Chemical Mixing Induced by Internal Gravity Waves in Intermediate-mass Stars

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Abstract

Internal gravity waves can cause mixing in the radiative interiors of stars. We study this mixing by introducing tracer particles into 2D hydrodynamic simulations. Following the work of Rogers & McElwaine, we extend our study to different masses (3, 7, and 20 $M_{\odot}$) and ages (ZAMS, midMS, and TAMS). The diffusion profiles of these models are influenced by various parameters such as the Brunt–Väisälä frequency, density, thermal damping, the geometric effect, and the frequencies of waves contributing to these mixing profiles. We find that the mixing profile changes dramatically across age. In younger stars, we noted that the diffusion coefficient increases toward the surface, whereas in older stars the initial increase in the diffusion profile is followed by a decreasing trend. We also find that mixing is stronger in more massive stars. Hence, future stellar evolution models should include this variation. In order to aid the inclusion of this mixing in 1D stellar evolution models, we determine the dominant waves contributing to these mixing profiles and present a prescription that can be included in 1D models.

1. Introduction

Chemical mixing plays a major role in stellar evolution. It can transport the chemical elements generated in the nuclear burning region to the surface, creating observed abundance variations. In massive stars, it influences the lifetime of the star by bringing fresh fuel into the burning region leading to a more massive helium core. Standard stellar evolution theory considers few transport mechanisms or instabilities in the stable radiative zone, and yet, is very successful in explaining many of the observed properties of stars, such as the mass–luminosity relation, the existence of the main sequence, and the evolution toward the giant branch (Zahn 1994).

However, a series of observed anomalies have suggested the need to consider additional mixing processes near the convective-radiative boundary and in the radiation zone; some among them are the N/C and $^{13}$C/$^{12}$C enrichment in low-mass stars on the upper red giant branch (RGB; Charbonnel 1994), N abundances in B stars (Gies & Lambert 1992), He abundances in O and B stars near the main sequence (Liubimkov 1975; Lyubimkov 1977, 1989), He discrepancy in O type stars (Herrero et al. 1992), He and N enrichments in OB supergiants (Walborn 1976), Li abundances in Population II low-mass giants (Pilachowski et al. 1993), and C, N, O abundances in globular cluster giants (Kraft 1994). Some of the additional physical processes that plausibly cause mixing in these regions are convective overshoot at the convective-radiative boundary (Zahn 1991; Herwig 2000), rotation (Zahn 1992; Maeder & Zahn 1998; Heger et al. 2000; Maeder & Meynet 2000), shear-induced turbulence (Zahn 1992; Talon & Zahn 1997; Maeder 2003; Mathis et al. 2004; Kulenthirarajah & Garaud 2018; Mathis et al. 2018; Park et al. 2020) internal gravity waves (IGWs; Press 1981; Garcia Lopez & Spruit 1991; Charbonnel & Talon 2007; Rogers & McElwaine 2017; hereafter RM17), and magnetic fields (Heger et al. 2005; Maeder & Meynet 2005). Over the years stellar evolution models focused on the inclusion of these additional mechanisms and using the different prescriptions given by Kippenhahn et al. (1970), Endal & Sofia (1976), Zahn (1992), Maeder & Zahn (1998), Herwig (2000), Spruit (2002), etc. These mechanisms are implemented in stellar evolution models such as MESA, FRANCE, STERN, GENEc, and STAREVOL (Siess et al. 2000; Eggenberger et al. 2008; Brett et al. 2011; Paxton et al. 2011; Chiefi & Limongi 2013; Paxton et al. 2013, 2015, 2018, 2019). These models were successful in explaining many observed anomalies such as the observed nitrogen enhancement in the early universe (Hirschi 2007), surface enrichment of He and C in main-sequence stars (Heger & Langer 2000), the blue side of the Li dip, and low Li abundances in subgiants (Palacios et al. 2003).

Mixing by convective overshooting is one of the oldest problems studied in stellar astrophysics. Overshooting occurs when the motion of matter extends beyond the boundary determined by either the Ledoux or Schwarzschild stability criteria and continues into the stable layer. Convective matter overshoots outward from the convective core to the radiative envelope in stars more massive than the Sun, while for solar-type stars (0.85 $\leq M/ M_{\odot} \leq 1.2$) the process is inward, from the convective envelope, leading it to also be called undershooting; in either case, the phenomenon can play an important role in stellar evolution. Studies by Alongi et al. (1991) showed that convective undershooting modifies the chemical abundance and also explains the bump in the luminosity function of RGB stars in globular clusters. Convective core overshooting extends the lifetime of core H burning by increasing the availability of fuel within the core, leading to a more massive He core and enhancing the luminosity in the later evolutionary track (Maeder 1976; Schroder et al. 1997).
With the recent advancements in asteroseismology, it has been found that the distinct signatures in the period spacings of gravity mode spectra can provide information on the extent to which chemical elements are mixed and the nature of mixing in the transition layer between a convective and radiative zone and in the radiative interiors (Monteiro et al. 2000; Noels et al. 2010; Christensen-Dalsgaard et al. 2011; Pedersen et al. 2018; Deheuvels 2020). Asteroseismic studies also reveal a more massive core than expected by the standard stellar evolution theory suggesting the need for extra mixing in the earlier evolutionary stages (Charpinet et al. 2011; Giammichele et al. 2018). Calibration of mixing profiles based on asteroseismic modeling provides an important input for the improvement of stellar evolution models (Pedersen et al. 2021).

Rotation strongly influences stellar evolution and is considered to be a major ingredient in stellar models and may account for the observed abundance anomalies in massive stars. Eddington (1925) proposed that meridional circulation can induce mixing in stellar interiors and later studies have indicated that this circulation could explain the C to N ratio in many early-type stars (Paczyński 1973). Internal mixing by rotation could explain the Li and Be abundances in low-mass stars (Pinsonneault et al. 1989), N/C enhancement seen in OB stars (Lyubimkov 1996), the overabundance of He in O stars (Herrero et al. 1992), Li abundances in evolved stars (Canto Martins et al. 2011), and the surface enrichment of O7–8 giants (Martins et al. 2017). More mixing is contributed by differential rotation that generates turbulent motions in stellar interiors, which give rise to various rotationally induced instabilities like Goldreich–Schubert–Fricke instability (Goldreich & Schubert 1967), ABD instability (Spruit et al. 1983), and shear instabilities (Zahn 1992; Bruggen & Hillebrandt 2001; Prat & Lignieres 2013; Garaud 2020; Chang & Garaud 2021; Park et al. 2021; Prat & Mathis 2021). These instabilities play a major role in mixing the CNO materials close to the surface in subgiant and giant branch models (Pinsonneault et al. 1989). Although models that included rotation could explain many of the observed anomalies, they failed to account for some of the observed features like the abundance anomalies in red giants (Palacios et al. 2006), the flat solar rotational profile measured by helioseismology (Brown et al. 1989; Mattig & Zahn 1997), and the nitrogen abundance in massive stars (Brott et al. 2011; Aerts et al. 2014). Models including rotationally induced transport mechanisms such as the meridional circulation and shear instabilities predicted a rapidly rotating stellar core in subgiants (Ceillier et al. 2013), red giants (Eggenberger et al. 2012; Marques et al. 2013; Cantiello et al. 2014) and γ Doradus main-sequence intermediate-mass stars (Ouazzani et al. 2019) contradicting the core rotation revealed by asteroseismic observations. This also suggests the need to consider additional transport mechanisms in the stellar interiors.

Apart from rotation, magnetism could also be a source of extra mixing in stars. Maeder & Meynet (2005) studied a magnetic model with the inclusion of meridional circulation and found a significant enrichment in N and He compared to rotating models without an internal magnetic field. Later studies argued that it is likely for magnetic buoyancy to transport materials in AGB and RGB stars (Busso et al. 2007; Nordhaus et al. 2008; Vescovi et al. 2020).

Recently, thermohaline mixing, which occurs because of the molecular weight inversion, was proposed to influence the surface abundances in low-mass red giants (Charbonnel & Zahn 2007; Eggleton et al. 2006). This could explain the 3He, Li, C, and N abundance in the low-mass stars above the RGB bump and the high Li abundances in low-mass AGB stars. (Charbonnel & Lagarde 2010; Stancliffe 2010; Lagarde et al. 2011). Cantiello & Langer (2010) investigated the role of this mixing along with rotational mixing and internal gravity fields in low-mass stars. They confirmed that this mixing could explain the decrease in He abundance in RGB stars with an initial mass less than 1.5M☉.

IGWs can also cause extra mixing in the radiative interiors (Press 1981; Montalbán & Schatzman 1993; Montalbán 1994; Montalbán & Schatzman 1996; Rogers & McElwaine 2017). IGWs are naturally occurring waves that propagate in stably stratified fluids with gravity as the restoring force. In stars, IGWs are generated at the convective–radiative interface either by bulk excitation through red Reynolds stress (Kumar et al. 1999; Belkacem et al. 2009; Samadi et al. 2010; Leconte & Quataert 2013) or by direct excitation through red plumes (Hurlburt et al. 1986; Montalbán & Schatzman 2000; Pincon et al. 2016). Press (1981) considered that the turbulent motion in the convective zone is characterized by eddies and studied the turbulent mixing by IGWs in stars with a convective envelope. Press (1981) proposed that IGWs could explain the solar neutrino discrepancy. Garcia Lopez & Spruit (1991) argued that the turbulence generated by the IGWs propagating in radiative interiors can explain the Li gap in F-type stars. Montalbán (1994) used plume morphology based on convective penetration (Zahn 1991) to describe the perturbation at the boundary and explained the observed Li abundance in the Sun (Montalbán & Schatzman 1996). RM17 studied the mixing by IGWs in massive stars and determined that it can be treated as a diffusive process with the diffusion profile set by the square of the wave amplitude. Theoretical models, including rotation and IGWs, were successful in providing insight into the surface Li abundance in low-mass stars (Talon & Charbonnel 2005; Charbonnel & Talon 2007).

In this paper, we focus on the mixing by IGWs in stars with a convective core and a radiative envelope. We extend the studies of RM17 to obtain the mixing profiles for stars of higher masses and different ages. We achieve this by running 2D simulations using a background reference model obtained from Modules for Experiments in Stellar Astrophysics (MESA; Paxton et al. 2011, 2013, 2015, 2018, 2019). We then determine the dominant wave contributing to these mixing profiles using the prescription given by RM17. Section 2 explains the 2D simulations and the tracer particle simulations done to obtain the mixing profiles. Section 3 introduces our results on the mixing profiles for the different models, including a brief description of the theoretical calculations used in this work, and Section 4 summarizes our findings.

2. Background and Numerical Methods

2.1. Two-dimensional Simulation

We generated the stellar models for three masses (3, 7, and 20 M☉) at three ages (zero age main sequence (ZAMS), core hydrogen mass fraction, XH = 0.7), mid-main sequence (midMS), XH = 0.35), and terminal age main sequence (TAMS), XH = 0.01) from MESA. We set the mixing length parameter to 1.8 and the convective overshoot profile to exponential, implemented the mass loss through van Loon
stellar wind scheme and considered zero rotation in our models. The inlists used to generate the models are given in Zenodo at doi:10.5281/zenodo.2596370.

We calculated the Brunt–Väisälä frequency, $N$ based on the work of Rogers et al. (2013),

$$N^2 = \frac{\bar{g}}{\bar{T}} \left( \frac{dT}{d\bar{T}} - (\gamma - 1)\bar{\rho} \right),$$

where $\bar{g}$, $\bar{T}$, $\gamma$, and $\bar{\rho}$ are the reference state gravity, temperature, adiabatic index, and negative inverse density scale height. The location of the convective–radiative interface is determined by the sign of the Brunt–Väisälä frequency, where

$$N^2 > 0$$

is the radiation zone and

$$N^2 < 0$$

is the convection zone. The background density and the Brunt–Väisälä frequency profiles of all the models considered in this work are shown in Figure 1.

To study IGWs in stellar interiors, we solved the Navier–Stokes equations in the anelastic approximations using 2D hydrodynamic simulations considering an equatorial slice of the star with stress-free, isothermal, and impermeable boundary conditions (Rogers et al. 2013). The numerical model followed in this work is similar to that of Rogers et al. (2013) and the 2D simulations are run by R.P. Ratnasingam (more details on the simulations can be found in Ratnasingam 2020, R. P. Ratnasingam et al. 2022 in preparation).

Figure 2 shows the time snapshots of vorticity for all the models considered in this work.

The thermal diffusivity ($\kappa$) and viscosity ($\nu$) are set to constant values shown in Table 1. Our objective was to attain the highest Reynolds number,

$$Re = \frac{v_{rms}L}{\nu},$$

for each model studied. Here $v_{rms}$ is the root mean squared velocity averaged over the convection zone and $L$ is the characteristic length scale (the radial extent of the convection zone in this case). We also aimed to attain convective velocity ratios for different masses from our simulations which are comparable to those predicted by the mixing-length theory (MLT) velocities in MESA for any given age. (We chose to compare across masses as the uncertainties in the MLT velocities in MESA are larger across ages.) We, therefore, chose the values such that the above are satisfied while maintaining numerical stability. The simulation is run for an average time of approximately, $2.7 \times 10^7$ s for the models studied.

The simulation domain extends up to 90% of the total stellar radius for all the 3 and 7 $M_\odot$ models and up to 80% of the total stellar radius for all the 20 $M_\odot$ models. The cutoff radius is determined such that the density does not vary more than $\sim 6$ orders of magnitude as we move from the inner to the outer boundary to maintain numerical stability. As evident from Figure 1, this is satisfied only until $0.9R_*$ for the 3 and 7 $M_\odot$ models and up to $0.8R_*$ for the 20 $M_\odot$ models. We, therefore, chose these respective domains for our simulations. For our analysis, we chose the velocity data from a time, $4 \times 10^6$ s for all the 3 and 7 $M_\odot$ models and from $6 \times 10^6$ s for all the 20 $M_\odot$ models. The total time window considered is given in terms of convective turnover times in Table 1. We then used this velocity data which is saved at a regular time interval to study the mixing by IGWs in stellar interiors.

### 2.2. Tracer Particle Simulation

To measure the mixing by IGWs in stellar interiors, we introduce $N$ tracer particles into our simulation and track them over time $T$. This procedure is carried out in post-processing and we use the relations given by RM17 to calculate the diffusion coefficient $D(r, \tau)$ at radius $r$, for a given time difference, $\tau$.

$$D(r, \tau) = \frac{Q(r, \tau)}{2\tau n(r, \tau)} - \frac{P(r, \tau)^2}{2\tau n(r, \tau)^2},$$

where $n(r, \tau)$, is the number of sub-trajectories starting at $r$ with a duration of $\tau$, $P(r, \tau)$ is the sum of the lengths of the sub-trajectories and $Q(r, \tau)$ is the sum of the square of these sub-trajectories. More details on the calculation of $n$, $P$, $Q$, and $D(r, \tau)$ can be found in RM17.

We then plotted the diffusion coefficients calculated using the above equation as a function of radius. We varied different parameters such as the number of particles, radial grid size, and velocity time steps in our simulation to check for numerical convergence and obtained the diffusion coefficient for each set of parameters. Figure 3 shows the radial diffusion profiles with (a) different velocity time steps $\Delta \tau$, (b) different radial grid sizes, and (c) different numbers of particles $N$, for a 7 $M_\odot$, ZAMS model. In each case, the profiles appear converged with respect to the variables changed. We extended the same treatment to all the other stellar models and found the radial diffusion profile to be already converged for a time resolution of 1000 s, radial resolution of 500, and particle resolution of 10,000. This is consistent with RM17, who found the mixing profile robust to parameter changes. Henceforth, we choose these values for all our further analysis and obtain the radial diffusion profile at a time difference$^6$ of $1.3 \times 10^7$ s for all three masses.

### 3. Results

We found the general trend of the diffusion profile to be increasing from the convective–radiative interface toward the surface as can be seen in Figure 3 consistent with the results of RM17. However, as the star ages, its properties, such as the density and the change in the Brunt–Väisälä frequency, are evident as shown in Figure 1. These changes also affect the diffusion coefficient. Here, we investigated the dependence of age and mass on the radial diffusion profiles.

$^5$ We found that the IGWs show a steady-state evolution from this value in our 2D hydrodynamic simulation. Steady-state evolution refers to a state where the amplitudes of the IGWs remain constant over time.

$^6$ The smaller $\tau$ has contributions from more time steps compared to a larger value of $\tau$. As an example, consider $T = 100$ with time step $1$. Then, for $\tau = 5$, it has contributions from $5 - 0$, $6 - 1$, $7 - 2$, and so on, whereas $\tau = 97$ can result only from $100 - 3$, $99 - 2$, and $98 - 1$. 

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3.1. Age Dependencies

Figure 4 shows the radial diffusion profiles at ZAMS (blue), midMS (green), and TAMS (pink) for the 3, 7, and 20 $M_{\odot}$ models. In general, we find that the mixing profile varies significantly across the ages for all the masses studied. The amplitude of the diffusion profile depends on several factors such as the wave driving, density stratification, thermal diffusivity, the Brunt–Väisälä frequency, and the geometric effect. Among these, density stratification and thermal diffusivity dominate in both ZAMS and midMS stars; hence, the diffusion coefficient increases with stellar radius following the density stratification modulated by the thermal diffusion.

However, the mixing profile at TAMS shows an increasing trend from the convective–radiative interface followed by a decreasing trend toward the surface, which is considerably different from that of the younger stars. To understand this behavior, we looked at the following second-order differential equation for wave propagation,

\[
0 = \frac{\partial^2 \alpha}{\partial r^2} + \left[ \frac{N^2}{\omega^2} - 1 \right] \frac{m^2}{r^2} \alpha + \frac{1}{2} \left[ \frac{\partial h_{\rho}}{\partial r} - h_{\rho}^2 + \frac{h_{\rho}}{r} \right] \alpha + \frac{1}{4 r^2} \alpha, \tag{6}
\]

which is obtained by reducing the linearized 2D hydrodynamic equations considering no thermal or viscous diffusion with $\alpha = \nu \bar{\rho}^2 r^2$ and $m$ is the 2D Fourier basis wavenumber. In younger stars, the first two terms dominate over most of their
radii. However, in older stars, the density term,
\[
\frac{1}{2} \left( \frac{\partial h_\rho}{\partial r} - \frac{h_\rho^2}{r} + \frac{h_\nu}{r} \right),
\]
becomes dominant at larger radii.

We define turning point as the radius at which the ratio of the oscillatory term,
\[
\left[ \frac{N^2}{\omega^2} - 1 \right] \frac{m^2}{r^2},
\]
becomes equal to 1 (Ratnasingam et al. 2020) and it is located at a lower fraction of the total radius in older stars. Waves lose their wave-like behavior when this ratio is less than 1, and as a result, they experience extra damping. This leads to waves becoming evanescent toward the surface and leads to the diffusion profile we see in Figure 4. The shaded region in the plot indicates the location of turning points for the TAMS models using the range of frequencies (4–14 μHz) determined in Section 3.4.

Another factor contributing to the diffusion profiles of TAMS models is the Brunt–Väisälä frequency spike near the convective–radiative interface left behind by a steep composition gradient as the star evolves from ZAMS (Figure 1). This peak damps many waves near the convective–radiative interface and traps the higher frequencies resulting in fewer waves contributing to mixing, thereby leading to a decrease in the diffusion coefficient. In general, TAMS models have a significantly reduced diffusion coefficient than the ZAMS and midMS models.
3.2. Mass Dependencies

Figure 5 shows the diffusion profiles as a function of radius for 3 $M_\odot$ (green), 7$M_\odot$ (pink), and 20 $M_\odot$ (blue) at different ages. As evident from the figure, the mixing is stronger in massive stars, and this can be accounted for by the stronger convective driving in massive stars. Another factor contributing to the increase in the diffusion coefficient with mass is the Brunt–Väisälä frequency. As noted in Figure 1, the Brunt–Väisälä frequency decreases with increasing mass. This leads to lower damping of waves in stars with higher mass and hence results in stronger mixing than lower mass stars.

3.3. Parameterization of the Diffusion Coefficient

RM17 determined the diffusion profile in the radiation zone to be set by the square of the wave amplitude given by

$$D = A_{\text{wave}}^2(\omega, l, r),$$  \hspace{1cm} (9)

where the coefficient $A$ was speculated to depend on the diffusivities, rotation, and dimensionality and was found to be $\sim 1$ s by RM17.

To test this theory against the new data, we calculated the wave amplitudes using the linear theory given by Ratnasingam et al. (2018) where they solved the anelastic, linearized hydrodynamic equations within the WKB approximation.
without considering the rotational, thermal, and viscous effects. The equation is given by

$$w = -r v_l N_0, \quad v_0(\omega, l, r)$$

where $\rho_0$, $r_0$, and $N_0$ are the density, radius, and the Brunt–Väisälä frequency at the initial reference point. $v_0(\omega, l, r)$ is the initial wave amplitude for a given frequency and wavenumber. The radial velocity is related to the tangential velocity by the following relation:

$$w = -v_l N_0, \quad v_0(\omega, l, r)$$

The above can be approximated to $w N_0$ for frequencies much smaller than the Brunt–Väisälä frequency. We, therefore, assume the wave amplitude to be equal to the rms velocity at the reference point averaged over the time window considered (see Section 2.1) multiplied by a factor of $w N_0$ to obtain the theoretical radial diffusion profiles. The term $\exp\left(-\frac{r}{N}\right)$ in the above equation is the attenuation factor multiplied to the wave amplitude as the radiative damping is considered within the quasi-adiabatic limit (Zahn et al. 1997). The damping coefficient $T$ according to Kumar et al. (1999) is given as

$$T(\omega, l, r) = \int_{r_0}^{r} \frac{16\sigma T^3}{3 \rho^2 \kappa c_p} \left(\frac{l(l+1)}{r N_0^2 - \omega^2}\right) \left(1 - \frac{\omega^2}{N_0^2}\right) dr,$$

where $\sigma$, $T$, $c_p$, $\kappa$, and $l$ are the Stefan–Boltzmann constant, temperature, specific heat capacity at constant pressure, opacity, and wavenumber. RM17 studied a $3 M_\odot$ midMS model considering up to 70% of the total stellar radius without taking into account the effect of the Brunt–Väisälä frequency

**Figure 5.** The diffusion coefficient as a function of fractional radius for 3, 7, and $20 M_\odot$ at (a) ZAMS (b) midMS, and (c) TAMS. The vertical dashed line represents the convective–radiative interface for each model.

**Figure 6.** Mixing profile near the convective–radiative interface from the simulation (blue) and the Gaussian fit (pink line) with the overshooting depth (0.18$H_p$) indicated by the pink vertical dashed line for a $7 M_\odot$ ZAMS model. The convective–radiative interface is given by the vertical blue dashed line.

| Model       | Overshooting Depth (units of $H_p$) |
|-------------|-------------------------------------|
| $3 M_\odot$ ZAMS | 0.22                               |
| $3 M_\odot$ midMS | 0.20                               |
| $3 M_\odot$ TAMS | 0.17                               |
| $7 M_\odot$ ZAMS | 0.18                               |
| $7 M_\odot$ midMS | 0.105                              |
| $7 M_\odot$ TAMS | 0.12                               |
| $20 M_\odot$ ZAMS | 0.14                               |
| $20 M_\odot$ midMS | 0.11                               |
| $20 M_\odot$ TAMS | 0.22                               |

The following relation:

$$\frac{v_w}{v_r} = \left(\frac{N^2}{\omega^2} - 1\right)^{\frac{1}{2}}.$$  (11)

The above can be approximated to $\frac{N}{\omega}$ for frequencies much smaller than the Brunt–Väisälä frequency. We, therefore, assume the wave amplitude to be equal to the rms velocity at the reference point averaged over the time window considered (see Section 2.1) multiplied by a factor of $\frac{N}{\omega}$ to obtain the theoretical radial diffusion profiles. The term $\exp\left(-\frac{r}{N}\right)$ in the above equation is the attenuation factor multiplied to the wave amplitude as the radiative damping is considered within the quasi-adiabatic limit (Zahn et al. 1997). The damping coefficient $T$ according to Kumar et al. (1999) is given as

$$T(\omega, l, r) = \int_{r_0}^{r} \frac{16\sigma T^3}{3 \rho^2 \kappa c_p} \left(\frac{l(l+1)}{r N_0^2 - \omega^2}\right) \left(1 - \frac{\omega^2}{N_0^2}\right) dr,$$  (12)

where $\sigma$, $T$, $c_p$, $\kappa$, and $l$ are the Stefan–Boltzmann constant, temperature, specific heat capacity at constant pressure, opacity, and wavenumber. RM17 studied a $3 M_\odot$ midMS model considering up to 70% of the total stellar radius without taking into account the effect of the Brunt–Väisälä frequency.
on the wave amplitude. We extend their analysis to stellar models presented in this work by considering a modified relation to calculate the wave amplitude (Equation (10)) based on the linear theory given by Ratnasingam et al. (2018).

### 3.4. Determining the Dominant Frequencies Contributing to the Mixing Profiles

In order to incorporate this mixing into 1D stellar evolution codes, we needed to determine the dominant waves contributing to the mixing profiles, so we launched waves from a radius outside the convective–radiative interface and calculated the theoretical diffusion coefficient using Equations (9)–(12) for a set of frequencies (1–40 $\mu$Hz) and wavenumbers (1–10) for each stellar model. The initial reference points where the waves are launched are highly influenced by the overshooting motions. We, therefore, initially determined the overshooting depth for each model by fitting the following Gaussian function to the mixing profile near the convective–radiative interface,

$$ D = D_0 \exp \left[ \frac{(x - cr + f_0 H_p)^2}{2(f_1 H_p)^2} \right], $$

where $D_0$ is the amplitude, $cr$ is the radius of the convection zone, $H_p$ is the pressure scale height, and $f_0$ and $f_1$ are the overshooting parameters. We measured the overshooting depth as the radius up to which we could get a good fit of the Gaussian profile. Figure 6 shows the Gaussian fit along with the mixing profile near the convective–radiative interface for a $7M_\odot$ ZAMS model as an example. Here, we obtained the

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**Figure 7.** Diffusion coefficient as a function of fractional radius for the 3, 7, and 20 $M_\odot$ at ZAMS (left panel) and midMS models (right panel) from the simulation (blue line) and from the linear theory with waves launched at $1.3H_p$ for the dominant frequencies (pink line). The dotted profiles show the theoretical profiles at different frequencies.
mixing profile (blue) near the convective–radiative interface from the simulation and then fitted this profile with the Gaussian function (pink) given by Equation (13). The overshooting depth determined is indicated by the pink vertical dashed line. We repeated this procedure for all the models and the overshooting depth for the different models found are given in Table 2. We then launched the waves at a radius equal to 1.37 times the overshooting depth in all the models studied. More details on the overshooting profiles along with the comparison of the overshooting depth determined from the theory and simulation will be discussed in an upcoming paper.

In order to implement a prescription for wave mixing into a 1D code, it would be helpful to narrow down the range of frequencies and wavenumbers contributing to the mixing profile. We, therefore, compared the theoretical profiles calculated using Equations (9)–(12) at different frequencies and wavenumbers with our simulation diffusion profiles for all the models to determine if a simpler prescription, with limited waves, could be found. We observed that the waves with higher wavenumbers provide a smaller contribution toward the diffusion coefficient since they experience higher thermal damping as expected from Equation (12), and therefore, we discard their contributions and consider only $l = 1$ waves in our further calculations. We show the theoretical diffusion profiles corresponding to the dominant frequencies that provide the best fit to the profiles from the simulations in Figure 7. The figure also shows the theoretical profiles at different frequencies as an example (dotted profiles in Figure 7). In general, the mixing profiles obtained from the linear theory corresponding to the dominant frequencies are in good agreement with the simulations diffusion profiles for all ZAMS (Figures 7(a)–(c)) and midMS (Figures 7(d)–(f)) models.

We found the dominant frequencies for the different models studied to be in the range of 4–9 $\mu$Hz at wavenumber $l = 1$; with the lower frequencies being dominant for massive stars. This can be attributed to the thermal damping given by Equation (12). Even though the lower frequencies are generated with larger amplitude near the convective–radiative interface, these waves are highly affected by thermal damping. As noted in Figure 1, the average Brunt–Väisälä frequency decreases with mass, causing the effect of damping to be less dominant in massive stars and thereby resulting in lower dominant frequencies. We also noted that the waves experience extra damping near the convective–radiative interface in all the midMS models because of the Brunt–Väisälä frequency peak as noted in Figure 1. The theoretical profiles do not match the numerical simulations well at the surface, nor the interface. At the surface, this is because the radial velocity is forced to zero in our hydrodynamic simulations, causing the amplitude of our numerical profile to drop near the surface, which is not necessarily physical. At the interface, convective overshooting means the region is not totally dominated by waves (Rogers et al. 2006). In our models, the deviation of the theoretical diffusion profile from that of the simulation near the interface, particularly in the case of ZAMS can be explained by these overshooting motions, as they influence the determination of the initial reference point at which the waves are to be launched.

We followed the same procedure to calculate the theoretical diffusion profiles for the TAMS models. We found that none of the theoretical profiles could explain the profile from the numerical simulation accurately. Figure 8 shows the best match that we could get from our analysis for the different TAMS models (pink dotted–dashed profiles). The pink vertical dashed line represents the turning point for the frequencies shown. We can clearly see that the profiles start to diverge as they approach the turning point beyond which the waves become evanescent. As stated previously, the waves lose their wave-like behavior at a lower fraction of the total stellar radius because of the density term in Equation (6) being dominant for a major fraction of the

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7 We considered various initial reference points beyond the overshoot depth to launch the waves and found that at this value, the theoretical profiles showed a reasonable agreement with that of the simulation profiles for all the models studied.
radius in older stars. Therefore, the WKB approximation applied to the equation for wave propagation (Equation (6)) is not valid in the TAMS models and hence the theoretical description outlined in RM17 and Section 3.3 is not valid in older stars. More analyses need to be carried out in the future for a better understanding of the diffusion profiles of the TAMS.

Figure 9. The frequency distribution of the kinetic energy density for 3 $M_\odot$ (green), 7 $M_\odot$ (pink), and 20 $M_\odot$ (blue) at ZAMS (left column), midMS (middle column), and TAMS (right column) in the radiation zone at 1.3 times the overshoot depth (top row), 0.3$R_*$ (middle row), and 0.6$R_*$ (bottom row). The vertical dashed lines indicate the dominant frequencies shown in Figures 7 and 8.

Figure 10. (a) Radial diffusion profile for the 7 $M_\odot$ ZAMS model at different time differences ($\tau$). (b) The square of the wave amplitude (summed over frequencies (1–40 $\mu$Hz) and wavenumbers (1–20)) from the simulation (pink) along with diffusion profile (blue) at $\tau = 3 \times 10^7$ s.
models. However, at this stage, it appears that a substantially lower diffusion coefficient, which is virtually flat throughout the radiation zone is a decent approximation of wave mixing at the late stages of stellar evolution.

We also computed the kinetic energy spectrum, \( \hat{E}_{\text{kin}} \),

\[
\hat{E}_{\text{kin}} = \frac{1}{2} \hat{\delta}(v_r^2 + \hat{v}_\theta^2),
\]

(14)

where \( \hat{v}_r \) and \( \hat{v}_\theta \) are the Fourier transforms of radial and tangential velocities. Figure 9 shows the frequency distribution of the kinetic energy for \( l = 1 \) at three different radii where the top panels (a)-(c) present the spectra at 1.3 times the overshoot depth (radius at which the waves are launched), the middle panels (d)-(f) at 0.3R\(_s\), and the bottom panels (g)-(i) at 0.6R\(_s\) for all the models studied. The vertical dashed lines indicate the dominant frequencies shown in Figures 7 and 8. We note that the dominant frequencies lie close to where the kinetic energy density peaks, thereby justifying our choice of frequencies. This is more evident from the middle and bottom panels of Figure 9. We are not concerned with the TAMS models as we have already shown that the linear theory does not explain their mixing profiles accurately.

3.5. Determination of the Parameter A

We conducted a number of tests to determine the value of the parameter “A” from our simulations. We found that the simulation should be run for longer convective turnover times for the correct estimate of this parameter. Regardless of how long the simulations were run, the mixing profiles maintained the same trends discussed in Sections 3.1 and 3.2. But, we noted that the amplitudes of the profiles decrease further and converge at higher time differences. This is shown in Figure 10(a) for the 7 M\(_{\odot}\) ZAMS model run for 87 convective turnover times. We see that the amplitude of the mixing profile converges at \( \sim 10^7 \) s. We then compared this profile to the square of wave amplitude (here the amplitude is summed over a range of frequencies (1–40 \( \mu \)Hz) and wavenumbers (1–20)\(^2\)) obtained from the simulation (pinker in Figure 10(b)). As evident from the figure, both the profiles match to a good extent, giving us the value of the parameter “A” \( \sim 1 \). We expect all the models to show similar behavior once the simulation is run for longer convective turnover times. Our finding is in agreement with that of RM17. A better estimate of this parameter can only be obtained by the comparison of our theoretical prescription with that of the observations.

4. Conclusion

We studied the mixing by IGWs in stars of different masses and ages by introducing tracer particles into our 2D hydrodynamic simulations. Initially, we carried out a convergence test for all our models to check if they agreed with the studies of RM17. We found that all our models attained numerical convergence with respect to the time, particle, and radial resolution. We then focused our attention on the diffusion profiles as a function of mass and age.

One of our main conclusions is that the mixing profile varies significantly across age with the mixing stronger in younger stars. The different trends observed in the mixing profiles of TAMS models can be accounted for by the turning point, which is located at a lower fraction of the total stellar radius and the Brunt–Väisälä frequency spike in these older stars. We also found that mixing by IGWs is stronger for stars of higher masses. The stronger convective driving in massive stars along with the lower average Brunt–Väisälä frequency result in higher amplitude waves within the radiative zone, and therefore, more mixing.

We then tested our simulation results against the prescription given by RM17 for the inclusion of these mixing profiles in one-dimensional stellar evolution models. We found that their theory agrees well with the simulation for all ZAMS and midMS models with the dominant waves contributing to these mixing profiles in the range of 4–9 \( \mu \)Hz for wavenumber \( l = 1 \). We also found that the dominant frequency decreases with increasing mass, but remains approximately the same across different ages for a given mass as can be noted in Figure 7. When run for a longer time, we find that the amplitude of the mixing profile converges such that \( A \sim 1 \). It is still unclear what physically sets this parameter. The linear theory however failed to explain the mixing profiles of TAMS models because the waves cannot be described by the WKB approximation. Studies attempting to find a prescription for the TAMS models will be forthcoming.

Future work will focus on determining the effect of rotation on the mixing by IGWs in the radiation zone by extending our analysis to models of different rotation rates. We aim to find out how rotation influences the turning point in older stars.

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*The wave amplitudes were negligible at higher wavenumbers, hence we neglected their contributions in our calculation.*
