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PANEL ON FIRE RESEARCH AND SAFETY
MARCH 1-7, 2000**

VOLUME 2

Sheilda L. Bryner, Editor



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A CONVECTIVE HEAT TRANSFER MODEL FOR LARGE EDDY FIRE SIMULATIONS

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Abstract

A model for the calculation of convective heat transfer to surfaces is presented. The model is designed to be used in conjunction with the large eddy simulation fire dynamics model developed at The National Institute of Standards and Technology. It is based on the approximate solution of the three-dimensional time dependent laminar boundary layer equations together with self-consistent boundary conditions. The approach involves the use of a suitable coordinate transformation to account for variable property effects in the boundary layer. A brief derivation of the required transformation is included as it does not seem to be in the standard heat transfer and combustion texts.

INTRODUCTION

The purpose of this work is the development of a model of convective heat transfer to approximately plane surfaces that can be used in conjunction with the large eddy simulation (LES) models of fire dynamics currently in use at The National Institute of Standards and Technology (NIST) [1]. At present, the convective heat transfer is either ignored or is represented by an empirical heat transfer coefficient. In either case, the LES code predicts an effective "surface" temperature $T_e(x, z, t)$ on a surface defined locally by a value of a "normal" coordinate $y = 0$. Similarly, the code predicts a surface velocity vector (u_e, w_e) that accounts for the transport between the last interior point in the computational domain and the physical boundary. This information represents the best estimate the LES model can give of the state of motion outside the boundary layer adjacent to any surface.

The approach taken here is to use this information together with an approximate solution to the three dimensional time dependent boundary layer equations to obtain the local heat transfer to each surface. The crucial simplification that makes the solution possible lies in the assumption that the components of the velocity field in the boundary layer parallel to each surface can be represented by a constant fraction $c(u_e, w_e)$ of the external velocity field. The heat transfer problem then reduces to the solution of the coupled mass and energy conservation equations. The temperature $T_e(x, z, t)$ is interpreted as the temperature "at infinity" with respect to the local boundary layer normal coordinate y . The actual wall temperature as predicted by a conjugate heat transfer analysis is denoted by $T_w(x, z, t)$.

The approximate boundary layer model retains the same overall mathematical structure as the full boundary layer equations. In particular, the velocity component normal to the surface is determined by conservation of mass, rather than a normal component of the momentum equation. The

transverse components of the velocity still come from transverse momentum equations, but here the result of the LES calculation are used rather than local boundary layer equations. Approximations of this type have a long history in laminar heat transfer and combustion problems. Indeed, the approach taken here is motivated by a well-known heat transfer formula originally derived by Lighthill [2]. Thus, to the extent that the wall region of the thermal boundary layer can be considered laminar, the present model should give reasonable solutions if the LES predictions of the near-wall velocity components parallel to the surface are reliable.

The use of the Howarth Transformation removes the effects of variable transport properties, reducing the equations to an equivalent constant density heat transfer problem. This reduced system is further transformed into an equivalent heat conduction problem in a suitably defined Lagrangian coordinate system. The relative simplicity of the final system of equations permits the convective heat transfer to a complex array of surfaces to be calculated. Little more computation is required than that needed for the heat conduction to the interior of the solid boundaries that define the surfaces.

The remainder of the paper is organized as follows. The next section presents a derivation of the three-dimensional time-dependent Howarth transformation, applied to the boundary layer equations. This is rather difficult to find in textbooks, and is crucial for the analysis to follow. The third section analyzes the Howarth Transformed model equations and shows their equivalence to the heat conduction equation in a suitably chosen coordinate system. The final section contains a discussion of alternative methods of solving the equation and extracting the wall heat transfer from the results.

THE HOWARTH TRANSFORMATION

The starting point is the three-dimensional time dependent form of the low Mach number boundary layer equations. These take a slightly different form depending upon the orientation of the surface with respect to gravity. Since we are ultimately concerned with the energy and mass conservation equations, and these differences arise only in the momentum equations, they will be omitted from the present analysis. Let y be the coordinate normal to the surface pointing *into* the gas, with v the corresponding velocity. The geometry is shown schematically in Figure 1. Then, if (x, z) are local cartesian coordinates in the surface layer, with (u, w) the corresponding velocity components and ρ the density, the conservation of mass takes the form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0 \quad (1)$$

In what follows, much use is made of the fact that the convective derivative of any physical quantity is unchanged by the Howarth Transformation. In the present notation it takes the form:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} \quad (2)$$

Using this construct, the energy conservation equation for a non-reacting radiatively transparent

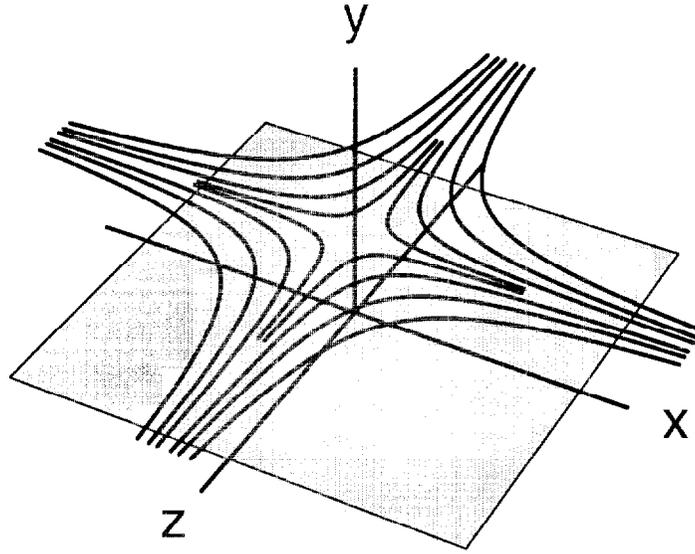


FIGURE 1: Schematic showing streamlines from LES simulation at outer edge of boundary layer. The actual surface is shaded with the coordinate y pointing into the gas.

ceiling layer is:

$$\rho C_p \frac{DT}{Dt} = \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) \quad (3)$$

The specific heat is denoted by C_p , the thermal conductivity by k , and the temperature in the ceiling layer is T . These equations are supplemented by the low Mach number version of the equation of state:

$$\rho T = \rho_w T_w = \rho_e T_e \quad (4)$$

The essence of the transformation is the choice of a normal coordinate η and a fictitious normal velocity component V that preserves the convective derivative operator defined by equation (2) and allows the energy and mass conservation equations to take an incompressible form. To this end we introduce η as:

$$\eta = \int_0^y \frac{\rho}{\rho_o} dy \quad (5)$$

Here, the subscript “ o ” denotes a reference state that can be taken as the initial density before any heating takes place. We seek to recast the equations in terms of the independent variables $x = X$, $z = Z$, η , and t . The transformation rules are:

$$\frac{\partial}{\partial t} |_{x,z,y} = \frac{\partial}{\partial t} |_{x,z,\eta} + \frac{\partial \eta}{\partial t} |_{x,z,y} \frac{\partial}{\partial \eta} \quad (6)$$

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial X} + \frac{\partial \eta}{\partial x} \Big|_{y,z,t} \frac{\partial}{\partial \eta} \quad (7)$$

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial Z} + \frac{\partial \eta}{\partial z} \Big|_{y,x,t} \frac{\partial}{\partial \eta} \quad (8)$$

$$\frac{\partial}{\partial y} = \frac{\rho}{\rho_o} \frac{\partial}{\partial \eta} \quad (9)$$

The normal velocity V is now defined so that the convective derivative transforms into itself.

$$V = \frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} + w \frac{\partial \eta}{\partial z} + \frac{\rho}{\rho_o} v \quad (10)$$

Using the transformation rules it is readily seen that the convective operator given by equation (2) is preserved as:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial X} + V \frac{\partial}{\partial \eta} + w \frac{\partial}{\partial Z} \equiv \frac{\tilde{D}}{\tilde{D}t} \quad (11)$$

Next, the temperature dependence of the viscosity μ , thermal conductivity k , and specific heat C_p are specified by assuming that C_p , the Prandtl number $Pr = (\mu C_p)/k$, and the product $\rho\mu$ are constant. Away from the firebed, the primary gases will be either undiluted air or nitrogen. For these constituents, the above approximations are accurate to within ten percent up to $1000^\circ K$. Applying these relationships and the transformation rules to the energy conservation equation yields:

$$\frac{\tilde{D}T}{\tilde{D}t} = \frac{\nu_o}{Pr} \frac{\partial^2 T}{\partial \eta^2} \quad (12)$$

The quantity ν_o is the kinematic viscosity evaluated at the reference state.

The last step is the demonstration that the conservation of mass takes the incompressible form. To see this we again use the definition of η to rewrite equation (1) in the form:

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho w)}{\partial z} + \frac{\partial}{\partial y}(\rho v + \rho_o \frac{\partial \eta}{\partial t}) = 0 \quad (13)$$

The last term in equation (13) can be rewritten as:

$$\rho_o \frac{\partial V}{\partial y} - (u \frac{\partial \rho}{\partial x} + w \frac{\partial \rho}{\partial z}) - \rho_o (\frac{\partial u}{\partial y} \frac{\partial \eta}{\partial x} + \frac{\partial w}{\partial y} \frac{\partial \eta}{\partial z}) \quad (14)$$

Using this expression together with equation (9), equation (13) becomes:

$$\rho (\frac{\partial u}{\partial x} - \frac{\partial \eta}{\partial x} \frac{\partial u}{\partial \eta}) + \rho_o \frac{\partial V}{\partial y} + \rho (\frac{\partial w}{\partial z} - \frac{\partial \eta}{\partial z} \frac{\partial w}{\partial \eta}) = 0 \quad (15)$$

Finally, using the transformation rules one more time, equation (15) takes the desired form:

$$\frac{\partial u}{\partial X} + \frac{\partial V}{\partial \eta} + \frac{\partial w}{\partial Z} = 0 \quad (16)$$

The final transformed set then consists of equations (16) and (12). They are respectively the “incompressible” form of the mass and energy conservation laws in the boundary layer.

MODEL EQUATIONS

Up to this point, only the boundary layer approximation has been made. The assumptions regarding both the thinness of the layer where the molecular viscosity and thermal conductivity are important and the dependence of these quantities on temperature are well founded. The solution of these equations however, requires considerable computational effort unless some further approximations are made. As noted in the Introduction, the crucial step consists of replacing the in-plane components of the velocity vector that appear in the convective derivative by $c(u_e, w_e)$. Then using equation (16) to obtain a consistent approximation for V , the convective derivative takes the form:

$$\frac{\tilde{D}}{\tilde{D}t} \approx \frac{\partial}{\partial t} + c \left[u_e \frac{\partial}{\partial X} + w_e \frac{\partial}{\partial Z} - \eta \left(\frac{\partial u_e}{\partial x} + \frac{\partial w_e}{\partial z} \right) \frac{\partial}{\partial \eta} \right] \equiv \frac{\hat{D}}{\hat{D}t} \quad (17)$$

The conservation equations can now be transformed without further approximation into the heat conduction equation. The starting point is the observation that since u_e and w_e are independent of η , the introduction of surface Lagrangian coordinates (x_o, z_o) removes the corresponding convective terms from equation (12). We now introduce the dimensionless temperature Θ as:

$$\Theta \equiv \frac{T}{T_e} = \Theta(t, \eta, x_o, z_o) \quad (18)$$

$$\frac{dX}{dt}(t, x_o, z_o) = c u_e(X, Z, t), \quad X(t_o) = x_o \quad (19)$$

$$\frac{dZ}{dt}(t, x_o, z_o) = c w_e(X, Z, t), \quad Z(t_o) = z_o \quad (20)$$

Using the fact that T_e must be approximately constant in this system of coordinates if the LES represents an essentially inviscid mixing process, equation (12) now takes the form:

$$\frac{\partial \Theta}{\partial t} - \alpha(t) \eta \frac{\partial \Theta}{\partial \eta} = \frac{\nu_o}{Pr} \frac{\partial^2 \Theta}{\partial \eta^2} \quad (21)$$

$$\alpha(t) \equiv c \left(\frac{\partial u_e}{\partial x}(X(t), Z(t), t) + \frac{\partial w_e}{\partial z}(X(t), Z(t), t) \right) \quad (22)$$

The quantity $\alpha(t)$ is the surface strain rate evaluated in the moving surface Lagrangian coordinate system. It plays an important role in the remaining transformations, and hence in the final formulae

for wall shear and heat transfer. The final step is the introduction of a stretched normal coordinate λ and time τ as follows:

$$\lambda = \eta f(t) \quad (23)$$

$$\tau = \int_{t_o}^t f^2(t') dt' \quad (24)$$

$$f(t) = \exp\left(\int_{t_o}^t \alpha(t') dt'\right) \quad (25)$$

Note that the surface strain rate appears exponentially in the definition of both the time and length scales. Thus, the results are *extremely* sensitive to variations in α . It is this sensitivity which gives rise to the enormous enhancement of the wall shear and heat transfer in flows with strong mixing.

With these transformations, the energy equation takes its final form:

$$\frac{\partial \Theta}{\partial \tau} = \frac{\nu_o}{Pr} \frac{\partial^2 \Theta}{\partial \lambda^2} \quad (26)$$

The heat flux to the wall q_w can be written explicitly as a function of Θ as follows:

$$q_w(X(t), Z(t), t) = k_w T_e \left(\frac{\rho_w}{\rho_o}\right) \exp\left(\int_{t_o}^t \alpha(t', x_o, z_o) dt'\right) \frac{\partial \Theta}{\partial \lambda}(0, \tau(t, x_o, z_o)) \quad (27)$$

Equation (27) shows how three factors contribute to the wall heat transfer. The convection of the heated gas is accounted for by the Lagrangian coordinates (x_o, z_o) , the effect of the strain rate history by the presence of the integral over α along the Lagrangian trajectory, and the molecular diffusion of heat by the normal derivative of Θ at the surface.

SOLUTION OF MODEL EQUATIONS

The solution of the boundary layer equations in the present formulation breaks up naturally into three parts. First, the Lagrangian coordinates and the transformation connecting the (t, y) and (τ, λ) coordinate systems must be advanced in time. Second, the solution to the diffusion equations expressing the transformed conservation laws must be solved for the time interval of interest. Finally, the results must be inserted back into the rectangular grid employed by the LES code and the condensed phase analysis so that these can be updated. As part of this last step, new Lagrangian elements must be added or deleted as needed.

The procedure to be followed must be considered in the context of the solution of the LES equations. Thus, although the general solution of the heat conduction equation (26) can be written down in the form of a convolution integral, it is unlikely that such a result would be employed in practice. Instead, consider the advancement of the boundary layer solution following the completion of a time step in the LES code. The new values of the wall velocities u_e and w_e together with the wall temperatures T_w and external temperature T_e are available.

The first step is to update the Lagrangian coordinates $X(t)$ and $Z(t)$ of each of a large number of fluid elements. The techniques needed to accomplish this are already employed to track the thermal elements used to represent the combustion generated energy release in the LES code. The value of the strain rate α on each trajectory can now be updated, along with the increment in the timelike coordinate $\tau(t)$. Next, the solution to the heat conduction equation for each fluid element is updated the required increment in time. Again, this represents no more work than is already required to advance the wall temperatures in the LES code by solving the solid phase heat conduction equation for each wall cell. The last step requires an interpolation procedure to estimate the convective heat flux to each wall cell in the rectangular grid employed in the LES code. With this information, the external temperature T_e needed at the next time step by the LES code can be found. The required value of T_e is the one which yields the same wall heat flux when the LES code is used to estimate the wall heat transfer. The LES code uses the eddy viscosity and a constant Prandtl number to estimate the heat transfer to the wall. The temperature gradient calculated at the wall by that code will depend on the choice of T_e . Inevitably, the LES temperature gradient will be much smaller and the “eddy conductivity” much higher than that predicted by the boundary layer equations. Requiring both predictions of the heat flux to be identical at all wall cells then closes the system of equations. At this point, the number of elements in each wall cell can be determined. New elements are introduced into cells that are no longer occupied and those elements that have left the region of interest can be removed from the list of those under consideration.

The numerical values of the heat transfer predicted by the model are affected by the choice of the convective constant c . However, it is not difficult to decide and test a plausible range of values for this parameter. Since the velocity will increase monotonically to its external value in the laminar sublayer described by this model, a plausible choice should be near $c = 1/2$. This choice can be optimized by comparing it with known exact solutions like the flat plate and stagnation point heat transfer formulae [3]. The corresponding solutions can be determined analytically from the present model. The results for the wall heat flux q (assuming constant properties) are:

$$q = k (T_e - T_w) \sqrt{\frac{2 c Pr}{\nu \pi} \left(\frac{du_e}{dx} \right)} \quad \text{stagnation point} \quad (28)$$

$$q = k (T_e - T_w) \sqrt{\frac{c u_e}{\nu x} \left(\frac{Pr}{\pi} \right)} \quad \text{flat plate} \quad (29)$$

A choice of $c = 0.45$ yields a 9.5 percent underprediction for the stagnation point and an 8.2 percent overprediction for the flat plate using a value of 0.7 for the Prandtl number Pr . Time dependent effects should act to reduce the relative errors since the corresponding term in the energy equation is not approximated.

CONCLUDING REMARKS

A convective heat transfer model is presented based on the idea that a three-dimensional time dependent laminar sublayer connects solid boundaries with a turbulent fire induced flow field. The

boundary layer equations governing the energy and mass transport in this layer are reduced to an approximate form which requires little more than the solution to the heat conduction equation to obtain the heat flux to a planar boundary. In its present state, it does not account for mass transfer from walls, although that extension is relatively straightforward. Hopefully, this represents the beginning of a systematic effort to put the prediction of heat, mass, and momentum transport near solid boundaries at a level of sophistication currently available in the interior of enclosure fire domains. Ultimately, any such undertaking will involve consideration of many other phenomena which can be relevant in fire scenarios. However, one has to begin any such effort somewhere, and this seems to be a useful place to start.

ACKNOWLEDGEMENT

Since this paper is offered as a contribution to the Symposium in honor of Prof. Howard Emmons, a personal remark may be forgiven. I was guided from my graduate school days as his teaching fellow, thru a junior faculty position at Harvard University, an industrial consulting job, and finally my present tenure at NIST, by his kindness, patience, and wisdom. It will be a long time before we see his equal again.

References

- [1] McGrattan, K.B., Baum, H.R., and Rehm, R.G., "Large Eddy Simulations of Smoke Movement", *Fire Safety J.*, Vol. 30, pp. 161-178, (1998).
- [2] Lighthill, M.J., "Contributions to the theory of heat transfer through a laminar boundary layer", *Proc. Roy. Soc. London A*, Vol. 202, pp. 359-377, (1950).
- [3] Schlichting, H., *Boundary Layer Theory*, McGraw-Hill, New York, pp. 263-272, (1955).