# A Higher-Order Projection Method for the Simulation of Unsteady Turbulent Nonpremixed Combustion in an Industrial Burner *

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There are a number of computational techniques for the simulation of reacting flow in furnaces and combustors at steady state conditions that have been developed over the last ten to twenty years. A large number of these are based are on the SIMPLE method of Patankar and Spalding [13], although other base methodologies have also been employed[5, 8]. In recent years development efforts have focused on extending these methodologies to three-dimensional flows[3, 5], or to the modeling of burners which utilize non-gaseous fuels, especially coal[5].

The modeling of unsteady reacting flows, on the other hand, has not received the same level of attention, although there has been some work in this area; see, for example, Benesch and Kremer[2]. The ability to model transient effects in burners, however, is becoming increasingly important for a number of reasons. The problem of ensuring the safe performance of an industrial burner, for example, is much more difficult during the startup or shutdown phases of operation. Further, the peak formation of pollutants is much more dependent on transient behavior, in particular, on peak temperatures, than on average operating conditions.

*This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract W-7405-Eng-48. Support under contract W-7405-Eng-48 was provided by the Applied Mathematical Sciences Program and the HPCC Grand Challenge Program of the Office of Scientific Computing at DOE and by the Defense Nuclear Agency under IACRO 94-831. Dr. Colella is also partially supported by DARPA and the National Science Foundation under grant DMS-8919074; and by a National Science Foundation Presidential Young Investigator award under grant ACS-8958522; and by the Department of Energy High Performance Computing and Communications Program under grant DE-FGO3-92ER25140.

The goal of this paper is to present a new methodology for the modeling of unsteady, nonpremixed, reacting flow in industrial burners. The algorithm uses the second-order projection method for unsteady, low-Mach number reacting flow developed by Lai[10] and accounts for species diffusion, convective and radiative heat transfer, viscous transport, turbulence, and chemical kinetics. The time step used by the method is restricted solely by an advective CFL condition. The methodology is applicable only in the low-Mach number regime ($M < .3$); this condition is typically met in industrial burners. The projection method for low-Mach number reacting flow is an extension of the higher-order projection method for incompressible flow of Bell, Colella, and Glaz [1] to the low-Mach number equations of reacting flow[12].

The main goal of this work is to introduce and investigate the use of the second-order projection method in the simulation of burners. As such, we have so far only applied the methodology to axisymmetric flow in natural gas-fired burners. We also assume the perfect gas law as the equation of state. In addition, we use some techniques for modeling other aspects of the flow that have been been replaced by other methodologies in recent years. In particular, we use a one-step reduced kinetics mechanism[9], a four-flux method to model radiative transport [6], a $k-\epsilon$ model for turbulent transport[7], and a simple turbulent combustion model[11].

The model for reacting flow to which the techniques presented in this paper are applied, then, is outlined as follows:

1. velocity ($u, v, w =$ radial, axial, and tangential components of velocity)

$$\rho \begin{pmatrix} \frac{Du}{Dt} - \frac{w^2}{r} \\ \\ \frac{Dv}{Dt} \\ \\ \frac{Dw}{Dt} + \frac{uw}{r} \end{pmatrix} = -\nabla p + \nabla \cdot \tau$$

where

$$\tau = \tau_{lam} - R_{ij},$$

$$\tau_{lam} = \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\delta_{ij} \nabla \cdot U \right),$$

and

$$-R_{ij} = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\delta_{ij} \nabla \cdot U \right) - \frac{2}{3}\delta_{ij}\rho k$$

2. species mass fractions, $m_l$ ($l = pr(product),\ fu(fuel),\ ox(oxidizer)$):

$$\rho \frac{Dm_l}{Dt} = \nabla \cdot \left( \left( D + D_t \right) \rho \nabla m_l \right) - st_l R_{fu}$$

where $st_l$ is the mass of species $l$ consumed in reaction per mass of fuel consumed;

3. temperature, $T$:

$$\begin{aligned}\rho c_{p,mix}\frac{DT}{Dt} &= \nabla\cdot\left(\left(k+k_t\right)\nabla T\right)-\nabla\cdot q_{rad}+H_{fu}R_{fu}\\ &\quad+\nabla\cdot\sum_l \rho h_l(T)\left(D+D_t\right)\nabla m_l-\rho\sum_l\frac{Dm_l}{Dt}h_l(T),\end{aligned}$$

where $c_{p,mix}$ is the specific heat of the gas mixture, $h_l$ is the specific enthalpy of species $l$, and $H_{fu}$ is the specific heat of reaction of the fuel;

4. radiation model:

$$-\nabla\cdot q_{rad}=2\alpha\left(F_r+F_z-2\sigma T^4\right)$$

where $F_r, F_z$ satisfy

$$\begin{aligned}\frac{1}{r}\frac{d}{dr}\left(\frac{r^2}{1+r\left(\alpha+s\right)}\frac{dF_r}{dr}\right)+\alpha\left(\sigma T^4-F_r\right)+\frac{1}{2}s\left(F_z-F_r\right)=0\\ \frac{d}{dz}\left(\frac{1}{\alpha+s}\frac{dF_z}{dz}\right)+\alpha\left(\sigma T^4-F_z\right)+\frac{1}{2}s\left(F_r-F_z\right)=0,\end{aligned}$$

and where $\alpha$ and $s$ are absorption and scattering coefficients.

5. kinetics model ($R_{fu}$ = mass rate of fuel consumed in reaction per volume):

$$R_{fu}=\max\left(\rho^2 m_{fu}m_{ox}A\exp\left(-E/RT\right),R_{fu,turb}\right)$$

where

$$R_{fu,turb}=\frac{\epsilon}{k}\min\left(\bar{A}\rho m_{fu},\bar{A}\rho m_{ox}/st_{ox},-\bar{A}'\rho m_{pr}/st_{pr}\right)$$

and

$$A=10^{10}\frac{m^3}{kg\cdot sec},\ \frac{E}{R}=1.84\times10^4\ {}^{\circ}K,\ \bar{A}=4.0,\ \bar{A}'=2.0$$

6. turbulent kinetic energy, $k$, and dissipation, $\epsilon$:

$$\begin{aligned}\rho\frac{Dk}{Dt} &= \nabla\cdot\left(\left(\frac{\mu_t}{\sigma_k}+\mu\right)\nabla k\right)-\\ &\quad G-\frac{\mu_t}{\rho^2}\left(\nabla\rho\cdot\nabla p\right)-\rho\epsilon\\ \rho\frac{D\epsilon}{Dt} &= \nabla\cdot\left(\left(\frac{\mu_t}{\sigma_\epsilon}+\mu\right)\nabla\epsilon\right)-\\ &\quad C_1\frac{\epsilon}{k}\left(G+\frac{\mu_t}{\rho^2}\left(\nabla\rho\cdot\nabla p\right)\right)-C_2\rho\frac{\epsilon^2}{k}\end{aligned}$$

where

$$G=R_{ij}\frac{\partial U_{ij}}{\partial x_j}$$

7. turbulent viscosity, thermal conductivity, mass diffusivity:

$$\mu_t = C_\mu \rho \frac{k^2}{\epsilon}, \qquad k_t = \frac{c_{p,mix}\mu_t}{\sigma_t}, \qquad D_t = \frac{\mu_t}{\rho \sigma_t}$$

8. turbulence model constants
   $C_\mu = .09,\ C_1 = 1.44,\ C_2 = 1.92,\ \sigma_k = 1.0,\ \sigma_\epsilon = 1.3,\ \sigma_t = .7$

9. divergence constraint ($U = (u, v)$):

$$\nabla \cdot U = \frac{\rho}{\bar{p}} \left( \left( \frac{D}{Dt} T \right) R_{mix} + T\mathcal{R} \sum_l \frac{1}{mw_l} \left( \frac{D}{Dt} m_l \right) \right),$$

   where $\mathcal{R}$ is the universal gas constant, $R_{mix}$ is the gas constant of the mixture, $mw_l$ is the molecular weight of species $l$, and $\bar{p}$ is the ambient pressure.

The overall strategy of the low-Mach number projection method in advancing the solution from time $t^n$ to $t^n + \Delta t = t^{n+1}$ is that of a predictor-corrector scheme. In the predictor step, values of $k, \epsilon, w, T$, and $m_i$ are computed at time $t^{n+1}$. In addition, values of $u$ and $v$ are predicted at $t^{n+1}$. In the corrector step, the divergence constraint is imposed on $u$ and $v$ through the solution of an elliptic equation. The solution of the elliptic equation also provides the value of the pressure at $t^n + \Delta t/2$.

The predictor step of the algorithm is itself a predictor-corrector. There are four main steps in this part of the methodology: 1) computing discrete approximations of the convective terms in the governing equations at time $t^n + \Delta t/2$ using the explicit higher-order upwind method of Colella[4]; 2) predicting the values of all flow quantities at $t^{n+1}$ using Crank-Nicholson differencing; 3) computing the divergence of the radiative flux at time $t^n + \Delta t/2$; 4) correcting the values of all the flow quantities to provide the solution at time $t^{n+1}$ again using Crank-Nicholson differencing. In the case of $u$ and $v$, this solution does not satisfy the divergence constraint; the solution of the elliptic equation mentioned above then reimposes this constraint. In steps 2) and 4) the equations for each of the flow quantities $k, \epsilon, m_i, T, U = (u, v)$, and $w$ are solved sequentially so that only linear systems of equations result from the Crank-Nicholson differencing. The solution of these linear systems is accelerated using multigrid techniques.

We now discuss some preliminary results from a simulation using our methodology. The geometry of the sample burner is shown in Figure 1. The temperature is initially 2500$^o$K in a cylindrical patch next to the inlet with radius and height of 2.3 cm and 300$^o$K elsewhere. The inlet conditions are a temperature of 300$^o$K, an axial velocity $v_{in}$ =12.2 m/sec, no radial velocity, and a swirl number of .5 with solid body rotation; swirl is only imparted to the air. The initial velocity in the burner has no tangential component and satisfies the divergence constraint for the given inlet conditions and initial temperature distribution. The inlet turbulence quantities are $k_{in} = .005 v_{in}^2$ and $\epsilon_{in} = C_\mu k_{in}^{3/2}/(.03 D_{in})$. The inlet fuel/air mole ratio is 1:19.25. The walls are maintained at 300$^o$K. Figures 2, 3, and 4 display results for these initial and boundary conditions on a 64×256 uniform grid.

**Key words**: numerical modeling, low-Mach number combustion, turbulent combustion, unsteady flows, industrial burners

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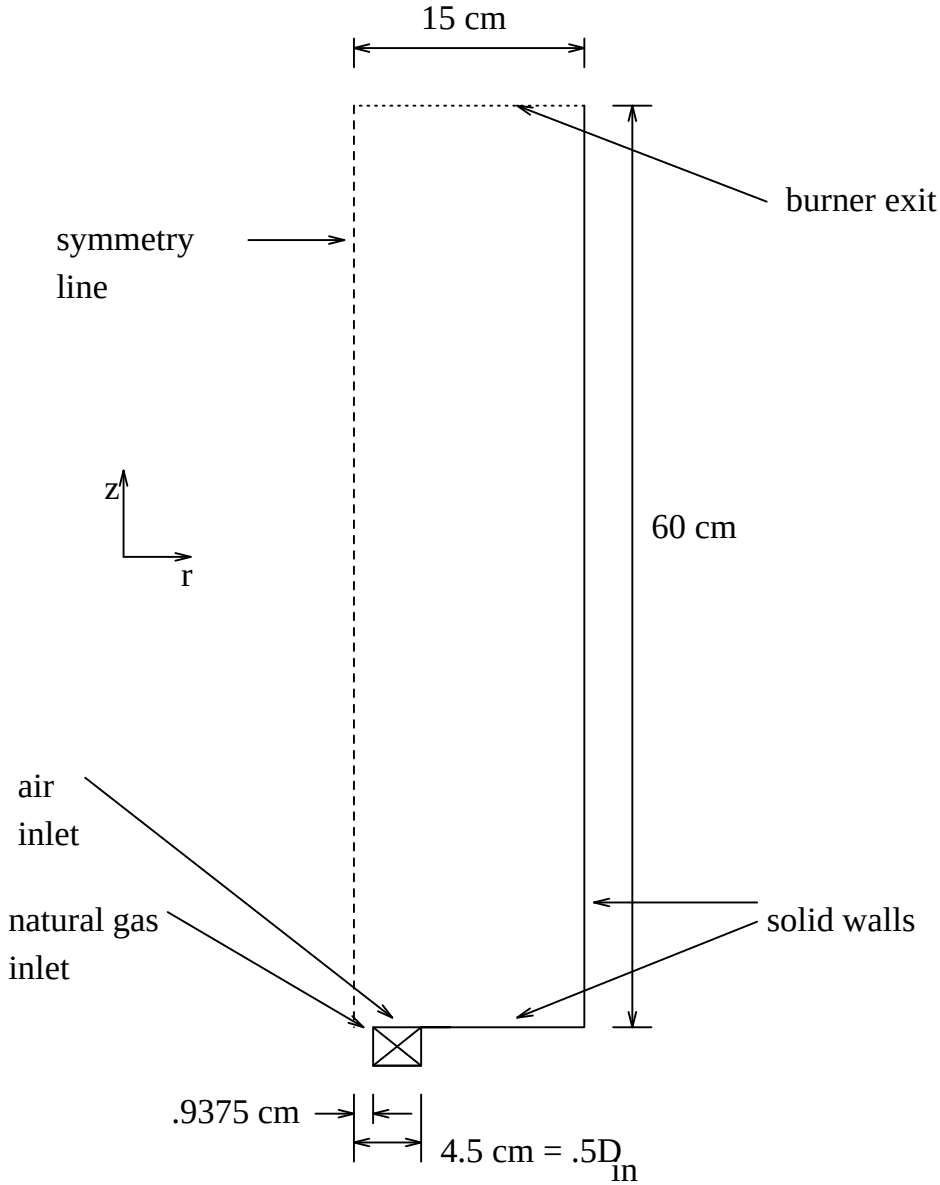


Sample Problem:
Burner Configuration

Figure 1: See text for detailed description.

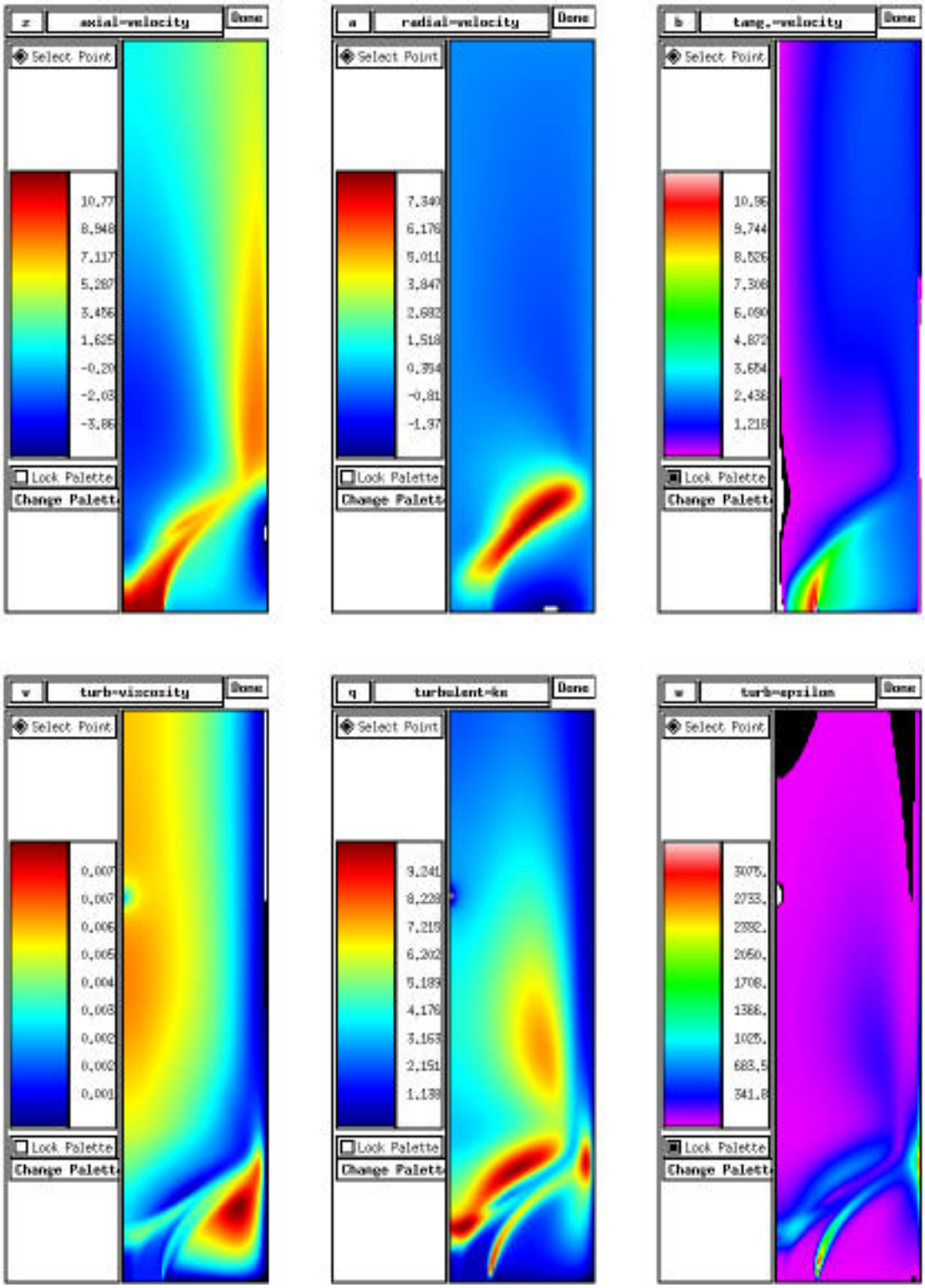


Figure 2: Solution of sample problem on a 64x256 grid at .927 sec. Radial, axial, and tangential components of velocity (m/sec) are displayed above. Turbulent viscosity (kg/m·sec), turbulent kinetic energy ($m^2/sec^2$), and turbulent dissipation rate($m^2/sec^2$) are displayed below.

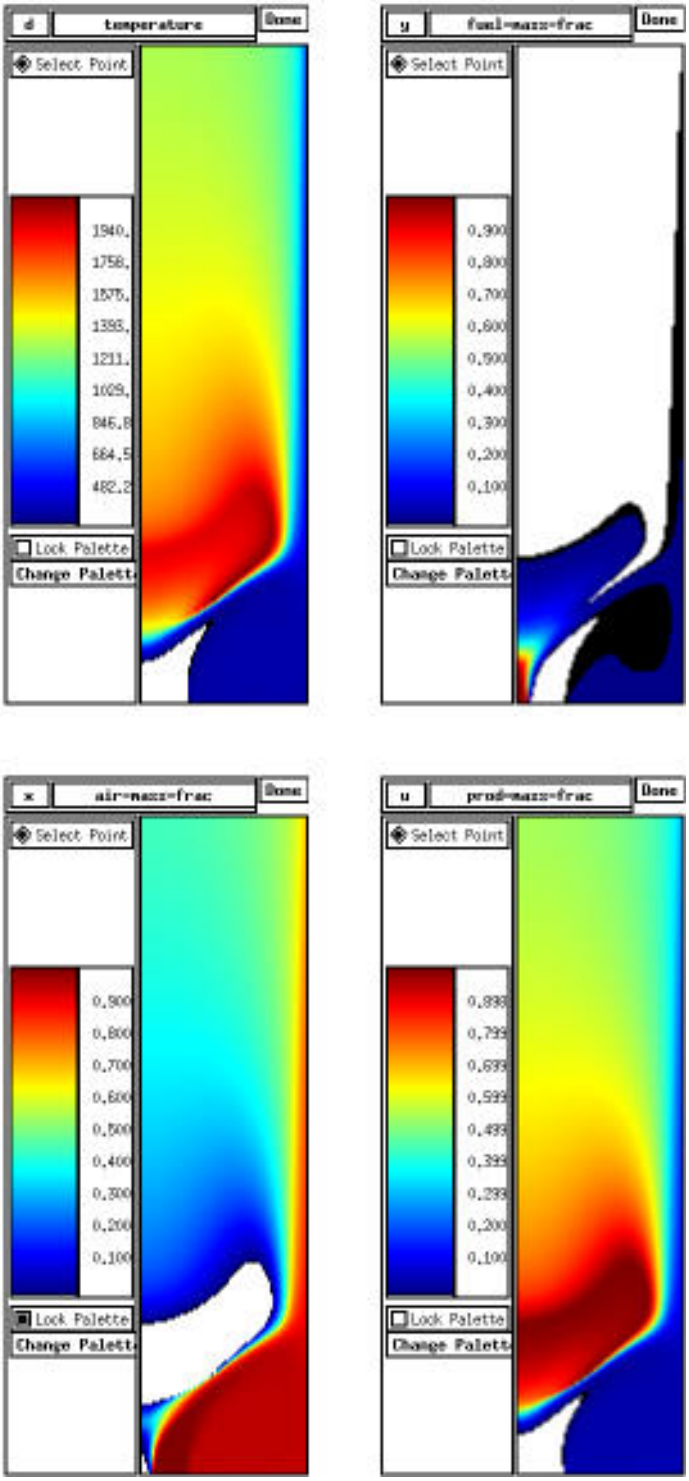


Figure 3: Solution of sample problem on a 64x256 grid at .927 sec. Temperature (deg-K) and mass fractions of fuel, air, and product are displayed.

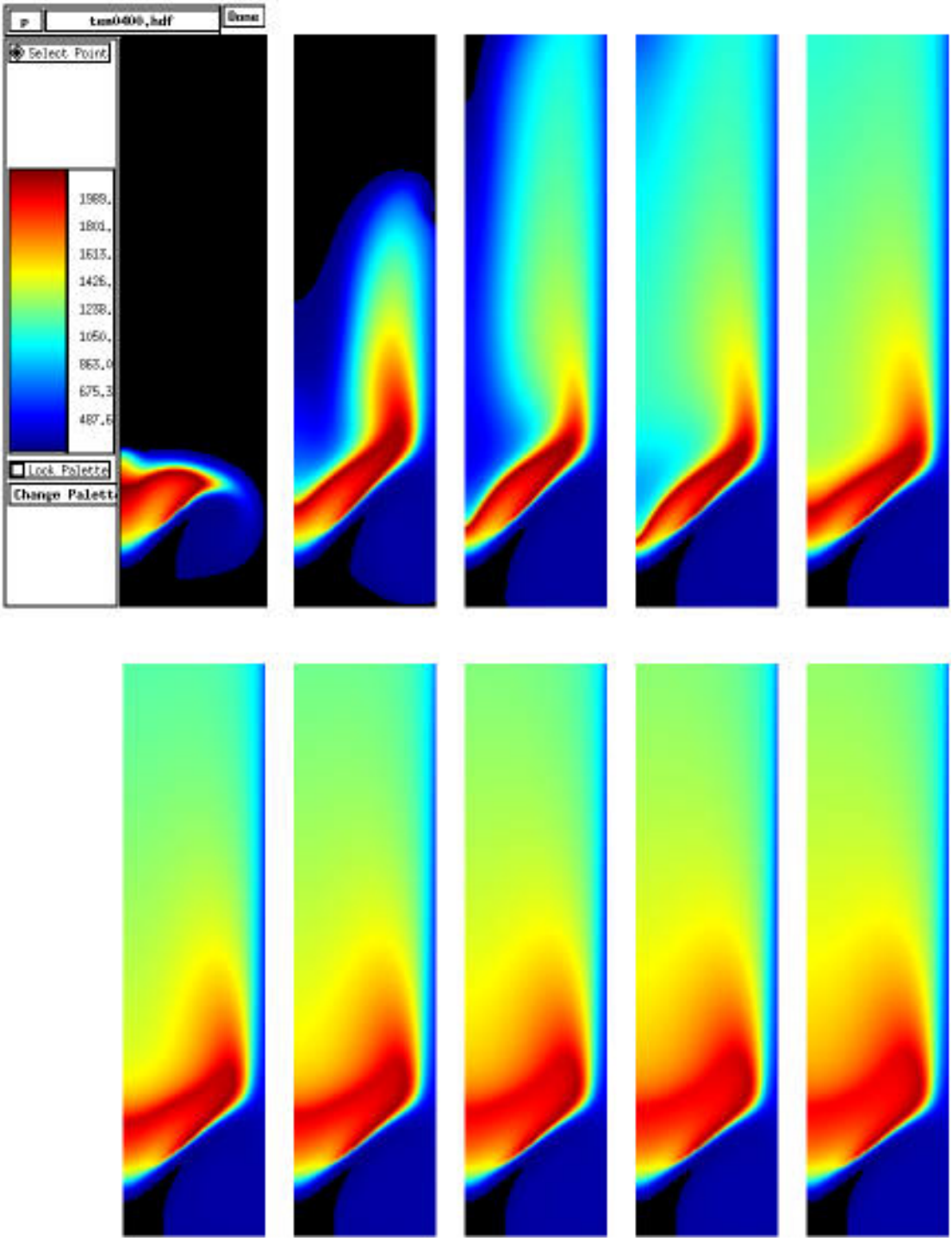


Figure 4: Temperature (deg-K) from solution of sample problem on a 64x256 grid at $t$ = .035, .110, .184, .258, .332, .406, .481, .555, .629, and .703 sec.