutines that can be linked to workstation-based thermal analysis codes in order to predict package performance during regulatory and other accident fire scenarios.

INTRODUCTION

Radioactive materials packages such as spent nuclear fuel casks that carry larger "Type B" quantities must be qualified under appropriate regulations such as Title 10, Code of Federal Regulations, Part 71 in the United States or Safety Series 6 published by the International Atomic Energy Agency. Package designers must assure that their design will survive without release of contents, a regulatory 30 minute pool fire. If the designer can assure that the regulatory tests are successful on the first attempt, then costs for redesign and retesting can be avoided. The CAFE fire model gives the package designer a computer workstation fire model based on fire physics that can increase the likelihood of successful testing.

The CAFE code is a complete fire model that includes all of the dominant physics present in fires. The primary limitation of CAFE is that it is a two-dimensional fire model which applies boundary conditions to three-dimensional objects. This problem is solved by sectioning a three-dimensional object into multiple two-dimensional cutting planes and applying the fire model to each of those planes, thereby simulating the three-dimensional character of the fire-object interaction.

FEATURES OF CAFE

CAFE has been developed and exists presently both as a stand alone version and as a subroutine set that links to the commercial Patran/P-Thermal code available from MSC Corporation. The features of the CAFE implementation are general enough that adaptation to other thermal computer codes is possible. The CAFE code is written in FORTRAN 77 and has the following features:

- Finite difference method
- Vorticity-velocity flow solver including a vorticity transport equation
- Pressure based flow solver including x- and y-direction momentum equations
- Two species transport equations (fuel and oxygen)
- Energy transport equation for the fire temperature distribution
- One equation turbulence (eddy diffusivity) model
- Chemical reaction model with Arrhenius reaction rates
- Fractional area and volume surface treatment
- Variable coordinates
- Variable thermophysical properties
- Heat transfer by conduction, convection and radiation
- Radiation heat transfer modeled by Rosseland conduction term
- Heat transfer to structures
- Arbitrary location, size, and shape of structures
- Arbitrary gravity vector orientation (x or y direction)
- Dimensioned for multiple x-y planes (will do many two-

dimensional cross sections)
- General boundary conditions - will allow two-dimensional wind simulations.
- *Restart capability*
- Runs with or without flow solver active at every time step
- Runs from an input file
- Both graphical and text output of system variables

Features that are specific to the CAFE/P-Thermal link are:
- Multiple object surfaces (independent fire models)
- Fire model uses P-Thermal surface temperatures for solid surface temperatures.
- three-dimensional unstructured grid to two-dimensional finite difference grid temperature interpolation algorithm.
- three-dimensional to two-dimensional grid mapping is under user control. User can specify direction in which to map the corresponding unstructured and structured grid surfaces.
- User can select any portion of any surface to map between the grids.
- Fire (flame) direction is user selectable.
- *CAFE initiates from either a restart file or stagnant pre-fire conditions.*
- CAFE time and P-Thermal time steps are independent and under user control.
- Graphical output of all CAFE surface /fire models is available.

CAFE uses two optional solvers, a variant of the vorticity-velocity method, and a pressure based method, as the computational-fluid-dynamic (CFD) flow solver in its fire model. Both flow solvers are general enough that any shape or size of structure and any type of two-dimensional fire, including those with wind, can be modeled. Figure 1 illustrates a typical CAFE application, wherein a fire engulfs cylinders in a crosswind.
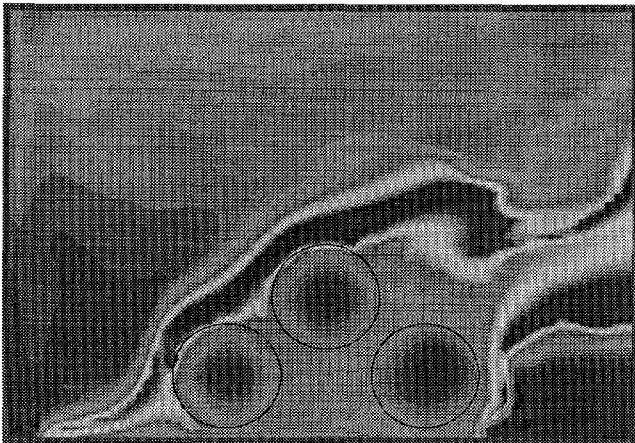

Figure 1. Temperature contours of cylinders in a crosswind. Cylinders are approximately 1 m diameter.

The hot spots are periodic vortices that are typical of large fires. CAFE can be run in different modes depending upon the users need. High fidelity calculations that include puffing phenomena and transient swirling vortices can be resolved with the code as shown the figure above. In contrast lower fidelity calculations that model the fire as a steady state phenomenon can also be utilized. Switching between the

various levels of solution fidelity is a matter of choosing time step size and solution convergence parameters. High fidelity fire models consume more computer time, so that the user must decide when it is warranted.

Recent improvements to the CAFE code have been the implementation of a pressure based flow solver and the Fractional Area and Volume Ratios (FAVOR) treatment for curved surfaces (see Sicilian, 1987).

Future CAFE work is projected to include a user friendly graphical interface so that the user can run P-Thermal directly from PATRAN without setting up input files. Additional development will include enhanced two equation k-ε turbulence modeling, and improved automated mapping of three-dimensional unstructured to two-dimensional structured grids. The extension of the two-dimensional flow solver to three dimensions is also being considered.

The remainder of this paper will describe the equations and numerical methods that are employed in the CAFE code, and an example problem of CAFE linked to the P/Thermal code.

The Governing Equations

In CAFE there are three main categories of equations
- The CFD flow solver
    - The vorticity-velocity method
    - The pressure-based method
- The transport equations
    - Fuel and oxidizer transport
    - Energy transport
    - Turbulence (eddy diffusivity) transport
- The constitutive relationships
    - Equation of state
    - Chemical Reaction Rate Equations
    - Eddy diffusivity relationships
    - Radiation transport (Rosseland conduction)
    - Mass and energy transport diffusion coefficients

THE FLOW SOLVERS

The Navier-Stokes equations have always proved to be exceedingly difficult to solve because of the tight coupling between the pressure term, the momentum flux, and the continuity equation. Researchers have devised many methods to overcome the numerical difficulties associated with the solution to the governing equations. To this end two principle methods have evolved to solve the flow equations, pressure based methods and vorticity based methods. Both methods have been implemented in CAFE. The original version of CAFE used only the vorticity-based solver and later the pressure based solver was included. The vorticity-based solver has the advantage of larger time steps and the pressure based solver has the advantage full implementation of desirable CFD features such as variable grid geometry and the FAVOR curved surface treatment.

Pressure based methods utilize an elliptic pressure equation to solve for the pressure distribution and then solve the momentum equation for the flow distribution. Iterations are often required between the equations to generate a final converged solution. The details of the CAFE pressure based solver are described later in this report. The advantage of the pressure based solver is that source code exists which includes many of the CFD features required in a general flow solver. In addition the

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extension to three dimensions is more straightforward with pressure based solvers.

In contrast the vorticity methods do not require a pressure solution at all, rather the flow is derived from the vorticity distribution, and the definition of vorticity combined with the continuity equation. The vorticity distribution is found from a parabolic transport equation for vorticity, which is derived by taking the curl of the momentum equation. The main advantage of the vorticity method is that the continuity equation is satisfied automatically, whereas in pressure based methods great pains are taken to insure that continuity is satisfied to some degree of precision. From the perspective of the CAFE code, the vorticity based methods are superior because they provide a flow solver that is transient, capable of taking very large time steps, and satisfies continuity to a high degree of precision. However a disadvantage of the vorticity method is that a significant amount of code development is required in order to implement the full generality of a CFD code.

Vorticity-Velocity Flow Solvers

The first CFD flow solver in CAFE is a variant of the vorticity-velocity method. To be precise it should be called the angular momentum - continuity method. To the authors' knowledge, this method has not been used before; thus it is a novel approach to solving the flow equations. Before presenting this method a review of the historical velocity-vorticity method is in order so that the reader is aware of the underlying differences.

Existing vorticity based methods can be further subdivided into those that utilize the vorticity-stream function method (Gatski, 1991) and those that use the vorticity-velocity method (Roache, 1972). The vorticity-stream function method was the earliest approach and it is still in use today, but is difficult to apply due to awkward boundary condition specification. The vorticity-velocity method is more recent and can be subdivided into first and second order approaches. In the first order approach (alternatively called the div-curl method, Osswald, et al, 1987), the velocity field is determined by solving the coupled problem of the divergence constraint and the definition of the curl of the velocity vector. In contrast, the second order approach (Gatski, 1991) determines the velocity distribution by solving a set of Poisson equations that are derived by taking the curl of the definition of vorticity and using the continuity equation. The first order approach has received scant attention in the literature, whereas the second order approach is quite common, primarily because it has been in use for a much longer period of time. CAFE utilizes a variant of the first order velocity-vorticity method.

The first order (div-curl) velocity-vorticity method relies on the solution to the following equations.

The vorticity transport equation

$$\frac{\partial \psi}{\partial t} + \nabla \Psi V = \nu \nabla^2 \psi - \nabla \times \rho g$$

The definition of vorticity, ψ,

$$\nabla \times V = \psi$$

The continuity equation

$$\nabla \cdot V = 0$$

In these equations, t is time, V is the velocity vector, ν is the kinematic viscosity, ρ is the fluid density, and g is the gravitational constant.

The first equation, vorticity transport, is solved by standard methods applicable to parabolic partial differential equations (Roache, 1972). The second and third equations are solved by expanding the equations on a finite difference (or other self consistent) grid and then manipulating the resulting matrices directly. The method of matrix manipulation varies from one author to the next. Historically the equations above have only been applied to incompressible flows, (ρ is a constant). In a fire the density varies considerably depending upon position whereas the pressure is relatively constant.

The governing equations for the variable density vorticity method are very similar to the incompressible version, and are shown below.

The angular momentum (akin to vorticity) transport equation

$$\frac{\partial \omega}{\partial t} + \nabla \omega V = \mu \nabla^2 \omega - \frac{1}{2}(\nabla \rho) \times \nabla V^2 - \nabla \times \rho g$$

where μ is the fluid viscosity and angular momentum, ω, is difined by

$$\nabla \times \rho V = \omega$$

The continuity equation is

$$\nabla \cdot \rho V = 0$$

In the equations above, angular momentum has replaced vorticity (i.e. angular velocity). This is done because the mass flux ρV appears in the continuity equation, rather than velocity V, and that substitution makes the matrix manipulations required for the solver much more straightforward.

Rather than writing out the form of the matrix and showing how it can be manipulated the actual numerical method will be presented. Figure 2 is a diagram of two adjacent computational mesh cells. The cells are configured in the conventional staggered grid arrangement wherein scalar variables (density, temperature, etc.) are defined at cell centers, fluxes (momentum, velocity, etc.) are defined at cell interfaces and rotation vectors (angular momentum, vorticity, etc.) are defined at cell corners.
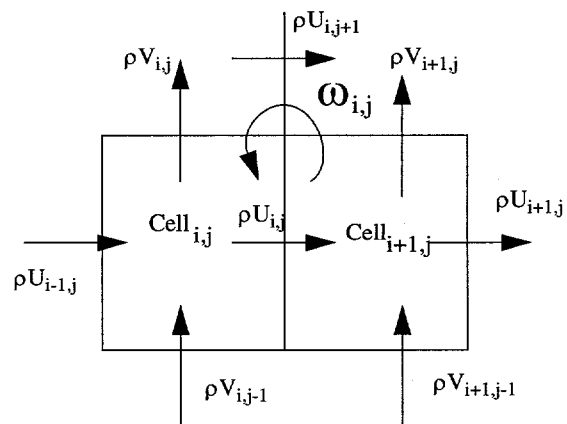

Figure 2. The mesh cell, linear and angular momentum definitions in CAFE

With the use of the terminology depicted in Figure 2. the expressions for the definition of angular velocity and continuity can be written as:

Angular momentum

$$\frac{\left(\rho V_{i+1,j} - \rho V_{i,j}\right)}{dX_{i,j}} - \frac{\left(\rho U_{i,j+1} - \rho U_{i,j}\right)}{dY_{i,j}} = \omega_{i,j}$$

The continuity equation

$$\frac{\rho U_{i,j} - \rho U_{i-1,j}}{dX_{i,j}} + \frac{\rho V_{i,j} - \rho V_{i,j-1}}{dY_{i,j}} = 0$$

These expressions are combined into a tri-diagonal expression for the x-direction mass flux along each level, 'j'. The right hand side of the equation contains y-direction mass fluxes evaluated at the bottom surface of level 'j', and the x-direction interfacial mass flux above cells i,j and i+1,j. The resulting form of the equations at each 'j' level are shown in the equations below

$$A\rho U_{i-1,j} + B\rho U_{i,j} + C\rho U_{i+1,j}$$

$$= D\rho V_{i,j-1} + E\rho V_{i+1,j-1} + F\rho U_{i+1,j+1} + \omega_{i,j}$$

Where the constants are

$$A = \frac{-1}{dX_{i,j}}, B = \frac{1}{dY_{i,j}} + \frac{2}{dX_{i,j}},$$

$$C = \frac{-1}{dX_{i,j}}, D = \frac{1}{dX_{i,j}}, E = \frac{-1}{dX_{i,j}}, F = \frac{1}{dY_{i,j}}$$

These equations are solved by iteration, typically by marching upward from the bottom surface and then down from the top surface. These up-down marching iterations are made until the error in vorticity is negligibly small. When marching, the entire line is solved for the x-direction mass fluxes using the (tri-diagonal) Thomas algorithm (Anderson, 1995). Beginning at the bottom surface, the right hand side of the equation contains the y-direction mass fluxes evaluated at the bottom surface, and those are know from the boundary conditions. The right hand side also contains the x-direction mass flux for the i,j+1 cell. This variable is unknown at the beginning of the iteration and is typically set to the closest known value, say from the last time step, or zero, if starting the calculation cold. Each line is solved for the x-direction mass fluxes using the Thomas algorithm, the fluxes are substituted into the continuity equation to evaluate the y-direction mass fluxes at the upper surface of the line of computational cells. Then the next line is solved in the same manner until the uppermost line is reached. At the top surface, only an expression for the continuity equation is used because it is not possible to satisfy both continuity and vorticity at that location. This same marching procedure is repeated in the downward direction, line by line to the bottom surface, and then marched alternately in the left and right directions. The actual equations are slightly different for each direction that is being marched. This alternating direction marching scheme converges rapidly to produce solutions that are correct to machine accuracy for mass conservation and

to errors of order 10^{-6} in angular momentum, provided there is no structure present.

When structure is present the continuity equation must be used for all computational cells that are adjacent to structure. With structure the iterative solver produces solutions accurate from 10^{-6} to 10^{-17} in both mass and angular momentum conservation.

The main disadvantage of the vorticity-velocity method is the overwhelming complexity that arises when implementing variable grid size along with the fractional area and volume ratio (FAVOR) method for the curved surface treatment. Rather than spend a great deal of time developing new code it was decided that existing pressure based methods, for which source code exists, would be easier to modify and implement for the variable grid and FAVOR methods.

The CAFE Pressure Based Flow Solver

The pressure based method in CAFE is identical to the incompressible algorithm in the two-dimensional code Flow2d, Suo-Anttila, 1993. Although the fully compressible algorithm has been documented in the reference, the incompressible algorithm has not been documented and will be described here.

The numerical methods in the CAFE pressure based flow solver are similar to other CFD codes wherein the flow solver is a SIMPLE algorithm derivative (Pantankar and Spaulding, 1972). The code solves two momentum equations, one continuity equation, a two-dimensional gas energy equation, a two-dimensional structure energy equation, a user defined number of species transport equations, and a two-dimensional Poisson equation for the pressure distribution--all of which are bound to a gas equation-of-state. The coordinate system can be either cartesian (x-y), cylindrical (r-z), or user-defined, with the limitation that the coordinates are assumed to be orthogonal. The conventional staggered-grid formalism is used, which means that all fluxes such as momentum or heat flux are defined at node interfaces, whereas scalar variables such as temperature, density, species, and pressure are defined at node centers.

Predictor-corrector types of algorithms have been used in CFD calculations for many years. The incompressible, primitive variable codes such as SIMPLE and MAC (Harlow and Welch, 1971) and their derivatives are of this variety. Typically in predictor-corrector algorithms one first solves a momentum equation to obtain an estimate of the velocity distribution. Next, a Poisson equation for pressure is solved to obtain a correction for the pressure field. This correction is then used with the momentum equations to produce a corrected velocity field such that the continuity equation is satisfied. Variants of this method exist but the technique is the same--one solves the appropriate equations for an approximate solution and then corrects the solution such that certain governing conditions are satisfied. The methods of correction can be either single, multi-step, or iterative, depending upon the precise formulation and the degree of accuracy desired. The CAFE predictor - corrector method will be presented below.

The governing equations solved in CAFE are the momentum equations, continuity equation, a Poisson pressure correction equation and a momentum correction equation.

The CAFE momentum equation is solved in its conservative form

$$\frac{\partial}{\partial t}\rho u^* + \left[\frac{1}{a}\nabla \bullet ua \, \rho u^*\right] = -\nabla P^n - \rho u^n F + \nabla \mu \nabla u^* - \rho g$$

where ρ is the gas density, u is the gas velocity, P is the gas pressure, F is a drag coefficient, and μ is the gas viscosity including the turbulent eddy viscosity, and g is gravity. The superscript * refers to an estimate of the momentum flux, and n refers to the beginning of the time step value. The area weighing effect of variable porosity due to the presence of structure, the FAVOR curved surface treatment, and non-cartesian (r-z) coordinate systems is included in the area factor **a** in the equation above. The brackets [ ] refer to a vector operation that satisfies the following identity

$$[\nabla \bullet u\, \rho u] = \rho u \bullet \nabla u + u \nabla \bullet \rho u$$

from which the non-conservative form of the momentum equation can be readily derived.

The continuity equation in CAFE is solved to obtain the mass divergence which is required as a source term in the pressure corrector equation

$$\frac{\partial \rho^*}{\partial t} + \frac{1}{a}\nabla \bullet \rho u^* a = 0$$

The Poisson equation for pressure correction is derived from the momentum and continuity equations. Since only a correction to the momentum field is needed, the finite difference form of the predictor momentum equation (indicated by the * superscript) can be subtracted from the end-of-time-step momentum equation (indicated by the n+1 superscript) resulting in the "momentum correction equation." Then the Poisson pressure correction equation is created by taking the dot product of the ∇ operator and the momentum correction equation, and then substituting the corrector continuity equation. The result of these operations is:

$$\nabla^2 P^{n+1} = \frac{\rho^{n+1}-\rho^*}{\Delta t^2} + \nabla \bullet u \frac{\rho^{n+1}-\rho^*}{\Delta t} + \nabla^2 P^n$$

Here n+1 refers to the end-of-time step value, n is the beginning of time step value, * is the end of time step predictor value, and Δt is the time step size. The end of time step density appears in this equation and that is obtained from the assumption of uniform (or hydrostatic) pressure everywhere in the computational mesh combined with the equation of state.

Note that in this expression the drag, gravity, and viscous drag terms no longer appear. This is because those terms are left either in their predictor or beginning of time step form rather than carried through into the final end of time step form shown above. Leaving those terms in their explicit or predictor form results in a negligible loss of accuracy because the time steps are normally short compared to changes in the magnitude of the flow field during a time step.

The solution of the pressure correction equation is used with the momentum correction equation to obtain the final end-of-time-step momentum field.

$$\frac{\rho u^{n+1}-\rho u^*}{\Delta t} = -\nabla(P^{n+1}-P^*) + \frac{u^*}{\Delta t}(\rho^{n+1}-\rho^*)$$

Once the end of time step momentum field has been obtained all of the transport equations for energy, species and turbulence can be updated for their end of time step values.

Summarizing, the method of solution in CAFE is:

1. Solve the momentum equations to obtain the predictor momentum distribution.

2. Integrate the continuity equation to obtain the predictor density distribution.

3. Solve the Poisson equation for a new pressure field that satisfies continuity equation.

5. Solve the momentum corrector equations for the corrected end of time step momentum field.

6. Solve the energy equation for the end of time step gas temperature.

7. Solve the structure energy equation for the end of time step structure temperature.

8. Solve the transport equations for the end of time step scalar variables.

This sequence of calculations is then repeated for the next time step. Note that this solution algorithm does not require an iteration for solution stability. Stability, and solution accuracy, is achieved by time step control rather than iteration.

FRACTIONAL AREA AND VOLUME RATIO (FAVOR) TREATMENT

The FAVOR method has been used for many years with success in finite difference codes (such as FLOW3D, Flow Sciences Los Alamos) in order to improve the treatment of curved surfaces. Earlier versions of CAFE used the 'stair step' method to represent curved surfaces. Increasing the fidelity of solid surface curvature with the stair step method required an increase in the number of computational nodes, with a consequent increase in computational run time. An improved treatment which includes the inclusion of diagonal surfaces within a computational node allows an increase in fidelity without an increase in the number of computational nodes. The FAVOR method is only applicable to the pressure-based flow solver in CAFE. It has not yet been implemented into the vorticity-velocity based flow solver. The basic concepts of the FAVOR method are depicted in Figure 3 below.

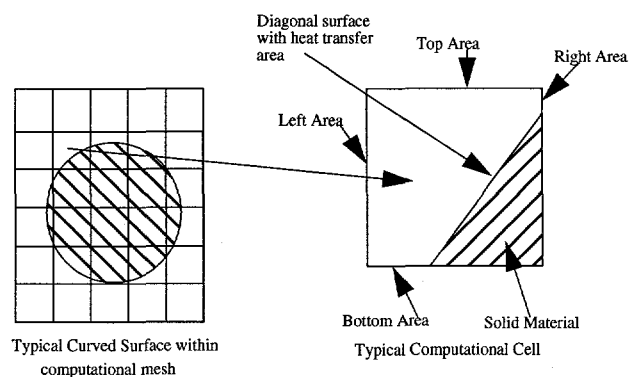Typical Curved Surface within computational mesh

Typical Computational Cell

Figure 3. The fractional area and volume ratio method in CAFE

The cell surface flow areas, top, left right and bottom, are either completely open or partially blocked as are the right and bottom areas shown in the example. The computational cell volume when structure is present is a fraction of the total cell volume. Numerically the FAVOR method appears as an area weighting component in the convective terms of the conservation equations.

In the energy equation there exists two temperatures in a partially filled computational cell, the gas temperature and the solid material temperature. Numerically this is handled by solving two energy equations simultaneously, one for the structure and one for the gas. The equations are coupled to each other by heat transfer through the diagonal surface in the cell. A simplification is made with regard to the conduction distance for heat transfer within partially filled cells, cell size and fractional volume weighting is used rather than distance weighting.

THE TRANSPORT EQUATIONS

A set of transport equations are solved for the various chemical species that are present. The transport equations for chemical species are solved in their conservative form

$$\frac{\partial \rho\, m_i}{\partial t} + \nabla \rho V m_i = \nabla \rho D_{i,j} \nabla m_i + S$$

where ρ is the fluid density, m_i is the mass fraction, V is the velocity vector, $D_{i,j}$ is the diffusion coefficient of species i thorough the bulk fluid j, and S is a mass source term.

A separate gas energy equation is solved in its conservative form shown in the equation below

$$\frac{\partial \rho\, CT}{\partial t} + \nabla \rho CVT = \nabla K \nabla T + Q_v$$

where ρ is the fluid density, C is the specific heat, T is the temperature, V is the velocity vector, K is the fluid conductivity, and Q_v is an volumetric energy source term.

A transport equation is solved in its conservative form for the kinetic energy of turbulence

$$\frac{\partial \rho k}{\partial t} + \nabla \rho V k = \nabla \left(\mu + \frac{\varepsilon}{\rho}\right) \nabla k + \frac{\varepsilon}{\rho} (\nabla \times V)^2 - \frac{C_d \rho k^{\frac{3}{2}}}{1}$$

where ρ is the fluid density, k is the turbulent kinetic energy, ε is the eddy diffusivity, C_d is a constant, and C_d=0.164 if 1 is the ordinary mixing length.

There are several constitutive relationships that are used in CAFE.

THE CONSTITUTIVE RELATIONSHIPS

There is the equation of state

$$P = \rho RT$$

where P is a user defined base pressure, and R is gas constant for air. Currently the molecular weight w is fixed for the entire calculation and is typically set to the value for air. The base pressure can vary during a

flow calculation because the user may assign boundary conditions that cause a net inflow or outflow of mass into the computational domain. Pressure is also affected the mean flow velocity. Since the velocities in a fire of any size are typically less than 20 m/s the maximum possible effect on the solution may be estimated from Bernoulli's equation. The drop in static pressure for a gas moving at 20 m/s is 200 Pa compared to a static gas at atmospheric pressure (0.1 MPa). This corresponds to 0.2% variation in the local gas density and a similar error in the gas velocity. Thus little error is introduced by assuming the gas pressure is governed by the hydrostatic formula for the standard atmosphere,

$$\frac{\partial P}{\partial Y} = -\rho g$$

The chemical reaction rate for mass and energy sources is governed by a second order reaction rate formula

$$R_i = A e^{\left(\frac{B}{RT}\right)} X_o X_f$$

where A and B are user adjustable constants for the Arrhenius reaction rate between oxygen and hydrocarbon fuel, and X_o and X_f are the mole fractions of oxygen and fuel.

The relationship between turbulent kinetic energy and eddy diffusivity is

$$\varepsilon = C_k l(k)^{\frac{1}{2}}$$

Radiation transport by the Rosseland diffusion approximation is valid as long as the mean beam length for radiation diffusion is of the order of the mesh length or less. The most recent experimental data for radiation beam lengths within sooty, fuel fires, is approximately 2-3 cm which is well within the range for computational cells that model large hydrocarbon fires. Thus the formula for the thermal conductivity of the fire is

$$K_r = \frac{16 L \sigma}{3\left(1 + \frac{(1+E)}{E}\right)} T^3$$

where, K_r is the radiative contribution to the gas conductivity. L is the mean beam length of the radiation, E is the emissivity of the gas, and σ is the Stefan-Boltzman constant.

THE ELLIPTIC SOLVER

The equations in CAFE all have elliptic character to some degree, that is, the solution at any given point depends upon the solution over the whole domain. The elliptic solver method chosen for CAFE is a combined form of a tri-diagonal line solver in one direction and an alternating direction explicit (ADE) method in the other direction. The ADE method is an iterative technique that requires at least two passes (up and down for example). After finite differencing all of the equations can be represented by a set of matrices in the following forms.

$$a(i, k)P_{i-1, k} + b(i, k)P_{i, k} + c(i, k)P_{i+1, k}$$
$$= d(i, k) + e(i, k)P_{i, k+1} + f(i, k)P_{i, k-1}$$

The matrices on the left hand side of the equals sign are solved using a tri-diagonal solver. The terms on the right hand side are solved by marching from one boundary, where the solution is known, to the opposite boundary updating the solution for P at each level. When the opposite boundary is reached the direction is reversed and the procedure is repeated. At least two iterations, one up then down, are required to obtain a solution. Additional iterations for increased accuracy can be made by user input options that specify the number of iterations. If the number of iterations exceeds 9 then additional sweeps in the left and right directions are made where the line solver and the ADE method are swapped in the x- and y-directions.

CAFE BOUNDARY AND INITIAL CONDITIONS

The boundary conditions that are used in CAFE determine the nature of the fire that is being modeled. There are many options that can be used such as velocity, velocity gradient, species, temperature, temperature gradient, vorticity and others. By distributing and overlaying combinations of these boundary conditions, almost any combustion configuration can be simulated. In simulating a pool fire the boundary conditions are typically set to an air inflow rate that will achieve complete stoichiometric combustion in a vertical dimension equal to approximately one pool diameter. Since the flame height in a typical pool fire is approximately two pool diameters that will insure that plenty of excess oxygen is present without unrealistic infiltration rates. At the bottom of the computational grid, 100% fuel vapor is injected at a rate typical of an open pool fire (i.e. approximately 0.06 Kg/m^{2}s).

When starting CAFE for the first time the combustion Arrhenius coefficients are set to low values such that fuel vapor will burn at room temperature. Thus when air is injected from the sides and fuel vapor from the bottom, combustion will begin as soon as the gases come into contact. The fire will grow with time to a fully developed state. At that time the fire calculation can be terminated and a restart file is written. All further fires are started from the restart file. This saves computer time and also insures that the fire is engulfing the object at the beginning of the (P-Thermal) calculation. Establishing an engulfing condition is important when running CAFE because the fire code will only be called when the solid object has heated a user-specified number of degrees. If the object is not engulfed, there will be no heating and the CAFE code will never be called.

When starting CAFE from a restart file, the user can make some changes to the input file that will take effect during the calculation. For example, the combustion, turbulence, heat transfer parameters, and boundary conditions can all be changed. Things that cannot be changed are those that would leave some computational cells undefined, such as changes in the number of nodes, object position, or size.

THE CFD ACCELERATOR

One potential problem that is anticipated by PATRAN/P-Thermal users is the calculation intensive nature of CFD types of codes. Typically the user wants the temperature distribution within a solid package and desires that CAFE supply the appropriate boundary conditions. Thus the user is not interested in allocating most of the

computer time to calculating boundary conditions, but rather wants the computer time spent on calculating the temperature distribution within the object of interest. An algorithm has been implemented that allows CFD acceleration so that most of the computer time is spent within the solid conduction model rather than the CAFE model.

CAFE can run with or without the CFD flow solver active. If the flow solver is not active, then CAFE will read a restart file for the steady flow distribution and only advance the energy, species and turbulence transport solutions in time. This type of calculation will allow the user to predict a surface temperature distribution which includes convective effects of the flow.

If the flow solver is turned on, then a fully time dependent CFD solution will be made available to the conduction solver code. The user can decide how often to use the flow solver vs. the conduction solution. If the flow solver is used for each conduction (P-Thermal) time step, the result will be a highly accurate but time intensive computation. In order to accelerate the CFD part of the calculation, the user chooses a maximum object surface temperature change that will switch on the CFD solver for a preset amount of time. The CFD solver will then advance the flow solution until a new quasi-steady solution has been found. Then a new set of surface heat transfer coefficients and temperatures are then evaluated and passed back to solid conduction model which then advances that solution further in time. By selecting a minimum surface temperature change, the user can control how often CAFE is called. In addition, the user can control how far to advance the CAFE flow solution in time to generate a new quasi steady solution.

EXAMPLE CALCULATION WITH THE FAVOR METHOD

The FAVOR curved surface treatment is a new development this year and has been chosen as a validation calculation. Heated air flow over a solid cylinder was chosen as the example because it tests both the CFD flow solver and the FAVOR curved surface treatment simultaneously. There have been numerous experiments of heated cross flow over circular cylinders and the experimental results can be summarized as Reynolds number correlations. A typical Nusselt number correlation for cross flow over a circular cylinder is that of Hilpert (Holman, 1990) shown in the equation below:

$$Nu = 0.51 Re^{\frac{1}{2}} Pr^{\frac{1}{3}}$$

where Nu is the Nusselt number, Re is the Reynolds number based upon cylinder diameter, and Pr is the Prandtl number of the fluid. The correlation is valid for the Reynolds number range 40 to 1000.

When setting up a CFD run, it is important to understand the limitations of the chosen computational mesh. In a heat transfer calculation the rate of temperature rise of an object is controlled by the boundary layer thickness, which, in a CFD calculation, cannot be thinner than a single computational cell width. It can be shown with a few definitions and algebraic manipulations that the Nusselt number is equivalent to the ratio of the correlation length scale divided by the boundary layer thickness. Thus for a given computational cell size the upper limit for the applicable Reynolds number range can be calculated from the Nusselt number correlation. For this example, a computational mesh of 40 x 60 nodes was chosen with a cell size of 1 mm. Using a circular cylinder of 12 mm and the experiment correlation above yields a maximum Reynolds number of 480 for the range of applicability of the

computational mesh. If flow velocities that correspond to Reynolds numbers higher than 480 are used, the CFD calculation will be unable to resolve the boundary layer temperature gradients and thus the heat transfer to the cylinder will be underpredicted. For flow rates at and below a Reynolds number of 480 the CFD calculation should be able to predict the correct temperature rise of the cylinder. In this example a flow rate corresponding to the maximum Reynolds number of 480 was chosen and the temperature rise rate of the cylinder was predicted. Likewise the temperature rise rate of a circular cylinder based upon the Nusselt number correlation was also predicted. Both predictions are shown in Figure 4 below.
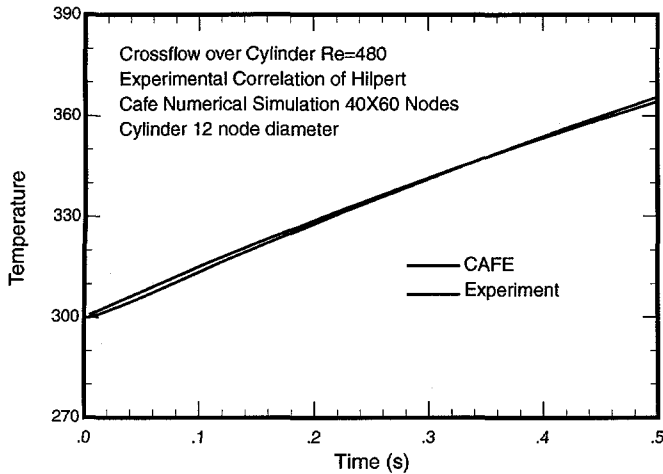

Figure 4. A comparison of CAFE and the experimental correlation of Hilpert for crossflow over a cylinder.

As shown in Figure 4 the prediction and the correlation have excellent agreement. Thus the FAVOR method and the pressure based flow solver has been validated. It is important to consider that the mesh in this example is very coarse, 40 x 60 and the cylinder is coarser yet, only 12 nodes in diameter, yet the CAFE code is capable of reproducing the correct heat transfer rate.

CAFE INPUT FILES.

There is one input file needed when running the CAFE code which can be edited with any text editor. The code is executed and output will be generated which can be viewed with PATRAN. In addition the UNIX X-windows routine Xplot can be used to display any CAFE specific output the user may wish to view.

A typical CAFE run consists of two parts. First, to ignite the fire, the the code is run with a low values of Arrhenius coefficients to achieve ignition. This startup problem is run until the object is fully engulfed and a restart file is written. The first phase is often run with a stand-alone version of CAFE. Next the fully linked version of CAFE/P-Thermal is run to complete the problem using the restart file as a starting point.

The process of actually linking a user subroutine to P-Thermal is relatively straight forward but it does entail several steps that will be described. P-Thermal can be run within PATRAN and many users find it convenient to do so. However CAFE in its present form must be run in batch mode with P-Thermal. Running in batch mode requires the user to generate a neutral file and then run the patq program to generate the required P-Thermal input files and the qtran.f main program. Next

qtran.f is compiled to produce qtran.o. Then the user must compile CAFE with the upatq command. The output of upatq is upatq.a which must be renamed ulib.a. Then the qlink command is executed to produce qtran.exe which is the final executable form of P-Thermal with CAFE. P-Thermal requires a template file for assigning values to user chosen surfaces.

EXAMPLE PROBLEM

An example problem wherein a 1 m diameter shipping container is suspended in the center of a 5 m diameter pool fire approximately 1 meter in elevation is presented below. A comparison between a traditional boundary condition and CAFE model boundary condition is shown.

Traditionally a simple σT^4 boundary condition has been employed where T is the regulatory fire temperature. The result when using that type of boundary condition is shown in Figure 5. In contrast, the CAFE code produces a non uniform heat flux on the package that results in a distributed temperature profile as shown in Figure 6.
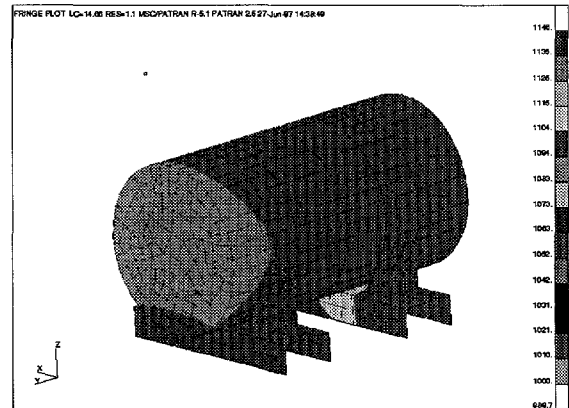

Figure 5. The temperature contours on a package with uniform σT^4 boundary condition. The package is approximately 1 m in diameter.
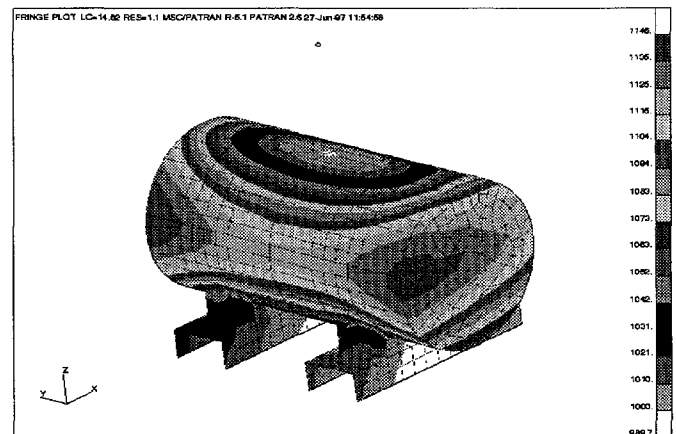

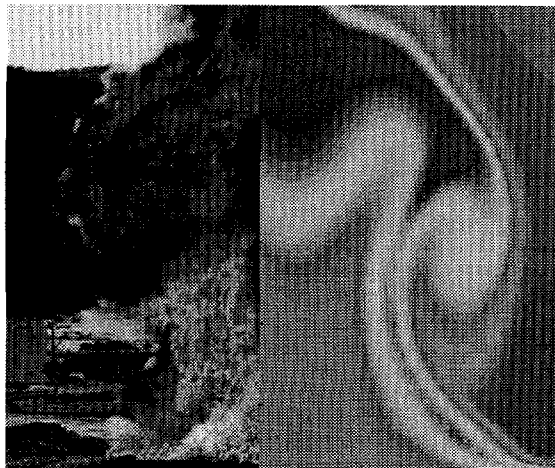Figure 6. The CAFE predicted temperature contours on a package exposed to an engulfing fire.

Figure 7. The temperature contours in a CAFE fire, without wind. The contours illustrate the puffing phenomenon. For comparison an actual fire photo is included at the left.

The nearly uniform temperature in Figure 5 is what one would expect from the traditional boundary condition. A comparison of the gray-scale temperatures in Figures 5 and 6 demonstrates the effects produced with a fire model when compared to the traditional σT^4 approach.

The CAFE model that predicts the surface heat transfer can be run at various levels of fire model fidelity. The highest model fidelity is to calculate the heat transfer with short CAFE time steps so that transient flow phenomena such fire puffing are resolved. Lower levels of fidelity are obtained by using longer CAFE time steps, wherein transient flow phenomena are replaced by steady flow conditions. The fire model is still accurate at lower levels of modeling fidelity but may yield slightly different results. The computer time requirements are greater for high model fidelity, thus the user can choose what level of fire modeling fidelity suits his needs. Figure 7 is a snapshot at one instant of time that shows the puffing vortices associated with a large fire and the short timestep high fidelity modeling option.

CONCLUSIONS AND DISCUSSION

A computer workstation based regulatory pool fire model that includes the dominant physics of fires has been successfully implemented and tested. The model can be applied to the design of Type B radioactive materials packages to predict their performance during fire testing and under accident conditions.

The parameters used in the code are based on current estimates of fire physical parameters such as absorption length and Arrhenius reaction rates. When compared to existing fire data, the current model yields reasonably good agreement. A program to develop further experimental data is in progress in cooperation with the University of Nevada, Reno. A carefully instrumented massive inertial calorimeter will be tested in a large pool fire. Data from these tests will be used to refine the parameters in the CAFE model and other fire models.

As currently implemented, the CAFE model stands as a separate set of computer routines. With proper interfacing, the model can be coupled to other thermal analysis codes of interest. Interfaces to other codes will be investigated on an as-needed basis.

Package designers interested in applying the code to their designs should contact the code developers for information on adapting the software to their particular workstation and problem.

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