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Evan H. Anders,[1] Adam S. Jermyn,[2] Daniel Lecoanet,[3] and Benjamin P. Brown[4]

[1]CIERA, Northwestern University
[2]CCA, Flatiron Institute
[3]ESAM & CIERA, Northwestern University
[4]APS Dept and LASP, University of Colorado, Boulder

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ABSTRACT

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1. INTRODUCTION

Convection is a crucial heat transport mechanism over some fraction of the stellar radius for all stars at some point in the stellar lifetime [CITE]. These motions drive the magnetic dynamo of the Sun and other stars [CITE], leading to the host of emergent phenomena known as stellar activity. Furthermore, convective motions impinge upon nearby stable layers, exciting gravity waves [CITE]. Convection is also responsible for mixing chemical compositions, which becomes increasingly important in the cores of evolved stars [CITE]. A complete and nuanced understanding is therefore crucial for understanding stellar structure, evolution, and observations.

One particular aspect of stellar convection which remains poorly understood even after decades of study is the class of mechanisms generally referred to as "convective overshoot." Useful parameterizations of the way in which convective motions extend beyond the nominally Schwarzschild- or Ledoux- stable boundaries of the convective zone have historically been elusive. Improved models of this "overshoot" could help to resolve many discrepancies between observations and theoretical model. In the Sun and solar-type stars, better models of convective boundaries could help solve the mystery of low abundances of Li at the surface of solar-type stars (Pinsonneault 1997; Dumont et al. 2021), the "solar modeling problem" (Basu & Antia 2004; Bahcall et al. 2005; Zhang & Li 2012; Vinyoles et al. 2017; Asplund et al. 2021) and problems in helioseismic profiles near the base of the convection zone (Christensen-Dalsgaard et al. 2011). There is also ample evidence that we do not understand the nature of convective mixing at the boundary of core convection zones (Claret & Torres 2018; Jermyn et al. 2018; Viani & Basu 2020; Martinet et al. 2021; Pedersen et al. 2021) which could have profound implications for the post-main sequence evolution and remnants of massive stars Farmer et al. (2019); Higgins & Vink (2020). In order to ensure that models can be evolved on fast (human) timescales, 1D stellar evolution codes rely on simple parameterizations of convective overshoot and mixing beyond convective boundaries (Shaviv & Salpeter 1973; Maeder 1975; Herwig 2000; Paxton et al. 2011, 2013, 2018, 2019). While some preliminary work has been done to couple 3D dynamical convective simulations with 1D stellar evolution codes [CITE], these calculations are currently prohibitively expensive to perform e.g., at every timestep in a stellar evolution calculation. In short, an improved theoretical understanding of the behavior of convective boundaries which can inform easy-to-calculate parameterizations is essential.

Convective overshoot and penetration have been studied in laboratory experiments and numerical simulations for decades, and has been reviewed by many authors (Marcus et al. 1983; Zahn 1991; Browning et al. 2004; Rogers et al.

Corresponding author: Evan H. Anders
evan.anders@northwestern.edu

2006; Viallet et al. 2015; Korre et al. 2019). A slew of simulations in Cartesian (Musman 1968; Moore & Weiss 1973; Hurlburt et al. 1986, 1994; Singh et al. 1995; Saikia et al. 2000; Brummell et al. 2002; Rogers & Glatzmaier 2005; Käpylä et al. 2007; Tian et al. 2009; Kitiashvili et al. 2016; Lecoanet et al. 2016; Käpylä et al. 2017; Couston et al. 2017; Toppaladoddi & Wettlaufer 2018; Käpylä 2019; Cai 2020) and spherical (Browning et al. 2004; Rogers et al. 2006; Brun et al. 2017; Pratt et al. 2017; Dietrich & Wicht 2018; Higl et al. 2021) geometry have been studied. Despite this lengthy list of experiments, no consensus model of convective overshoot or penetration has emerged. Throughout the remainder of this work, we will use terminology from this hydrodynamical literature. "Convective penetration" refers to convective motions which extend beyond the nominal Schwarzschild boundary of the convection zone *and* flatten the temperature gradient towards the adiabatic. "Convective overshoot" refers to the motions that extend beyond the convective boundary but do not modify the thermal structure. Our main focus in this paper will be on convective penetration.

Zahn (1991) theorized that convective penetration should depend only on how steeply the radiative temperature gradient varies at the convective boundary. Some simulations (Hurlburt et al. 1994; Rogers et al. 2006) have shown at least partial agreement with this theory. A semianalytic model of solar overshoot (Rempel 2004) also agreed with the early ideas of Zahn. Furthermore, some select simulations have found hints that convective overshoot or penetration may be sensitive the magnitude of the flux in some way (Singh et al. 1998; Hotta 2017; Käpylä 2019). These results suggest that the gradients of fluxes near convective boundaries deserve further examination.

In this work, we design two numerical experiments to test the theory of Zahn (1991). We use a modified incompressible, Boussinesq model to study the simplest possible system, and re-derive his theory in our simplified limit. The results of our simulations are in full agreement with Zahn's theory.

> *Specifically, we find that the depth of convective penetration depends on the gradient of the radiative flux near the convective boundary.*

Thus, the penetration depth can be approximated so long as the radiative conductivity, or likewise the opacity, is known at the convective boundary.

We present these findings as follows. In Sec. 2, we describe our modified Boussinesq equations, re-derive the theory of Zahn (1991), and retrieve predictions for our two experimental designs from that theory. In Sec. 3, we describe our simulation setup and parameters. In Sec. 4, we present the results of these simulations, with a particular focus on the depth of the penetrative regions. In Sec. 5, we create and discuss a solar MESA model which uses this theory to determine the bottom of the solar convection zone. Finally, we discuss how future simulations can put finer constraints on this theory in Sec. 6.

2. THEORY

Throughout this work, we will utilize a modified version of the Boussinesq equations of motion, similar to the model derived by Spiegel & Veronis (1960) and utilized by e.g., Korre et al. (2019). In dimensional form,

$$\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0 \tag{1}$$

$$\partial_t\boldsymbol{u} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u} = -\frac{1}{\rho_0}\boldsymbol{\nabla}p + \frac{\rho'}{\rho_0}\boldsymbol{g} + \nu\boldsymbol{\nabla}^2\boldsymbol{u} \tag{2}$$

$$\partial_t T + \boldsymbol{u}\cdot\boldsymbol{\nabla}T + w\nabla_{\rm ad} + \boldsymbol{\nabla}\cdot[-k\boldsymbol{\nabla}\overline{T}] = \chi\boldsymbol{\nabla}^2 T' + Q \tag{3}$$

$$\frac{\rho'}{\rho_0} = -|\alpha|T. \tag{4}$$

In this model, ρ_0 is a (constant) background density and ρ' are fluctuations which act only in the buoyancy force and varies linearly with the temperature T according to the coefficient of thermal expansion, $\alpha = \partial\ln\rho/\partial T$. Furthermore, $\boldsymbol{u}$ is the velocity vector, ν and χ are respectively the viscous and thermal diffusivity, Q is a bulk internal heating term [CITE], and $\nabla_{\rm ad}$ is the adiabatic temperature gradient (we define $\nabla_{\rm ad}$ as a positive value to align with stellar structure conventions; this means marginal stability is achieved when $\partial_z T = -\nabla_{\rm ad}$). We modify the model of Spiegel & Veronis (1960) to allow the mean temperature profile $\overline{T}$ to carry a radiative flux $F_{\rm rad} = -k\boldsymbol{\nabla}\overline{T}$, where k is a radiative diffusivity which can vary with height. We assume that the classical thermal diffusion term $\chi\boldsymbol{\nabla}^2 T'$ only acts on the fluctuations away from the mean temperature profile, $T' \equiv T - \overline{T}$.

The basis of the theory of Zahn (1991) is that the size of the convection zone is determined by the horizontally-averaged energetics and buoyancy breaking. We assume convection reaches a time-stationary, equilibrium state; we vertically integrate Eqn. 3 and take a horizontal average to find

$$F_{\text{tot}} = F_{\text{rad}} + F_{\text{conv}} = \int Q dz + F_{\text{bot}}, \tag{5}$$

with $F_{\text{conv}} = \overline{wT}$ and F_{bot} the flux at the bottom of the convective domain and F_{tot} the total flux, which can vary in height according to integral of Q. We next assume that convection penetrates above the nominal schwarzschild boundary of the convection zone and mixes the temperature gradient towards the adiabatic in that region. Thus, in that region, the convective flux can be found,

$$F_{\text{conv}} = F_{\text{tot}} - F_{\text{rad,ad}} = F_{\text{tot}} - k\boldsymbol{\nabla}_{\text{ad}}. \tag{6}$$

By definition, in this region, $\boldsymbol{\nabla}_{\text{ad}} > \boldsymbol{\nabla}_{\text{rad}}$, where $\boldsymbol{\nabla}_{\text{rad}} = F_{\text{tot}}/k$, so this requires that $F_{\text{conv}} < 0$ in the convective penetration region. We next assume that the temperature and velocity are highly correlated in the penetrative region with very similar horizontal fluctuations,

$$w(x, y, z) = W(z)h(x, y), \qquad T'(x, y, z) = \delta T(z)h(x, y). \tag{7}$$

We here assume that $\overline{h} = 0$ and $\overline{h^2} \neq 0$. We can then express the convective flux in terms of these vertically-varying profiles and an average over the horizontal structure of the flows,

$$F_{\text{conv}} \equiv \overline{wT} = \overline{h^2}\, W(z)\, \delta T(z). \tag{8}$$

In the penetrative region, since $F_{\text{conv}} < 0$, $W(z)$ and $\delta T(z)$ must be oppositely signed and the convective flows should eventually come to a stop through buoyancy breaking. This is achieved through a balance between advection and buoyancy in the vertical momentum equation (Eqn. 2 with Eqn. 4),

$$\frac{1}{2}\frac{dw^2}{dz} = |\alpha| g T'. \tag{9}$$

Multiplying both sides by $h(x, y)$, taking a horizontal average, and then substituting $\delta T(z)$ using Eqn. 8, we retrieve a simple ordinary differential equation,

$$\frac{\overline{h^3}}{6|\alpha|g\overline{h^2}} dW^3 = F_{\text{conv}} dz. \tag{10}$$

This equation can be integrated over the depth of the convection zone from $W = 0$ to $W = W_0$ at the convective boundary, as well as over the penetration zone from $W = W_0$ to where $W = 0$. We assume however that the horizontal structure h of the flux-carrying flows is not identical in the convection zone (CZ) and the penetration zone (PZ). Integrating Eqn. 10 over the CZ and PZ and taking a ratio of these two equations, we find

$$-\frac{(\overline{h}^3/\overline{h^2})_{\text{PZ}}}{(\overline{h^3}/\overline{h^2})_{\text{CZ}}} = \frac{\int_{\text{PZ}} F_{\text{conv}} dz}{\int_{\text{CZ}} F_{\text{conv}} dz}. \tag{11}$$

In order to move further with this theory, it is necessary to specify the vertical shape of F_{conv}, which is in turn set by Q, ∇_{ad}, and k. We will assume that ∇_{ad} has a constant value and that the internal heating Q is localized near the bottom of the CZ so that a constant convective flux F_{cz} is carried in the bulk convection zone. As a result, the vertical profile of F_{rad} and F_{conv} is determined completely by the behavior of $k(z)$ near the convective boundary. We will study two cases in this work: a discontinuous jump in $k(z)$ at the convective boundary, and a piecewise-linear profile of $k(z)$ whose derivative may be discontinuous at the convective boundary.

2.1. *Case I: Discontinuous radiative conductivity*

We first consider a radiative conductivity $k(z)$ which is discontinuous, with a value of k_{CZ} in the convection zone and larger value k_{RZ} in the PZ and radiative zone (RZ). The values of k are chosen so that the convective flux follows

$$F_{\text{conv}}(z) = \begin{cases} F_{\text{cz}} & z \leq L_{\text{cz}}, \\ -\mathcal{P}_D^{-1} F_{\text{cz}} & z > L_{\text{cz}} \end{cases}. \tag{12}$$

Here, $\mathcal{P}_D^{-1}$ is the "penetration parameter" (subscript D for discontinuous case). Plugging this functional form of the flux into Eqn. 11, and integrating the convection zone from $z = 0$ to $z = L_{\rm cz}$ and the penetration zone from $z = L_{\rm cz}$ to $z = L_{\rm cz} + \delta_{\rm p}$,

$$\frac{\delta_{\rm p}}{L_{\rm cz}} = \mathcal{P}_D \frac{(\overline{h}^3/\overline{h^2})_{\rm PZ}}{(\overline{h^3}/\overline{h^2})_{\rm CZ}}. \tag{13}$$

We then see that the size of the penetration region is linearly proportional to $\mathcal{P}_D$ and is a function of the horizontal structure of the convective dynamics in the PZ and the CZ. This makes sense; As $\mathcal{P}_D$ grows, the magnitude of $F_{\rm conv}$ in the PZ shrinks, and so too does the breaking force of buoyancy.

2.2. *Case II: Piecewise linear radiative conductivity*

We next assume that $k(z)$ is not discontinuous at the CZ-PZ boundary, but that its derivative may be. As a result, the convective flux in the vicinity of the boundary takes the form

$$F_{\rm conv}(z) = \begin{cases} (\partial_z k)_{\rm cz} \nabla_{\rm ad}(L_{\rm cz} - z) & z \leq L_{\rm cz} \\ -\mathcal{P}_L^{-1}(\partial_z k)_{\rm cz}\nabla_{\rm ad}(z - L_{\rm cz}) & z > L_{\rm cz} \end{cases}, \tag{14}$$

where we assume that $(\partial_z F_{\rm rad})_{\rm cz} = (\partial_z k)_{\rm cz}\nabla_{\rm ad}$ is a constant. Again, solving Eqn. 11 with this functional form of the flux, we retrieve

$$\frac{\delta_{\rm p}}{L_{\rm cz}} = \sqrt{\mathcal{P}_L \frac{(\overline{h}^3/\overline{h^2})_{\rm PZ}}{(\overline{h^3}/\overline{h^2})_{\rm CZ}}}, \tag{15}$$

which is identical to the prediction of Zahn (1991) when we take $\mathcal{P}_L = 1$. In this work, we will test the predictions of Eqns. 15 and 13. Our aim is to see if the predicted scalings with $\mathcal{P}$ are realized in direct numerical simulations, and to measure preliminary values for $\frac{(\overline{h}^3/\overline{h^2})_{\rm PZ}}{(\overline{h^3}/\overline{h^2})_{\rm CZ}}$ in local simulations.

3. SIMULATION DETAILS

We nondimensionalize Eqns. 1-4 on the length scale of the convection zone, the timescale of freefall across that convection zone, and the temperature scale of the internal heating over that freefall time,

$$\begin{gathered} T^* = (\Delta T)T = Q_0 \tau T, \qquad \partial_{t^*} = \tau^{-1}\partial_t = \left(\frac{\alpha g Q_0}{L_{\rm cz}}\right)^{1/3}\partial_t, \qquad \boldsymbol{\nabla}^* = L_{\rm cz}^{-1}\boldsymbol{\nabla}, \qquad \boldsymbol{u}^* = u_{\rm ff}\boldsymbol{u} = \left(\alpha g Q_0 L_{\rm cz}^2\right)^{1/3}\boldsymbol{u}, \\ k^* = (L_{\rm cz}^2\tau^{-1})k, \qquad Q^* = Q_0 Q, \qquad \mathcal{R} = \frac{u_{\rm ff}L_{\rm cz}}{\nu}, \qquad \mathrm{Pr} = \frac{\nu}{\chi}. \end{gathered} \tag{16}$$

Here, quantities with $*$ (e.g., T^*) refer to the "dimensionful" quantities of Eqns. 1-4, and going forward quantities without these (e.g., T) will be dimensionless. The equations of motion are therefore

$$\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0 \tag{17}$$

$$\partial_t\boldsymbol{u} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u} = -\boldsymbol{\nabla}\varpi + T\hat{z} + \mathcal{R}^{-1}\boldsymbol{\nabla}^2\boldsymbol{u} \tag{18}$$

$$\partial_t T + \boldsymbol{u}\cdot\boldsymbol{\nabla}T + w\boldsymbol{\nabla}_{\rm ad} + \boldsymbol{\nabla}\cdot[-k\boldsymbol{\nabla}\overline{T}] = (\mathrm{Pr}\mathcal{R})^{-1}\boldsymbol{\nabla}^2 T' + Q. \tag{19}$$

We construct a domain in the range $z \in [0, L_z]$ where in this work we choose $L_z \geq 2$ so that the domain contains at least two convection zone length scales according to the Schwarzschild criterion. We decompose the temperature field into a background and fluctuations, $T(x, y, z, t) = T_0(z) + T_1(x, y, z, t)$. For boundary conditions, we impose impenetrable, no-slip boundary conditions at the top and bottom of the box so that $\boldsymbol{u} = 0$ at $z = [0, L_z]$. We also impose a fixed-flux boundary at the bottom of the box ($\partial_z T_1 = 0$ at $z = 0$) and a fixed temperature boundary at the top of the domain ($T_1 = 0$ at $z = L_z$).

We impose an order unity internal heating which spans one fifth of the convection zone,

$$Q = \begin{cases} 0 & z < 0.1 \text{ or z} \geq 0.1 + \delta_{\rm H}, \\ |Q_{\rm mag}| & 0.1 \leq z \leq 0.1 + \delta_H \end{cases}. \tag{20}$$

The integrated value of the flux through the system from the heating is therefore $F_H(z > 0.1 + \delta_H) = \int_0^z Q_{\rm mag} dz = Q_{\rm mag}\delta_H$. Throughout this work we choose $Q_{\rm mag} = 1$ and $\delta_H = 0.2$ so $F_H = 0.2$. We offset this heating from the bottom boundary to $z = 0.1$ to avoid heating within the bottom impenetrable boundary layer where velocities go to zero and k is small; this prevents strong temperature gradients from establishing there. We assume that the (adiabatic) temperature gradient at the bottom boundary carries some flux, $F_{\rm bot} = \zeta F_H$ and we choose $\zeta = 10^{-3}$ so that most of the flux in the convection zone is carried by the convection.

In our equations, we expect the volume-average convective velocities to depend on the magnitude of the heating, $\langle \boldsymbol{u} \rangle \approx Q_{\rm mag}^{1/2} \approx 1$, so the characteristic convective frequency $f_{\rm conv} \approx \langle \boldsymbol{u} \rangle L_{\rm cz} \approx 1$. We want to allow the stiffness of the radiative-convective interface to be a control parameter. The stiffness is defined,

$$\mathcal{S} \equiv \frac{N^2}{f_{\rm conv}} \approx N^2, \tag{21}$$

where N^2 is the Brunt-Väisälä frequency in the radiative zone. In our nondimensionalization, $N^2 = \nabla_{\rm ad} - \nabla_{\rm rad}$ where $\nabla_{\rm rad} = F_{\rm tot}/k$, so by choosing a value of the stiffness we set the magnitude of the background temperature gradient, T_0 which in turn sets the value of k in the radiative zone.

The crucial place in which our model differs from that of prior work is that we define a "penetration parameter," $\mathcal{P}$, which determines the size of the convective penetration region. We define

$$\mathcal{P} = -\frac{F_{\rm conv}|_{\rm CZ}}{F_{\rm conv}|_{PZ}}, \tag{22}$$

where $F_{\rm conv}|_{PZ}$ is the negative convective flux carried in a perfectly adiabatic convective penetration region. We construct our experiments so that $\mathcal{P}$ and $\mathcal{S}$ can be varied separately. We suspect that many past experiments have implicitly set $\mathcal{P} \approx \mathcal{S}^{-1}$.

Aside form $\mathcal{S}$ and $\mathcal{P}$, the two remaining control parameters that control our experiments determine the degree of turbulence. The value of $\mathcal{R}$ roughly corresponds to the value of the peak Reynolds number measured in the simulations, and we set the ratio of the diffusivities $\mathrm{Pr} = 0.5$ throughout this work. Astrophysical convection is in the limit of $\mathrm{Pr} \ll 1$; we choose a modest value of Pr which slightly separates the scales between thermal and viscous structures while still allowing us to achieve convection with large Reynolds and Péclet numbers.

3.1. *Case I: Discontinuous radiative conductivity*

Most of the simulations in this paper study simulations with a discontinuous radiative conductivity,

$$k_D(z) = \begin{cases} k_{\rm CZ} & z < 1 \\ k_{\rm RZ} & z \geq 1 \end{cases}. \tag{23}$$

Leaving $\mathcal{S}$ and $\mathcal{P}_D$ as free parameters and requiring that the adiabatic gradient can carry the $F_{\rm bot}$ at $z = 0$ and that the radiative gradient can carry the flux for $z \geq 1$ specifies this system fully,

$$k_{\rm RZ} = \frac{\delta_H}{\mathcal{S}\mathcal{P}_D}, \qquad k_{\rm CZ} = k_{\rm RZ}\frac{1}{1 + \zeta + \mathcal{P}_D^{-1}}, \qquad \nabla_{\rm ad} = Q_{\rm mag}\mathcal{S}\mathcal{P}_D(1 + \zeta + \mathcal{P}_D^{-1}), \qquad \nabla_{\rm rad} = \nabla_{\rm ad} - Q_{\rm mag}\mathcal{S}. \tag{24}$$

We study three sweeps through the ($\mathcal{P}_D$, $\mathcal{S}$, $\mathcal{R}$) parameter space in this paper (one in which we vary each parameter while holding the other parameters constant). We use "Reference values" of $\mathcal{P}_D = 4$, $\mathcal{S} = 10^3$, and $\mathcal{R} = 400$; all of our parameter space sweeps pass through this point in the three-dimensional parameter space. As in section 2.1, we expect $\delta_p \propto \mathcal{P}_D$.

3.2. *Case II: Piecewise linear radiative conductivity*

We additionally study a select few simulations where the radiative conductivity's gradient is piecewise discontinuous,

$$\partial_z k = \partial_z k_0 \begin{cases} 1 & z < 1 \\ \mathcal{P}_L^{-1} & z \geq 1 \end{cases} \tag{25}$$

Since k varies with height, the value of $\mathcal{S}$ and $\mathcal{P}$ also vary with height; we specify their values at $z = 2$. by this choice, we require

$$\partial_z k_0 = \frac{\delta_H}{L_{\rm cz}\mathcal{S}\xi}, \qquad k_b = \frac{\delta_H \zeta}{\mathcal{S}\xi}, \qquad \nabla_{\rm ad} = Q\mathcal{S}\xi, \tag{26}$$

where $\xi \equiv 1 + \mathcal{P}_L(1+\zeta)$. In these simulations, we hold $\mathcal{S} = 10^3$ and $\mathcal{R} = 800$ while varying $\mathcal{P}_L$. As in section 2.2, we expect $\delta_p \propto \mathcal{P}_L^{1/2}$.

3.3. *Numerics*

We time-evolve equations 17-19 using the Dedalus pseudospectral solver (Burns et al. 2020)[1] using timestepper RK443 [CITE]. All fields are represented as spectral expansions of n_z Chebyshev coefficients in the vertical (z) direction and as (n_x,n_y) Fourier coefficients in the horizontal (x,y) directions; our domains are therefore horizontally periodic. The aspect ratio of our domains is two so that $x \in [0, L_x]$ and $y \in [0, L_y]$ with $L_x = L_y = 2L_z$. To start our simulations, we add random noise temperature perturbations with a magnitude of 10^{-3} to a background temperature profile $\overline{T}$; we discuss the choice of $\overline{T}$ in appendix A. We produce the figures in this paper using matplotlib [CITE]. All of the Python scripts used to run the simulations in this paper and to create the figures in this paper are publicly available in a git repo, found at [CITE].

4. RESULTS

5. A MODIFIED SOLAR MODEL

6. DISCUSSION

1 We'd like to thank

APPENDIX

A. ACCELERATED EVOLUTION

B. TABLE OF SIMULATION PARAMETERS

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