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TURBULENCE IN STARS. III. UNIFIED TREATMENT OF DIFFUSION, CONVECTION, SEMICONVECTION, SALT FINGERS, AND DIFFERENTIAL ROTATION

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ABSTRACT

The goal of this paper is to propose a unified treatment of diffusion, convection, semiconvection, salt fingers, overshooting, and rotational mixing.

The detection of SN 1987A has served, among other things, to highlight the incompleteness of our understanding of such phenomena. Moreover, the variety of solutions proposed thus far to deal with each phenomenon separately, the uncertainty about the Ledoux-Schwarzschild criteria, the extent of overshooting, the effect of a μ gradient, the role of differential rotational mixing, etc., have added further urgency to the need of a unified, rather than a case-by-case, treatment of these processes. Since at the root of these difficulties lies the fact that we are dealing with a highly nonlinear, turbulent regime under the action of three gradients ∇T (temperature), ∇C (concentration), and $\nabla \boldsymbol{U}$ (mean flow), it is not surprising that such difficulties have arisen.

In this paper we propose a unified treatment based on a turbulence model. A key difference with previous models is that we do not employ heuristic arguments to determine the five basic timescales that enter the problem and that entail a corresponding number of adjustable constants. These timescales are computed using renormalization group (RNG) techniques. The model comes in three flavors: (*a*) all the turbulent variables are treated nonlocally; (*b*) the turbulent kinetic energy K and its rate of dissipation ϵ are nonlocal, while the remaining turbulence variables (fluxes, Reynolds stresses, etc.) are treated locally; and (*c*) all turbulence variables are local. In the latter case, one must specify a mixing length. Some of the results are as follows:

1. The local model entails the solution of two algebraic equations, one being the flux conservation law. By solving them, we obtain the desired $\nabla - \nabla_{ad}$ versus ∇_μ relations for semiconvection and salt fingers. We also derive other variables of interest, turbulent diffusivities, Peclet number, turbulent velocity, etc.
2. Schwarzschild and Ledoux criteria for instability are replaced by a new criterion that is physically equivalent to the requirement that turbulent mixing can exist only so long as the turbulent kinetic energy is positive. In addition to ∇, ∇_{ad}, and ∇_μ, the new criterion depends on the turbulent diffusivities for temperature and concentration that only a turbulence model can provide.
3. We derive the dynamic equations necessary to quantify the extent of overshooting OV in the presence of a μ barrier.
4. We prove that $\mathrm{OV}(\nabla_\mu) < \mathrm{OV}(\mu = \mathrm{const.})$. Although this result is physically understandable, no direct proof has been available as yet.
5. We derive the turbulent diffusivity for a passive scalar, one that does not affect a preexisting turbulence, e.g., a sedimentation of He. We show that it differs from that of an active scalar, e.g., a μ field causing semiconvection and/or salt fingers. Such diffusivity is a function of the temperature gradient (stable/unstable) and shear (rotational mixing).
6. We show that the turbulent diffusivities of momentum (entering the angular momentum equation), of heat (entering the model of convection), and concentration (entering the diffusion equation and/or semiconvection and salt fingers) are different from one another and should not be taken to be the same, as has been done thus far.
7. We consider the effect of shear. We solve the local turbulence problem analytically and derive the turbulent diffusivities for momentum, heat, and concentration in terms of the three gradients of the mean fields, ∇T, ∇C, and $\nabla \boldsymbol{U}$. Since shear is itself a source of turbulent mixing, one could expect it to enhance the diffusivities. However, its interaction with salt fingers and semiconvection is a subtle one, and the opposite may occur, a phenomenon for which we offer a physical interpretation and a validation with laboratory data.
8. A comparison is made with previous models.

Subject headings: diffusion — stars: interiors — stars: rotation — turbulence

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1. INTRODUCTION

1.1. *General Considerations*

There seems to be little disagreement that phenomena like (1) turbulent convection, (2) semiconvection, (3) salt fingers, (4) overshooting with and without a μ gradient, (5) turbulent diffusion of a passive scalar (e.g., sedimentation of heavy elements), and (6) rotational mixing would greatly benefit from a predictive rather than descriptive, and prognostic rather than diagnostic, treatment. The uncertainties brought about by the constructional limitations of the phenomenological approaches used thus far have rekindled the need for a unified treatment of the above processes.

As noted by Langer (1992), many derived properties disagree in several fundamental ways with results of stellar evolution; the discrepancies are larger than possible error bars and cannot be overcome by adjusting free parameters. Specifically, we can cite the fact that the progenitors of type II supernovae were generally thought to be red giants whereas SN 1987A showed a blue progenitor. For interesting reviews, see Weiss (1989), Ritossa (1996), Woosley et al. (1999), and Heger, Langer, & Woosley (1999). While there is general agreement that low metallicity favors a blue progenitor and moderate mass losses favor a red one, the role of mixing induced by semiconvection is still under discussion. For example, Dent, Bressan, & Chiosi (1996a, 1996b) proposed a phenomenological model for the turbulent semiconvective diffusivity that contains an adjustable parameter. While this allowed them to fit W–R stars, blue/red supergiants counts, etc., the model failed to reproduce the blue supergiant progenitor of SN 1987A, and perhaps more worrisome was the extreme sensitivity of the results to the adjustable parameter. The most recent work by the same group (Salasnich, Bressan, & Chiosi 1998) employs a simpler parameterization: the ratio of the turbulent diffusivity for semiconvection to the thermal diffusivity is denoted by α_2^{-1}. To obtain the correct evolutionary H–R diagram for a 20 solar mass star which then loops to the blue region via a strong mass loss, the value of α_2 must be $50 \leq \alpha_2 \leq 10^2$, which implies that the diffusion timescale is much shorter than the thermal timescale. These values of α_2 are considerably smaller than the value $\alpha_2 = 10^4$ first suggested by Woosley, Pinto, & Ensman (1988). Langer, El Eid, & Baratte (1989) employed a model of semiconvection (Langer, Sugimoto, & Fricke 1983; Langer, El Eid, & Fricke 1985; Langer et al. 1989), which contains an adjustable parameter $\alpha_{\rm sc}$ to represent the efficiency of semiconvection (somewhat akin to the mixing-length theory [MLT] α). The blue progenitor can be obtained only if $0.05 \geq \alpha_{\rm sc} \geq 0.008$ (see Fig. 1 of Langer et al. 1989). With this $\alpha_{\rm sc}$, the model is however unable to reproduce the *IUE* data concerning the high N/C ratio (8 ± 4), since it yields N/C = 0.7–1.8. To accommodate this result, Langer (1991) invoked an additional source of mixing, rotational mixing. For a recent critical summary of the solved and unsolved problems presented by SN 1987A see Woosley et al. (1998). We shall comment on these models in § 23.

The inability to match different data is a symptom of deeper problems of methodological nature and of internal consistency. Not only does the need arise for a predictive model for each of the processes 1–6, but one must be able to correctly account for the feedback mechanisms—for example, how does semiconvection affect overshooting, and does differential rotation increase or decrease semiconvection and salt fingers?

The main feature of the model adopted here is that it abandons the *bottom-up* approaches used thus far and adopts a *top-down* approach. Bottom-up models are those that employ linear stability analysis (e.g., Kato 1966; Nakakita & Umezu 1994; Umezu 1998) and the criteria of stability/instability that ensue from them to describe the turbulent regime. The Ledoux versus Schwarzschild dichotomy and the indeterminacy in the parameters α_2 and $\alpha_{\rm sc}$ is a consequence of such approaches. Since in astrophysics one does not have the luxury of witnessing the transition from laminarity to turbulence, as one does in a controlled laboratory setting, the validity of the bottom-up approach is justifiably questionable. Linear stability analysis can only give the rate at which velocity, temperature, kinetic energy, etc., grow in time, but this corresponds to a clearly unphysical circumstance that never occurs, since the nonlinear interactions distribute the (would-be divergent) energy among eddies of widely different sizes so as to attain a physically meaningful stationary state, which is what is ultimately needed in stellar calculations. On these grounds alone, it seems unavoidable that one adopts a top-down approach, one that begins with the recognition that we are facing a turbulent stellar state and are required to quantify it—for example, by predicting the behavior of the turbulent kinetic energy (TKE) as a function of some stability parameter like the Richardson number. The point at which the TKE vanishes is where turbulent mixing vanishes. We recall that linear stability analysis predicts that there should be no turbulent mixing beyond $\mathrm{Ri} = \frac{1}{4}$, while laboratory, oceanographic, and large eddy simulation (LES) data indicate that turbulent mixing does exist past $\mathrm{Ri} = \frac{1}{4}$. As a concrete example, we recall that the depth of the ocean mixed layer is underestimated by the $\mathrm{Ri} = \frac{1}{4}$ rule. Turbulence models correctly predict that turbulence survives past Ri = 1–1.5, while linear stability analysis predicts that it does not. And yet the criterion $\mathrm{Ri} = \frac{1}{4}$ has been enforced in all studies of shear-driven (rotational) mixing in stars (for a discussion see Canuto 1998).

In semiconvection, mixing is due to the unstable temperature gradient, while ∇_μ is a sink. Using the bottom-up approach, Langer et al. (1983, 1985, 1989) computed the semiconvection turbulent diffusivity K_c using $K_c = \frac{1}{3} lv = \frac{1}{3} l^2 \tau^{-1}$. With the timescale τ taken from Kato's linear stability analysis, one obtains

$$K_c \chi^{-1} = \frac{1}{6} \alpha_{\rm sc} \frac{1}{R_\mu - 1} , \quad R_\mu \equiv \frac{\nabla_\mu}{\nabla - \nabla_{\rm ad}} , \tag{1}$$

where χ is the radiative conductivity and R_μ is a stability parameter analogous to the Richardson number. The efficiency parameter $\alpha_{\rm sc}$ is not predicted by the model, and we have already discussed the sensitivity of the results to it. The turbulence model presented here provides a deterministic relation free of adjustable parameters.

In a top-down approach, the Ledoux-Schwarzschild criteria are replaced by the criterion (K_h is the turbulent heat diffusivity)

$$K_h (\nabla - \nabla_{\rm ad}) > K_c \nabla_\mu , \tag{2}$$

which follows from the requirement that for turbulent mixing to exist, the source from the unstable temperature gradient $\nabla - \nabla_{\rm ad} > 0$ must be larger than the sink due to the μ gradient. Only a turbulence model can provide the diffusivities $K_{h,c}$, as we now discuss.

1.2. *Turbulent Diffusivities*

Empirical models do not allow to construct the full functional dependence of the turbulent diffusivities. Since the dimensions of the diffusivities are cm^2 s^{-1}, one needs two variables. Over the years, three expressions have been suggested:

1. Richardson law: $\quad \text{Diffusivity} \sim l^{4/3}\epsilon^{1/3}\,, \qquad (3a)$

2. Prandtl law: $\quad \text{Diffusivity} \sim K^{1/2} l\,, \qquad (3b)$

3. Turbulence modeling: $\quad \text{Diffusivity} \sim K\tau \sim K^2\epsilon^{-1}\,, \qquad (3c)$

where l is a typical length scale, K is the turbulent kinetic energy, ϵ is the rate of dissipation of K, and $\tau = 2k/\epsilon$ is the dissipation timescale. Richardson law (a precursor of Kolmogorov law) highlights the diffusive nature of large eddies, while Prandtl law is reminiscent of mean free path arguments. Both expressions entail a poorly defined length scale l whereas equation (3c) does not, since it entails K and ϵ, for which we shall derive two differential equations. This avoids the need of an l. On that basis alone, equation (3c) is preferable to both equations (3a) and (3b). Even so, equation (3c) is not yet satisfactory. In fact, consider the turbulent Prandtl number

$$\sigma_t = \frac{K_m}{K_h} \qquad (4)$$

of the momentum K_m and heat K_h turbulent diffusivities for stable stratification (radiative regions) when shear is the source of turbulence. If we limit the functional dependence to the forms (3a)–(3c), we obtain σ_t = constant, whereas it is known (Webster 1964; Wang, Large, & McWilliams 1996) that σ_t increases with stratification. Therefore, equations (3a)–(3c) are incomplete.

1.3. *Structure Functions*

The complete form must be of the type

$$K_{m,h,c} = 2\,\frac{K^2}{\epsilon}\,S_{m,h,c}\,, \qquad (5)$$

where the dimensionless structure functions $S_{m,h,c}$ for momentum, heat, and concentration are different from one another and thus

$$K_m \neq K_h \neq K_c\,. \qquad (6)$$

We shall derive the structure functions and show that they are of the general form

$$S_{m,h,c}(\nabla \boldsymbol{U},\, \alpha_T \nabla T,\, \alpha_c \nabla C \,|\, K, \epsilon)\,, \qquad (7)$$

where $\alpha_{T,C}$ are the volume expansion coefficients. They represent the effect on the density field ρ of a variation of the temperature and c fields. The turbulent variables K and ϵ provide a unit of time $\tau = 2k/\epsilon$ to measure shear (time^{-1}). Equation (6) implies that the momentum diffusivity that enters the angular momentum equation is not the same as the heat diffusivity and that both are different from the diffusivity that enters the concentration equations. We must also remark that in some cases ratios like that in equation (4) may be as large as 20 (e.g., see Fig. 6). Phenomenological models cannot yield the structure functions, and that explains why the diffusivities $K_{m,h,c}$ are often assumed to be the same (e.g., Talon et al. 1997).

Finally, we must distinguish between passive and active scalars, a difference that is essential but often overlooked. Semiconvection and salt fingers are the manifestations of a μ-field that is active in the sense that it can weaken and/or enhance turbulence. This implies that its effect on the density field cannot be neglected; $\alpha_c \neq 0$. On the other hand, the sedimentation of metals in stars and/or the dispersion of a contaminant driven by a wind field are examples of processes that entail passive scalars, since they do not affect the turbulent field that makes them turbulent. In that case, $\alpha_c = 0$. In either case, the diffusivity can still be describe by equations (5) and (7). However, for a passive scalar, equation (7) becomes

$$S_c(\nabla \boldsymbol{U},\, \alpha_T \nabla T,\, 0 \,|\, K, \epsilon)\,. \qquad (8)$$

1.4. *Turbulence*

In addition to the known difficulties of turbulence, we have to account for three interacting fields, temperature, velocity, and concentration. The gradients of their mean components,

$$\nabla T,\, \nabla \boldsymbol{U},\, \nabla C\,, \qquad (9)$$

act as sources/sinks of instabilities. The three fields have also turbulent components

$$T'',\, u_i'',\, c'' \qquad (10)$$

that give rise to the following nonzero correlation functions:

$$\overline{\rho u_i'' u_j''},\, \overline{\rho u_i'' T''},\, \overline{\rho u_i'' c''},\, \overline{\rho T''^2},\, \overline{\rho c''^2},\, \overline{\rho T'' c''}\,. \qquad (11)$$

The first three are the fluxes of momentum (Reynolds stresses), temperature (convective flux), and concentration (mass flux). The fourth and the fifth are proportional to the potential energies of the fluctuating temperature and concentration fields, while the last term represents the correlation between the T'' and c'' fluctuating fields. The first three terms in expression (11) enter the dynamic equations for the mean variables

$$\frac{\partial}{\partial t} U_i + \cdots = -\frac{\partial}{\partial x_j}\,\overline{\rho u_i'' u_j''}\,, \qquad (12a)$$

$$\frac{\partial T}{\partial t} + \cdots = -\frac{\partial}{\partial x_j}\,\overline{\rho u_i'' T''}\,, \qquad (12b)$$

$$\frac{\partial C}{\partial t} + \cdots = -\frac{\partial}{\partial x_j}\,\overline{\rho u_i'' c''}\,, \qquad (12c)$$

but the equations for the three second-order moments in equations (12a)–(12c) depend on the last three correlations in expression (11). Thus, the mean variables T, C, and $\boldsymbol{U}$ are coupled by turbulence.

Under certain circumstances one can write

$$R_{ij} \equiv \bar{\rho}^{-1}\overline{\rho u_i'' u_j''} = -K_m S_{ij}\,, \qquad (13a)$$

$$J_i \equiv \bar{\rho}^{-1}\overline{\rho u_i'' T''} = K_h \beta_i\,, \qquad (13b)$$

$$\Phi_i \equiv \bar{\rho}^{-1}\overline{\rho u_i'' c''} = -K_c\,\frac{\partial C}{\partial x_i}\,, \qquad (13c)$$

where $K_{m,h,c}$ are the turbulent diffusivities of momentum, temperature, and concentration (cm^2 s^{-1}), while the shear and the superadiabatic temperature gradients are defined as

$$S_{ij} = \tfrac{1}{2}(U_{i,j} + U_{j,i}) , \quad (14a)$$

$$\beta_i = -\frac{\partial T}{\partial x_i} + \left(\frac{\partial T}{\partial x_i}\right)_{\rm ad} . \quad (14b)$$

For a discussion of equations (13a) and (13b) in the three-dimensional case, specifically regarding solar data see (Canuto & Christensen–Dalsgaard 1998). To show how difficult it is to generalize equation (13a) using only phenomenology, let us observe that equation (13a) does not account for vorticity,

$$V_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i}\right) , \quad (15)$$

which is known to contribute to the Reynolds stresses. However, since V_{ij} is an antisymmetric while R_{ij} is symmetric, one cannot add V_{ij} to the right-hand side of equation (13a). The only way to proceed is to add to equation (13a) a symmetric tensor of the form

$$R_{ik} V_{jk} + R_{jk} V_{ik} , \quad (16)$$

which, at the very least, complicates the final expression for R_{ij}. An additional shortcoming of equation (13a) is the absence of the heat flux J_i, which, on physical grounds, is expected to contribute to R_{ij}. Thus, instead of equation (13a) one expects a relation of the form

$$R_{ij} = -K_m S_{ij} + A(R_{ik} V_{jk} + R_{jk} V_{ik}) + B(g_j J_i + g_i J_j) , \quad (17)$$

where g_i is the gravity vector. Phenomenological models are unable to provide K_m, A, and B. It is important to stress that it is the presence of the last two terms in equation (17), namely,

$$\text{Vorticity} + \text{Buoyancy} , \quad (18)$$

that allows us to reproduce the solar data alluded to before. As for equation (13b), in the case of stable stratification it predicts a negative heat flux: while this is the general rule, it is not always so. Positive fluxes have been measured even in stably stratified flows but equation (13b) is unable to reproduce them. This brief summary shows why one cannot use phenomenological arguments to provide a quantitatively reliable model for the turbulent diffusivities.

1.5. *Structure of the Paper*

In Paper I (Canuto & Dubovikov 1998), we considered only one external stirring force, an unstable temperature profile given by the first term in expression (9), which corresponds to the case of convection. In Paper II (Canuto 1998), a formalism was presented to deal with two nonzero gradients, the first two in expression (9). In this paper we present a formalism to include all three gradients of expression (9).

In §§ 2–8 we derive the general nonlocal model to evaluate the mean fields and the turbulent variables. In § 9 we retain only two nonlocal equations, for K and ϵ, while the other turbulence variables are given analytically. In §§ 11–13 we discuss the general features of semiconvection and salt fingers. In § 16 we discuss qualitative results of the model. In §§ 18 and 19 we give the analytic solution of the local without mean flow. We also solve the flux conservation law and obtain the $\nabla - \nabla_{\rm ad}$ versus ∇_μ relation for both semiconvection and salt fingers. In § 20 we discuss the effect of a μ gradient on the overshooting distance OV and show that a μ gradient decreases the OV. In § 21 we give the analytic expressions for the turbulent diffusivities in the presence of all three gradients in expression (9), including the case of a passive scalar. In § 22 we present numerical solutions to exhibit the effect of shear on the diffusivities. In § 23 we discuss previous models of semiconvection. In § 24 we present some conclusions.

Notation.—Here ν is the kinematic viscosity, χ_θ is the radiative diffusivity ($K_r = c_p \rho \chi_\theta$, $K_r = 4acT^3/3\kappa_{\rm op}\rho$, where $\kappa_{\rm op}$ is the opacity), and χ_c is the kinematic diffusivity for the c field. The units are cm^2 s^{-1}. Expressions for ν, $\chi_{\theta,c}$ can be found in equations (62), (16), and (61) of Spruit (1992); $\chi_{\theta,c}$ are there called $\kappa_{t,s}$. See also Table 1 of Stevenson (1979). In the case of massive stars, ν is contributed primarily by radiation, $\nu = 2aT^4/15c\kappa_{\rm op}\rho^2$ (Kippenhahn, Ruschenplatt, & Thomas 1980; Merryfield 1995). As shown in equations (13), the turbulent diffusivities are denoted by K_m, K_h, and K_c.

2. CONTINUITY EQUATION

Following the formalism presented elsewhere (Canuto 1997a), the total velocity, density, and pressure fields are split into a mean and a fluctuating part as follows:

$$u_i = U_i + u_i'' , \quad \rho = \overline{\rho} + \rho' , \quad p = P + p' , \quad \overline{p'} = \overline{\rho'} = 0 , \quad (19a)$$

$$\overline{\rho u_i''} = 0 , \quad \overline{u_i''} = -\overline{\rho}^{-1}\overline{\rho' u_i''} , \quad U_i = \overline{\rho}^{-1}\overline{\rho u_i} . \quad (19b)$$

The averaging process is known as the mass (or Favre) average and is different from the Reynolds average. The relation between the two is discussed in Canuto (1997a). Using the equation for the density ρ,

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 , \quad \frac{d\rho}{dt} + \rho \frac{\partial u_i}{\partial x_i} = 0 , \quad \frac{d}{dt} \equiv \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i} , \quad (20)$$

we obtain, upon mass averaging,

$$\frac{D\overline{\rho}}{Dt} + \overline{\rho}\frac{\partial U_i}{\partial x_i} = 0 , \quad \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + U_i \frac{\partial}{\partial x_i} . \quad (21)$$

3. MOMENTUM EQUATIONS

Next we consider the Navier-Stokes equations,

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = F_i , \quad (22)$$

where F_i is the sum of pressure forces, body forces, and viscous forces:

$$F_i \equiv -\frac{\partial p}{\partial x_i} - \rho g_i + F_i^{\rm vis} , \quad F_i^{\rm vis} \equiv \frac{\partial \sigma_{ij}}{\partial x_j} , \quad (23)$$

where σ_{ij} is the viscous stress tensor,

$$\sigma_{ij} = \nu\rho\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\nu\rho\delta_{ij}\frac{\partial u_k}{\partial x_k} . \quad (24)$$

Mass-averaging equation (22), we obtain the dynamic equation for the large-scale flow $\boldsymbol{U}$,

$$\overline{\rho}\frac{DU_i}{Dt} = -\frac{\partial}{\partial x_j}(P\delta_{ij} + \tau_{ij}) - \overline{\rho} g_i , \quad (25)$$

where τ_{ij} are the turbulent Reynolds stresses,

$$\tau_{ij} \equiv \overline{\rho u_i'' u_j''} = \bar{\rho} R_{ij} . \tag{26}$$

The kinetic energy of the large-scale field,

$$K_u = \tfrac{1}{2} U_i U_i , \tag{27}$$

satisfies the equation ($a_{ij,k} \equiv \partial a_{ij}/\partial x_k$, $P_{,i} \equiv \partial P/\partial x_i$)

$$\bar{\rho} \frac{DK_u}{Dt} = -U_i(P_{,i} + \tau_{ij,j} + \bar{\rho} g_i) . \tag{28}$$

It was shown in Canuto (1997a) that the Reynolds stresses R_{ij} satisfy the dynamic equations

$$\bar{\rho}\left(\frac{DR_{ij}}{Dt} + D_{ij}\right) = A_{ij} + B_{ij} - \pi_{ij} + \frac{2}{3} \overline{\rho' d} \delta_{ij} - \bar{\rho} \epsilon_{ij} , \tag{29}$$

where the nonlocal term representing the flux of Reynolds stresses is given by

$$D_{ij} = \bar{\rho}^{-1} \frac{\partial}{\partial x_k} \left(\bar{\rho} R_{ijk} + \frac{2}{3} \delta_{ij} \overline{p' u_k''} - \overline{\sigma_{ik} u_j} - \overline{\sigma_{jk} u_i}\right) \tag{30}$$

and R_{ijk} represents the flux of the Reynolds stresses

$$R_{ijk} \equiv \bar{\rho}^{-1} \tau_{ijk} = \bar{\rho}^{-1} \overline{\rho u_i'' u_j'' u_k''} . \tag{31}$$

The source term due to shear is represented by

$$-A_{ij} = \bar{\rho}(R_{ik} U_{j,k} + R_{jk} U_{i,k}) \tag{32}$$

while the source (sink) term due to stratification is represented by

$$\bar{\rho} B_{ij} = (\overline{\rho' u_j''} \delta_{ik} + \overline{\rho' u_i''} \delta_{jk}) P_{,k} . \tag{33}$$

The fluctuating pressure p' gives rise to the pressure-velocity correlation

$$\Pi_{ij} = \overline{u_i'' p'_{,j}} + \overline{u_j'' p_{,i}} , \quad \pi_{ij} \equiv \Pi_{ij} - \tfrac{1}{3} \delta_{ij} \Pi_{kk} . \tag{34}$$

Finally, compressibility introduces a pressure-dilatation term

$$\frac{2}{3} \overline{p' u''_{i,i}} \equiv \frac{2}{3} \overline{p' d} , \quad d \equiv \frac{\partial u_i''}{\partial x_i} , \tag{35}$$

where d is the "dilatation," while ϵ_{ij} is the dissipation tensor,

$$\epsilon_{ij} = \tfrac{2}{3} \bar{\rho} \epsilon \delta_{ij} , \tag{36}$$

for which we shall derive an independent dynamic equation (see below). The trace of equation (29) yields the equation for the turbulent kinetic energy K,

$$K \equiv \tfrac{1}{2} \bar{\rho}^{-1} \overline{\rho u_i'' u_i''} = \tfrac{1}{2} R_{ii} , \tag{37}$$

$$\bar{\rho}\left(\frac{DK}{Dt} + D_f\right) = -\bar{\rho} R_{ij} U_{i,j} + \bar{\rho}^{-1} \overline{\rho' u_i''} P_{,i} + \overline{p' d} - \bar{\rho} \epsilon , \tag{38}$$

where D_f is the nonlocal transport of K:

$$D_f \equiv \bar{\rho}^{-1} \frac{\partial}{\partial x_i} \left(\frac{1}{2} \bar{\rho} R_{kki} + \overline{p' u_i''} - \overline{\sigma_{ij} u_j}\right) . \tag{39}$$

4. CONCENTRATION EQUATIONS

If we denote by ρ the total density of the fluid, and consider a two-fluid model, the density of one component is ρc while that of the other is $\rho(1-c)$, c being the concentration. While ρ satisfies equations (20), the equation satisfied by ρc is given by (no external sources)

$$\frac{\partial(\rho c)}{\partial t} + \frac{\partial(\rho c u_i)}{\partial x_i} = (\rho J_i)_{,i} , \tag{40}$$

or, alternatively,

$$\rho \frac{dc}{dt} = (\rho J_i)_{,i} , \tag{41}$$

where J_i is the diffusion flux. The two-fluid components ρc and $\rho(1-c)$ have diffusion flux densities $cu_i - J_i$ and $(1-c)u_i + J_i$, respectively, so that their sum is u_i. If we define a diffusion velocity u_i^d as follows,

$$J_i = -c u_i^d , \tag{42}$$

Equation (40) can be rewritten as

$$\frac{\partial \rho_*}{\partial t} + \frac{\partial(\rho_* v_{*i})}{\partial x_i} = 0 , \tag{43}$$

$$\rho_* = \rho c , \quad v_{*i} = u_i + u_i^d , \tag{44}$$

which bears a close similarity to the first of equations (20). The vector J_i has been discussed by Chapman & Cowling (1970) and by Landau & Lifshitz (1987). We shall write it as

$$J_i = \chi_c\left(\frac{\partial c}{\partial x_i} + \kappa_T T^{-1} \frac{\partial T}{\partial x_i} + \kappa_p p^{-1} \frac{\partial p}{\partial x_i}\right) . \tag{45}$$

Often, in the cited literature, J includes the density ρ and has the opposite sign; χ_c is called D, but for symmetry reasons we prefer to call it χ_c; both κ_T and κ_P are dimensionless functions (Chapman & Cowling 1970). Different authors employ different notations, e.g., equation (2.1) of Aller & Chapman (1960), equation (3) of Schatzman (1969), equation (1) of Michaud (1970), and equation (1) of Vauclair & Vauclair (1982). As one can see from equation (45), J_i is contributed not only by the gradient of the concentration, a reasonable approximation under laboratory situations, but also by temperature and pressure gradients, first introduced by Chapman (1917), which may be important in stellar interiors.

Following the procedure of averaging discussed in Canuto (1997a), we have

$$\overline{\rho c} = \bar{\rho} C , \quad \overline{\rho c u_i} = \bar{\rho} C U_i + F_i(\text{conc}) , \tag{46}$$

where C is mean concentration and F_i(conc) is concentration flux:

$$C \equiv \bar{c} , \quad F_i(\text{conc}) = \overline{\rho u_i'' c''} = \bar{\rho} \Phi_i . \tag{47}$$

Taking the mass average of equation (41), we obtain the equation for the mean concentration C:

$$\bar{\rho} \frac{DC}{Dt} = \frac{\partial \bar{J}_i}{\partial x_i} - \frac{\partial(\bar{\rho} \Phi_i)}{\partial x_i} , \tag{48}$$

or, more explicitly,

$$\bar{\rho} \frac{DC}{Dt} = \left(\bar{\rho} \chi_c \frac{\partial C}{\partial x_i}\right)_{,i} - (\bar{\rho} \Phi_i)_{,i} + \{\bar{\rho} \chi_c [\kappa_T (\ln T)_{,i} + \kappa_p (\ln P)_{,i}]\}_{,i} . \tag{49}$$

It has been common practice (Cloutman & Eoll 1976; Chaboyer & Zahn 1992; Chaboyer, Demarque, & Pinsonneault 1995; Ventura et al. 1998; Maeder & Zahn 1998) to neglect the last two terms, which is probably a justifiable approximation when one deals with a highly turbulent regime.

5. EQUATION FOR THE MEAN TEMPERATURE

We begin with the equation for the entropy S (Landau & Lifshitz 1987),

$$\rho T \frac{dS}{dt} = -\frac{\partial}{\partial x_i}(q_i + \rho\tilde{\mu}J_i) + \rho J_i \frac{\partial \tilde{\mu}}{\partial x_i} + \sigma_{ij}\frac{\partial u_i}{\partial x_j}, \quad (50)$$

where $\tilde{\mu}$ is the chemical potential and

$$q_i = F_i^r - \rho J_i\left(\tilde{\mu} - T\frac{\partial \tilde{\mu}}{\partial T}\bigg|_{p,c}\right) - \rho J_i \kappa_T \frac{\partial \tilde{\mu}}{\partial c}\bigg|_{p,T}, \quad (51)$$

where F_i^r is the radiative flux. In the absence of diffusion $q_i = F_i^r$, but here q_i depends also on the gradients of the concentration as well as on the gradient of $\tilde{\mu}$. Next, we work out the entropy change dS/dt. We have

$$\frac{dS}{dt} = \frac{\partial S}{\partial T}\bigg|_{c,p}\frac{dT}{dt} + \frac{\partial S}{\partial c}\bigg|_{T,p}\frac{dc}{dt} + \frac{\partial S}{\partial p}\bigg|_{c,T}\frac{dp}{dt}, \quad (52)$$

and since

$$T\frac{\partial S}{\partial T}\bigg|_{c,p} = c_p, \quad \frac{\partial S}{\partial c}\bigg|_{T,p} = -\frac{\partial \tilde{\mu}}{\partial T}\bigg|_{p,c},$$
$$\rho^2\frac{\partial S}{\partial p}\bigg|_{c,T} = \frac{\partial \rho}{\partial T}\bigg|_{p,c}, \quad (53)$$

equation (50) becomes

$$\rho c_p \frac{dT}{dt} = \frac{dp}{dt} + \rho T\frac{\partial \tilde{\mu}}{\partial T}\bigg|_{p,c}\frac{dc}{dt} - \frac{\partial}{\partial x_i}(q_i + \rho\tilde{\mu}J_i)$$
$$+ \rho J_i\frac{\partial \tilde{\mu}}{\partial x_i} + \sigma_{ij}\frac{\partial u_i}{\partial x_j}, \quad (54)$$

where we have taken $T\rho^{-1}\partial\rho/\partial T|_{p,c} = -1$ (no radiation pressure). Use of equation (41) gives

$$\rho c_p \frac{dT}{dt} = \frac{dp}{dt} - h\frac{\partial(J_i\rho)}{\partial x_i} - \frac{\partial q_i}{\partial x_i} + \sigma_{ij}\frac{\partial u_i}{\partial x_j}, \quad (55)$$

where h is defined as

$$h = \tilde{\mu} - T\frac{\partial \tilde{\mu}}{\partial T}\bigg|_{p,c}. \quad (56)$$

Next, we employ the definition of the generalized flux q_i given above (eq. [51]). We obtain

$$\rho c_p \frac{dT}{dt} = \frac{dp}{dt} - \frac{\partial}{\partial x_i}F_i^r + \sigma_{ij}\frac{\partial u_i}{\partial x_j} + \rho\chi_c\frac{\partial c}{\partial x_k}\frac{\partial h}{\partial x_k}$$
$$+ \left(\rho J_i \kappa_T\frac{\partial \tilde{\mu}}{\partial c}\bigg|_{p,T}\right)_{,i} \quad (57a)$$

or, alternatively,

$$c_p\left[\frac{\partial}{\partial t}\rho T + \frac{\partial}{\partial x_i}(\rho u_i T)\right] = \frac{dp}{dt} - \frac{\partial F_i^r}{\partial x_i} + \sigma_{ij}\frac{\partial u_i}{\partial x_j}$$
$$+ \rho\chi_c\frac{\partial c}{\partial x_k}\frac{\partial h}{\partial x_k}$$
$$+ \left(\rho J_i\kappa_T\frac{\partial \tilde{\mu}}{\partial c}\bigg|_{p,T}\right)_{,i}. \quad (57b)$$

The last two terms are due to diffusion, and the remaining terms are identical to those of Canuto (1997a). The last term is likely to be much smaller than the previous one, and thus we can neglect it (even though the retention of it would not cause conceptual difficulties). The neglect can be justified in the following way. Even at the lowest order in J_i, that is, retaining only the first term in equation (45), this term would be proportional to the product of two "molecular" variables, $\chi_c \kappa_T$, while the previous terms are linear in such parameters. Merryfield (1995) has carried out a two-dimensional numerical simulation of semiconvection using this approximation. It was also shown that for an individual species i, $h_i = 5kT/2m_i$, while for a binary mixture one can use the definition of $\mu = \mu_1/m_1 - \mu_2/m_2$ (Landau & Lifshitz 1987), where μ's are the mean molecular weights of the two species. Thus,

$$h = \frac{5}{2}\frac{kT}{\mu_{1,2}}, \quad \mu_{1,2} = (\mu_1^{-1} - \mu_2^{-1})^{-1}. \quad (58)$$

For $\mu_1 \equiv \mu(\mathrm{He})$ and $\mu_2 = \mu(\mathrm{H})$, one then has (Merryfield 1995)

$$h = -\tfrac{25}{8}RT. \quad (59)$$

Next, we take the mass average of equation (57b). Making use of the results derived in Canuto (1997a) and recalling that $\overline{\sigma_{ij}u_{j,i}} = \bar{\rho}\epsilon$, we obtain

$$\bar{\rho}c_p\frac{DT}{Dt} = -(F_i^c + \overline{F_i^r} - \overline{p'u_i''})_{,i} + \frac{DP}{Dt}$$
$$+ \overline{u_i''}P_{,i} - \overline{p'd} + \bar{\rho}\epsilon - \frac{25}{8}\chi_c R\overline{\rho c_{,k}T_{,k}} \quad (60)$$

where F_i^c is the convective flux,

$$F_i^c = c_p\overline{\rho T''u_i''} = \bar{\rho}H_i = c_p\bar{\rho}J_i. \quad (61)$$

In the last term we have kept only the largest term. The $\overline{u_i''}$ term in equation (60) can be written using equation (19b). Adding equation (60) to equation (38) yields

$$\frac{DP}{Dt} = \bar{\rho}R_{ij}U_{i,j} + \bar{\rho}\frac{D}{Dt}(c_pT + K)$$
$$+ (F_i^c + \overline{F}_i^r + F_i^{\mathrm{ke}})_{,i} - \frac{25}{8}\chi_c R\overline{\rho c_{,k}T_{,k}}, \quad (62)$$

where F_i^{ke} is the flux of turbulent kinetic energy (summation over the indices j),

$$F_i^{\mathrm{ke}} = \tfrac{1}{2}\overline{\rho u_j''u_j''u_i''}. \quad (63)$$

A further simplification occurs if we add to both sides of equation (62) the term $\bar{\rho}DK_u/Dt$ given by equation (28). We obtain

$$\frac{\partial P}{\partial t} = \bar{\rho}\frac{D}{Dt}(c_pT + K + K_u + G)$$
$$+ (F_i^c + \overline{F}_i^r + F_i^{\mathrm{ke}} + \bar{\rho}R_{ij}U_j)_{,i}$$
$$-\frac{25}{8}\chi_c R\bar{\rho}C_{,k}T_{,k}, \quad (64)$$

where $g_i\bar{\rho}U_i = \bar{\rho}U_iG_{,i} = \bar{\rho}DG/Dt$. Equation (64) is the generalized Bernoulli equation with turbulence, diffusion, and radiation.

6. TURBULENCE

As already discussed, we need to evaluate the second-order moments defined in expressions (11). The equation for the first of them has already been given by equation (29). As for the correlation

$$\phi = \tfrac{1}{2}\overline{\rho c''^2} , \tag{65}$$

we first note that using equation (40), ρc^2 satisfies the dynamic equation ($J_{i,i} \equiv \partial(\rho J_i)/\partial x_i$)

$$\frac{\partial(\rho c^2)}{\partial t} + \frac{\partial(\rho u_i c^2)}{\partial x_i} = 2cJ_{i,i} . \tag{66}$$

Taking into account the relations

$$\overline{\rho c^2} = \overline{\rho} C^2 + \overline{\rho c''^2} , \tag{67a}$$

$$\overline{\rho u_i c^2} = \overline{\rho} U_i C^2 + U_i \overline{\rho c''^2} + \overline{\rho u_i'' c''^2} + 2C\overline{\rho u_i'' c''} , \tag{67b}$$

the mass average of equation (66) yields the following for ϕ:

$$\frac{\partial \phi}{\partial t} + D_f(\phi) + \frac{1}{2}\frac{\partial(\overline{\rho}C^2)}{\partial t} = -\frac{1}{2}(\overline{\rho}U_i C^2)_{,i} - (\phi U_i)_{,i} - [CF_i(\text{conc})]_{,i} + \overline{cJ}_{i,i} . \tag{68}$$

Using equations (21) and (48), equation (68) can be reduced to the following form:

$$\frac{D\phi}{Dt} + D_f(\phi) = -\phi U_{i,i} - F_i(\text{conc})C_{,i} + \overline{cJ}_{i,i} - C\overline{J}_{i,i} . \tag{69}$$

Finally, introducing the new function Φ,

$$\tfrac{1}{2}\overline{\rho c''^2} = \overline{\rho}\Phi . \tag{70}$$

Equation (69) simplifies further to

$$\overline{\rho}\left[\frac{D\Phi}{Dt} + D_f(\Phi)\right] = -\frac{\partial C}{\partial x_i} F_i(\text{conc}) + \overline{cJ}_{i,i} - C\overline{J}_{i,i} , \tag{71}$$

where F_i (conc) is defined in equations (47) and the nonlocal transport of Φ is given by

$$D_f(\Phi) = \frac{1}{2}\overline{\rho}^{-1}\frac{\partial}{\partial x_i}(\overline{\rho u_i'' c''^2}) . \tag{72}$$

The last two terms in equation (71) will be computed as follows:

$$\overline{cJ}_{i,i} - C\overline{J}_{i,i} = C\overline{J}_{i,i} + \overline{c''J}_{i,i} - C\overline{J}_{i,i} = \overline{c''J}_{i,i} = \overline{c''J''_{i,i}} , \tag{73}$$

which, using equation (45), becomes (whenever the equation is rather complicated, we may employ angular brackets instead of an overbar for ease of notation)

$$\overline{\rho}\chi_c\left[\left\langle c''\frac{\partial^2 c''}{\partial x_j^2}\right\rangle + \left\langle c''\frac{\partial}{\partial x_i}\left(\kappa_T T^{-1}\frac{\partial T''}{\partial x_i}\right)\right\rangle + \left\langle c''\frac{\partial}{\partial x_i}\left(\kappa_T P^{-1}\frac{\partial p''}{\partial x_i}\right)\right\rangle\right] . \tag{74}$$

Assuming, as seems natural, a higher degree of correlation of c'' among themselves than with the temperature and pressure fluctuations, we approximate expression (74) as follows:

$$\overline{\rho}\chi_c\left\langle c''\frac{\partial^2 c''}{\partial x_j^2}\right\rangle = 2\overline{\rho}\tau_c^{-1}\Phi , \tag{75}$$

where τ_c is the correlation timescale discussed below. Thus, we finally have:

$$\frac{D\Phi}{Dt} + D_f(\Phi) = -\overline{\rho}^{-1}F_i(\text{conc})C_{,i} - 2\tau_c^{-1}\Phi . \tag{76}$$

Next, we consider the third term in equation (11) and make use of equations (47). Multiply equation (40) by u_i and equation (22) by c. Adding the results, we obtain

$$\frac{\partial(\rho c u_i)}{\partial t} + \frac{\partial(\rho c u_i u_j)}{\partial x_j} = F_i c + u_i J_{k,k} . \tag{77}$$

Recalling that

$$\begin{aligned}\overline{\rho c u_i} &= \overline{\rho}U_i C + \overline{\rho u_i'' c''} = \overline{\rho}U_i C + F_i(\text{conc}) , \\ \overline{\rho c u_i u_j} &= \overline{\rho}U_i U_j C + C\tau_{ij} + U_k \\ &\quad\times [\delta_{ik}F_j(\text{conc}) + \delta_{jk}F_i(\text{conc})] \\ &\quad+ \overline{\rho u_i'' u_j'' c''} ,\end{aligned} \tag{78}$$

substitution into the mass-averaged form of equation (77) gives, after several steps,

$$\frac{D\Phi_i}{Dt} + D_f(\Phi_i) = -R_{ij}C_{,j} - \Phi_j U_{i,j} + \overline{\rho}^{-1}A_i , \tag{79}$$

where the function A_i is given by

$$A_i \equiv \overline{F_i c} - \overline{F}_i C + \overline{u_i'' J_{k,k}} . \tag{80}$$

Recalling the definition of F_i (equation [23]), we have after some algebra

$$\overline{F_i c} - \overline{F}_i C = -g\overline{\rho}\Lambda_i\overline{c''} - \left\langle c''\frac{\partial p''}{\partial x_i}\right\rangle , \tag{81}$$

where the dimensionless function Λ_i is given in terms of the pressure scale height H_p

$$\Lambda_i = H_p P^{-1}\frac{\partial P}{\partial x_i} , \quad H_p = P(g\overline{\rho})^{-1} . \tag{82}$$

Since by definition

$$\overline{\rho}\overline{c''} = -\overline{\rho' c''} , \tag{83}$$

use of the expansion

$$\frac{\rho'}{\overline{\rho}} = -\alpha_T T'' + \alpha_c c'' , \tag{84}$$

where the expansion coefficients are defined as

$$\alpha_T \equiv \alpha = -\left(\frac{\partial \ln\rho}{\partial T}\right)_{p,c} , \quad \alpha_c = \left(\frac{\partial \ln\rho}{\partial C}\right)_{p,T} , \tag{85}$$

gives

$$\overline{c''} = \alpha\overline{T''c''} - \alpha_c\overline{c''^2} . \tag{86}$$

The $\overline{c''^2}$ term will be approximated with 2Φ given by equation (70), while $\overline{T''c''}$ will be computed later on. Thus, we have

$$A_i = -g\overline{\rho}\Lambda_i(\alpha\overline{T''c''} - 2\alpha_c\Phi) - \left\langle c''\frac{\partial p''}{\partial x_i}\right\rangle + \overline{u_i'' J_{k,k}} . \tag{87}$$

To evaluate the last term in equation (87), we use equation (40) and consider the quantity

$$L_i \equiv \chi_c \overline{\rho u_i'' \Delta} , \qquad (88)$$

where

$$\Delta \equiv \frac{\partial}{\partial x_k}\left(\frac{\partial c}{\partial x_k} + \kappa_T T^{-1} \frac{\partial T}{\partial x_k} + \kappa_p p^{-1} \frac{\partial p}{\partial x_k}\right) = \overline{\Delta} + \Delta'' . \qquad (89)$$

Since by definition $\overline{\rho u_i''} = 0$, the only nonzero contribution is

$$L_i = \chi_c \overline{\rho_i'' \Delta''} , \qquad (90)$$

where

$$\Delta'' = \frac{\partial}{\partial x_k}\left(\frac{\partial c''}{\partial x_k} + \kappa_T T^{-1} \frac{\partial T''}{\partial x_k} + \kappa_p P^{-1} \frac{\partial p''}{\partial x_k}\right) ; \qquad (91)$$

here we have kept only the largest terms in the (unwritten) expansion. This is why in the last term in equation (91) we have P in the denominator. Thus, we have

$$L_i = \chi_c \left\langle \rho u_i'' \frac{\partial^2 c''}{\partial x_j{}^2} \right\rangle + \cdots . \qquad (92)$$

This term is analogous to part of the term η_i in equation (34*b*) of Canuto (1992), namely,

$$\eta_i = \chi_\theta \left\langle u \frac{\partial^2 \theta}{\partial x_k^2} \right\rangle \qquad (93)$$

where the radiative conductivity χ_θ plays the role of χ_c and c'' is the analog of the temperature fluctuations θ; u_i'' was denoted by u_i. Using the arguments developed in the cited reference, we shall write

$$L_i = \tfrac{1}{2} \chi_c \Phi_{i,kk} , \qquad (94)$$

which represents the dissipation of $\overline{u_i'' c''}$ due to the diffusivity χ_c. We have neglected the extra terms due to temperature and pressure gradients because we believe that equation (94) is the largest contribution. The last term we must compute is the pressure correlation term

$$\Pi_i^c = \left\langle c'' \frac{\partial p''}{\partial x_i} \right\rangle . \qquad (95)$$

Using the analogy with the temperature case (Canuto 1992, eq. [43a], [43b]), we shall write

$$\Pi_i^c = \tau_{\rm pc}^{-1} \Phi_i . \qquad (96)$$

Finally, the complete equation for Φ_i is

$$\frac{D\Phi_i}{Dt} + D_f(\Phi_i) = -R_{ij} C_{,j} - \Phi_j U_{i,j} - g\Lambda_i(\alpha \overline{T'' c''} - 2\alpha_c \Phi) - \tau_{\rm pc}^{-1} \Phi_i + \frac{1}{2} \chi_c \Phi_{i,kk} . \qquad (97)$$

Next, we consider the fourth function in equation (11), which we generalize to

$$\psi = \tfrac{1}{2} \overline{\rho T''^2} = \overline{\rho} \Psi . \qquad (98)$$

First we recall that, except for the last two diffusion terms, the temperature equation (57b) can be treated as in Canuto (1997a), where the equation for ψ is given by eq. (26f). Thus, we must add the last but one term in equation (57b),

$$-\frac{25}{8} \chi_c R c_p^{-1} \rho T \frac{\partial c}{\partial x_k} \frac{\partial T}{\partial x_k} . \qquad (99)$$

Keeping only the largest terms, the dynamic equation for Ψ becomes

$$\frac{D\Psi}{Dt} + \overline{\rho}^{-1} D_f = c_p^{-1} H_i \beta_i - 2\tau_\theta^{-1} \Psi + \chi_\theta \Psi_{,kk} - \frac{25}{16} \chi_c R c_p^{-1} \overline{\rho} \frac{\partial C}{\partial x_k} \frac{\partial \overline{T}^2}{\partial x_k} , \qquad (100)$$

where the convective flux H_i is defined in equation (61). Here β_i is the superadiabatic gradient

$$\beta_i = T H_p^{-1} (\nabla - \nabla_{\rm ad}) . \qquad (101)$$

Next, we consider the second term in equation (11), namely, the convective flux (eq. [61]. Here, too, the relevant dynamic equation was already derived in Canuto (1997a), equation (24a), to which we must add the last but one term of equation (57b). The result is

$$\frac{DH_i}{Dt} + c_p D_f(H_i) = c_p R_{ij} \beta_j - H_j U_{i,j} - c_p g \Lambda_i \overline{T''} - \tau_{p\theta}^{-1} H_i + \frac{1}{2} \times \chi_\theta H_{i,kk} - \frac{25}{8} R \chi_c U_i \frac{\partial C}{\partial x_k} \frac{\partial \overline{T}}{\partial x_k} , \qquad (102)$$

where the pressure term gives rises to the relaxation term $\tau_{p\theta}^{-1}$. Finally, we use the fact that

$$\overline{\rho T''} = -\overline{\rho' T''} \qquad (103)$$

and the expansion (84) to obtain

$$\overline{T''} = \alpha \overline{T''^2} - \alpha_c \overline{c'' T''} , \qquad (104)$$

so that equation (102) becomes

$$\frac{DH_i}{Dt} + c_p D_f(H_i) = c_p R_{ij} \beta_j - H_j U_{i,j} - c_p g \Lambda_i (2\alpha \Psi - \alpha_c \overline{c'' T''}) - \tau_{p\theta}^{-1} H_i + \frac{1}{2} \chi_\theta H_{i,kk} - \frac{25}{8} R \chi_c U_i \frac{\partial C}{\partial x_k} \frac{\partial \overline{T}}{\partial x_k} . \qquad (105)$$

Finally, let us consider the last term in equations (11), the correlation between T'' and c''. We recall that in general

$$\frac{dc}{dt} = \frac{DC}{Dt} + \frac{Dc''}{Dt} + u_i''\left(\frac{\partial C}{\partial x_i} + \frac{\partial c''}{\partial x_i}\right) , \qquad (106)$$

and thus from equation (41)

$$\rho\left(\frac{DC}{Dt} + \frac{Dc''}{Dt} + u_i'' \frac{\partial C}{\partial x_i} + u_i'' \frac{\partial c''}{\partial x_i}\right) = J_{k,k} . \qquad (107)$$

Subtracting the mass average of equation (107) from itself, we obtain

$$\frac{Dc''}{Dt} + (u_i'' - \overline{u_i''}) \frac{\partial C}{\partial x_i} = \left\langle u_i'' \frac{\partial c''}{\partial x_i} \right\rangle - u_i'' \frac{\partial c''}{\partial x_i} + \rho^{-1} J_{k,k} - \langle \rho^{-1} J_{k,k} \rangle . \quad (108)$$

Multiplying equation (108) by T'' and mass averaging, we obtain

$$\left\langle T'' \frac{Dc''}{Dt} \right\rangle + (\overline{T''u_i''} - \overline{T''}\,\overline{u_i''})C_{,i} = \langle \rho^{-1} T'' J_{k,k} \rangle - \overline{T''} \langle \rho^{-1} J_{k,k} \rangle + \cdots , \quad (109)$$

where by " ⋯ " (higher order terms) we mean all the terms that entail correlations higher than the second-order terms under consideration. For example, if we neglect the higher orders, we must also neglect $\overline{u_i''}$ in equation (109): in fact, because of the second relation in equations (19b), $\overline{u_i''}$ is already a second-order quantity. As for the equation for T'', we employ equations (27) and (32) of Canuto (1993; with obvious change in notation), to which we must add the last but one term of equation (57b). Keeping only the largest terms, we have

$$\frac{DT''}{Dt} = u_i'' \beta_i - (u_i'' T'' - \overline{u_i'' T''})_{,i} + \chi_\theta T''_{,kk} - \frac{25}{8} R c_p^{-1} \chi_c U_i \left(\frac{\partial c''}{\partial x_k} \frac{\partial \overline{T}}{\partial x_k} + \frac{\partial C}{\partial x_k} \frac{\partial T''}{\partial x_k} \right) . \quad (110)$$

Once we multiply by c'' and mass-average, we obtain

$$\left\langle c'' \frac{DT''}{Dt} \right\rangle = \overline{c'' u_i''} \beta_i + \chi_\theta \left\langle c'' \frac{\partial^2 T''}{\partial {x_k}^2} \right\rangle + \text{higher order terms} . \quad (111)$$

Adding equation (109) to equation (111), we obtain

$$\frac{D}{Dt} (\overline{T''c''}) = \beta_i \Phi_i - c_p^{-1} H_i \frac{\partial C}{\partial x_i} - \tau_{c\theta}^{-1} \overline{T''c''} , \quad (112)$$

where we have taken

$$\chi_c \left\langle c'' \frac{\partial^2 T''}{\partial {x_k}^2} \right\rangle + \langle \rho^{-1} T'' J_{k,k} \rangle - \overline{T''} \langle \rho^{-1} J_{k,k} \rangle = -\tau_{c\theta}^{-1} \overline{T''c''} . \quad (113)$$

Since it is quite hard to provide an exact evaluation of the terms in equation (113), we have followed a previous suggestion of considering that the effect of these terms is a damping of the $\overline{T''u_i''}$ fluctuations on a timescale $\tau_{p\theta}$ whose evaluation will be discussed in Appendix B.

7. NONLOCAL MODEL

To simplify the use of the equations we have derived, we list them here beginning with the equations for the mean quantities:

Large-scale flow U_i:

$$\overline{\rho} \frac{DU_i}{Dt} = -\frac{\partial}{\partial x_j} (P\delta_{ij} + \overline{\rho} R_{ij}) - \overline{\rho} g_i . \quad (114)$$

Mean temperature T:

$$\frac{\partial P}{\partial t} = \overline{\rho} \frac{D}{Dt} (c_p T + K + K_u + G) + (F_i^c + \overline{F}_i^r + F_i^{\text{ke}} + \overline{\rho} R_{ij} U_j)_{,i} + f(\chi_c) , \quad (115)$$

where $f(\chi_c)$ represents the last term in equation (64).

Mean concentration C:

$$\overline{\rho} \frac{DC}{Dt} = \left(\overline{\rho} \chi_c \frac{\partial C}{\partial x_i} \right)_{,i} - (\overline{\rho} \Phi_i)_{,i} + [\overline{\rho} \chi_c (\kappa_T T^{-1} T_{,i} + \kappa_p P^{-1} P_{,i})]_{,i} . \quad (116)$$

Reynolds stresses $\overline{\rho u_i'' u_j''} = \overline{\rho} R_{ij}$:

$$\overline{\rho} \left(\frac{D}{Dt} R_{ij} + D_{ij} \right) = A_{ij} + B_{ij} - \pi_{ij} - \frac{2}{3} \overline{\rho} \epsilon \delta_{ij} , \quad (117)$$

where

$$-A_{ij} \equiv \overline{\rho} (R_{ik} U_{j,k} + R_{jk} U_{i,k}) , \quad (118a)$$

$$B_{ij} = -(c_p^{-1} \alpha H_i - \alpha_c \Phi_i) P_{,j} + (i \to j, j \to i) . \quad (118b)$$

The pressure-velocity correlation π_{ij} is discussed in Appendix A.

Turbulent kinetic energy $K = \frac{1}{2} R_{ii}$:

$$\frac{DK}{Dt} + D_f(K) = -R_{ij} U_{i,j} - \overline{\rho}^{-1} (\alpha c_p^{-1} H_i - \alpha_c \Phi_i) P_{,i} - \epsilon . \quad (119)$$

In both equations (117) and (119) we have not included the dilatation term $\overline{p'd}$, which, however, can be accounted for using equations (45c) and (35c) of Canuto (1997a).

Convective flux $c_p \overline{\rho u_i'' T''} = \overline{\rho} H_i$:

$$\frac{DH_i}{Dt} + c_p D_f(H_i) = c_p R_{ij} \beta_j - H_j U_{i,j} - c_p \overline{\rho}^{-1} (2\alpha \Psi - \alpha_c \overline{c''T''}) P_{,i} - \tau_{p\theta}^{-1} H_i + \frac{1}{2} \chi_\theta H_{i,kk} \quad (120)$$

Temperature fluctuations $\frac{1}{2} \overline{\rho T''^2} = \overline{\rho} \Psi$:

$$\frac{D\Psi}{Dt} + \overline{\rho}^{-1} D_f(\Psi) = c_p^{-1} H_i \beta_i - 2\tau_\theta^{-1} \Psi + \chi_\theta \Psi_{,kk} . \quad (121)$$

Concentration variance $\frac{1}{2} \overline{\rho c''^2} = \overline{\rho} \Phi$:

$$\frac{D}{Dt} \Phi + D_f(\Phi) = -\Phi_i C_{,i} - 2\tau_c^{-1} \Phi . \quad (122)$$

Concentration flux $\overline{\rho c'' u_i''} = \overline{\rho} \Phi_i$:

$$\frac{D\Phi_i}{Dt} + D_f(\Phi_i) = -R_{ij} C_{,j} - \Phi_j U_{i,j} - \overline{\rho}^{-1} \times (\alpha \overline{T''c''} - 2\alpha_c \Phi) P_{,i} - \tau_{\text{pc}}^{-1} \Phi_i + \frac{1}{2} \chi_c \Phi_{i,kk} . \quad (123)$$

Temperature-concentration correlation $\overline{T''c''}$:

$$\frac{D(\overline{T''c''})}{Dt} + D_f = \beta_i \Phi_i - c_p^{-1} H_i C_{,i} - \tau_{c\theta}^{-1} \overline{T''c''} \ . \quad (124)$$

The equations for the timescale τ_{pc}, $\tau_{c\theta}$, τ_c, $\tau_{p\theta}$, τ_θ are given below.

8. THE RENORMALIZATION GROUP METHOD OF DETERMINING THE TIMESCALES τ_{pc}, $\tau_{c\theta}$, τ_c, $\tau_{p\theta}$, τ_θ

To make the above equations predictive, one must know the dissipation timescales of the different turbulent variables, namely, τ_{pc}, $\tau_{c\theta}$, τ_c, $\tau_{p\theta}$, τ_θ. Not surprisingly, this is one of the most difficult problems, since one-point closure models, like the one we have used, are incapable of providing them. Thus far, two types of models have been employed, namely, engineering and geophysical models.

8.1. *Engineering and Geophysical Models*

Since in most situations the kinematic diffusivities of heat and/or concentrations are very small, they give rise to timescales $l^2(\chi_\theta^{-1}, \chi_c^{-1})$ which are considerably larger than the dynamic timescale τ characterizing the turnover time of a large eddy:

$$\tau \sim K\epsilon^{-1} \sim K^{-1/2} l \ . \quad (125)$$

Under these conditions, it is expected that ($\kappa = 1, \ldots, 5$)

$$\tau_\kappa = (\tau_{pc}, \tau_{c\theta}, \tau_c, \tau_{p\theta}, \tau_\theta)\tau^{-1} \sim C_\kappa = \text{constant} \ . \quad (126)$$

Examples of the constants C_κ can be found in Canuto (1994).

8.2. *Astrophysics*

In this case equations (126) can only be valid in the case of very efficient convection when radiative losses are unimportant. In the most crucial and interesting case of inefficient convection, ∇ detaches itself from ∇_{ad} and tends toward ∇_r owing to the increasing dominance of radiative losses that weaken the efficiency of convection as a heat transport mechanism. Since the efficiency of convection is described by the Peclet number (Pe), the above timescales should depend on Pe in such a way that when $\mathrm{Pe} \gg 1$, they satisfy equation (126), while in the opposite case of $\mathrm{Pe} < 1$, they become smaller than the dynamical timescale τ. Thus, instead of equation (126), one should write

$$(\tau_{pc}, \tau_{c\theta}, \tau_c, \tau_{p\theta}, \tau_\theta)\tau^{-1} = f(\mathrm{Pe}) \ ,$$
$$f(x) = \text{constant} \quad \text{for } x \gg 1, \quad f(x) < 1 \quad \text{for } x \ll 1 \ . \quad (127)$$

Without a theory, the construction of the function $f(x)$ is a major hurdle. Grossman & Taam (1996) and Xiong (1985a, 1985b, 1986) have suggested empirical functions of the type

$$f(x) = \frac{ax}{1 + bx} \ , \quad (128)$$

but even so, there is no a priori reason why the constants a and b should be the same for all the ratios considered in equation (126). Since we have five timescales, this means 10 adjustable parameters, which, at the very least, are hard to control. As the authors just cited have stressed, this is the major shortcoming of their methodology. They prevent the proliferation of constants by demanding that all length scales (which are equivalent to timescales) be taken proportional to a master length scale which itself, however, is not determined by the model and must be fixed empirically.

In the present formalism we try to overcome these difficulties by adopting results obtained from the renormalization group (RNG) formalism.

8.3. *The RNG method*

We recall that the Peclet number is actually a function of the form

$$\mathrm{Pe} \sim \frac{\nu_t}{\chi} \ , \quad \nu_t(k) = \int_k^\infty \psi(k')dk' \ , \quad (129)$$

where the turbulent viscosity $\nu_t(k)$, which depends on the eddy size $\sim k^{-1}$, is the key quantity. From the first model by Heisenberg to the most modern ones (Lesieur 1991), $\nu_t(k)$ is expressed as a UV property, since it is contributed by all eddies smaller than k^{-1}. The construction of the function $\nu_t(k)$ has improved considerably through the use of the RNG-based techniques. As discussed elsewhere in detail (Canuto & Dubovikov 1996, 1998 and references therein), the RNG-based model yields the following expressions for the five τ_κ of equation (126):

$$(\tau_{p\theta}, \tau_{pc})\tau^{-1} = a\mathrm{Pe}(1 + b\mathrm{Pe})^{-1} \ , \quad a = \frac{1}{4\pi^2} \ ,$$
$$b = 5a(1 + \sigma_t^{-1}) \ , \quad (130)$$

$$(\tau_\theta, \tau_c)\tau^{-1} = a\mathrm{Pe}(1 + a\mathrm{Pe}\ \sigma_t^{-1})^{-1} \ , \quad a = \frac{4}{7\pi^2} \ , \quad (131)$$

$$\tau_{c\theta}\tau^{-1} = a\mathrm{Pe}_\theta(1 + b\sigma_{t\theta}^{-1}\mathrm{Pe}_\theta)^{-1} \quad a = \frac{4}{7\pi^2}\left(1 + \frac{\mathrm{Pe}_\theta}{\mathrm{Pe}_c}\right)^{-1} ,$$
$$b = 15(7\pi^2)^{-1}\left(1 + \frac{\sigma_{t\theta}}{\sigma_{tc}}\right)\left(1 + \frac{\mathrm{Pe}_\theta}{\mathrm{Pe}_c}\right)^{-1} . \quad (132)$$

The final result does justify empirical models of the type shown in equation (128), with the advantage that the parameters a and b are no longer free, and in most cases they are not even constant, since they depend on the turbulent Prandtl number σ_t, which itself is a function of Pe (Canuto & Dubovikov 1996):

$$\gamma_2 \sigma_t^{-1} = 1 + \frac{2}{5}\pi^2\gamma_2 \mathrm{Pe}^{-1} \times \left\{\left[1 + \frac{5}{2\pi^2}\mathrm{Pe}(\sigma_t^{-1} + \gamma_1^{-1})\right]^{-\Gamma} - 1\right\} . \quad (133)$$

The constants are given by

$$2\gamma_1 = (\gamma^2 + 4\gamma)^{1/2} - \gamma \ , \quad \gamma_2 = \gamma_1 + \gamma \ ,$$
$$\Gamma = \gamma_1/\gamma_2 \ , \quad \gamma = 0.3 \ . \quad (134)$$

Equation (133) has the following limits:

$$\mathrm{Pe} \gg 1{:}\ \sigma_t = 0.72 \ , \quad \mathrm{Pe} \ll 1{:}\ \sigma_t \sim \mathrm{Pe}^{-1} \ . \quad (135)$$

As one can observe, in the large Pe limit we recover equation (126), but the various constants are different, as indeed is known from several studies of engineering flows. We have used only one symbol for both Pe_θ, Pe_c and $\sigma_{t\theta}$, σ_{tc}, but, clearly, in each specific case one must insert the corresponding Pe and σ_t. The Peclet numbers are defined as

$$\mathrm{Pe}_{\theta,c} = \frac{4\pi^2}{125}\frac{K^2}{\epsilon}\left(\frac{1}{\chi_\theta}, \frac{1}{\chi_c}\right). \tag{136}$$

9. K-ϵ MODEL

A widely used turbulence model is the nonlocal K-ϵ model, in which both K and ϵ are treated nonlocally while the remaining turbulence variables are treated locally. The equations for the mean variables are unchanged. Thus, we have two nonlocal equations:

Kinetic energy K:

$$\frac{DK}{Dt} + D_f = -R_{ij}U_{i,j} + g\lambda_i(\alpha J_i - \alpha_c \Phi_i) - \epsilon . \tag{137}$$

Dissipation rate ϵ:

$$\frac{D\epsilon}{Dt} + D_f = -c_s R_{ij}U_{i,j} + c_1 g\lambda_i(\alpha J_i - \alpha_c \Phi_i)\epsilon K^{-1} - c_2\epsilon^2 K^{-1} . \tag{138}$$

while the other turbulence variables are given by the following local expressions:

Convective flux $F_i^c = c_p \overline{\rho u_i'' T''} = c_p \bar{\rho} J_i$:

$$\tau_{p\theta}^{-1} J_i = R_{ij}\beta_j - J_k U_{i,k} - (\bar{\rho}T)^{-1}(2\alpha\Psi - \alpha_c T\overline{c''T''})P_{,i} . \tag{139}$$

Temperature fluctuations $\frac{1}{2}\overline{\rho T''^2} = \bar{\rho}\Psi$:

$$\Psi = \tfrac{1}{2}\tau_\theta J_i \beta_i . \tag{140}$$

Concentration variance $\frac{1}{2}\overline{\rho c''^2} = \bar{\rho}\Phi$:

$$\Phi = -\tfrac{1}{2}\tau_c \Phi_i C_{,i} . \tag{141}$$

Concentration flux $\overline{\rho c'' u_i''} = \bar{\rho}\Phi_i$:

$$\tau_{\mathrm{pc}}^{-1}\Phi_i = -R_{ij}C_{,j} - \Phi_j U_{i,j} - \bar{\rho}^{-1}(\alpha\overline{T''c''} - 2\alpha_c\Phi)P_{,i} . \tag{142}$$

Temperature-concentration correlation $\overline{T''c''}$:

$$\tau_{c\theta}^{-1}\overline{T''c''} = \beta_i\Phi_i - J_i C_{,i} . \tag{143}$$

Reynolds stresses (Appendix A):

$$b_{ij} = R_{ij} - \tfrac{2}{3}K\delta_{ij} , \tag{145a}$$

$$2\tau_{\mathrm{pv}}^{-1}b_{ij} = -\tfrac{8}{15}KS_{ij} - (1-p_1)\Sigma_{ij} - (1-p_2)Z_{ij} + \beta_5 B_{ij} . \tag{145b}$$

10. TURBULENT DIFFUSIVITIES

Solving equations (141)–(143), we obtain

$$(\delta_{ij} + \eta_{ij})\Phi_j = -d_{ik}\frac{\partial C}{\partial x_k} , \tag{146}$$

where

$$d_{ik} = \tau_{\mathrm{pc}}(R_{ik} + \alpha g \tau_{c\theta}\lambda_i J_k) , \tag{147a}$$

$$\eta_{ij} = \tau_{\mathrm{pc}}\left[U_{i,j} - g\lambda_i\left(\alpha\tau_{c\theta}\beta_j + \tau_c\alpha_c\frac{\partial C}{\partial x_j}\right)\right], \tag{147b}$$

$$\lambda_i = -(g\bar{\rho})^{-1}\frac{\partial P}{\partial x_i} . \tag{147c}$$

We recall that the pressure gradient must be computed consistently with equation (114). Equation (146) begins to acquire a familiar form, but to obtain an explicit form for Φ_i, we must apply the Hamilton-Cayley theorem. The result is

$$\Phi_i = -(K_c)_{ij}\frac{\partial C}{\partial x_j} , \tag{148}$$

where the turbulent concentration diffusivity tensor $(K_c)_{ij}$ is given by

$$(K_c)_{ij} = A(A_0\delta_{ik} + A_1\eta_{ik} + \eta_{im}\eta_{mk})d_{kj} , \tag{149}$$

with

$$A_0 = 1 + L_1 - L_2 , \quad A_1 = -1 - L_1 , \quad A = (A_0 + L_3)^{-1} , \tag{150}$$

$$L_1 = \eta_{ii} , \quad 2L_2 = -L_1^2 + \eta_{ij}\eta_{ji} ,$$
$$6L_3 = L_1^3 + 2\eta_{im}\eta_{mk}\eta_{ki} - 3L_1\eta_{ij}\eta_{ji} . \tag{151}$$

From equations (141) and (143), we then obtain the expressions for the concentration variance and $\overline{T''c''}$ correlation:

$$\Phi = \frac{1}{2}\tau_c(K_c)_{ij}\frac{\partial C}{\partial x_i}\frac{\partial C}{\partial x_j} , \tag{152}$$

$$\overline{T''c''} = -\tau_{c\theta}[J_i + \beta_k(K_c)_{ki}]\frac{\partial C}{\partial x_i} . \tag{153}$$

Analogously, inserting equations (140), (148), and (153) into equation (139), we obtain an expression for the convective flux J_i which is structurally similar to equations (146)–(147c),

$$(\delta_{ik} + \mu_{ik})J_k = c_{ik}\beta_k , \tag{154}$$

where

$$c_{ik} = \tau_{p\theta}\left[R_{ik} + \alpha_c g\tau_{c\theta}\lambda_i(K_c)_{kj}\frac{\partial C}{\partial x_j}\right], \tag{155a}$$

$$\mu_{ij} = \tau_{p\theta}\left[U_{i,j} - g\lambda_i\left(\tau_\theta\alpha\beta_j + \tau_{c\theta}\alpha_c\frac{\partial C}{\partial x_j}\right)\right]. \tag{155b}$$

Using the Hamilton-Cayley theorem, we can solve equation (154). The convective flux is given by

$$J_i = (K_h)_{ij}\beta_j . \tag{156}$$

The turbulent heat diffusivity tensor $(K_h)_{ij}$ has the following form:

$$(K_h)_{ij} = B(B_0\delta_{ik} + B_1\mu_{ik} + \mu_{im}\mu_{mk})c_{kj} , \tag{157}$$

with

$$B_0 = 1 + M_1 - M_2 , \quad B_1 = -1 - M_1 ,$$
$$B = (B_0 + M_3)^{-1} , \tag{158}$$

$$M_1 = \mu_{ii} , \quad 2M_2 = -M_1^2 + \mu_{ij}\mu_{ji} ,$$
$$6M_3 = M_1^3 + 2\mu_{im}\mu_{mk}\mu_{ki} - 3M_1\mu_{ij}\mu_{ji} . \tag{159}$$

Finally, equations (148) for Φ_i and (156) for J_i must be substituted in equation (A7) in order to obtain the tensor B_{ij}. Once that is done, the result is substituted in equation (145b) and the Reynolds stresses can then be obtained in terms of the gradients of the mean variables. The solution of equation (145b) entails a system of algebraic equations. We recall that there are only five independent components of R_{ij}, since the kinetic energy K satisfies a separate differential equation, equation (119).

The two turbulence variables, K and $\tau = 2K/\epsilon$, are solutions of equations (137) and (138).

11. TURBULENT DIFFUSIVITIES: ONE-DIMENSIONAL CASE

The one-dimensional case is particularly interesting, since it allows a completely analytical solution of the problem and is of direct interest in stellar structure computations where one considers only the radial direction r. Using equations (148) and (156), one obtains the solutions

$$\bar{\rho} J \equiv \overline{\rho w'' T''} = \bar{\rho} K_h \beta , \tag{160a}$$

$$\bar{\rho} \Phi_Z \equiv \overline{\rho w'' c''} = -\bar{\rho} K_c \frac{\partial C}{\partial z} , \tag{160b}$$

where the turbulent diffusivities $K_{h,c}$ are given by

$$K_h = \nu_T A_h , \quad K_c = \nu_T A_c , \tag{161}$$

and the turbulent viscosity is given by

$$\nu_T \equiv \tau \overline{w}^2 , \tag{162a}$$

$$A_h = \pi_4(1 + \eta x + \pi_1 \pi_2 x R_\mu) D^{-1} , \tag{162b}$$

$$A_c = \pi_1(1 + \mu x - \pi_2 \pi_4 x) D^{-1} , \tag{162c}$$

$$D = (1 + \eta x)(1 + \mu x) + \pi_1 \pi_2^2 \pi_4 x^2 R_\mu , \tag{162d}$$

$$\eta = \pi_1(\pi_2 - \pi_3 R_\mu) , \quad \mu = \pi_4(\pi_5 - \pi_2 R_\mu) , \tag{162e}$$

where we have introduced the following dimensionless functions:

$$x = \tau^2 N_h^2 , \tag{163a}$$

$$\pi_{1,2,3,4,5} = (\tau_{\rm pc}, \tau_{c\theta}, \tau_c, \tau_{p\theta}, \tau_\theta)\tau^{-1} . \tag{163b}$$

We have also introduced the timescales of the T and C fields:

$$N_h^2 = -g\alpha_T \beta = -gH_p^{-1}(\nabla - \nabla_{\rm ad}) , \tag{164a}$$

$$N_c^2 = g\alpha_c \frac{\partial C}{\partial z} = -gH_p^{-1} \nabla_\mu , \tag{164b}$$

$$\alpha_c \frac{\partial C}{\partial z} = -H_p^{-1} \nabla_\mu , \quad \nabla_\mu \equiv \frac{\partial \ln \mu}{\partial \ln P} . \tag{164c}$$

In oceanography, one also defines the Turner number R_ρ as (Kelley 1984)

$$R_\rho = \frac{g\alpha_c \partial C/\partial z}{g\alpha_T \partial T/\partial z} , \tag{165}$$

which weighs the relative importance of the two gradients. In the stellar case, the equivalent of R_ρ is the ratio

$$R_\mu = -\frac{g\alpha_c \partial C/\partial z}{g\alpha_T \beta} = \frac{N_c^2}{N_h^2} = \frac{\nabla_\mu}{\nabla - \nabla_{\rm ad}} . \tag{166}$$

Equation (161) is still not the final solution, since it depends on two unknown variables, ν_T and x, which we must express in terms of calculable variables like R_μ. To compute ν_T, we need an expression for w^2. For that, we use the equation for the Reynolds stresses, equations (145b), (A7)–(A9), and (165). We obtain

$$\nu_T = \tfrac{1}{3} \epsilon \tau^2 [1 + \tfrac{2}{15} (A_h - A_c R_\mu) x]^{-1} . \tag{167}$$

Next, we need an equation for x. We shall take the local limit of the kinetic energy equation, equation (39), which reads

$$\epsilon = g\alpha_T J - g\alpha_c \Phi_3 = \nu_T N_h^2 (A_c R_\mu - A_h) . \tag{168}$$

Substituting equation (168) into (167), we obtain the equation for x:

$$x(A_c R_\mu - A_h) = \tfrac{15}{7} , \tag{169}$$

which changes equation (167) to

$$\nu_T = \frac{7}{15} \epsilon \tau^2 = \frac{28}{15} \frac{K^2}{\epsilon} . \tag{170}$$

Thus, ν_T is expressed in terms of K and ϵ. Finally, using the expressions for $A_{h,c}$, equations (162b) and (162c), equation (169) becomes

$$A(x) x^2 + B(x) x - \tfrac{15}{7} = 0 , \tag{171}$$

where $A(x)$ and $B(x)$, which can depend on x (see below), are given by

$$A = \pi_1(\mu - \pi_2 \pi_4) R_\mu - \pi_4(\eta + \pi_1 \pi_2 R_\mu) - \tfrac{15}{7}(\eta\mu + \pi_1 \pi_2^2 \pi_4 R_\mu) , \tag{172a}$$

$$B = \pi_1 R_\mu - \pi_4 - \tfrac{15}{7}(\eta + \mu) . \tag{172b}$$

Thus, x is expressed entirely as a function of R_μ. Finally, we have

$$K_h = \frac{28}{15} \frac{K^2}{\epsilon} A_h , \quad K_c = \frac{28}{15} \frac{K^2}{\epsilon} A_c , \tag{173}$$

where we still have to determine K and ϵ, which in principle are solutions of the two dynamic equations (137) and (138). Equation (137) has already been used in the local form, that is, equation (168). The equation for ϵ, equation (138), has not yet been used, and it can be taken to be local or not. Below, we give the solution corresponding to the case where equation (138) is taken to be local, which means

$$\epsilon = \frac{K^{3/2}}{\Lambda} , \tag{174}$$

where Λ is a mixing length; the specification of Λ is the price that one has to pay for not solving equation (138). From the definition of x, equation (163a), and the definition $\tau = 2K\epsilon^{-1}$, we obtain, using equation (174),

$$K = 4\Lambda^2 N_h^2 x^{-1} , \tag{175}$$

and thus the final expressions for the diffusivities $K_{h,c}$ follow from equations (173) and (174).

$$K_h = \frac{56}{15} \Lambda^2 \left(\frac{N_h^2}{x}\right)^{1/2} A_h , \quad K_c = \frac{56}{15} \Lambda^2 \left(\frac{N_h^2}{x}\right)^{1/2} A_c . \tag{176}$$

Thus, the problem is completely solved analytically. In fact, both diffusivities are now expressed in terms of the gradients β and ∇_μ. Clearly, for $N_h^2 < 0$ (corresponding to unstable stratification), x must be taken as the negative solution of equation (171), since K is positive (eq. [175]). Numerical solutions are presented in § 18.

12. SEMICONVECTION AND SALT FINGERS: GENERALITIES

Using the previous formalism, one can study semiconvection and salt fingers, since they can be viewed as diffusion processes. For example, when there is a nonzero gradient of the mean molecular weight μ, it is because of the presence of species whose main concentrations have gradients opposite to that of the mean temperature and whose kinematic diffusivities are also different from the radiative one. On Earth, the most common example is that of salt and temperature in the ocean, a phenomenon that is referred to as thermohaline and/or thermosolutal convection. When both T and the mean salinity S increase from the ocean surface toward the bottom, the result is cold fresh water over warm salty water. The S field is stable, the T field is unstable (heavy at the top), and one refers to the phenomenon as *diffusive convection* (Turner & Stommel 1964; Turner 1973; Marmorino & Caldwell 1976; Turner 1985; Kelley 1984, 1990; Schmitt 1994). Examples are several lakes, water underneath an ice island, and the Red Sea.

In astrophysics, diffusive convection is called *semiconvection*, and it has been studied by several authors (Stothers 1970; Spiegel 1972; Stothers & Chin 1975, 1976; Stevenson 1979; Langer et al. 1983, 1985, 1989; Spruit 1992; Grossman & Taam 1996; Umezu 1998). Yet there does not seem to be a generally agreed upon procedure to treat the phenomenon. Stothers (1970) critically analyzed 11 different prescriptions and concluded that only two were physically acceptable: one used by Schwarszchild & Härm (1958), who adopted the K Schwarzschild criterion, and the other by Sakashita & Hayashi (1959), who adopted the Ledoux criterion (Ledoux 1947). In the absence of a turbulence model, Langer et al. (1983, 1985, 1989), suggested a phenomenological model that we shall discuss below. Merryfield (1995) found that none of his two-dimensional numerical simulations exhibited any close resemblance to the models by Stevenson and/or the Spruit models and that the closest similarity is with a Langer et al. model. Xiong (1985a, 1985b, 1986) and Grossman & Taam (1996) have carried out a nonlinear study of semiconvection. However, no study has included the effect of a mean flow (differential rotation) on semiconvection.

Semiconvection is characterized by the following conditions:

$$\nabla - \nabla_{\rm ad} > 0\ , \quad \nabla_\mu > 0\ , \quad \nabla_r > \nabla\ , \tag{177}$$

and thus

$$\nabla_r > \nabla > \nabla_{\rm ad}\ . \tag{178}$$

When both the T and S fields increase from the bottom to the top of the ocean, the result is warm salty water over cold fresh water. Since the T field is stable while the S field is unstable (heavy at the top), the latter causes an instability called *salt fingers*. An example is the Atlantic Ocean underneath the Mediterranean outflow of very salty water. In astrophysics, this instability occurs when a layer with a higher μ lies above a region of lower μ—for example, when the He flash does not occur at the center of a star. Salt fingers were first suggested by Stothers & Simon (1969) and later studied by Ulrich (1972) and by Kippenhahn et al. (1980). The μ field causes the instability, while $\nabla - \nabla_{\rm ad}$ plays the role of a stabilizing gradient. The salt fingers phenomenon is characterized by the following conditions:

$$\nabla_{\rm ad} - \nabla > 0\ , \quad \nabla_\mu < 0\ , \quad \nabla > \nabla_r\ , \tag{179}$$

and thus

$$\nabla_{\rm ad} > \nabla > \nabla_r\ . \tag{180}$$

For both semiconvection and salt fingers, the stability parameter

$$R_\mu = \frac{\nabla_\mu}{\nabla - \nabla_{\rm ad}} > 0 \tag{181}$$

is positive. Finally, in the case of binary stars, the accreted material has a higher μ but a lower T than the material underneath, (Proffitt 1989).

13. STABILITY CRITERIA

We begin by recalling that dynamical stability is governed by the Brunt-Väisälä frequency N (Kippenhahn & Weigert 1991):

$$\frac{d^2\delta z}{dt^2} = -N^2\delta z\ , \tag{182}$$

where

$$N^2 = -\frac{g}{\rho}\frac{\partial \rho}{\partial z} = N_h^2 - N_c^2 = gH_p^{-1}[\nabla_\mu - (\nabla - \nabla_{\rm ad})]\ . \tag{183}$$

A system is stable or unstable depending on whether $N^2 > 0$ or $N^2 < 0$:

$$\text{Ledoux stable:}\quad \nabla_\mu > \nabla - \nabla_{\rm ad}\ , \tag{184a}$$

$$\text{Ledoux unstable:}\quad \nabla - \nabla_{\rm ad} > \nabla_\mu\ . \tag{184b}$$

Since equations (184a) and (184b) apply to both semiconvection and salt fingers, we have

Semiconvection:

$$\begin{aligned}
&\nabla - \nabla_{\rm ad} > 0\ , \quad \nabla_\mu > 0\ , \quad N_h^2 < 0\ , \quad N_c^2 < 0\ , \quad R_\mu > 0\ ,\\
&\text{Ledoux stable:}\quad N^2 > 0\ , \quad \nabla_\mu > \nabla - \nabla_{\rm ad}\ , \quad R_\mu > 1\ ,\\
&\text{Ledoux unstable:}\quad N^2 < 0\ , \quad \nabla - \nabla_{\rm ad} > \nabla_\mu\ , \quad R_\mu < 1\ .
\end{aligned} \tag{185}$$

Salt fingers:

$$\begin{aligned}
&\nabla_{\rm ad} - \nabla > 0\ , \quad \nabla_\mu < 0\ , \quad N_h^2 > 0\ , \quad N_c^2 > 0\ , \quad R_\mu > 0\ ,\\
&\text{Ledoux stable:}\quad N^2 > 0\ , \quad \nabla_{\rm ad} - \nabla > |\nabla_\mu|\ , \quad R_\mu < 1\ ,\\
&\text{Ledoux unstable:}\quad N^2 < 0\ , \quad |\nabla_\mu| > \nabla_{\rm ad} - \nabla\ , \quad R_\mu > 1\ .
\end{aligned} \tag{186}$$

As these relations show, nothing has yet been said about turbulence, which has not been used in any of the previous expressions that only establish the criteria for dynamical stability/instability. The uncomfortable uncertainty still surrounding the Ledoux versus the Schwarzschild criteria is due to the lack of separation of the above relations that do not involve turbulence and the ones that follow that do involve turbulence.

We begin by using equations (13a) and (84) to rewrite equation (137) as

$$\frac{DK}{Dt} + D_f(K) = K_m N_u^2 - g\bar{\rho}^{-1}\overline{\rho' w''} - \epsilon\ , \tag{187}$$

where

$$F_\rho \equiv \overline{\rho' w''} \tag{188}$$

is the "mass flux," and the time scale N_u is related to the presence of shear, which we have included for the sake of generality. In analogy with equations (164b) and (164c), we have defined

$$N_u^2 \equiv 2S_{ij}S_{ij} , \tag{189}$$

where S_{ij} is the mean shear, equation (14a). In analogy with $K_{h,c}$, the "momentum diffusivity" is represented by K_m. Quantifying the strength of shear by the dimensionless parameter Ω (Hamilton, Lewis, & Ruddick 1989),

$$\Omega = K_m N_u^2 \epsilon^{-1} - 1 , \tag{190}$$

we have, in the stationary and local case,

$$\overline{\rho' w''} = \bar{\rho} g^{-1} \Omega \epsilon . \tag{191}$$

If we further write the mass flux is

$$\overline{\rho' w''} = -K_\rho \frac{\partial \rho}{\partial z} , \tag{192}$$

use of equation (183) gives the following expression for the "mass diffusivity" K_ρ:

$$K_\rho = \Omega \frac{\epsilon}{N^2} . \tag{193}$$

An alternative expression for K_ρ follows from equations (84), (160a) and (160b), and (164b) and (164c), which yield

$$\frac{g}{\rho} \overline{\rho' w''} = K_h N_h^2 - K_c N_c^2 . \tag{194}$$

Using equations (192) and (183), we obtain the expression for K_ρ in terms of K_h and K_c:

$$K_\rho = N^{-2}(K_h N_h^2 - K_c N_c^2) . \tag{195}$$

Finally, use of equation (166) gives the final expression for K_ρ:

$$K_\rho = (K_h - K_c R_\mu)(1 - R_\mu)^{-1} . \tag{196}$$

Clearly, if one assumes $K_h = K_c$, it follows that

$$K_\rho = K_c = K_h . \tag{197}$$

We shall distinguish two cases.

13.1. *No Shear*: $\Omega = -1$

In this case, equation (191) shows that we have a downward mass flux

$$\overline{\rho' w''} < 0 . \tag{198}$$

13.1.1. *Semiconvection, Stable Case*: $N^2 > 0, R_\mu > 1$

Equations (193) and (196) imply that

$$K_\rho < 0 , \tag{199}$$

$$\frac{K_h}{K_c} > R_\mu \equiv \frac{\nabla_\mu}{\nabla - \nabla_{\rm ad}} > 1 , \tag{200}$$

The last two conditions in equation (200) can be written as a unique relation:

$$\frac{K_h}{K_c} (\nabla - \nabla_{\rm ad}) > \nabla_\mu > \nabla - \nabla_{\rm ad} . \tag{201}$$

A region that is Ledoux stable (last inequality) but Schwarzschild unstable, $\nabla - \nabla_{\rm ad} > 0$, is known as "vibrationally unstable" (Kippenhahn & Weigert 1991, eq. [6.20]). The *requirement of dynamical stability sets the lower limit for* ∇_μ, *while the requirement of turbulent mixing sets the upper limit of* ∇_μ. This is a natural result, since transgressing the upper limit would mean that ∇_μ, which acts like sink, is too strong for turbulent mixing to survive. The Schwarzschild instability criterion corresponds to taking, in the first inequality in equation (201), the turbulent μ number as

$$\sigma_\mu = \frac{K_h}{K_c} \to \infty , \tag{202}$$

which is not consistent with model results (Fig. 6) or with available data. Finally, we notice that equation (201) implies that

$$K_h > K_c , \tag{203}$$

which, as we show below, is predicted by the full model and in agreement with the data.

13.1.2. *Semiconvection, Unstable Case*: $N^2 < 0, R_\mu < 1$

Equations (193) and (196) imply that

$$K_\rho > 0 , \tag{204a}$$

$$\nabla - \nabla_{\rm ad} > \frac{K_c}{K_h} \nabla_\mu , \tag{204b}$$

$$\nabla - \nabla_{\rm ad} > \nabla_\mu , \tag{204c}$$

where the second inequality expresses Ledoux instability. Once again, if one adopts equation (202), equation (204b) becomes the Schwarzschild instability criterion, which is different from equation (204c). This may have been the source of the problem in the choice of the two criteria.

13.1.3. *Salt Fingers, Stable Case*: $N^2 > 0, R_\mu < 1$

Equations (193) and (196) imply that

$$K_\rho < 0 , \tag{205a}$$

$$|\nabla_\mu| > \frac{K_h}{K_c} (\nabla_{\rm ad} - \nabla) , \tag{205b}$$

$$\nabla_{\rm ad} - \nabla > |\nabla_\mu| . \tag{205c}$$

In this case we have

$$K_c > K_h . \tag{206}$$

13.1.4. *Salt Fingers, Unstable Case*: $N^2 < 0, R_\mu > 1$

Equations (193) and (196) imply that

$$K_\rho > 0 , \tag{207a}$$

$$|\nabla_\mu| > \frac{K_h}{K_c} (\nabla_{\rm ad} - \nabla) , \tag{207b}$$

$$|\nabla_\mu| > \nabla_{\rm ad} - \nabla . \tag{207c}$$

13.2. *Nonzero Shear*, $\Omega > 0$

An analogous set of conditions can be worked in this case. We only recall that equation (191) shows that we have an upward mass flux

$$\overline{\rho' w''} > 0 . \tag{208}$$

14. THE CASE OF A PASSIVE SCALAR

Mixing (diffusion) in stellar interiors has been studied for many years (Pinsonneault 1997), but the nonlinear, turbulent nature of the problem makes it very difficult to study. In the absence of turbulence, diffusion was studied by Aller & Chapman (1960), Michaud (1970), Vauclair & Vauclair (1982), and Bahcall & Pinsonneault (1992). Schatzman (1969), (1996) and Schatzman & Baglin (1991) attempted to include turbulence via an enhanced diffusion coefficient. The effect of a mean shear was not included. Zahn (1974), Chaboyer & Zahn (1992), and Maeder (1997) used phenomenological expressions for shear-induced mixing, which are discussed in Canuto (1998).

A nonzero α_c in equation (84) implies that the c field affects the overall density field. On the other hand, a passive scalar does not change the density field; rather, it is carried along by the preexisting turbulence, to which it does not contribute. The case of a passive scalar is thus recovered by taking $\alpha_c = 0$. As one can, however, observe from equations (47) and (48), even with $\alpha_c = 0$, the c field is turbulent.

15. THE PRINCIPLE OF WEAKENING OF THE SINK

To characterize the relative strength of two opposing gradients, one acting like a source, the other like a sink, it is useful to introduce a stability parameter. The most frequent case is that of shear (source) in the presence of stable stratification ($\partial T/\partial z > 0$) acting as a sink of turbulence. The stability parameter is the Richardson number,

$$\mathrm{Ri} = \frac{g\alpha\, \partial T/\partial z}{(\partial U/\partial z)^2} , \tag{209}$$

where U is the mean flow. Turbulence can be sustained only for values of Ri less than a critical value $\mathrm{Ri}^{\mathrm{cr}}$

$$\mathrm{Ri} < \mathrm{Ri}^{\mathrm{cr}} , \tag{210}$$

above which it dies out (Canuto 1998). In stars there is the additional consideration that the sink may be weakened by nonturbulent processes such as radiative losses, which tend to erode the temperature gradient. Since such losses can be characterized by a Peclet number ($\mathrm{Pe}_\theta = wl\chi_\theta^{-1}$), we expect equation (210) actually to be of the form

$$\mathrm{Pe}_\theta(1 + \mathrm{Pe}_\theta)^{-1}\mathrm{Ri} < \mathrm{Ri}^{\mathrm{cr}} , \tag{211}$$

which implies that when radiative losses are important ($\mathrm{Pe}_\theta < 1$), the effective Ri is actually $\mathrm{Pe}_\theta\,\mathrm{Ri}$, which, by virtue of being smaller than Ri, more easily satisfies equation (210), thus allowing a wider margin of turbulence (Canuto 1998).

In the case of semiconvection, ∇_μ is stabilizing while $\nabla - \nabla_{\mathrm{ad}}$ is destabilizing, and the analog of equation (210) is then taken to be

$$R_\mu < R_\mu^{\mathrm{cr}} , \tag{212}$$

or, more explicitly,

$$R_\mu^{\mathrm{cr}}(\nabla - \nabla_{\mathrm{ad}}) > \nabla_\mu . \tag{213}$$

The Ledoux instability criterion assumes that

$$R_\mu^{\mathrm{cr}} = 1 , \tag{214}$$

which, as we shall discuss below, is an over restrictive assumption not supported by the available data, which instead suggest $R_\mu^{\mathrm{cr}} > 1$. In further analogy with equation (211), we expect that when the kinematic diffusivity of the c field becomes large, there will be a weakening of the sink ∇_μ and thus a relation of the type (Pe_c is the Peclet number of the c field)

$$\mathrm{Pe}_c(1 + \mathrm{Pe}_c)^{-1}R_\mu < R_\mu^{\mathrm{cr}} , \tag{215}$$

or, for small Pe_c

$$R_\mu^{\mathrm{cr}}(\nabla - \nabla_{\mathrm{ad}}) > \mathrm{Pe}_c\,\nabla_\mu . \tag{216}$$

A $\mathrm{Pe}_c < 1$ thus facilitates the possibility of $\nabla - \nabla_{\mathrm{ad}}$ being able to overcome the μ barrier. Whether the kinematic diffusivity χ_c is sufficiently large to give rise to small Pe_c depends clearly on the problem at hand.

In the case of salt fingers, the source of instability is the μ gradient, while the T gradient acts like a sink. We can still use equation (212), since it is a positive quantity in this case also. In analogy with the above discussion,

$$R_\mu^{\mathrm{cr}}\,\nabla_\mu > \mathrm{Pe}_\theta(\nabla_{\mathrm{ad}} - \nabla) , \tag{217}$$

which shows again that radiative losses favor the changes that ∇_μ will overcome the sink $\nabla_{\mathrm{ad}} - \nabla$.

These results are physically intuitive, and it will be shown below that the model of turbulence developed here satisfies the above results.

16. QUALITATIVE RESULTS

Before presenting the numerical solutions of the model, we present some qualitative results. Using the definitions of $K_{h,c}$, equations (176) and (169), we derive the relations

$$\frac{K_h}{K_c} = R_\mu - \frac{15}{7}\frac{1}{xA_c} . \tag{218}$$

In semiconvection, equations (164b) and (163a) give $x < 0$, and since in the stable case $R_\mu > 1$, we conclude that (see eq. (203))

$$K_h > K_c , \tag{219}$$

which is in accordance with the measurements (Kelley 1984). In salt fingers, we use the equivalent expression

$$\frac{K_c}{K_h} = R_\mu^{-1}\left(1 + \frac{15}{7}\frac{1}{xA_h}\right) . \tag{220}$$

Since $x > 0$ and $R_\mu < 1$, it follows that (see eq. [206])

$$K_c > K_h , \tag{221}$$

which is in agreement with the measurements (Hamilton et al. 1989, Fig. 2). Furthermore, in semiconvection, the flux ratio

$$R_F = \frac{\alpha_c \Phi_3}{\alpha_T J} = R_\mu\left(R_\mu - \frac{15}{7}\,x^{-1}A_c^{-1}\right)^{-1} \tag{222}$$

is predicted to be ($x < 0$)

$$R_F < 1 , \tag{223}$$

also in agreement with the data (Kelley 1990, Fig. 2). Similarly, in salt fingers we derive that the flux ratio,

$$R_F = \frac{\alpha_T J}{\alpha_c \Phi_3} = \frac{K_h}{K_c}\,R_\mu^{-1} = \left(1 + \frac{15}{7}\,x^{-1}A_h^{-1}\right)^{-1} , \tag{224}$$

is predicted to be ($x > 0$)

$$R_F < 1 , \tag{225}$$

in accord with the measurements (Turner 1967, Fig. 4; Schmitt 1979, Fig. 4; McDougall & Taylor 1984, Fig. 4; Taylor & Buchens 1989, Fig. 6; Ozgokmen, Esenkov, & Olson 1998, Fig. 13). Since R_F is the ratio of the potential energy gained by the T field to the energy lost by the C field, it must be less than unity, otherwise the system would be gaining energy.

17. THE $\nabla_\mu \to 0$ LIMIT

We now show that the expression for K_h for the case of semiconvection in the limit $\nabla_\mu \to 0$ reduces to the standard expression for the convective flux (Canuto & Mazzitelli 1991). Equation (169) becomes $|x|\,A_h(x) = \mathrm{constant}$, so that equation (176) yields

$$K_h \sim (\nabla - \nabla_{\rm ad})^{1/2} A_h^{3/2} \sim (\nabla - \nabla_{\rm ad})^{1/2} \pi_4^{3/2} . \quad (226)$$

In the Pe > 0 limit, $\pi_4 \sim$ constant and thus $K_h \sim (\nabla - \nabla_{\rm ad})^{1/2}$, which coincides with the standard model. In the opposite limit, Pe < 1, $\pi_4 \sim$ Pe, and we have instead

$$K_h \sim (\nabla - \nabla_{\rm ad})^{1/2} {\rm Pe}^{3/2} , \quad (227)$$

which also coincides with previous results (Canuto 1996, eqs. [32e]–[32g]). Furthermore, since

$$\begin{aligned} {\rm Pe} &\sim K^2 \epsilon^{-1} \sim (\nabla - \nabla_{\rm ad})^{1/2} |x|^{-1/2} \sim (\nabla - \nabla_{\rm ad})^{1/2} \\ &\times A_h^{1/2} \sim (\nabla - \nabla_{\rm ad})^{1/2} \pi_4^{1/2} \sim (\nabla - \nabla_{\rm ad})^{1/2} {\rm Pe}^{1/2} , \quad (228) \end{aligned}$$

we have Pe $\sim (\nabla - \nabla_{\rm ad})$. The final form of K_h is then

$$K_h \sim (\nabla - \nabla_{\rm ad})^2 , \quad (229)$$

in agreement with the standard result for inefficient convection.

18. SEMICONVECTION: $\nabla - \nabla_{\rm ad}$ VERSUS ∇_μ RELATION

The final expressions for the diffusivities are given by equations (176), (171), and (162a)–(162e). The functions A and B in equation (171) may or may not depend on x itself. This comes about because the dimensionless functions π (eq. (163b)), given in Appendix B, depend on Pe, which is defined by equation (B7):

$${\rm Pe}_{\theta, c} = \frac{4\pi^2}{125} \frac{K^2}{\epsilon} \left(\frac{1}{\chi_\theta}, \frac{1}{\chi_c}\right) , \quad (230)$$

where χ and χ_c are the molecular diffusivities of the T and C fields, respectively. For the results presented below, we only consider the case of large ${\rm Pe}_c$ and thus we retain only ${\rm Pe}_\theta$ for the T field, which we shall call Pe for simplicity. Using equation (175), we derive

$${\rm Pe} = \Gamma U (-x)^{-1/2} , \quad x < 0 , \quad (231)$$

where the dimensionless function U and the dimensionless constant Γ's are defined by

$$U = \left(\frac{\nabla - \nabla_{\rm ad}}{\nabla_r - \nabla_{\rm ad}}\right)^{1/2} ,$$

$$\Gamma \equiv \frac{8\pi^2}{125} [g \Lambda^4 H_p^{-1} (\nabla_r - \nabla_{\rm ad}) \chi^{-2}]^{1/2} . \quad (232)$$

We note that

$$0 \le U \le 1 . \quad (233)$$

Here Γ represents the "efficiency of convection": the more efficient the heat transport by convection, the smaller the role of the radiative losses represented by χ and thus the larger the Γ. Thus, Pe depends on x, and if the π's depend on Pe, they also depend on x. In the case of large convective efficiencies, Pe ≫ 1, the π's are constant.

Next, consider the temperature equation. In the stationary limit, and in the absence of a mean flow, equation (115) becomes

$$\nabla + H_p (T K_r)^{-1} F_c = \nabla_r^* , \quad (234)$$

where $F^r = K_r H_p^{-1} T \nabla$, and where we have neglected the kinematic term $f(\chi_c)$. The modified radiative gradient ∇_r^* includes the flux of turbulent kinetic energy

$$\nabla_r^* = \nabla_r - H_p (T K_r)^{-1} F^{\rm ke} , \quad (235)$$

where $K_r = c_p \rho \chi$. For the convective flux, $F_c = c_p \overline{\rho w'' T''} \equiv c_p \bar{\rho} J$, we have from equation (160a)

$$J = K_h \beta . \quad (236)$$

Equation (234) becomes

$$U^2 (1 + K_h \chi^{-1}) = 1 + (\nabla_r^* - \nabla_r)(\nabla_r - \nabla_{\rm ad})^{-1} , \quad (237)$$

where $K_h \chi^{-1}$ represents the ratio of turbulent to radiative heat diffusivity χ. Using equation (176), we have

$$\frac{K_h}{\chi} = \frac{175}{3\pi^2} \Gamma (-x)^{-1/2} A_h(x) U . \quad (238)$$

Equation (234) then becomes the equation for the variable U:

$$U^3 + p(U^2 - 1) = q , \quad (239)$$

where

$$q \equiv p (\nabla_r^* - \nabla_r)(\nabla_r - \nabla_{\rm ad})^{-1} , \quad (240a)$$

$$p^{-1} = \frac{175}{3\pi^2} \Gamma (-x)^{-1/2} A_h(x) . \quad (240b)$$

Since R_μ depends on U, we must write

$$R_\mu = r_\mu U^{-2} , \quad r_\mu = \frac{\nabla_\mu}{\nabla_r - \nabla_{\rm ad}} , \quad (241)$$

so that the variables r_μ and Γ can be considered given. In terms of the variable U, the turbulent diffusivities are given by

$$\frac{K_h}{\chi} = \left(1 + \frac{q}{p}\right) U^{-2} - 1 , \quad K_c = K_h \sigma_\mu^{-1} , \quad (242)$$

where σ_μ is the turbulent Prandtl μ number

$$\sigma_\mu = \frac{K_h}{K_c} = \frac{A_h}{A_c} . \quad (243)$$

The turbulent kinetic energy K is given by equation (175) as

$$K = \left(\frac{125}{4\pi^2}\right)^2 {\rm Pe}^2 \left(\frac{\chi}{\Lambda}\right)^2 , \quad (244)$$

while the rms vertical velocity is given by

$$(\overline{w^2})^{1/2} = \left(\frac{14}{15}\right)^{1/2} \left(\frac{125}{4\pi^2}\right) {\rm Pe} \left(\frac{\chi}{\Lambda}\right) . \quad (245)$$

The turbulent pressure $p_t = \rho \overline{w^2}$ is then easily evaluated.

In conclusion, in semiconvection, the $\nabla - \nabla_{\rm ad}$ versus ∇_μ relation is obtained by solving equation (239). The function x is a solution of equations (171)–(172b), in which R_μ must be taken as in equation (241) and depends on U itself. The functions π are defined in equation (163b) and are given in Appendix B as a function of the Peclet number, which in turn is a function of both x and U via equation (231). The result is

$$\nabla - \nabla_{\rm ad} \text{ versus } r_\mu \text{ for different } \Gamma . \quad (246)$$

We have solved the above equations for $q = 0$ and different values of the parameter Γ. In Figure 1 we show the Peclet number versus r_μ for different values of the convective efficiency Γ. In Figure 2 we present the turbulent kinetic energy K (in units of $\chi^2 \Lambda^{-2}$) versus r_μ, and in Figure 3 we show the ratio K_h/χ versus r_μ. In Figure 4 we exhibit K_h/χ versus Γ for different r_μ. As expected on physical grounds, the $r_\mu = 0$ case in Figure 4 corresponds to the standard convection model (e.g., Canuto & Mazzitelli 1991). The

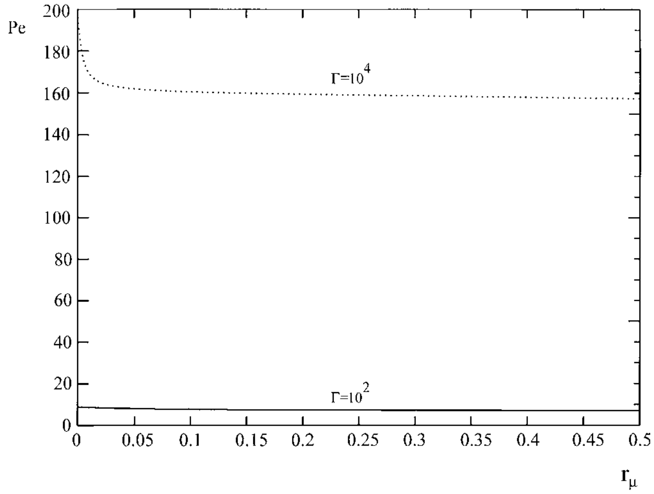

FIG. 1.—Semiconvection. Peclet number vs. r_μ, for two values of the convective efficiency parameter Γ (eq. [232]).

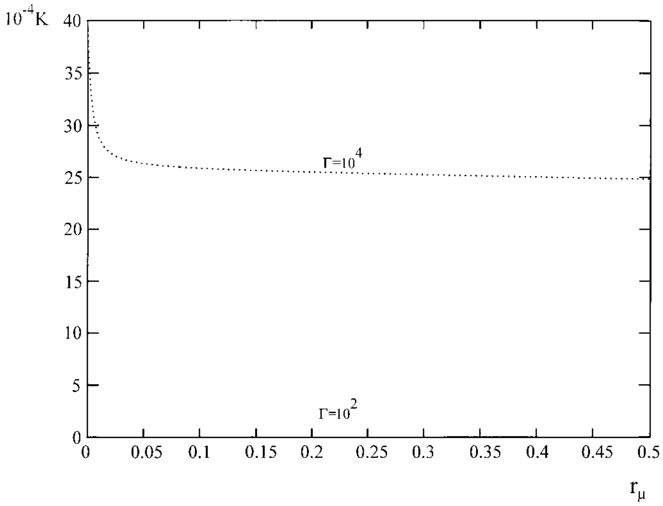

FIG. 2.—Semiconvection. Turbulent kinetic energy K in units of $\chi^2\Lambda^{-2}$ vs. r_μ (eq. [244]).

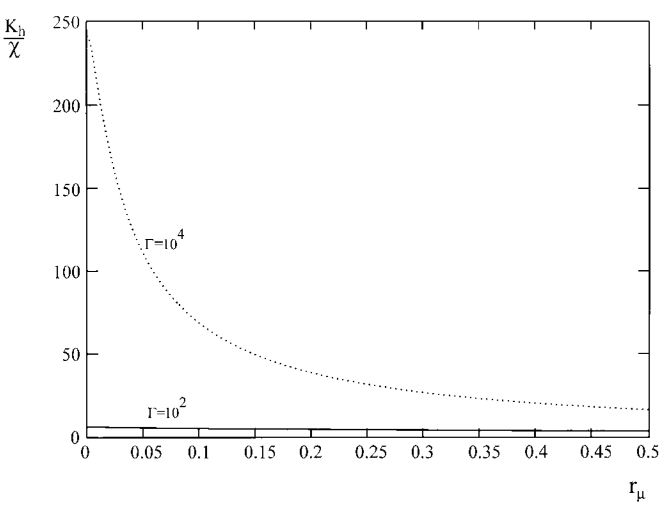

FIG. 3.—Semiconvection. Turbulent heat diffusivity K_h/χ (eq. [242]) versus r_μ for the $q = 0$ case.

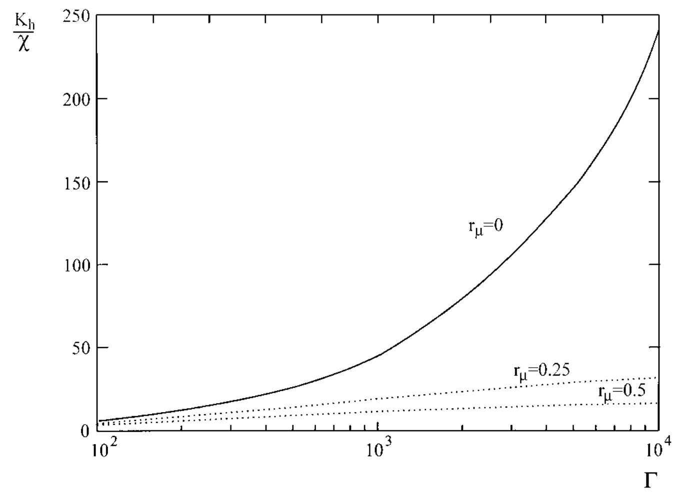

FIG. 4.—Semiconvection. The ratio K_h/χ vs. Γ for different values of r_μ. The $r_\mu = 0$ case corresponds to the standard local model of convection.

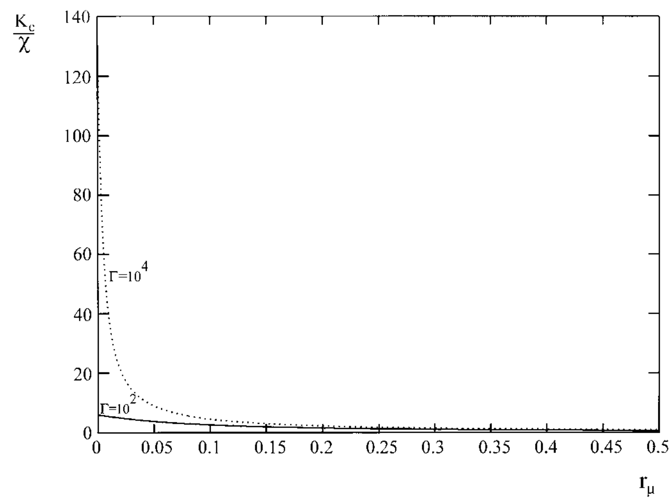

FIG. 5.—Semiconvection. Turbulent concentration diffusivity K_c/χ vs. r_μ (eq. [242]).

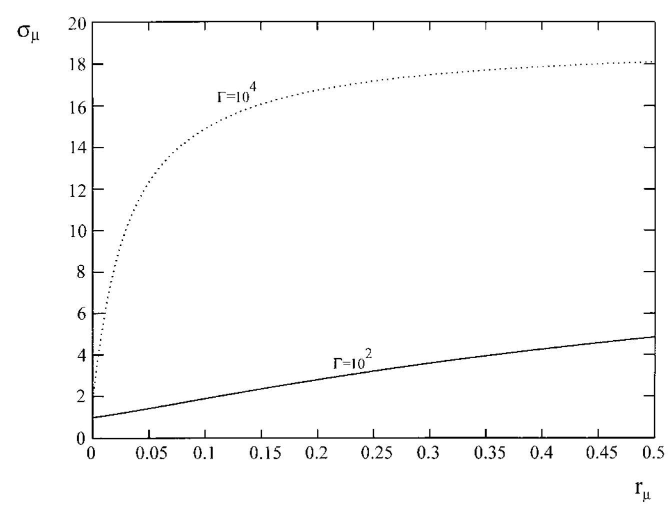

FIG. 6.—Semiconvection. The ratio K_h/K_c vs. r_μ (eq. [243]). The behavior is in agreement with the data by Kelley (1984).

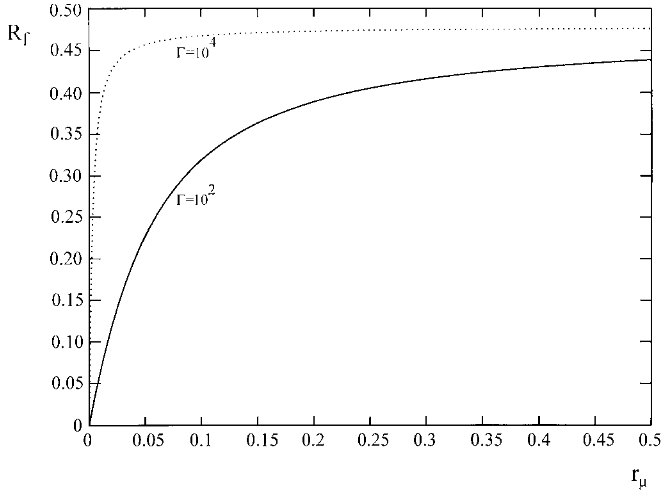

FIG. 7.—Semiconvection. The flux ratio in eq. (222) vs. r_μ. The behavior agrees with the data by Kelley (1990).

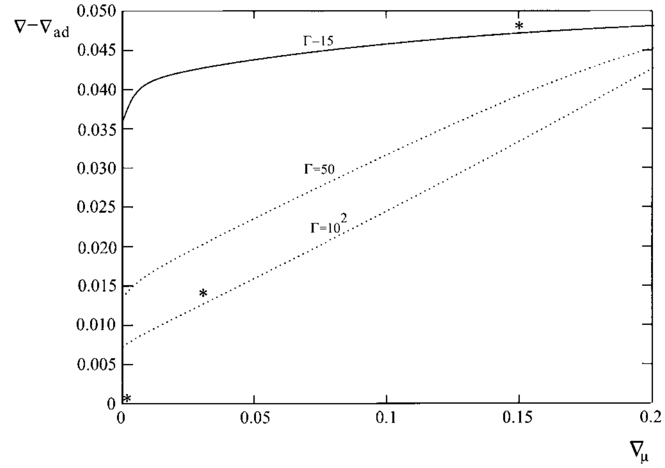

FIG. 9.—Semiconvection. The function $\nabla - \nabla_{ad}$ vs. ∇_μ for $\nabla_r - \nabla_{ad} = 0.05$. The asterisks correspond to the values computed by Grossman & Taam (1996).

larger the r_μ, that is, the larger the μ barrier, the lower the heat diffusivity. The turbulent diffusivity of the c field K_c/χ is shown versus r_μ in Figure 5, while the ratio σ_μ given in equation (243) is shown in Figure 6; σ_μ is near unity only for values of ∇_μ close to zero, while for large r_μ the ratio reaches an asymptotic value, in agreement with the data (Kelley 1984, Fig. 2). In Figure 7 we show the flux ratio in equation (222); the behavior agrees with the measurements (Kelley 1990, Fig. 2).

The variable of most direct astrophysical interest is $\nabla - \nabla_{ad}$ versus ∇_μ. In Figure 8 we present $(\nabla - \nabla_{ad})(\nabla_r - \nabla_{ad})^{-1}$ versus r_μ for different Γ. The whole region is Schwarzschild unstable. The Ledoux-unstable region is to the left of the dashed line, while the Ledoux-stable region is to the right of it. This latter region is often referred to as "vibrationally unstable" (Kippenhahn & Weigert 1991, chap. 6, eq. [6.20]), and several authors (e.g., Maeder & Conti 1994) refer only to it as semiconvection. For large Γ, the curves lie mostly outside the Ledoux-unstable region, while the smaller Γ is, the larger the portion of the Ledoux-unstable region. In Figure 9, we plot $\nabla - \nabla_{ad}$ versus ∇_μ for $\nabla_r - \nabla_{ad} = 0.05$ (Grossmann & Taam 1996). The asterisks correspond to their values.

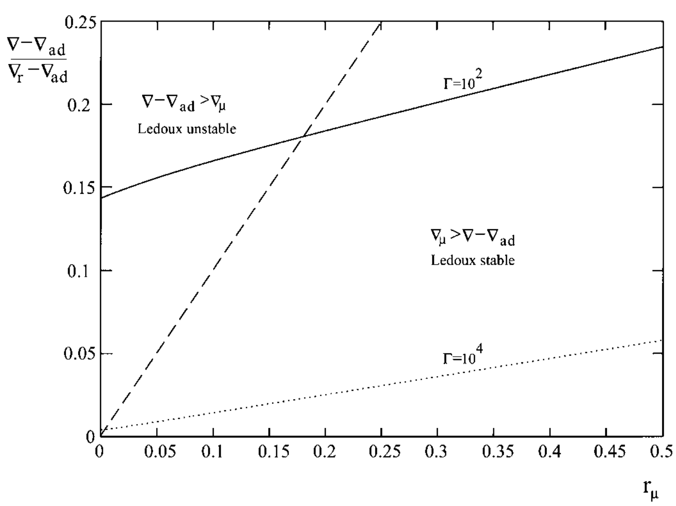

FIG. 8.—Semiconvection. The variable $\nabla - \nabla_{ad}$ versus ∇_μ (both normalized to $\nabla_r - \nabla_{ad}$) for different values of Γ. The whole region is Schwarzschild unstable. The Ledoux-unstable region is to the left of the dashed line, while the Ledoux-stable region is to the right of it. See eqs. (184a) and (184b). The latter region is often referred to as "vibrationally unstable."

19. SALT FINGERS: THE $\nabla_{ad} - \nabla$ VERSUS $|\nabla_\mu|$ RELATION

Since from equation (186) we have that $\nabla_{ad} - \nabla > 0$, $\nabla_\mu < 0$, $R_\mu > 0$, $N_h^2 > 0$, equation (163a) implies that $x > 0$, so that $K > 0$ equation (175),

$$K = 4gH_p^{-1}\Lambda^2(\nabla_{ad} - \nabla)x^{-1} . \tag{247}$$

At the same time the Peclet number becomes

$$\mathrm{Pe} = \Gamma U x^{-1/2} , \tag{248}$$

where in this case

$$U = \left(\frac{\nabla_{ad} - \nabla}{\nabla_{ad} - \nabla_r}\right)^{1/2} , \quad \Gamma \equiv \frac{8\pi^2}{125}\,[g\Lambda^4 H_p^{-1}(\nabla_{ad} - \nabla_r)\chi^{-2}]^{1/2} \tag{249}$$

The equation for the variable U (we consider only the case $q = 0$) is given by

$$U^3 + p(U^2 - 1) = 0 , \tag{250}$$

$$p^{-1} = \frac{175}{3\pi^2}\,\Gamma x^{-1/2} A_h(x) , \tag{251}$$

and

$$\frac{K_h}{\chi} = \frac{175}{3\pi^2}\,\Gamma x^{-1/2} A_h(x) U , \quad K_c = K_h \sigma_\mu^{-1} , \tag{252}$$

where, as before,

$$\sigma_\mu = \frac{K_h}{K_c} = \frac{A_h}{A_c} . \tag{253}$$

In this case, we have

$$R_\mu = r_\mu U^{-2} , \quad r_\mu = \frac{|\nabla_\mu|}{\nabla_{ad} - \nabla_r} . \tag{254}$$

Finally, equations (244) and (245) are formally unchanged.

In Figure 10 we present the Peclet number Pe versus r_μ for two values of Γ. We recall that the smaller r_μ, the smaller is the source, that is, the μ gradient. In Figure 11 we present

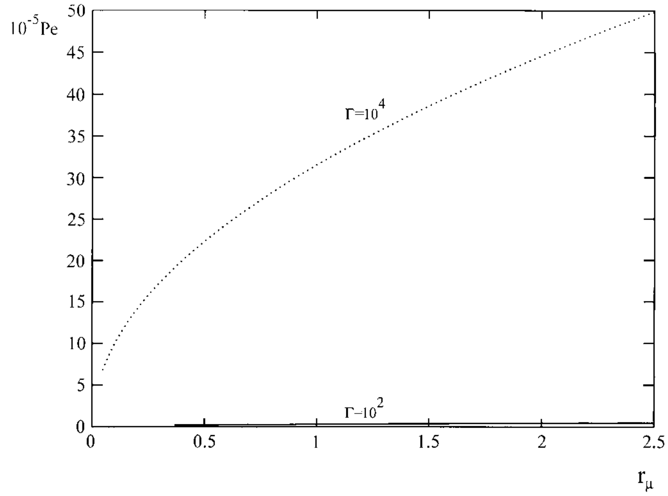

FIG. 10.—Salt fingers. Peclet number Pe vs. r_μ for two values of Γ; see eqs. (247)–(254).

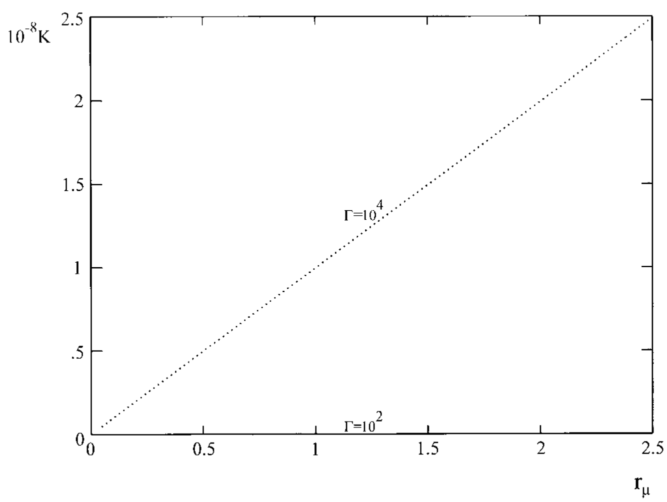

FIG. 11.—Salt fingers. Turbulent kinetic energy K in units of $\chi^2\Lambda^{-2}$ vs. r_μ (eqs. [247]–[254]).

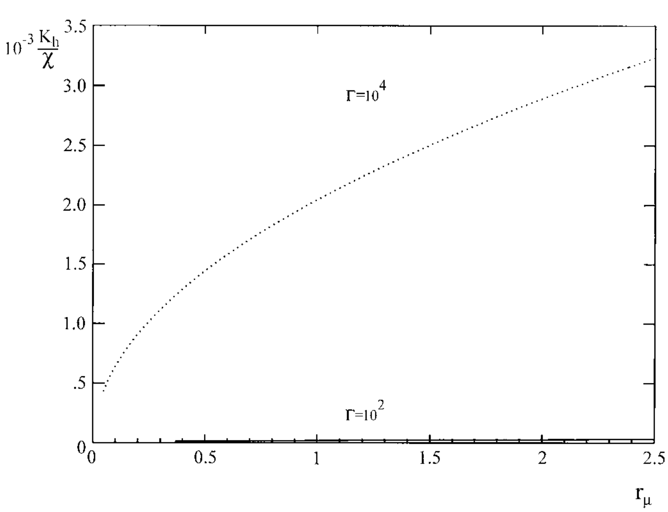

FIG. 12.—Salt fingers. Turbulent heat diffusivity K_c/χ vs. r_μ (eq. [252])

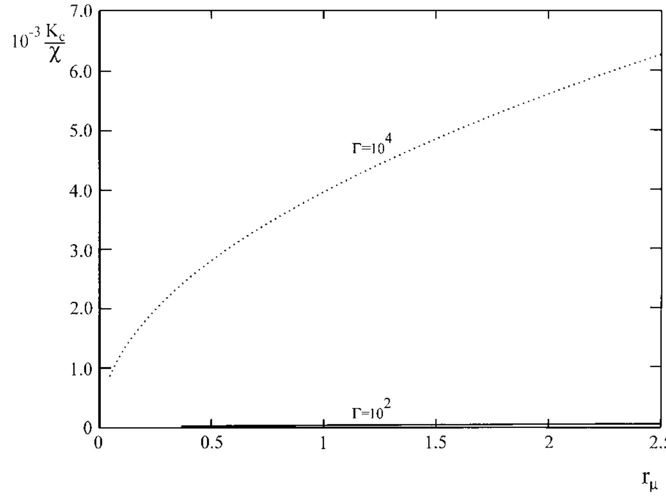

FIG. 13.—Salt fingers. Turbulent concentration diffusivity K_c/χ vs. r_μ (eq. [252]).

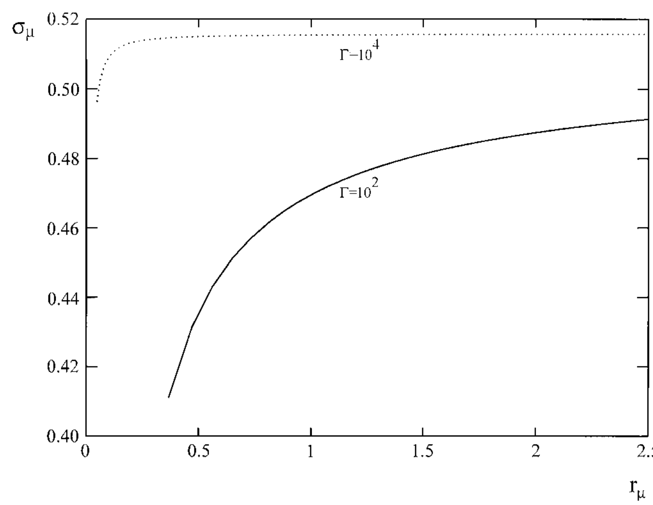

FIG. 14.—Salt fingers. The ratio K_c/K_h vs. r_μ (eq. [253])

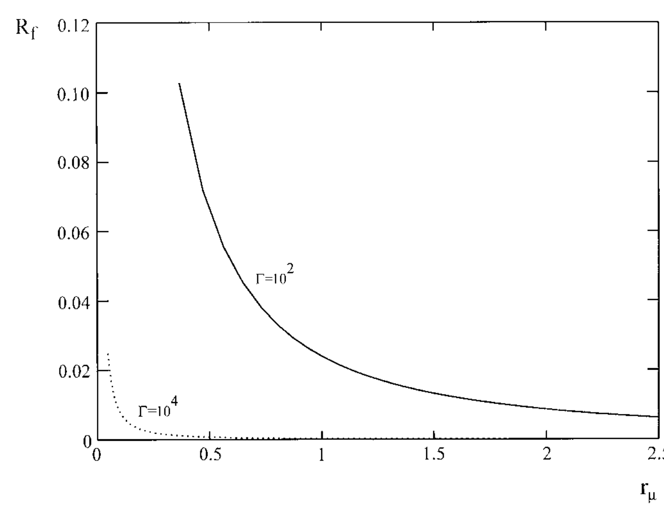

FIG. 15.—Salt fingers. Flux ratio R_F vs. r_μ (eq. [224]). The behavior is in agreement with the data.

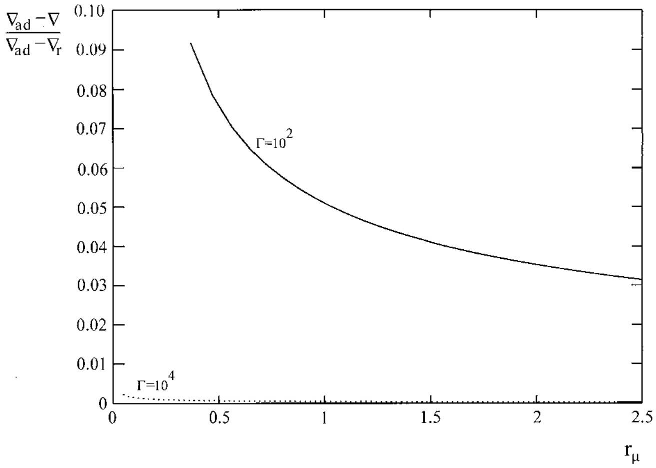

FIG. 16*a*

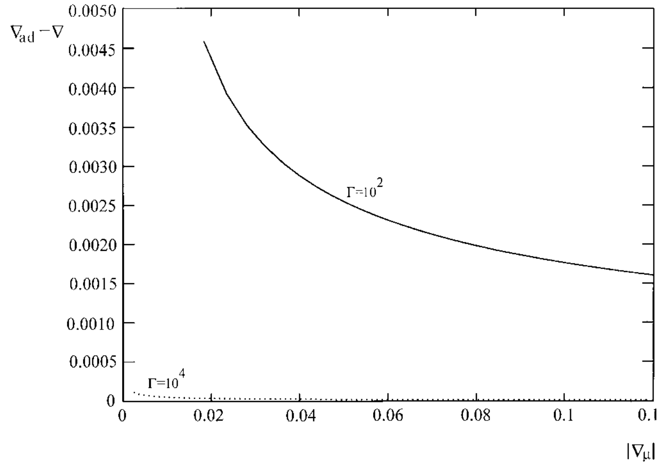

FIG. 16*b*

FIG. 16.—Salt fingers. (*a*) Temperature gradient $\nabla_{\rm ad} - \nabla$ vs. r_μ. For a small r_μ (small ∇_μ) and a large Γ (low radiative losses), the negative convective flux is relatively important and ∇ is far from ∇_r. When radiative losses are important, χ is large, Γ is low, convection is less efficient as a sink, and ∇ is closer to ∇_r. (*b*) $\nabla_{\rm ad} - \nabla$ vs. $|\nabla_\mu|$ for $\nabla_{\rm ad} - \nabla_r = 0.05$.

the turbulent kinetic energy K (in units of $\chi^2\Lambda^{-2}$), whereas in Figure 12 we show the temperature turbulent diffusivity K_h/χ versus r_μ. In Figure 13 we exhibit the c field turbulent diffusivity K_c/χ. As expected, because the latter is the driving instability, we have $K_c > K_h$, as already discussed in equation (206), a result that is in agreement with the measured data. The ratio $\sigma_\mu = K_h/K_c$ is displayed in Figure 14. The flux ratio R_F defined in equation (224) is displayed in Figure 15; as predicted by qualitative arguments, the ratio is found to be less than unity, in agreement with the data. In Figure 16*a*, we present the variable of direct astrophysical interest, $\nabla_{\rm ad} - \nabla$ (in units of $\nabla_{\rm ad} - \nabla_r$) versus r_μ. For a large r_μ (large ∇_μ) and a large Γ (small radiative losses), the (negative) convective flux is relatively important and ∇ is far from ∇_r. When χ is large (Γ small), convection is less important as a sink and ∇ is closer to ∇_r. The numerical results reflect these expectations. In Figure 16*b* we plot $\nabla_{\rm ad} - \nabla$ versus $|\nabla_\mu|$ for a typical value of $\nabla_{\rm ad} - \nabla_r = 0.05$.

20. OVERSHOOTING AND THE $\bar{\mu}$ BARRIER

It is frequently stated that semiconvection is "depressed" by penetrating convection, namely, overshooting. We believe that the logic of this statement is upside down. Overshooting is a dynamical consequence of Newton's law and, as such, is unavoidable. On the other hand, semiconvection is a ∇_μ effect whose existence is not required by any fundamental laws of physics. It is the result of a peculiar state of affairs in a star. Thus, we suggest that the logically consistent way to state the problem is as follows: given an overshooting distance, which cannot be zero, computed as if the medium were homogeneous, what effect has on it a μ gradient? It is the overshooting distance that gets depressed by semiconvection, not the other way around. In what follows, we shall prove the following general result:

$$\frac{({\rm OV})_{\nabla\mu}}{({\rm OV})_{\mu={\rm const}}} < 1 \ . \tag{255}$$

The relevant dynamic equations are given by equations (117)–(124). We shall neglect the large-scale flow $\boldsymbol{U}$, not because it is unimportant but because we first want to compare the results with the case without concentration gradients, namely, with equations (19a)–(19d) of Canuto & Dubovikov (1998), as well as with eqs. (2a)–(2d) of Canuto (1997b). To facilitate the comparison with previous work, we adopt the same notation:

$$\bar{\rho}^{-1}\overline{\rho T''^2} \equiv \overline{\theta^2} \ , \quad \bar{\rho}^{-1}\overline{\rho u_z''^2} \equiv \overline{w^2} \ . \tag{256}$$

Using equation (A12), we obtain

$$\frac{\partial K}{\partial t} + D_f = g\alpha J - \epsilon + X_1(c) \ , \tag{257a}$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\,\overline{\theta^2}\right) + D_f = \beta J - \tau_\theta^{-1}\,\overline{\theta^2} + \frac{1}{2}\,\chi\overline{\theta^2}_{,zz} \ , \tag{257b}$$

$$\frac{\partial J}{\partial t} + D_f = \beta\overline{w^2} + g\alpha\overline{\theta^2} - \tau_{p\theta}^{-1}J + \frac{1}{2}\,\chi J_{,zz} + X_3(c) \ , \tag{257c}$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\,\overline{w^2}\right) + D_f = -\tau_{\rm pv}^{-1}\left(\overline{w^2} - \frac{2}{3}\,K\right) + \frac{2}{3}\,g\alpha J - \frac{1}{3}\,\epsilon + X_4(c) \ . \tag{257d}$$

We have used the same symbol D_f to represent all nonlocal terms, but they are clearly different from each other. Explicit forms for the various D_f's can be found in Canuto & Dubovikov (1998). The new terms $X(c)$ are given by

$$X_1(c) = -g\alpha_c\,\Phi_z \ , \tag{258a}$$

$$X_3(c) = -g\alpha_c\,\overline{T''c''} + \tfrac{1}{2}\chi_c\,\Phi_{z,zz} \ , \tag{258b}$$

$$X_4(c) = \tfrac{2}{3}X_1(c) \ . \tag{258c}$$

The equations for Φ_3 and $\overline{T''c''}$ follow from equations (122)–(124):

$$\frac{D\Phi}{Dt} + D_f = -\,\Phi_z\,C_{,z} - 2\tau_c^{-1}\Phi \ , \tag{259a}$$

$$\frac{\partial \Phi_z}{\partial t} + D_f = -\overline{w^2} C_{,z} + g(\alpha \overline{T''c''} - 2\alpha_c \Phi) - \tau_{pc}^{-1} \Phi_z + \frac{1}{2} \chi_c \Phi_{z,zz} , \quad (259b)$$

$$\frac{D}{Dt} (\overline{T''c''}) + D_f = \beta \Phi_z - J C_{,z} - \tau_{c\theta}^{-1} \overline{T''c''} , \quad (259c)$$

For a qualitative treatment of the effect of the μ barrier on the extent of the OV, it is sufficient to consider the stationary, nondiffusive, local limit of equations (259a)–(259c), which become algebraic with the solutions

$$\Phi_z = -K_c C_{,z} , \quad K_c = \frac{d}{1 - \eta} , \quad d = \tau_{pc}(\overline{w^2} + \alpha g \tau_{c\theta} J) , \quad (260a)$$

$$\eta = g\tau_{pc}(\alpha\beta\tau_{c\theta} + \tau_c \alpha_c C_{,z}) , \quad (260b)$$

$$\overline{T''c''} = -\tau_{c\theta}(J + K_c \beta)C_{,z} \quad (260c)$$

$$\Phi = \tfrac{1}{2}\tau_c K_c (C_{,z})^2 . \quad (260d)$$

The functions X then become

$$X_1(c) = gK_c \alpha_c C_{,z} = -gK_c H_p^{-1} \nabla_\mu , \quad (261a)$$

$$X_3(c) = g\tau_{c\theta} \alpha_c (J + K_c \beta) C_{,z} = -\tau_{c\theta} g H_p^{-1} (J + K_c \beta) \nabla_\mu , \quad (261b)$$

$$X_4(c) = \tfrac{2}{3} g K_c \alpha_c C_{,z} = -\tfrac{2}{3} g K_c H_p^{-1} \nabla_\mu . \quad (261c)$$

Substituting back into equations (257a)–(257d), we obtain

$$\frac{\partial K}{\partial t} + D_f = g\alpha J - (\epsilon + gK_c H_p^{-1} \nabla_\mu) , \quad (262a)$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\overline{\theta^2}\right) + D_f = \beta J - \tau_\theta^{-1} \overline{\theta^2} + \frac{1}{2}\chi \overline{\theta^2}_{,zz} , \quad (262b)$$

$$\frac{\partial J}{\partial t} + D_f = \beta(\overline{w^2} - \tau_{c\theta} g H_p^{-1} K_c \nabla_\mu) + g\alpha\overline{\theta^2} - (\tau_{p\theta}^{-1} + \tau_{c\theta} g H_p^{-1} \nabla_\mu) J + \frac{1}{2}\chi J_{,zz} , \quad (262c)$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\overline{w^2}\right) + D_f = -\tau_{pv}^{-1}\left(\overline{w^2} - \frac{2}{3}K\right) - \frac{1}{3}\epsilon(1 + 2K_c \times gH_p^{-1}\epsilon^{-1}\nabla_\mu - 2g\alpha J \epsilon^{-1}) . \quad (262d)$$

The physical interpretation of these equations is clear: (1) In the kinetic energy equation, ∇_μ increases the dissipation rate ϵ, increases the sink, and lowers K; with less available kinetic energy, one expects *smaller overshooting.* (2) In the equation for the convective flux J, ∇_μ lowers the source of potential energy $\frac{1}{2}\overline{\theta^2}$ by lowering the kinetic energy $\overline{w^2}$, and it increases the damping of $\frac{1}{2}\overline{w^2}$, represented by the last but one term ($J < 0$). (3) In the equation for the energy $\overline{w^2}$, ∇_μ increases the overall sink, since $J < 0$; this leads to a lower $\overline{w^2}$ and to a *smaller overshooting.*

To give a more tangible feeling of what this entails, we employ the OV Criterion expressed by equation (4a) of (Canuto 1997b; we assume adiabaticity, a simplification that does not affect the present argument). We have

$$\frac{g}{c_p}\int_{r_1}^{r*} T^{-2} | L_N - L_r | dr = \frac{g}{c_p}\int_{r*}^{r} T^{-2} | L_N - L_r | dr + 4\pi \int_{r_1}^{r_2} T^{-1} r^2 \rho \epsilon_{\rm eff}\, dr , \quad (263)$$

where the "effective dissipation" $\epsilon_{\rm eff}$ is given by

$$\epsilon_{\rm eff} = \epsilon(1 + gK_c H_p^{-1}\epsilon^{-1}\nabla_\mu) \equiv Q\epsilon . \quad (264)$$

Here $r_{1,2}$ are the endpoints of the convective zone; $r_2 - r^*$ is the extent of the OV. Since the second term on the right-hand side has been increased by the presence of ∇_μ in $\epsilon_{\rm eff}$, the first term need not be large in order to compensate the left-hand side. The OV extent $r_2 - r^*$ may be small and equation (263) still be satisfied. Thus, ∇_μ decreases the extent of the OV.

To derive our result, we employ a relation for the decay of the velocity w in the OV, due to Unno, Kondo, & Xiong (1985):

$$w(r) = w(r^*) e^{x \ln (P/P_*)} , \quad P < P_* , \quad (265)$$

where r is an arbitrary point in the OV region, $r^* < r < r_2$. The key parameter is x, which can only be provided by a turbulence model. If we consider a polytrope of index m, $P \sim r^{-m}$, then

$$w(r) = w(r^*)\left(\frac{r^*}{r}\right)^{xm} . \quad (266)$$

Since by construction OV $= r_2 - r^* \ll r_2$, if we take $r = r_2$, we have

$$w(r_2) = w(r^*)\left(1 - \frac{\rm OV}{r_2}\right)^{xm} \approx w(r^*)\left(1 - xm\frac{\rm OV}{r_2}\right) . \quad (267)$$

Since $w(r_2) = 0$, the extent of the OV is r_2/xm, and since $H_p = r_2 m^{-1}$, we finally derive

$$\frac{\rm OV}{H_p} = \frac{1}{x} . \quad (268)$$

From the work of Unno et al. (1985) one can deduce that under the scaling $\epsilon \rightarrow Q\epsilon$, the variable x scales as

$$x \rightarrow Qx , \quad (269)$$

and thus in the presence of a ∇_μ, the decay law (eq. [268]) changes to

$$\frac{\rm OV}{H_p} = \frac{1}{x}\frac{1}{Q} , \quad (270)$$

and thus finally,

$$\frac{{\rm OV}(\nabla_\mu)}{{\rm OV}(\nabla_\mu = 0)} = \frac{1}{Q} < 1 , \quad (271)$$

which is the desired result: *the μ barrier increases the rate of dissipation of available turbulent kinetic energy and leads to a decrease of the extent of the* OV. The role of the dissipation ϵ in determining the core OV has been recently analyzed by Rosvick & VandenBerg (1998).

21. DIFFERENTIAL ROTATION: ITS EFFECT ON SEMICONVECTION AND SALT FINGERS

In this section, we study the effect of differential rotation on semiconvection and salt fingers. In what follows, we present the analytic solution of the turbulence equations in the presence of the three gradients (eq. [9]) which we shall take to be of the form given below in equation (278). We leave K and ϵ to be treated either locally or not. It is convenient to introduce the following variables:

$$n_i \equiv (\tau_c \tau_{c\theta} \tau^{-2}) g\alpha\tau^2 \beta_i , \quad (272a)$$

$$c_i \equiv g\tau_c^2 \alpha_c \frac{\partial C}{\partial x_i} , \quad (272b)$$

$$\psi_i \equiv \beta_5 K^{-1} \alpha g \tau_{pv} J_i = \tfrac{2}{5} \alpha g \epsilon^{-1} J_i , \quad (272c)$$

$$\phi_i \equiv \beta_5 K^{-1} \alpha_c g \tau_{pv} \Phi_i = \tfrac{2}{5} \alpha_c g \epsilon^{-1} \Phi_i , \quad (272d)$$

$$\lambda_i = -(g\bar{\rho})^{-1} P_{,i} , \quad (272e)$$

where n_i, c_i, ψ_i, and ϕ_i are dimensionless and where we have chosen $\beta_5 = \frac{1}{2}$ and $\tau_{pv}/\tau = \frac{2}{5}$ (Appendix B). The turbulence equations then take the following forms.

Reynolds stresses:

$$a_{ij} \equiv K^{-1} R_{ij} - \tfrac{2}{3}\delta_{ij} , \quad (273a)$$

$$2a_{ij} = -\tfrac{8}{15}\tilde{S}_{ij} - (1 - p_1)\tilde{\Sigma}_{ij} - (1 - p_2)\tilde{Z}_{ij} + \Psi_{ij} - T_{ij} , \quad (273b)$$

$$\Psi_{ij} \equiv \lambda_i \psi_j + \lambda_j \psi_i - \tfrac{2}{3}\lambda_k \delta_{ij} \psi_k , \quad (273c)$$

$$T_{ij} \equiv \lambda_i \phi_j + \lambda_j \phi_i - \tfrac{2}{3}\lambda_k \delta_{ij} \phi_k . \quad (273d)$$

Concentration flux:

$$(\delta_{ik} + \eta_{ik})\phi_k = -[p_4(a_{ik} + \tfrac{2}{3}\delta_{ik}) + p_5 \lambda_i \psi_k] c_k , \quad (274a)$$

$$\eta_{ij} = p_3 \tilde{U}_{i,j} - \lambda_i p_{11}(n_j + c_j) . \quad (274b)$$

Temperature flux:

$$(\delta_{ik} + \mu_{ik})\psi_k = p_6(a_{ik} + \tfrac{2}{3}\delta_{ik} - p_7 \lambda_i \phi_k) n_k , \quad (275a)$$

$$\mu_{ij} = p_8 \tilde{U}_{i,j} - \lambda_i (p_9 n_j + p_{10} c_j) . \quad (275b)$$

Here

$$\tilde{U}_{i,j} \equiv \tau_{pv} U_{i,j} , \quad \tilde{S}_{i,j} \equiv \tau_{pv} S_{ij} , \quad \tilde{\Sigma}_{ij} = \tau_{pv} \Sigma_{ij} , \quad \tilde{Z}_{ij} = \tau_{pv} Z_{ij} . \quad (276)$$

The functions p are defined as follows:

$$p_1 = 0.832 , \quad p_2 = 0.545 , \quad p_3 = \frac{5}{2}\frac{\tau_{pc}}{\tau} ,$$

$$p_4 = \frac{1}{5}\tau\tau_{pc}\tau_c^{-2} , \quad p_5 = \tau_{pc}\tau_{c\theta}\tau_c^{-2} , \quad p_6 = \frac{1}{5}\frac{\tau}{\tau_c}\frac{\tau_{p\theta}}{\tau_{c\theta}} ,$$

$$p_7 = 5\frac{\tau_{c\theta}}{\tau} , \quad p_8 = \frac{5}{2}\frac{\tau_{p\theta}}{\tau} , \quad p_9 = \frac{\tau_\theta}{\tau_c}\frac{\tau_{p\theta}}{\tau_{c\theta}} ,$$

$$p_{10} = \tau_{c\theta}\tau_{p\theta}\tau_c^{-2} , \quad p_{11} = \frac{\tau_{pc}}{\tau_c} . \quad (277)$$

There is a case in which we can give a complete algebraic solution of the previous turbulence equations. It corresponds to

$$\frac{\partial}{\partial x_i}(T, C) \rightarrow \delta_{i3}\frac{\partial}{\partial z}(T, C) , \quad \boldsymbol{U} = (U(z), V(z), 0) . \quad (278)$$

Shear and vorticity become

$$\tilde{S}_{ij} = \frac{1}{2}\begin{pmatrix} 0 & 0 & \partial\tilde{U}/\partial z \\ 0 & 0 & \partial\tilde{V}/\partial z \\ \partial\tilde{U}/\partial z & \partial\tilde{V}/\partial z & 0 \end{pmatrix} ,$$

$$\tilde{V}_{ij} = \frac{1}{2}\begin{pmatrix} 0 & 0 & \partial\tilde{U}/\partial z \\ 0 & 0 & \partial\tilde{V}/\partial z \\ -\partial\tilde{U}/\partial z & -\partial\tilde{V}/\partial z & 0 \end{pmatrix} . \quad (279)$$

Since we are dealing with only one component of the vectors n_i, c_i, we simplify the notation and write

$$n_3 \equiv n = n_0 g\alpha\beta\tau^2 , \quad n_0 = \tau_c\tau_{c\theta}\tau^{-2} , \quad (280a)$$

$$c_3 \equiv c = c_0 g\tau^2\alpha_c \frac{\partial C}{\partial z} , \quad c_0 = \left(\frac{\tau_c}{\tau}\right)^2 , \quad (280b)$$

$$\beta_3 = \beta . \quad (280c)$$

The dimensionless shear is given by

$$y = (\tau_{pv} N_u)^2 , \quad N_u^2 = \left(\frac{\partial U}{\partial z}\right)^2 + \left(\frac{\partial V}{\partial z}\right)^2 . \quad (281)$$

If we introduce the simplifying notation,

$$w \equiv \bar{\rho}^{-1}\rho u_z'' , \quad \theta \equiv T'' , \quad (282)$$

we obtain the following results:

Momentum flux:

$$\overline{uw} = -K_m \frac{\partial U}{\partial z} , \quad \overline{vw} = -K_m \frac{\partial V}{\partial z} , \quad K_m = 2\frac{K^2}{\epsilon} S_m . \quad (283)$$

Heat flux (in units of $c_p \rho$):

$$\overline{w\theta} = K_h \beta , \quad K_h = 2\frac{K^2}{\epsilon} S_h . \quad (284)$$

Concentration flux:

$$\overline{wc''} = -K_c \frac{\partial C}{\partial z} , \quad K_c = 2\frac{K^2}{\epsilon} S_c . \quad (285)$$

As one can notice, the turbulent diffusivities are indeed of the general form of equation (5) and satisfy equation (6). The dimensionless structure functions are given by

$$S_m = \frac{4}{15}\frac{\tau_{pv}}{\tau} A_m D^{-1} , \quad S_h = \frac{4}{15}\frac{\tau_{p\theta}}{\tau} A_h D^{-1} ,$$

$$S_c = \frac{4}{15}\frac{\tau_{pc}}{\tau} A_c D^{-1} , \quad (286a)$$

$$A_m = 12 + a_1 n^2 + a_2 nc + a_3 c^2 + a_4 n + a_5 c , \quad (286b)$$

$$A_h = (1 + b_1 c + b_2 n)(60 + b_3 y + b_4 c + b_5 n) , \quad (286c)$$

$$A_c = (1 + b_6 c + b_7 n)(60 + b_3 y + b_4 c + b_5 n) , \quad (286d)$$

$$D = 24 + d_1 yn^2 + d_2 ync + d_3 yc^2 + d_4 n^3 + d_5 n^2 c + d_6 nc^2 + d_7 c^3 + d_8 yn + d_9 yc + d_{10} n^2 + d_{11} nc + d_{12} c^2 + d_{13} y + d_{14} n + d_{15} c . \quad (286e)$$

As one can see, the dimensionless functions A, as well as D, depend on the gradients of the mean temperature, concentration and mean velocity represented by n, c, and y. The functions a_k, b_k, and d_k (Appendix C) depend on the timescales τ_c, τ_{pc}, etc., which in turn depend on the Peclet numbers. The apparent algebraic complexity of the functions $S_{m,h,c}$ is a small price to pay if one considers that the above equations are the solution of a fully turbulent problem in the presence of three external fields, T, $\boldsymbol{U}$, and C. It is in fact quite surprising that such a complex problem could be expressed via a set of algebraic relations. Finally, it is important to stress that these analytic solutions are already telling us a great deal, since equations (286a) exhibit the ratios

$$\frac{\tau_{pv}}{\tau}, \quad \frac{\tau_{p\theta}}{\tau}, \quad \frac{\tau_{pc}}{\tau} \tag{287}$$

as the dominant factors in the diffusivities. As shown in Appendix B, these ratios entail the dependence on the Peclet numbers and thus on the efficiency of convection. For large Peclet numbers, a_κ, b_κ, and d_κ become constant (Appendix C), and we suggest beginning with these values. The variables K and ϵ are in principle solutions of equations (137) and (138).

21.1. *Local Model*

In the case of a local model, equation (137) gives

$$-R_{ij}U_{i,j} + g\alpha\lambda_i J_i - g\alpha_c \lambda_i \Phi_i = \epsilon . \tag{288}$$

Using equations (283)–(285), we then obtain

$$(\tau N_u)^2 S_m - (\tau N_h)^2 S_h + (\tau N_c)^2 S_c = 2 . \tag{289}$$

The frequencies N_h, N_c, and N_u have been defined in equations (164a), (164b), and (281). Using the definition of y given in equation (281), we then have

$$y(S_m - \mathrm{Ri}\, S_h + \mathrm{Ri}\, R_\mu S_c) = \tfrac{8}{25} , \tag{290}$$

where we have used equation (166) and defined the Richardson number Ri as follows:

$$\mathrm{Ri} = \frac{N_h^2}{N_u^2} , \tag{291}$$

so that it is positive for stable stratification. The solution of the algebraic equation (290) yields the function y, or, equivalently, the timescale $\tau = 2K\epsilon^{-1}$, as a function of the two stability parameters:

$$y = y(\mathrm{Ri}, R_\mu) . \tag{292}$$

We recall that in equations (286b)–(286e) we must substitute

$$n = -\tfrac{25}{4} n_0\, y\, \mathrm{Ri} , \tag{293}$$

$$c = \tfrac{25}{4} c_0\, \mathrm{Ri}\, R_\mu\, y . \tag{294}$$

Once the function $y(\mathrm{Ri}, R_\mu)$ is obtained, one must solve the flux conservation law. In the stationary case, equation (115) becomes

$$F_i^c + F_i^r + F_i^{\mathrm{ke}} + \bar{\rho} U_j[(c_p T + K + K_u + G)\delta_{ij} + R_{ij}] = \text{constant} . \tag{295}$$

With the structure given in equation (278) of the U field, we obtain ($i = 3$)

$$F^c + F^r + F^{\mathrm{ke}} - K_m \bar{\rho} \frac{\partial}{\partial z} K_u = \text{constant} \tag{296}$$

where K_u is the kinetic energy of the mean field, equation (27). The analog of equation (234) is then

$$\nabla + K_h \chi^{-1}(\nabla - \nabla_{\mathrm{ad}}) - H_p(c_p T\chi)^{-1} K_m \frac{\partial}{\partial z} K_u = \nabla_r^* , \tag{297}$$

where we have exhibited the fact that the heat and momentum diffusivities are measured in units of the radiative conductivity $\chi(=K_r/c_p\rho)$, the length z in units of H_p, and the kinetic energy K_u in units of $c_p T$. Contrary to the case we studied earlier, without a specific expression for K_u, we cannot solve equation (297). We therefore exhibit the turbulent diffusivities K_m, K_h, and K_c leaving the solution of equation (297) to the specific stellar case one might consider. The diffusivities $K_{m,h,c}$ are obtained by combining equations (283)–(287) with the result

$$K_m = C_1 y^{-1/2} A_m D^{-1} , \tag{298a}$$

$$K_h = C_2 y^{-1/2} A_h D^{-1} , \tag{298b}$$

$$K_c = C_3 y^{-1/2} A_c D^{-1} , \tag{298c}$$

where

$$C_1 = \frac{16}{15} C_0 \left(\frac{\tau_{pv}}{\tau}\right)^2 , \tag{299a}$$

$$C_2 = \frac{16}{15} C_0 \left(\frac{\tau_{pv}}{\tau}\right)\left(\frac{\tau_{p\theta}}{\tau}\right) , \tag{299b}$$

$$C_3 = \frac{16}{15} C_0 \left(\frac{\tau_{pv}}{\tau}\right)\left(\frac{\tau_{pc}}{\tau}\right) , \tag{299c}$$

$$C_0 = N_u \Lambda^2 . \tag{299d}$$

The Peclet number and thus χ, characterizing radiative losses, enter through the timescales $\tau_{p\theta}$ and τ_θ, as well as in the functions a_k, b_k, and d_k in equations (286b)–(286e).

22. NUMERICAL RESULTS

Here we consider only the case of $\mathrm{Pe} \gg 1$ corresponding to negligible radiative losses. Thus, χ drops out of the problem as in the case of efficient convection, since for large Pe, the functions a_k, b_k, and d_k in equations (286b)–(286e) become Pe-independent and are given by equations (B9)–(B16). Substituting equations (286b)–(286e), (293), and (294) into equation (290), one obtains the variable y, equation (292), which is then used in equations (298a)–(298c) to compute the turbulent diffusivities K. In Figures 17–19 we plot the $K_{m,h,c}$ versus Ri for different R_μ. The right-hand panel corresponds to salt fingers, and the left-hand panel corresponds to semiconvection. Consider first the case of salt fingers. At a fixed Ri, the diffusivities increase as R_μ increases, which is physically understandable, since the instability is generated by salt, and thus the larger the

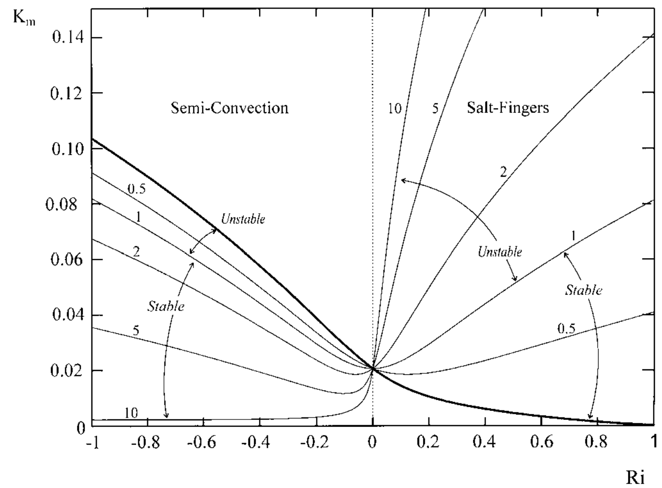

FIG. 17.—The effect of shear. Momentum turbulent diffusivity K_m (in units of $N_u \Lambda^2$) vs. Ri for different R_μ. See eqs. (298a). The thick line corresponds to the case of a passive scalar ($\alpha_c = 0$).

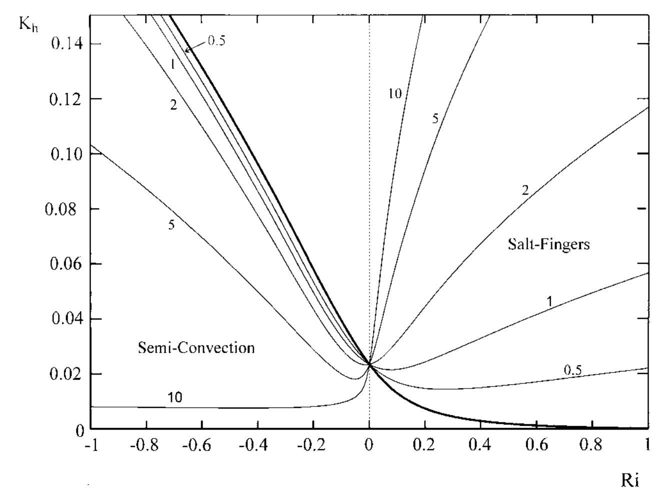

FIG. 18.—The effect of shear. Same as Figure 17, but for the heat turbulent diffusivity K_h vs. Ri for different R_μ. See eq. (298b). Same units as in Figure 17.

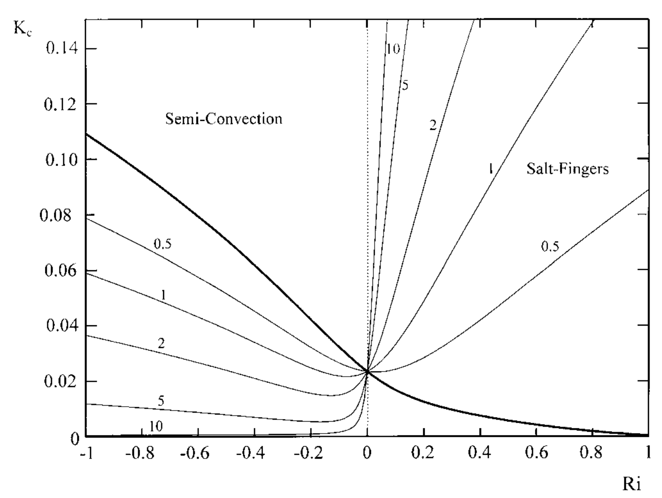

FIG. 19.—The effect of shear. Same as Figure 17, but for the concentration turbulent diffusivity K_c vs. Ri for different R_μ. See eqs. (298c). Same units as in Figure 17.

source, the larger the diffusivity. Next, consider the dependence on Ri. First, we must note the change of curvature in going from a passive (*thick curve*) to an active scalar. In the first case, the $K_{m,h,c}$ decrease with Ri, the stronger the level of stratification, the smaller the level of turbulence (Canuto 1998). The opposite occurs when $R_\mu > 0$. We notice that the smaller the shear (large Ri), the larger are the $K_{m,h,c}$, which at first sight may seem paradoxical: since both ∇_μ and shear contribute to the instability, one might expect that their effects add up. What we find is that the larger the shear, the smaller the diffusivity, which implies that *shear and salt fingers work in opposite directions.* Laboratory and analytical work (Linden 1971, 1974) have shown that in a steady shear the only instability that can grow is in the form of sheets aligned with the shear. More specifically, Kunze (1990, especially Fig. 15) has also shown that fingers are tilted so rapidly that they are damped before they produce significant fluxes. The two lower curves correspond to the stable case, while the upper three curves correspond to the unstable case (in the Ledoux sense); see equations (184a)–(186).

Consider now semiconvection. At a given Ri, the diffusivities decrease as R_μ increases, the opposite of the salt fingers case. This is in accordance with the fact that in this case ∇_μ acts as a sink of turbulent mixing (which is caused by an unstable temperature gradient), and thus the stronger the sink, the lower the level of turbulence, a circumstance that is reflected in the decrease of the diffusivities. As for the effect of shear, we notice that here, too, the smaller the shear (large negative Ri), the larger the diffusivities, which implies that shear prevents the mixing caused by the temperature instability. However, this is not true in general: the curves first decrease with increasing negative Ri, which indicates that for moderate negative Ri shear helps mixing, as one would expect, but the trend does not continue, since the curves change curvature. However, there is a saturation phenomenon, which does not occur in the salt finger case. At large R_μ (large sink), the help in mixing from shear saturates. Finally, the lowest three curves correspond to a stable situation, while the second and third correspond to an unstable situation (in the Ledoux sense); see equations (185) and (186). In Figures 20–22 we plot the ratios K_m/K_h, K_m/K_c, and K_h/K_c, which show quite clearly the validity of

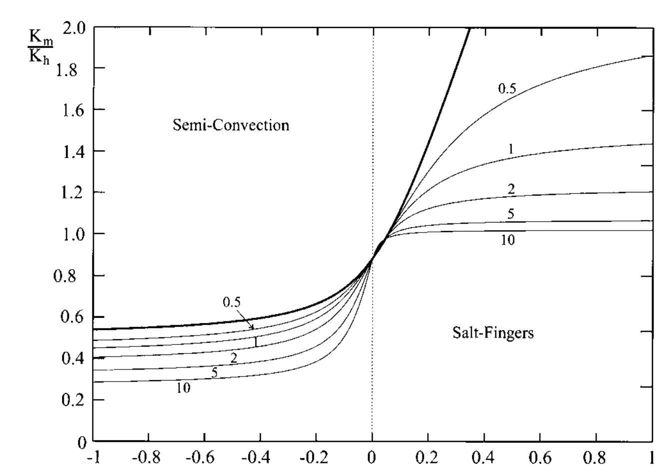

FIG. 20.—The effect of shear. The ratio K_m/K_h vs. Ri for different R_μ (see text).

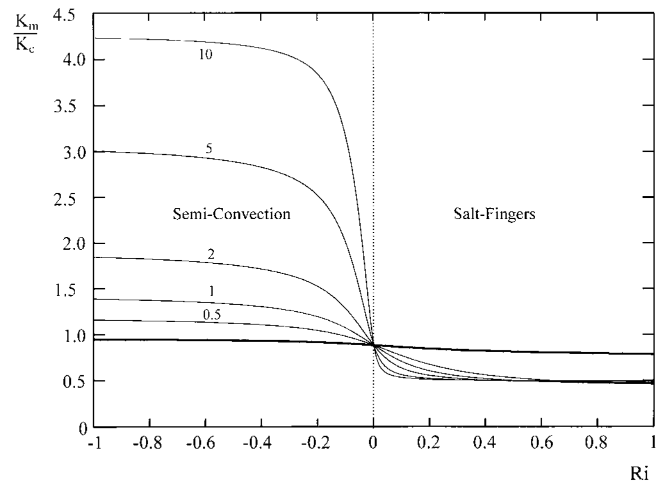

FIG. 21.—The effect of shear. The ratio K_m/K_c vs. Ri for different R_μ (see text).

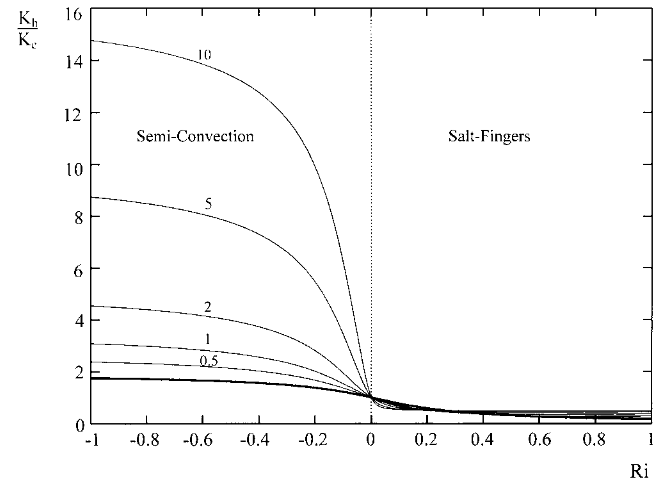

FIG. 22.—The effect of shear. The ratio K_h/K_c vs. Ri for different R_μ (see text).

equation (6), that is, the diffusivities are in fact different among themselves.

23. PREVIOUS MODELS

To obtain the turbulent diffusivities K, all previous models had to rely on some heuristic arguments, though for different reasons and in different degrees. The models of Xiong (1985a, 1985b, 1986) and Grossman & Taam (1996) have already been discussed in section § 8, and we shall therefore comment only on the recent work of Umezu (1998). We shall then discuss the work of Langer et al. (1983, 1985, 1989), Woosley et al. (1998), and Salasnich et al. (1998). These models were extensively used to study massive stars and the problem of the red/blue SN 1987A progenitor.

Umezu (1998) employed the results of Kato (1966), as well as those of a mixing-length model developed earlier by Nakakita & Umezu (1994). The results are presented in dual form, since the expression for the convective flux depends on a parameter B. In the model with $B = 0$, F_c is positive, while in the other case F_c is negative. We believe that only $B = 0$ is acceptable. We give three reasons for our conclusion. First, in semiconvection the T gradient is unstable and this induces a necessarily positive convective flux. The presence of a ∇_μ acts like a sink and lowers F_c, as is indeed shown on Figure 4, but F_c remains positive. A negative convective flux, in addition to a negative μ flux, would mean that both T and the μ fields act like sinks, but without a source turbulence cannot exist. The second argument is a direct consequence of the assumption of locality that underlies Umezu's model and mixing-length type models in general. Consider the turbulent kinetic energy equation,

$$\frac{\partial K}{\partial t} + D_f(K) = P - \epsilon\ , \tag{300}$$

where $D_f(K)$ represents the nonlocal process of diffusion of K, P is the total production of K, and ϵ is its rate of dissipation. P is given by

$$P = (g\alpha/c_p\bar{\rho})F_c - gK_c H_p^{-1}\nabla_\mu\ . \tag{301}$$

A local model is defined as one in which there is no diffusion (in addition to stationarity), and thus the local version of equation (300) is

$$P = \epsilon\ , \tag{302}$$

To balance $\epsilon > 0$, P must be positive, which means that $F_c > 0$. A negative convective flux is inconsistent with the underlying assumption of locality. The third argument is based on the fact that one can identify the form of the convective flux from the flux conservation law. The latter is the result of taking the stationary limit of the dynamic equation for the mean temperature. The basic equation for T is given by equation (57b), and the only effect of a c field (or μ field) is in the last two terms, which are proportional to kinematic diffusivities that are assumed small in a turbulent regime. Thus, no ∇_μ effect appears, and a flux conservation law discussed by Umezu (1998, his equation [14]),

$$\nabla + \mathrm{Pe}(\nabla - \nabla_{\mathrm{ad}}) + B\mathrm{Pe}\nabla_\mu = \nabla_r\ , \tag{303}$$

can only be consistent with the proceeding arguments if $B = 0$. This in turn means that the second term is the convective flux, which is by necessity positive, since $\nabla - \nabla_{\mathrm{ad}} > 0$.

Umezu (1998) also attempted to reproduce the low diffusivities required by Langer and collaborators and Deng et al. (1996*a*), 1996*b*. He concludes that this is an indication that the mixing length must be very small. As Figures 23 and 24 show, even a large convective efficiency, $\Gamma \sim \Lambda^2$, is compatible with a small α_{sc} provided $R_\mu \sim 10$. In many other respects, and for $B = 0$, the general trend of Umezu's results is in essential agreement with ours, even though a one-to-one comparison is not possible because his value $r_\mu = 100$ is larger than the one we have considered in this paper (though easily included). In conclusion, the shortcoming discussed in § 8 concerning the need to rely on some heuristic arguments to determine several timescales applies here as well.

Next, we consider the work of Langer et al. (1983, 1985, 1989. They adopt the viewpoint than when K_c/χ is much larger than unity, the diffusion timescale is short enough to produce rapid mixing, thus allowing them to treat it as homogeneous convection. Thus, they only treat the case of

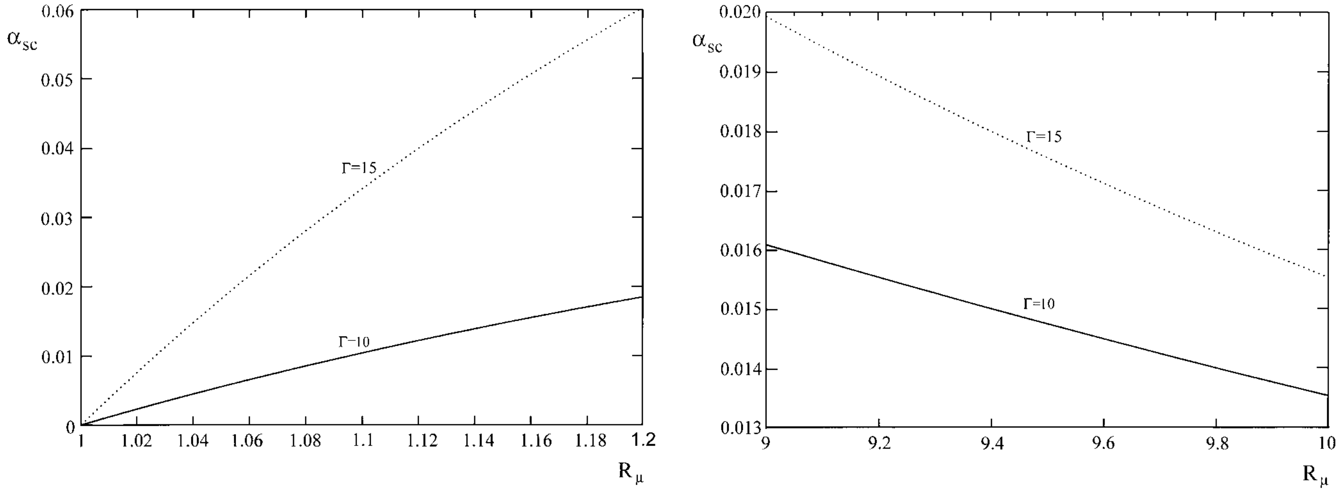

FIG. 23.—(*a*) Semiconvection efficiency parameter α_{sc} vs. R_μ as defined by Langer et al. (1983, 1985, 1989) computed from the present model (see text). (*b*) Same as (*a*), but for a different range of R_μ values.

slow mixing, and their model for K_c is given by equation (1) for the Ledoux stable region. Equating our expression for K_c/χ given by equation (242) and Figure 5 to the right-hand side of equation (1) gives the parameter α_{sc}, which we plot in Figure 23. Several considerations are in order. First, α_{sc} is not constant with respect to either R_μ or Γ. Second, it has a maximum where $\alpha_{sc} > 1$ and the values in Figure 23 represent the beginning and end portions of the α_{sc} versus R_μ curve. Third, these are the only regions in which we find values of α_{sc} which are of the same order as those used by Langer et al. (1983) and Woosley et al. (1998). Fourth, Γ does not appear in Langer et al.'s formulation, since it is assumed to be very large. On the other hand, Salasnich et al. (1998) have taken a simpler approach and written $K_c/\chi = \alpha_2^{-1}$. They find that $\alpha_2 = 50$–100. In Figure 24, we reproduce an expanded version of Figure 5 in order to exhibit the small K_c/χ regime. As in the previous case, values of the order of those required by Salasnich et al. (1998) can be reproduced by the present theory provided that $r_\mu > 2$–3. One may also notice that $K_c \sim r_\mu^{-n}$, $n > 1$, as assumed by Eggleton (1971, 1972).

In conclusion, at first sight the models and parameterizations used thus far do not appear inconsistent with the theoretical predictions, but a complete consistency check is still missing, since the values of R_μ, r_μ, and Γ must also match. It is also clear that the present model shows that the diffusivities K exhibit a texture, structure, and complexity that we formally represent as

$$K = K(R_\mu, \mathrm{Ri}, \Gamma) \tag{303}$$

that previous models could not account for, especially the effect of differential rotation.

24. CONCLUSIONS

We have presented a formalism to treat turbulent diffusion in the presence of three nonzero gradients, ∇T, ∇U, and ∇C. We have derived the nonlocal dynamic equations that govern the turbulence variables. We have then solved the local problem analytically and given the explicit expressions for the turbulent diffusivities. The whole turbulence problem is reduced to the solution of an algebraic equation. We have applied the formalism to study semiconvection and salt fingers. We have also solved the flux conservation equation and exhibited the behavior of the temperature gradient ∇ versus ∇_μ.

We have analyzed the Schwarzschild and Ledoux criteria and suggested an alternative criterion which is derived from the turbulence model. We have shown that the extent of overshooting is lowered by the presence of semiconvection, a result of general validity. Finally, we have encountered a new phenomenon: shear (differential rotation) and mixing caused by the ∇_μ gradient do not reinforce each other, as one might expect; rather, shear tends to weaken the ∇_μ mixing.

A comparison is made with some previous formulations of semiconvection diffusivities calibrated to the H-R diagrams of massive stars and to the phenomenon of SN 1987A. We show that, while not inconsistent with the turbulence model presented here, these models leave out several important features and are probably inadequate to include the nontrivial effect of shear. The formalism also yields the diffusivity corresponding to the case of a passive scalar. Perhaps the simplest and most immediate result is that

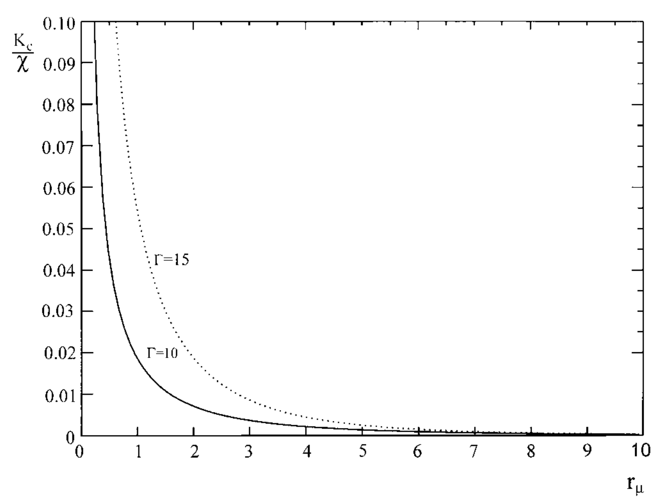

FIG. 24.—Expanded version of Figure 5 (see text)

momentum, heat, and concentration diffusivities are distinct quantities that cannot be assumed to be equal.

We finally stress that we have avoided the empiricism of all previous formulations in determining the turbulence timescales through the use of the RGN techniques discussed in § 8. The hope is that this formalism will now be tested on a specific case of stellar structure and evolution.

I would like to thank R. Stothers, N. Langer, and C. Chiosi for discussions concerning semiconvection and salt fingers, and Guang Yu for solving the equations numerically. I also want to thank W. Merryfield for useful correspondence on his work and S. Shore for advice on how to improve the paper.

APPENDIX A

REYNOLDS STRESS EQUATIONS

We introduce the traceless tensor

$$b_{ij} = R_{ij} - \tfrac{1}{3}\delta_{ij} R_{kk} = R_{ij} - \tfrac{2}{3}\delta_{ij} K \,, \tag{A1}$$

where K satisfies equation (137). Equation (117) then becomes

$$\frac{Db_{ij}}{Dt} + D_f(b) = -\frac{4}{3} K S_{ij} - \Sigma_{ij} - Z_{ij} + B_{ij} - \pi_{ij} \,, \tag{A2}$$

where the (traceless) tensors $\boldsymbol{\Sigma}$ and $\boldsymbol{Z}$ representing shear and vorticity are defined as

$$\Sigma_{ij} = b_{ik} S_{jk} + b_{jk} S_{ik} - \tfrac{2}{3}\delta_{ij} S_{kl} b_{kl} \,, \tag{A3}$$

$$Z_{ij} = b_{ik} V_{jk} + b_{jk} V_{ik} \,, \tag{A4}$$

where S_{ij} and V_{ij} are shear and vorticity:

$$S_{ij} = \tfrac{1}{2}(U_{i,j} + U_{j,i}) \,, \tag{A5}$$

$$V_{ij} = \tfrac{1}{2}(U_{i,j} - U_{j,i}) \,. \tag{A6}$$

The tensor B_{ij} is given by

$$B_{ij} = g(\alpha L_{ij} - \alpha_c M_{ij}) \,, \tag{A7}$$

$$L_{ij} = \lambda_i J_j + \lambda_j J_i - \tfrac{2}{3}\delta_{ij} \lambda_k J_k \,, \tag{A8}$$

$$M_{ij} = \lambda_i \Phi_j + \lambda_j \Phi_i - \tfrac{2}{3}\delta_{ij} \lambda_k \Phi_k \,. \tag{A9}$$

We recall that

$$\lambda_i = -(g\bar{\rho})^{-1} \frac{\partial P}{\partial x_i} \,. \tag{A10}$$

Finally, we have to treat the pressure-velocity tensor. Following the procedure described in Canuto (1994), we take

$$\bar{\rho}^{-1}\Pi_{ij} = 2\tau_{\rm pv}^{-1} b_{ij} - \tfrac{4}{5} K S_{ij} - p_1 \Sigma_{ij} - p_2 Z_{ij} + (1 - \beta_5) B_{ij} \,, \tag{A11}$$

where the numerical constants $p_{1,2}$ and β_5 are given in the text. The timescale τ_{pv} is discussed in Appendix B. Finally, equation (A2) becomes

$$\frac{Db_{ij}}{Dt} + D_f(b) = -2\tau_{\rm pv}^{-1} b_{ij} - \frac{8}{15} K S_{ij} - (1 - p_1)\Sigma_{ij} - (1 - p_2) Z_{ij} + \beta_5 B_{ij} \,. \tag{A12}$$

APPENDIX B

THE TURBULENT TIMESCALES

The $(\tau_{pv}, \tau_{p\theta}, \tau_\theta)$ versus τ relation is (Canuto & Dubovikov 1998):

$$\tau = 2K\epsilon^{-1}, \qquad \tau_{pv} = \tfrac{2}{5}\tau \,. \tag{B1}$$

For the T field we have

$$\frac{\tau_{p\theta}}{\tau} = \frac{1}{4\pi^2} \mathrm{Pe}_\theta \left[1 + \frac{5}{4\pi^2} \mathrm{Pe}_\theta (1 + \sigma_{t\theta}^{-1})\right]^{-1} \tag{B2}$$

$$\frac{\tau_\theta}{\tau} = \frac{4}{7\pi^2} \mathrm{Pe}_\theta \left[1 + \frac{4}{7\pi^2} \mathrm{Pe}_\theta \, \sigma_{t\theta}^{-1}\right]^{-1} \,. \tag{B3}$$

For the C field we have

$$\frac{\tau_{\mathrm{pc}}}{\tau}=\frac{1}{4\pi^2}\,\mathrm{Pe}_c\left[1+\frac{5}{4\pi^2}\,\mathrm{Pe}_c(1+\sigma_{tc}^{-1})\right]^{-1} \tag{B4}$$

$$\frac{\tau_c}{\tau}=\frac{4}{7\pi^2}\,\mathrm{Pe}_c\left[1+\frac{4}{7\pi^2}\,\mathrm{Pe}_c\,\sigma_{tc}^{-1}\right]^{-1}. \tag{B5}$$

For the T-C correlation, we have

$$\frac{\tau_{c\theta}}{\tau}=\frac{4}{7\pi^2}\,\mathrm{Pe}_\theta\left(1+\frac{\mathrm{Pe}_\theta}{\mathrm{Pe}_c}\right)^{-1}\left[1+\frac{15}{7\pi^2}\,\mathrm{Pe}_\theta\,\sigma_{t\theta}^{-1}\left(1+\frac{\sigma_{t\theta}}{\sigma_{tc}}\right)\left(1+\frac{\mathrm{Pe}_\theta}{\mathrm{Pe}_c}\right)^{-1}\right]^{-1}. \tag{B6}$$

The Peclet numbers $\mathrm{Pe}_{\theta,c}$ are defined as

$$\mathrm{Pe}_{\theta,c}=\frac{4\pi^2}{125}\,\frac{K^2}{\epsilon}\left(\frac{1}{\chi_\theta},\frac{1}{\chi_c}\right). \tag{B7}$$

The turbulent Prandtl numbers $\sigma_{t,\theta}$, σ_{tc} are themselves functions of the corresponding Peclet numbers and satisfy the general equation. Calling $\sigma_t^{-1}\equiv\Sigma$, we have

$$\gamma_2\Sigma=1+\frac{2}{5}\,\pi^2\mathrm{Pe}^{-1}(\gamma_2-\sigma)\left[\left(1+\frac{5}{2\pi^2}\,\mathrm{Pe}\,\frac{\gamma_1\Sigma+1}{\gamma_1+\sigma}\right)^{-\Gamma}-1\right], \tag{B8}$$

with $2\gamma_1=(\gamma^2+4\gamma)^{1/2}-\gamma$, $\gamma_2=\gamma_1+\gamma$, $\gamma=0.3$ and $\Gamma=\gamma_1/\gamma_2$. The Prandtl number $\sigma=\nu/\chi$ is usually $O(10^{-8})$ and thus negligible.

The Peclet number Pe_c can safely be taken much larger than unity, in which case both equation (B4) and equation (B5) become constant. When also $\mathrm{Pe}_\theta \gg 1$, we have

$$\sigma_t=0.72\,, \tag{B9}$$

and thus

$$\frac{\tau_{p\theta}}{\tau}=\frac{\tau_{\mathrm{pc}}}{\tau}=\frac{1}{5}\,(1+\sigma_t^{-1})^{-1}\,,\qquad \frac{\tau_\theta}{\tau}=\frac{\tau_c}{\tau}=\sigma_t\,,\qquad \frac{\tau_{c\theta}}{\tau}=\frac{2}{15}\,\sigma_t\,, \tag{B10}$$

or

$$\frac{\tau_{p\theta}}{\tau}=\frac{\tau_{\mathrm{pc}}}{\tau}=0.0837\,,\qquad \frac{\tau_\theta}{\tau}=\frac{\tau_c}{\tau}=0.72\,,\qquad \frac{\tau_{c\theta}}{\tau}=0.096\,. \tag{B11}$$

These values in turn imply that equations (277) become

$$p_1=0.832\,,\quad p_2=0.545\,,\quad p_3=0.2093\,,\quad p_4=0.0323\,,\quad p_5=0.0155\,,$$
$$p_6=0.2422\,,\quad p_7=0.4799\,,\quad p_8=0.2093\,,\quad p_9=0.8721\,,\quad p_{10}=0.0155\,,$$
$$p_{11}=0.1163\,,\quad p_{1m}=0.168\,,\quad p_{2m}=0.455\,. \tag{B12}$$

Thus

$$a_1=1.0494\,,\quad a_2=0.9239\,,\quad a_3=0.0163\,,\quad a_4=-10.4205\,,\quad a_5=-1.3656\,, \tag{B13}$$

$$b_1=-0.1008\,,\quad b_2=-0.1163\,,\quad b_3=0.5702\,,\quad b_4=-0.9689\,,\quad b_5=-7.2674\,,\quad b_6=-0.0155\,,\quad b_7=-0.7558 \tag{B14}$$

and

$$d_1=0.1111\,,\quad d_2=0.1042\,,\quad d_3=0.0017\,,\quad d_4=-0.3494\,,\quad d_5=-0.4353\,,\quad d_6=-0.0572\,,$$
$$d_7=-0.0007\,,\quad d_8=-1.0938\,,\quad d_9=-0.1435\,,\quad d_{10}=6.2271\,,\quad d_{11}=4.0950\,,\quad d_{12}=0.1034\,,$$
$$d_{13}=1.1857\,,\quad d_{14}=-30.5038\,,\quad d_{15}=-4.0196\,. \tag{B15}$$

The quantities n_0 and c_0 entering equations (280a) and (280b) as well as equations (293) and (294) are then

$$n_0=0.0691\,,\qquad c_0=0.5184\,. \tag{B16}$$

APPENDIX C

THE COEFFICIENTS IN EQUATIONS (286)

The functions a, b, c, and d entering equations (286b)–(286e) are given by

$$
\begin{aligned}
a_1 &= p_{11}[12p_9 + 8p_6 - 30p_6 p_8 - 5p_6(p_{1m} + 3p_{2m})] ,\\
a_2 &= -5(p_4 p_9 + p_6 p_{11} - 2p_4 p_6 p_7)(p_{1m} + 3p_{2m})\\
&\quad + 8(p_4 p_9 + 2p_6 p_{11} - 2p_5 p_6) + 12(p_{11} p_9 + p_{10} p_{11} - p_5 p_6 p_7)\\
&\quad - 30(p_3 p_4 p_9 + p_6 p_8 p_{11} - p_5 p_6 p_8 - p_3 p_5 p_6) ,\\
a_3 &= p_{10}[8p_4 + 12p_{11} - 30p_3 p_4 - 5p_4(p_{1m} + 3p_{2m})] ,\\
a_4 &= -p_6(8 - 30p_8 - 5p_{1m} - 15p_{2m}) - 12(p_9 + p_{11}) ,\\
a_5 &= -p_4(8 - 30p_3 - 5p_{1m} - 15p_{2m}) - 12(p_{10} + p_{11}) ,
\end{aligned} \tag{C1}
$$

$$
\begin{aligned}
&b_1 = p_4 p_7 - p_{11} , \qquad b_2 = -p_{11} , \qquad b_3 = 15p_{2m}^2 + 2p_{1m} - 5p_{1m}^2 - 6p_{2m} ,\\
&b_4 = -30p_4 , \qquad b_5 = -30p_6 , \qquad b_6 = -p_{10} , \qquad b_7 = p_6 p_7 - p_9 ,
\end{aligned} \tag{C2}
$$

$$
\begin{aligned}
d_1 &= p_{11}[p_{2m}^2(p_6 + 6p_9) + 2(p_{1m} - 3p_{2m})p_6 p_8 - p_{1m}^2(p_6 + 2p_9)] ,\\
d_2 &= (p_{1m}^2 - p_{2m}^2)(2p_4 p_7 p_6 - p_6 p_{11} - p_4 p_9)\\
&\quad + 2(p_{1m}^2 - 3p_{2m}^2)(p_4 p_6 p_7^2 - p_{11} p_9 - p_{10} p_{11})\\
&\quad + 2(p_{1m} - 3p_{2m})(p_3 p_4 p_9 + p_6 p_8 p_{11} - p_4 p_6 p_7 p_8 - p_3 p_4 p_6 p_7) ,\\
d_3 &= p_{10}[p_{2m}^2(p_4 + 6p_{11}) + 2(p_{1m} - 3p_{2m})p_3 p_4 - p_{1m}^2(p_4 + 2p_{11})] ,\\
d_4 &= -4p_6 p_{11}(2p_6 + 3p_9) ,\\
d_5 &= 4p_4 p_7 p_6^2(4 + 3p_7) - 4p_4 p_9(3p_{11} + 2p_6) - 4p_6 p_{11}(3p_9 + 3p_{10} + 2p_4 + 2p_6) ,\\
d_6 &= 4p_4^2 p_6 p_7(4 + 3p_7) - 4p_4 p_9(2p_4 + 3p_{11}) - 8p_4 p_6(p_{10} + p_{11}) - 12p_{10} p_{11}(p_4 + p_6) ,\\
d_7 &= -4p_4 p_{10}(2p_4 + 3p_{11}) ,\\
d_8 &= p_{1m}^2(2p_9 + 2p_{11} + p_6) - p_{2m}^2(6p_9 + 6p_{11} + p_6) - 2p_6 p_8(p_{1m} - 3p_{2m}) ,\\
d_9 &= p_{1m}^2(2p_{11} + 2p_{10} + p_4) - p_{2m}^2(6p_{11} + 6p_{10} + p_4) - 2p_3 p_4(p_{1m} - 3p_{2m}) ,\\
d_{10} &= 8p_6^2 + 4p_6(3p_9 + 7p_{11}) + 24p_9 p_{11} ,\\
d_{11} &= -8p_4 p_6 p_7(4 + 3p_7) + 4p_4(4p_6 + 7p_9 + 3p_{11}) + 4p_6(3p_{10} + 7p_{11}) + 24p_{11}(p_9 + p_{10}) ,\\
d_{12} &= 4p_{10}(7p_4 + 6p_{11}) + 4p_4(2p_4 + 3p_{11}) , \qquad d_{13} = 6p_{2m}^2 - 2p_{1m}^2 ,\\
d_{14} &= -24p_9 - 24p_{11} - 28p_6 , \qquad d_{15} = -24p_{11} - 24p_{10} - 28p_4 .
\end{aligned} \tag{C3}
$$

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