ACOUSTIC DISTURBANCES PRODUCED BY AN

UNSTEADY SPHERICAL DIFFUSION FLAME

Maurice L. Rasmussen University of Oklahoma

SUMMARY

The disturbances produced by a moving spherical diffusion flame are investigated within the framework of a linearized theory. After the flame position and species concentrations are determined, the problem of determining the associated density, pressure, temperature, and velocity fields is delineated. Explicit results for certain limiting situations are discussed.

INTRODUCTION

This paper deals with the acoustic disturbances produced by an unsteady spherical diffusion flame. The basic problem is envisaged as follows. Inside an initial sphere of radius \bar{r}_0 , a mixture of oxidant (or fuel) and product gases exists, and outside the sphere a mixture of fuel (or oxidant) and product gases exists, as depicted in Figure 1. At an initial instant the spherical surface that separates the two initial mixtures disappears, and the subsequent combustion and acoustic disturbances are to be determined. We assume that the combustion of the initially unmixed oxidant and fuel species is confined to a spherical Burke-Schumann flame surface.

This problem is associated with the theory of particle and liquid-droplet combustion at high pressures, such as treated by Spalding (Ref. 1) and Rosner (Ref. 2). An applicable situation occurs when bubbles of oxidant (or fuel) are injected into a medium of fuel (or oxidant). The bubbles burst, or are ignited, and the subsequent disturbance field is to be determined. This investigation also pertains to the general study of unsteady diffusion flames and to the broad subject of spherical explosions.

Most investigations of diffusion flames have dealt with steady flows, starting with the original work of Burke and Schumann (Ref. 3). A number of such problems are described in texts and review articles (Refs. 4 and 5). In particular, detailed mathematical expositions for steady linearized flows have been developed by Clarke (Refs. 6 and 7); the present work is something akin to this framework of analysis. Unsteady diffusion flames have not been as thoroughly treated. Clarke and Stegen (Ref. 8) considered unsteady perturbations on a two-dimensional flame sheet. Rasmussen (Refs. 9 and 10) developed a linearized theory for the one-dimensional motion induced by a diffusion flame. In this paper the related problem of a spherical diffusion flame is treated. Whereas the general form of the problem is nonlinear, the limiting acoustic approximation is of some interest. The explicit analytic results obtained within the linearized theory contain the embryonic behavior of the more complicated nonlinear problem. The linearized results, besides having their own intrinsic value, can be used to estimate the magnitude of convective terms and deviations from constant-property approximations. The gas dynamic interactions of the pressure, temperature, and velocity fields can be examined coherently within a linearized framework.

FORMULATION OF THE PROBLEM

Preliminary Remarks

We consider the basic combustion process that involves a mixture of oxidant (X), fuel (F), and product (P) species governed by the reaction equation

$$\chi X + f F \neq g P$$
(1)
$$t_r$$

where χ , f, and g are the stoichiometric coefficients. The corresponding molecular weights for the species are denoted by W_X , W_F , and W_P . The forward and reverse reaction times are denoted by t_f and t_r . The essence of combustion is that $t_f \rightarrow 0$ and $t_r \rightarrow \infty$. In this sense, the reaction associated with (1) moves only to the right, and this is the limiting situation considered here. This simple reaction model has been utilized previously (Refs. 5-10). In this limit a uniform <u>oxidant-product</u> mixture exists inside the initial spherical diaphragm, of radius r_0 , and a uniform fuel-product mixture outside (or vice versa).

In the framework of a linearized theory, we begin with a basic uniform medium composed of entirely the product species at pressure, density, and temperature conditions denoted by p_0 , ρ_0 , and T_0 . Inside the initial sphere we suppose that the pressure and temperature are perturbed such that $p = p_0(1+\Delta_p)$ and $T = T_0(1+\Delta_T)$. The corresponding oxidant and fuel mass fractions inside the initial sphere are denoted by $C_X = \Delta_X$ and $C_F = 0$. Outside the initial sphere the pressure and temperature are unperturbed, but the mass fractions are given by $C_X = 0$ and $C_F = \Delta_F$ (see Fig. 1). At a given instant, t = 0, the diaphragm disappears. We assume that the ambient temperature and density, T_0 and ρ_0 , are sufficient to initiate combustion spontaneously. Combustion of the oxidant and fuel occurs at an interface, and a diffusion flame is established. In the limit $t_f \rightarrow 0$, the diffusion flame collapses to a discontinuity surface, and all the reactions occur entirely on this surface. On either side of the surface there are no reactions, but binary diffusion takes place.

The limiting situation $t_f \rightarrow 0$ produces a singular perturbation problem. The outer problem corresponds to the flame envisaged as the discontinuity surface. The inner problem deals with the structure of the flame and is obtained by matching with the outer problem. This procedure has been established previously for steady-flow problems (Refs. 5-7) and for one-dimensional unsteady flow problems (Refs. 9 and 10). Here we restrict outselves to the lowest-order outer problem, with the flame treated as a discontinuity surface.

Basic Equations

When the mass fractions C_X and C_F are small, the pressure and thermal diffusion coefficients are small and are represented by nonlinear contributions. Consequently, since binary diffusion prevails on either side of the flame sheet, the diffusion-flux vectors are represented by Fick's law. As is usual in these problems, we assume the binary-diffusion coefficients are equal: $D_{XP} = D_{FP} = D$. We also assume that the components of the mixtures behave as thermally perfect gases. We now introduce dimensionless pressure, density, and temperature per-turbations p', ρ' , T' defined by

$$p = p_{o}(1+p')$$
, $\rho = \rho_{o}(1+\rho')$, $T = T_{o}(1+T')$ (2)

We have correspondingly for the mass fractions and velocity:

$$C_{X} = C_{X}'$$
, $C_{F} = C_{F}'$, $C_{P} = 1 - C_{X}' - C_{F}'$ (3)

$$\vec{v} = \vec{V}/a_{f_o}$$
, $a_{f_o}^2 = \gamma p_o/\rho_o$ (4)

where a_{f_Q} is the frozen speed of sound of the ambient medium and γ is the ratio of specific heats of the product species in the ambient medium. We represent the dimensionless space and time variables by

$$\vec{r} = a_{f_0} \vec{r} / \widetilde{v}_0$$
, $\tau \equiv a_{f_0}^2 t / \widetilde{v}_0$ (5)

where $\widetilde{\nu} \equiv (2\mu + \lambda)/\rho$, and μ and λ are the first and second coefficients of viscosity. Since the problem of interest is spherically symmetric we introduce a velocity potential, $\widetilde{v} = \nabla \varphi$, where $\nabla \equiv \partial/\partial r$ (the barred space variables are dimensional). The characteristic Prandtl and Schmidt numbers are defined as

$$P_{r} \equiv \rho \widetilde{v} c_{p} / k_{o}, \quad S_{c} \equiv \widetilde{v} / D_{o}$$
(6)

where c_{p_0} is the constant-pressure specific heat of the product species and k_0 is the thermal conductivity, the subscript naught denoting the ambient state. With the above definitions, the linearized equations for mass, momentum, species, energy, and thermal equation of state become

$$\frac{\partial \rho}{\partial \tau} + \nabla^2 \varphi = 0$$
 , $p = \gamma \left[\nabla^2 \varphi - \frac{\partial \varphi}{\partial \tau} \right]$ (7a,b)

$$D_{S}C_{X} = -S_{C} \times W_{X}R$$
, $D_{S}C_{F} = -S_{C}fW_{F}R$ (8a,b)

$$D_{p}T = \frac{\gamma - 1}{\gamma} P_{r} \frac{\partial p}{\partial \tau} + P_{r}Q R , \quad p = \rho + T + \alpha_{X}C_{X} + \alpha_{F}C_{F} \qquad (9a,b)$$

The primes denoting the perturbation variables have been omitted. In the above we have the operators D_p and D_s , the parameters of α_X and α_F , and the dimensionless heat of reaction Q defined as

$$D_{p} \equiv P_{r} \frac{\partial}{\partial t} - \nabla^{2} , \quad D_{S} \equiv S_{c} \frac{\partial}{\partial \tau} - \nabla^{2}$$
(10)

$$\alpha_{\rm X} \equiv \frac{\kappa_{\rm X}}{R_{\rm P}} - 1 , \quad \alpha_{\rm F} \equiv \frac{\kappa_{\rm F}}{R_{\rm P}} - 1$$
(11)

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$$Q = \left[\chi W_{X}(h_{X_{o}} - h_{P_{o}}) + fW_{F}(h_{F_{o}} - h_{P_{o}})\right]/c_{P_{o}}^{T}$$
(12)

where R_X , R_F and R_P are the specific gas constants. The symbol R denotes the dimensionless reaction rate. For the flame discontinuity sheet, R is given by

$$R = S(\tau) \delta(Z_n)$$
(13)

where $S(\tau)$ is the flame strength and $\delta(Z_n)$ is the Dirac delta function with Z the coordinate measured normal from the flame sheet. Derivations of these equations can be found in references 6, 9 and 10, and also in references 11 and 12 when there are no chemical reactions.

Continuity Conditions

All the physical flow variables are continuous at the flame sheet. Integration of equations (8a,b) and (9a) across the flame sheet shows that the following normal derivatives are discontinuous across the flame sheet:

$$\left[\frac{\partial}{\partial n} \left(\frac{C_{X}}{\chi W_{X} S_{C}}\right)\right]_{-}^{+} = \left[\frac{\partial}{\partial n} \left(\frac{C_{F}}{f W_{F} S_{C}}\right)\right]_{-}^{+} = -\left[\frac{\partial}{\partial n} \left(\frac{T}{Q P_{r}}\right)\right]_{-}^{+} = S(\tau)$$
(14)

where the bracket rotation denotes the jump in value across the discontinuity. These jump conditions suggest that the following new variables be defined that do have continuous normal derivatives across the flame:

$$\mathbf{C}^* \equiv \mathbf{C}_{\mathbf{F}} - \Psi \frac{\Delta_{\mathbf{F}}}{\Delta_{\mathbf{X}}} \mathbf{C}_{\mathbf{X}}$$
, $\mathbf{T}^* \equiv \mathbf{T} + \frac{P_{\mathbf{T}}Q}{S_{\mathbf{C}}\chi W_{\mathbf{F}}} \mathbf{C}_{\mathbf{X}}$ (15a,b)

where

$$\Psi \equiv \frac{t W_F \Delta_X}{\chi W_X C_F}$$
(16)

is the stoichiometric fuel-oxidant ratio. With the new variables C^{\times} and T^{\times} , the reaction rate can be eliminated from the set of equations. Equations (8a,b) can be combined and equation (9a) can be recast to read

$$D_{S}C^{*} = 0$$
 , $D_{P}T^{*} = \frac{\gamma - 1}{\gamma} P_{r} \frac{\partial p}{\partial \tau} + \frac{P_{r}Q(P_{r} - S_{c})}{S_{c} \chi W_{X}} \frac{\partial C_{X}}{\partial \tau}$ (17a,b)

The linearized state equation (9b) becomes

$$p = \rho + T^* - \alpha_F C^* - E C_X \text{ where } E \equiv \frac{P_r Q}{S_c \chi W_X} - \alpha_X - \alpha_F \Psi \frac{\Delta_F}{\Delta_X}$$
(18a,b)

Equation (17a) is uncoupled from the other equations and can be solved separately, yielding C_X and C_F as well as the flame position. A single equation for the velocity potential can then be found by eliminating T^* in equation (17b) by means of equation (18) and then utilizing equations (7a,b) to eliminate p and ρ . We obtain

$$L(\varphi) = (S_c - P_r) \left[\alpha_F C_{\tau\tau}^* + \frac{P_r Q}{S_c \chi W_X} C_{\chi\tau\tau} \right] + E D_P C_{\chi\tau}$$
(19)

where

$$L(\varphi) \equiv \gamma \nabla^{4} \varphi_{\tau} + \nabla^{2} \left[\nabla^{2} \varphi - (\gamma + P_{r}) \varphi_{\tau \tau} \right] + P_{r} \left[\varphi_{\tau \tau} - \nabla^{2} \varphi \right]_{\tau}$$
(20)

Equation (17a) for C* can be solved separately. The initial conditions are $C*(r > r_0, 0) = \Delta_F$ and $C*(r < r_0) = -\psi \Delta_F$. Further, C* is finite at the origin and infinity, and both C* and C* are continuous at r=r₀. The result is (Ref. 2):

$$\frac{C^{*}}{\Delta_{F}} = -\Psi + \frac{\Psi+1}{2} \left[\operatorname{erfc} \left(\frac{1-r_{*}}{\sqrt{4\tau_{*}}} \right) + \operatorname{erfc} \left(\frac{1+r_{*}}{\sqrt{4\tau_{*}}} \right) + \frac{2}{r_{*}} \sqrt{\frac{\tau_{*}}{\pi}} \left\{ e^{-(1-r_{*})^{2}/4\tau_{*}} - e^{-(1+r_{*})^{2}/4\tau_{*}} \right\} \right]$$
(21)

(22), (23)

where $r_{\star} \equiv r/r_{o}$ and $\tau_{\star} \equiv \tau/(r_{o}^{2}S_{c})$. (22), (2) The flame position $r = r_{s}(\tau)$ is determined from the condition $C^{\star}(r_{s},\tau) = 0$ but $r_{s}(\tau)$ cannot be obtained explicitly. For small τ_{\star} , however, we obtain

$$r_{s*}(\tau_{*}) = 1 + 2 A \tau_{*}^{\frac{1}{2}} - 2\tau_{*} + 2A \tau_{*}^{3/2} - (4 + \frac{8}{3} A^{2}) \tau_{*}^{2} + O(\tau_{*}^{5/2})$$
(24)

where

$$erf(A) \equiv (\Psi - 1) / (\Psi + 1).$$
 (25)

The position of the flame with time is a function of the initial conditions through the parameter Ψ , defined by (16). When $\Psi=1$, the initial conditions are stoichiometric, and the flame travels inward toward the origin, linearly with τ when τ is small. When $\Psi > 1$ the initial conditions are oxidant-rich and the flame initially moves outward from the origin and then subsequently toward the origin. The case of fuel-rich initial conditions corresponds to Ψ < 1, and the flame moves only toward the origin, the position varying like $\tau^{\frac{1}{2}}$ when τ is small. This behavior is contrary to the one-dimensional (Refs. 9 and 10) problem in which the flame remains stationary under stoichiometric initial conditions and moves either to the right or left depending on whether Ψ is greater than or less than unity. Figure 2 shows the position of the flame as a function of τ_* for Ψ = 1/2, 1, and 2. When Ψ =1, for instance, the flame reaches the origin and becomes extinguished when $\tau_{\downarrow} \cong 0.21$.

The spherical diffusion flame travels ultimately inward. Because the species outside the sphere is of infinite extent and the species inside the sphere is of finite extent, the species inside the sphere tends to be consumed. Consequently, the flame eventually will move inward in order to add a relative diffusion rate for the vanishing inside species and thus maintain stoichiometric combustion at the flame. When the flame reaches the origin, the species originally inside the sphere has been completely consumed and the flame becomes extinguished.

The mass fractions are determined from the function C^* . For $r < r_s$, we have $C_X/\Delta_X = -C^*/(\Psi\Delta_F)$ and $C_F=0$. For $r > r_s$, we have $C_X=0$ and $C_F=C^*$. These profiles are plotted in Figure 3 for $\Psi=1$ and $\tau_* < 0.21$. When the flame becomes extinguished at the origin, the species inside the original sphere has been completely consumed, in this case the oxidant. For times greater than the extinguish-time, the species outside the original sphere proceeds to establish a uniform state. The return to a uniform state is shown in Figure 4.

SOLUTION FOR $P_r = S_c$ and E = 0

Laplace-Transform Analysis

With C^{\star} and C_{x} known, equation (19) constitutes a fifth order non-homogeneous equation for φ . Because the position of the flame varies with time, the problem is difficult to solve. A great simplification occurs when we set $P_{r}=S_{c}$ and E=0. For most gases setting $P_{r}=S_{c}$ is a good approximation. The approximation E=0 is valid when ratios of specific heats of all the species are the same. These approximations correspond to the Shvab-Zeldovich approximation (Ref. 4). With these approximations, the problem is very similar to the binary diffusion problem of Reference 12, without pressure diffusion, and we proceed in similar fashion.

If $\overline{\varphi}(\mathbf{r},\mathbf{s})$ denotes the Laplace transform with respect to time of $\varphi(\mathbf{r},\tau)$, the solution of the transform of $L(\varphi) = 0$ is

$$\mathbf{r} \,\overline{\varphi}(\mathbf{r} < \mathbf{r}_{o}, \mathbf{s}) = -\frac{r\Delta_{p}}{\gamma s^{2}} + A_{1} \,\sinh \lambda_{1} \mathbf{r} + A_{2} \,\sinh \lambda_{2} \mathbf{r}$$
(26a)

$$r \overline{\varphi}(r > r_0, s) = B_1 \exp(-\lambda_1 r) + B_2 \exp(-\lambda_2 r)$$
 (26b)

where A1, A2, B1 and B2 are arbitrary constants of integration, and

$$\lambda_{1,2} \equiv \left[\frac{(\gamma + P_r)s^2 + P_r s + s}{2(1 + \gamma s)} \sqrt{[(\gamma - P_r)s + P_r]^2 + 4(P_r - 1)P_r s}\right]^{\frac{1}{2}}$$
(27)

where the plus sign holds for λ_1 and the negative sign for λ_2 . The Laplace transforms of the pressure and density are found from (7a,b):

$$\overline{p}(\mathbf{r},\mathbf{s}) = \gamma \left[(\mathbf{r}\overline{\varphi})_{\mathbf{r}\mathbf{r}} - \mathbf{s} \mathbf{r} \overline{\varphi} \right] / \mathbf{r}$$
(28)

$$\overline{\rho}(\mathbf{r} < \mathbf{r}_{o}, \mathbf{s}) = -(\Delta_{\rho}/\mathbf{s}) - (\mathbf{r}\overline{\phi})_{rr}/(rs)$$
(29a)

$$\overline{\rho}(\mathbf{r} > \mathbf{r}_{o}, \mathbf{s}) = -(\alpha_{F} \Delta_{F})/\mathbf{s} - (\mathbf{r}\overline{\phi})_{rr}/(\mathbf{r}\mathbf{s})$$
(29b)

The reduced temperature, T^* , is determined by means of equation (18). The velocity is determined by $v = \varphi_r$.

The constants A_1 , A_2 , B_1 , and B_2 are determined by requiring that $\overline{\rho}$, \overline{p} , \overline{v} , and \overline{T}_r^* be continuous at $r=r_0$. We find that

$$A_{1} = (1+\lambda_{1}r_{0})e^{-\lambda_{1}r_{0}} \Lambda_{1}/\lambda_{1} , \quad A_{2} = -(1+\lambda_{2}r_{0})e^{-\lambda_{2}r_{0}} \Lambda_{2}/\lambda_{2}$$
(30a,b)

$$B_{1} = (\sinh \lambda_{1} r_{o} - \lambda_{1} r_{o} \cosh \lambda_{1} r_{o}) \Lambda_{1} / \lambda_{1}$$
(31a)

$$B_2 = -(\sinh \lambda_2 r_0 - \lambda_2 r_0 \cosh \lambda_1 r_0) \Lambda_2 / \lambda_2$$
(31b)

where

$$\Lambda_{1} \equiv \left[(\Delta_{\rho} + \alpha_{F} \Delta_{F}) (\lambda_{2}^{2} - s)/s + \Delta_{p} \lambda_{2}^{2}/(\gamma s^{2}) \right] / (\lambda_{2}^{2} - \lambda_{1}^{2})$$
(32a)

$$\Delta_{2} \equiv \left[\left(\Delta_{\rho} + \alpha_{F} \Delta_{F} \right) \left(\lambda_{1}^{2} - s \right) / s + \Delta_{p} \lambda_{1}^{2} / (\gamma s^{2}) \right] / \left(\lambda_{2}^{2} - \lambda_{1}^{2} \right)$$

$$\Delta_{p} = \Delta_{\rho} + \Delta_{T} + \alpha_{x} \Delta_{x}$$
(32b)
(32b)
(32b)

The inversion of the transformed variables now remains.

Constant-Pressure Solution

When $P_r = S_c = 1$ we have the simplified results $\lambda_1 = \sqrt{s}$ and $\lambda_2 = s/\sqrt{1+\gamma s}$. Further when $\Delta p = 0$, the factor Λ_2 vanishes (hence $A_2=B_2=0$), and the pressure perturbation is identically zero, $p(r,\tau) = 0$. The remaining solution is entirely diffusive:

$$\mathbf{v}(\mathbf{r},\tau) = \frac{\Delta_{\rho} + \alpha_{F}\Delta_{F}}{2r^{2}\sqrt{\pi\tau}} \left[(\mathbf{rr}_{o}^{-2\tau})\mathbf{e}^{-(\mathbf{r}-\mathbf{r}_{o})^{2}/4\tau} + (\mathbf{rr}_{o}^{+2\tau})\mathbf{e}^{-(\mathbf{r}+\mathbf{r}_{o})^{2}/4\tau} \right]$$
(34)

$$\rho(\mathbf{r},\tau) = \Delta_{\rho} - (\Delta_{\rho} + \alpha_{F}\Delta_{F}) \left[\psi + (C^{\times}/\Delta_{F}) \right] / (1 + \psi)$$
(35)

$$T^{*}(r,\tau) = \Delta_{T^{*}} \lfloor 1 - (C^{*}/\Delta_{F}) \rfloor / (1+\psi)$$
(36)

where $C*/\Delta_F$ is given by equation (21), and $\Delta_{T*} \equiv \Delta_T + (Q\Delta_X/\chi W_X)$. Wave behavior does not occur in this special case.

The temperature at the flame sheet is determined from expression (36) by setting $C^* = C_X = 0$. We obtain

$$\Delta T_{f} = T * (r_{s}, \tau) = [\Delta_{T} + (Q\Delta_{x}/\chi W_{x})]/(1 + \psi)$$
(37)

The increment ΔT_f is the adiabatic flame temperature. It does not vary with time. The temperature is found from equation (15b) to be

$$T(r \leq r_{e},\tau) = \Delta T_{f} + (\Delta T_{f} - \Delta_{m}) C^{*}/(\psi \Delta_{m})$$
(38a)

$$T(r \ge r_s, \tau) = \Delta T_f \left[1 - (C^*/\Delta_F) \right]$$
(38b)

This temperature distribution is shown in Figure 5 for $\psi=1$ and $\Delta_{\tau}=0$.

Large-Time Behavior

An asymptotic approximation can be obtained for large times, and the results for density, pressure, velocity and T* are similar to those obtained in References 11 and 12. The major difference from these results occurs in the temperature distribution (as contrasted with the reduced temperature T*). When $\Delta_p \neq 0$, a gasdynamic expansion wave travels inward from the initial sphere, r_o , cooling the gas. This wave reflects from the origin and travels outward. The result after this reflected wave passes the position of the initial sphere is a reduction in temperature by an amount $(\gamma - 1)\Delta_p/\gamma$. This temperature residual is subsequently eliminated by thermal diffusion (Ref. 11). Thus for times long after the reflected wave passes the initial sphere, the net effect is to change the initial temperature increment such that

$$\Delta_{\rm T} \stackrel{\rightarrow}{\rightarrow} \Delta_{\rm T} - (\gamma - 1) \Delta_{\rm p} / \gamma \tag{39}$$

For large Reynolds numbers ($r_0 >> 1$), the wave processes are much faster than the diffusion processes, and under these circumstances formulas (36-38) hold

for the temperature long after the reflected wave passes the initial sphere, with the modification (39) noted. When $P_r \neq 1$, the time is also modified such that $\tau \rightarrow \tau/P_r$ in the function C*.

When $\Delta_p = 0$, but $P_r \neq 1$, there is a weak pressure wave generated that is proportial to (P_r-1) (Refs. 10 and 13). This wave does not affect the temperature distribution near the flame since Δ_T is left unaltered.

CONCLUDING REMARKS

The present analysis demonstrates the main features associated with unsteady spherical diffusion flames. It would be useful to continue the analysis without the approximations $P_r = Sc$ and E = 0. For the one-dimensional problem (Ref. 10) there are weak waves generated by the combustion at a stationary diffusion flame that are proportional to E. It would be interesting to investigate these waves for a moving spherical diffusion flame. The inner problem associated with the structure of the flame is also worthy of further attention.

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Figure 1.- Initial conditions and spherical configuration.



Figure 2.- Flame position as a function of time.



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Figure 3.- Oxidant and fuel concentrations before flame extinguishment.



Figure 4.- Fuel concentration after flame extinguishment.

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Figure 5.- Temperature distribution for constant-pressure solution.