The behaviour of the turbulent Prandtl number ($Pr_t$) for buoyancy-affected flows near a vertical surface is investigated as an extension study of Gibson & Leslie, *Int. Comm. Heat Mass Transfer*, Vol. 11, pp. 73-84 (1984). By analysing the location of mean velocity maxima in a differentially heated vertical planar channel, we identify an infinity anomaly for the eddy viscosity $\nu_t$ and the turbulent Prandtl number $Pr_t$, as both terms are divided by the mean velocity gradient according to the standard definition, in vertical buoyant flow. To predict the quantities of interest, e.g. the Nusselt number, a machine learning framework via symbolic regression is used with various cost functions, e.g. the mean velocity gradient, with the aid of the latest direct numerical simulation (DNS) dataset for vertical natural and mixed convection. The study has yielded two key outcomes: (i) the new machine learnt algebraic models, as the reciprocal of $Pr_t$, successfully handle the infinity issue for both vertical natural and mixed convection; and (ii) the proposed models with embedded coordinate frame invariance can be conveniently implemented in the Reynolds-averaged scalar equation and are proven to be robust and accurate in the current parameter space, where the Rayleigh number spans from $10^5$ to $10^9$ for vertical natural convection and the bulk Richardson number $Ri_b$ is in the range of 0 and 0.1 for vertical mixed convection.

**Keywords** Buoyant flow · Machine learning · Turbulence modelling · Wall-bounded turbulence.

1 **Introduction**

Buoyancy-affected flows near a heated surface have vast engineering applications. Examples include thermal energy systems, e.g. nuclear reactor containment [Hanjalic, 2002], building ventilations [Batchelor, 1954] and geophysical flows [Wells and Worster, 2008]. The turbulent fluid flow for these applications can be numerically simulated using the Reynolds-averaged Navier-Stokes (RANS) equations. However, the model-form uncertainties induced by the buoyancy effect have been a long-standing engineering problem. One major source of uncertainty is the approximation of the turbulence closure terms, which are the Reynolds stress tensor ($-\overline{u_i u_j}$) in the momentum equation and the turbulent
heating flux vector \((-\bar{u}\bar{\theta})\) in the temperature equation. These terms are commonly modelled by the linear eddy viscosity model (LEV) and standard gradient-diffusion hypothesis (SGDH). The bridge between LEVM and SGDH is the turbulence Prandtl number, which is usually defined analogous to the molecular Prandtl number \(Pr \equiv \nu/\alpha\). For uni-directional flows in a channel:

\[
Pr_t = \frac{\nu_t}{\alpha_t} \frac{\partial \theta}{\partial y} dU/dy = \frac{\nu_t}{\alpha_t} S = \frac{\nu_t}{\alpha_t} \Gamma,
\]

where \(\nu_t\) is the turbulent eddy viscosity, \(\alpha_t\) is the turbulent thermal diffusivity, the mean velocity gradient \(S = dU/dy\), and the mean temperature gradient \(\Gamma = d\theta/dy\).

Studies on the turbulent Prandtl number \(Pr_t\) via laboratory experiments, field observations and numerical simulations have a long history. Commonly, \(Pr_t\) is treated as a near unity constant (the classical Reynolds analogy, or \(\nu_t \approx \alpha_t\)) for air flow as a reasonable approximation. Reviews by [Reynolds, 1975] and [Kays, 1994] for engineering flows found evidence that \(Pr_t\) deviated from unity in the near-wall region. Thus, it has been suggested that \(Pr_t\) should not be a constant but a function of the distance from the wall or the turbulent Peclet number \(Pe_t = \frac{(\nu_t/\nu)Pr_t}{1}\). The presence of buoyancy adds complexity to the modelling of the \(Pr_t\), because of the increasing dissimilarity between turbulent transport of momentum and heat [Li, 2019]. The existing literature has mostly paid attention to the flow near a horizontal surface, in which \(Pr_t\) is modelled according to the stability conditions caused by heat flux. Popular models include \(Pr_t\) as functions of the stability parameter \(\zeta = y/L = y/(U^3/\kappa g \beta \bar{\theta})\) [Monin and Obukhov, 1954], the gradient Richardson number \(R_g = N^2/S^2\) or flux Richardson number \(R_f = G/P\) [Gibson and Lauder, 1978; Mellor and Yamada, 1982], where \(L\) is the Obukhov length, \(N = \sqrt{g\beta T}\) is the Brunt–Väisälä frequency, and \(P\) and \(G\) represent shear production and buoyancy production, respectively, in turbulent kinetic energy (TKE) budgets. Recently, a more unified framework based on the energy- and flux-budget [Zilitinkevich et al., 2013] or cospectral budget of momentum and heat fluxes [Li et al., 2015] has been introduced to analytically formulate the relationship between \(Pr_t\) and \(Pe_t\) [see Li, 2019 for a comprehensive review by the atmospheric community], where the subscript ‘neu’ indicates ‘neutral conditions’. The general observation is that \(Pr_t\) decreases as the flow become unstable. In contrast to the extensive literature of flow near a horizontal surface, the behaviour of \(Pr_t\) near a vertical surface has rarely drawn attention. [Gibson and Leslie, 1984] applied a parametrized model for a vertical setup related to \(R_f\) by parametrizing second-moment transport equations that were initially employed for the ground effect near a horizontal surface [Gibson and Lauder, 1978]. It is still not clear whether the aforementioned relations, developed by the atmospheric community, are applicable to the \(Pr_t\) in vertical setup; nevertheless, the budgets for second-order statistics are different. For instance, the buoyancy production \(G = g\beta u\bar{\theta}\) is calculated using the streamwise heat flux for a vertical configuration, whereas \(G\) is based on the wall-normal heat flux for buoyant flow near a horizontal surface. Furthermore, the existence of velocity maxima \((S \to 0)\) adds complexity to modelling \(Pr_t\) as it tends to infinity. Therefore, an understanding of the behaviour of \(Pr_t\) in a vertical setup warrants closer inspection.

There are several vertical configurations [Holling and Herwig, 2005]: flow along a plate, within an enclosed cavity, along a tube or pipe [Jackson et al., 1989] and that between two infinite differentially heated vertical walls. We choose the latter configuration (see Fig 1), a fully developed planar channel flow, because of the ideal one-dimensional averaged statistics and the availability of high-fidelity data (either direct numerical simulations (DNSs) or well-resolved large eddy simulations). Semi-works on the vertical setup include the vertical mixed convection (VMC) cases by Kasagi and Nishimura [1997] for global Reynolds number \(Re_C = 150\) with Rayleigh number \(Ra = 6.8 \times 10^5\) and the vertical natural convection (VNC) cases for \(Ra\) at \(O(10^6)\) [Phillips, 1996; Boudjemadi et al., 1997; Versteegh and Nieuwstadt, 1999]. Recent studies on VMC have focused on analysing the effect of near-wall large-scale structures [Fabregat et al., 2010; Wetzl and Wagner, 2019] using the same parameters. In contrast to the attention on Kasagi and Nishimura [1997], the DNS study carried out by Sutherland et al. [2015] at \(Re_C = 395\) with several \(Ra\) cases has received rare attention from modellers. Regarding vertical natural convection, DNS studies have more recently extended the \(Ra\) to \(O(10^8)\) [Kiš and Herwig, 2014; Ng et al., 2015]. This paper will use the newest DNS results [Sutherland et al., 2015; Ng et al., 2015] on the buoyancy-affected vertical channel to develop suitable models.

Applying machine learning techniques based on high-fidelity data to develop physically informed turbulence models is a burgeoning field [Kutz, 2017; Duraisamy et al., 2019]. Early studies have applied an optimization method (such as field inversion and the adjoint method) or a Bayesian approach to quantify and reduce the RANS-based uncertainties by modifying turbulent closure terms, model coefficients etc. [Ling et al., 2016] applied a deep neural network method to simple geometrical flows and it showed promising results. Another approach is gene expression programming (GEP) developed by [Weatheritt and Sandberg, 2016; 2017]. In the comparison of GEP with a deep neural network by Weatheritt et al., 2017, both approaches improved the prediction of the velocity fields for a jet-in-crossflow problem. Recently, similar training frameworks have been implemented for heat flux vector modelling [Milani et al., 2018; 2020; Sandberg et al., 2018; Weatheritt et al., 2020]. The models are developed by referring to second-order high-fidelity data in an a priori sense, called frozen training, and the a posteriori performance in RANS is sometimes unsatisfactory. Hence, a CFD-driven training approach [Zhao et al., 2020] was devised to seek better machine learnt candidate models.
by directly appraising \textit{a posteriori} performance during the training process. In this paper, we will utilize GEP with both \textit{frozen} and \textit{CFD-driven} training to find a proper model for $Pr_t$.

The primary objective of this paper is a close inspection of the behaviour of the turbulent Prandtl number for buoyancy-affected flow near a vertical surface, which has not shown sufficient attention, since the final study by Gibson and Leslie \cite{Gibson1984}. The paper is organized as follows. In §2, the location of velocity maxima based on the latest DNS data is shown. We highlight the need for variable $Pr_t$ in the whole domain due to the existence of an infinity anomaly for both vertical natural and mixed convection. The training framework is then presented in §3, where the detailed procedures of \textit{frozen} and \textit{CFD-driven} training are delineated. Here, we also present the preprocessing method on DNS-based eddy viscosity. In §4, the predictive accuracy of GEP-trained models is systematically assessed by investigating the dependency on the training dataset and cost functions. Finally, §5 concludes this paper.

2 Data source and flow features

In this section, we present the setup and the unified governing equations for VNC and VMC. Then, the DNS dataset used in the following modelling process is shown. Based on the DNS data, we discuss the behaviour of $Pr_t$, which encompasses several distinctive features, e.g., the existence of a singularity for the vertical buoyant flow.

2.1 Flow setup and governing equation

Fig. 1 shows a schematic with the three- and two-dimensional view of the setup used in this paper. The coordinate system $(x, y, z)$ denotes the streamwise (opposed to gravity direction), wall-normal and spanwise directions. When using Reynolds decomposition, the flow instantaneous quantities $(\tilde{u}, \tilde{v}, \tilde{w}, \tilde{P}, \tilde{\theta})$ are expressed as the sum of the mean part $(U, V, W, P, \Theta)$ and fluctuations $(u, w, p, \theta)$. The no-slip and no-penetration boundary conditions are imposed on the velocity and constant isothermal temperatures are set at the walls. Both streamwise ($x$) and spanwise ($z$) directions are periodic for velocity, pressure and temperature. This indicates $\partial/\partial y \gg \partial/\partial x$, $\partial/\partial x = \partial/\partial z = 0, V = W = 0$. Thus, the time- and area- averaged mean profiles $U(y)$ and $\Theta(y)$ only vary along the wall-normal direction. Consequently, the Reynolds-averaged mean equations of motion can be written as:

$$0 \simeq -\frac{1}{\rho} \frac{\partial P}{\partial x} + \frac{d}{dy} \left( \nu \frac{dU}{dy} - \overline{uw} \right) + g_1 \beta \left( \Theta - \Theta_0 \right),$$

(2)

$$0 \simeq \frac{d}{dy} \left( \frac{\alpha \frac{d\Theta}{dy} - \overline{w\theta}}{\nu} \right).$$

(3)

We treat density $\rho$ as a constant by employing the Oberbeck–Boussinesq approximation for the density variation with temperature in the momentum equations. Furthermore, for simplicity, we prefer to use $-\overline{u_i u_j}$ instead of $-\rho \overline{u_i u_j}$ and to use $-\overline{w\theta}$ instead of $-\rho \overline{w\theta}$.

The vertical channel is controlled by two streamwise body forces: the gravity force $g_1 = -g$ and a constant mean pressure gradient $-1/\rho \left( \partial P/\partial x \right)$. The following parameters that dominate the flow, Rayleigh number $Ra$, bulk Reynolds number $Re_b$, bulk Richardson number $Ri_b$ and Prandtl numbers $Pr = \nu/\kappa$ are, respectively, defined by,

$$Ra \equiv \frac{\beta \Delta \Theta (2h)^3}{\nu \kappa}, \quad Re_b \equiv \frac{2hU_b}{\nu}, \quad Ri_b \equiv \frac{Re_b^2 Pr}{4},$$

(4)

where the half-channel-width is $h$ (full width $H = 2h$), $g$ is the gravitational acceleration, bulk mean velocity $U_b = 1/(2h) \int_0^{2h} U(y)dy$, $\nu$ is the kinematic viscosity and $\kappa$ is the thermal diffusivity. The fluid properties are assumed to be constant. The temperature difference $\Delta \Theta = \Theta_h - \Theta_c$ is defined by the scaled temperature $\Theta_h = 0.5$ on the hot plate and $\Theta_c = -0.5$ on the cold plate (see Fig. 1). It is worth noting that the mean pressure gradient in mixed convection is defined as:

$$-\frac{1}{\rho} \frac{\partial P}{\partial x} = \frac{U_{\tau,h}^2 + U_{\tau,c}^2}{2h},$$

(5)

where the friction velocities are $U_{\tau,h} = \sqrt{\nu \frac{dU}{dy}|_{w,h}}$ at the hot wall and $U_{\tau,c} = \sqrt{\nu \frac{dU}{dy}|_{w,c}}$ at the cold wall. In addition, the global mean friction velocity is defined by the arithmetic mean of the one at each wall, that is, $U_{\tau} = (U_{\tau,h} + U_{\tau,c})/2$. For forced convection, $U_{\tau} = U_{\tau,h} = U_{\tau,c}$, and $(-1/\rho) \frac{\partial P}{\partial x} = U_{\tau}^2/h$. Lastly, the Nusselt number, the dimensionless heat transfer rate, is quantified as $Nu \equiv f_w(2h)/\Delta \Theta \kappa$ where $f_w \equiv \kappa |\frac{d\Theta}{dy}|_{w,h}$, $|\frac{d\Theta}{dy}|_{w,h}$ is the mean temperature gradient at the hot and cold walls.

There are two limit states for the current setup, namely, pure buoyancy-driven flow (referred to as natural or free convection) and pure shear-driven flow (referred to as forced convection), which can be quantified by the bulk Richardson...
number $Ri_b$. Increasing $Ri_b$ means adding a buoyancy effect; if $Ri_b = 0$, it means $g = 0$, and the flow is the canonical channel flow (forced convection), while as $Ri_b \to \infty$ (namely, $U_b = 0$), the flow is purely buoyancy-driven (natural convection). Fig. 1 (b) is a two-dimensional view of the vertical channel, from left to right: natural, mixed and forced convection. In each panel, the mean velocity $U(y)$ and mean temperature $\Theta(y)$ are plotted to show the velocity maxima for the three scenarios.

This paper employs different nondimensionalizations for natural, mixed or forced convection due to the distinctive features of shear-dominant and buoyancy-dominant flows. For natural convection, we choose the traditional full width $H$ as the length scale and $H/U_f$ (where the velocity scale is the free fall velocity $U_f = \sqrt{g\beta\Delta \Theta H}$ [Ng et al., 2015]) as time scale. For forced and mixed convection, the length scale is the half channel-width $h$, and the time scale is $h/U_\tau$.

Note that the mechanical turbulent dissipation rate $\varepsilon$ is normalized by $U_f^3/H$ for VNC and $U_\tau^4/\nu$ for VMC.

### 2.2 DNS dataset

In this study, 14 cases of the DNS dataset are used (see Table 1), which were carried out by Ng et al. [2015] (Set A, Case 1 ~ 7) for VNC and Sutherland et al. [2015] (Set B, Case 8 ~ 14) for VMC with $Pr = 0.709$ (for air flow). The cases cover the range of Reynolds and Rayleigh numbers $0 \leq Re_b \leq 1.471 \times 10^4$, $10^5 \leq Ra \leq 10^9$. We adopt the label $Rax_Rey$ [Pirozzoli et al., 2017] at $Ra = 10^8$, $Re_b = 10^7$. For instance, the flow case 11, $Ra_{6.5}~Re_{4.2}$, denotes $Ra = 3.6 \times 10^9 = 10^{9.3}$ and $Re_b = 1.471 \times 10^4 = 10^4.2$. Besides, $Ra = 0$ corresponding to pure Poiseuille flow (forced convection), and $Re_b = 0$ corresponding to VNC. Table 1 also provides a shorthand label, for instance, $Ra_{80}$ for the natural convection case at $Ra = 1.0 \times 10^8$ and $Ri_{50}$ for the mixed convection case at $Ri_b = 0.050$.

### 2.3 The behaviour of the turbulent Prandtl number in global coordinates

For the one-dimensional mean flow field, the governing equations only include the two components of the Reynolds stress tensor and heat flux vector, which are the Reynolds shear stress ($\overline{uv}$) and the wall-normal heat flux ($\overline{v\theta}$) for a planar channel flow. We adopted the well-established linear gradient LEVM and SGDH models as the starting point, which are, respectively,

\begin{align}
- \overline{uv} &= \nu_t \frac{dU}{dy}, \\
- \overline{v\theta} &= \alpha_t \left( \frac{d\Theta}{dy} \right)_y = \frac{\nu_t}{Pr_t} \frac{d\Theta}{dy}.
\end{align}

First and foremost, it is essential to discuss the signature of the mean velocity gradient $dU/dy$ and mean temperature gradient $d\Theta/dy$, $\overline{uv}, \overline{v\theta}$ in global coordinates. Gibson and Leslie [1984] listed the major features along the vertical
Appendix

Table 1: DNS dataset of flow cases, $Re_b = 2\beta g \Delta \Theta h / \nu^2$ is the bulk Reynolds number, $Ri_b = 2\beta g \Delta \Theta h / U_b^2$ is the bulk Richardson number. $Ray = \beta g \Delta \Theta (2b)^3 / (\alpha \nu w)$ is the Rayleigh number, $Nu = (2h/\Delta \Theta)|d\Theta / dy|_w$ is the Nusselt number. Set A, Case 1 ~ 7, Ng et al., [2015], Set B, Case 9 ~ 14, Sutherland et al., [2015]; more details are showed in Appendix A. In the Purposes column, the training and testing datasets are showed, in which the training represents the cases used to train a machine learnt model, and testing represents the cases used for cross-validation.

surface; they are mostly true only if the flow is in or near the buoyancy-driven/buoyancy-dominated regime. From DNS studies [see Versteegh and Nieuwstadt, 1999, Fig. 2 (c)] on the vertical natural convection, the adapted version is,

Figure 2: Division of region in VNC: (a), $y_1$ is the zero point of $\overline{w}$, and (b), $y_2$ is the zero point of $dU / dy$ in the region between the hot wall ($y/H = 0$) and the centreline ($y/H = 0.5$). The greyscale from light to dark that varies with the increase in $Ra$ from $10^5$ to $10^9$ is based on Ng et al., [2015]; see Table 1 for details on DNS cases. The $y_1$ and $y_2$ values for $Ra = 5.4 \times 10^5$ are explicitly shown in (a) and (b). (c), the variation in $y_1$ and $y_2$ with the change in $Ra$, where the Ref. $\times$ is a verification case in Versteegh and Nieuwstadt, [1999] at $Ra = 5.4 \times 10^5$.

(i) The temperature gradient $(d\Theta / dy)$ is negative everywhere, and the wall-normal heat flux $(\overline{w} \Theta)$ is positive everywhere;

(ii) The Reynolds shear stress $(\overline{wU})$ is negative for small $y_w$ and positive for large $y_w$, where $y_w$ is the nearest distance from the wall (or wall distance).

(iii) The turbulent Prandtl number $Pr_t$ has singularities and a negative region in the vicinity of the wall.

For a clear discussion regarding the division of the regions, we define $y_1$ as the zero point of $\overline{w}$ and $y_2$ as the zero point of $dU / dy$ in the region of the hot wall ($y = 0$) to the centerline ($y = h$). Fig. 2 (a) and (b) shows the exact position of $y_1$ and $y_2$, which results in the sign of key quantities (see Table 1). For the whole domain in global coordinates, a
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laminar sublayer exists within $0 < y_w < y_1$ and a turbulent layer within $y_2 < y_w < h$. The $y_1 < y_w < y_2$ region is actually the bridge between these two distinctive regions, which can be called the adjustment region [Wells and Worster, 2008]. Fig. 2(c) shows that the adjustment region shrinks with the increase in $Ra$ and might diminish when $Ra \to \infty$ [Hölling and Herwig, 2005]. Meanwhile, Ng et al. [2017] suggest that the thermal and viscous boundary layers undergo a transition from a classical laminar-like state to the ultimate shear-dominated state from moderate to high $Ra$. Therefore, given the diminishing of the adjustment region and the transition of the laminar sublayer, the whole domain could be turbulent in the ultimate state. From the point of view of the modeller, the adjustment region is the area where the LEVM [Versteegh and Nieuwstadt, 1999] is not valid near both walls. In other words, the infinity issue occurs in both $Pr_t$ (see Eq. 1 and Fig. 3(b)) and $\nu^\text{dns}$ in global coordinates. Collectively, the infinity issue at $Ra$ from $10^5$ to $10^6$ is a challenging question for symbolic regression and model generality in this study.

| region | $dU/dy$ | $d\Theta/dy$ | $\nu^\text{t}$ | $\nu$ | $Pr_t$ |
|--------|---------|--------------|---------------|------|--------|
| $0 < y_w < y_1$ | + | - | - | + | + |
| $y_1 < y_w < y_2$ | + | - | + | + | - |
| $y_2 < y_w < h$ | - | - | + | + | + |

Table 2: The sign of quantities along wall-normal direction until the centreline in global coordinates for VNC.

Figure 3: The distribution of turbulent Prandtl number ($Pr_t$) and eddy viscosity $\nu^\text{dns}$ at $Ra = 5.0 \times 10^6$ for VNC, where (a), $Pr_t$, in the near-wall positive region; (b), $Pr_t$ in global coordinates, where the present data are validated against Dol et al. 1999 ($\times$); (c), $\nu^\text{dns}$ in global coordinates. The grey patch depicts the adjustment region between $y_1$ and $y_2$.

For vertical mixed convection, Fig. 3(a) and (b) shows that when $Re_t = 0$ (forced convection), the profiles of $\nu^\text{t}$ and $dU/dy$ have symmetry and the zero points stay at the centreline ($y/h = 1$). With an increase in $Re_t$, both profiles gradually shift to the hotter wall side. Fig. 3(c) illustrates the zero points $y_1$ and $y_2$ are almost at the same position until $Re_t \simeq 0.10$. It is still not clear whether $y_1$ and $y_2$ are mathematically the same. Nevertheless, the mismatch between $y_1$ and $y_2$ is negligible. Thus, the LEVM is approximately valid in the whole domain for $0 \leq Re_t < 0.10$. The resulting adjustment region is illustrated in Fig. 5 for $Pr_t$ and Fig. 8 for $\nu^\text{dns}$. It is worth noting that $Pr_t$ is larger than unity within the viscous sublayer ($y^+ < 10$), which is quite different with respect to the buoyant horizontal channel [Pirozzoli et al., 2017]. Meanwhile, the discrepancy of $Pr_t$ between the hotter and colder wall at the same $y^+$ becomes larger with the increase in $Re_t$. To summarize, the most distinctive feature is the break of symmetry for the mean and second moment statistics for VMC compared with the pure shear or buoyancy-driven vertical flow and horizontal channel [Garcia-Villalba and del Alamo, 2011; Pirozzoli et al., 2017]. Moreover, The asymmetry causes several modelling issues, such as the implementation of wall distance $y_w$ or $y^+$ for the low-Re approach.

3 Modelling Methodologies

In this section, we present the modelling framework via GEP with frozen and CFD-driven training. Then, the RANS-based approximation method for recovering DNS-based input quantities is introduced.
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3.1 Training framework

For modelling scalar flux, the goal is to find a mathematical representation of \( \overline{u_i \theta} \). Based on dimensional arguments, Shih and Lumley [1993] showed that
\[
\overline{u_i \theta} = f \left( U_{i,j}, \Theta_i, k, \varepsilon, \overline{\theta^2}, \varepsilon_\theta \right),
\]
where \( \overline{\theta^2} \) denotes the temperature variance and \( \varepsilon_\theta \) denotes the dissipation rate in a thermal field. This can be further simplified by assuming a sole time scale (\( \overline{\theta^2}/\varepsilon_\theta \simeq k/\varepsilon \)), which means that the thermal to mechanical time ratio, \( R = \overline{\theta^2} \varepsilon/(k \varepsilon_\theta) \) is treated as a near unity constant [Dol et al., 1999]. Hence, we obtain
\[
\overline{u_i \theta} = f \left( U_{i,j}, \Theta_i, k, \varepsilon \right).\]

In light of Galilean invariance and nondimensionalization, a dimensionless velocity invariant \( I \) and a dimensionless temperature invariant \( J \) [Weatheritt et al., 2020] are used to construct the target scalar flux models,
\[
I = \left( \frac{c_\mu k}{\varepsilon} \right)^2 S_{ij} S_{ji} = \frac{1}{2} \left( \frac{c_\mu}{\varepsilon} \frac{k}{dU/dy} \right)^2, \tag{8}
\]
\[
J = \left( \frac{c_\mu k^{1.5}}{\varepsilon} \frac{d\Theta}{dy} \right)^2, \tag{9}
\]
where the mean stain rate tensor \( S_{ij} = \frac{1}{2} (U_{i,j} + U_{j,i}), c_\mu = 0.09 \). We adopt a variable turbulent Prandtl number \( Pr_t \) with the reciprocal form \( f(I, J) = Pr_t^{-1} \) and calculate the turbulent thermal diffusivity \( \alpha_t \),

\[
\alpha_t = \frac{\nu_t}{Pr_t} = f(I, J) \nu_t. \tag{10}
\]

Note that the commonly used SGDH adopts a constant turbulent Prandtl number \( Pr_t = 0.80 \sim 1.10 \) (equivalent to \( 1/f(I, J) \) in the models proposed here) for air.

### 3.1.1 Frozen training

The machine learning procedure employs an in-house symbolic regression tool based on GEP, which was initially developed and tested for Reynolds stress closures by [Weatheritt and Sandberg, 2016](#), and was recently used in scalar flux modelling [Weatheritt et al., 2020](#). In general, we treat the wall-normal heat flux \( \overline{v\theta} \) as a target term and regress by the constraint of cost function \( J(\varphi) \); see Eq. (11) where a square root error is calculated along the wall-normal direction of \( \varphi = \overline{v\theta} \), with superscript \( dns \) representing data from direct numerical simulation, and \( gep \) the value from simulation by GEP models.

\[
J(\varphi) = \int dy (\varphi^{dns} - \varphi^{gep})^2 dy \tag{11}
\]

This approach is called \textit{frozen} training [Zhao et al., 2020](#) as we are trying to optimize a closure against a fixed high-fidelity database. The detailed procedure can be found in Algorithm 1. Moreover, before running GEP, there are two preprocessing steps. One possible issue is the lack of a DNS-based dissipation rate \( \varepsilon \) suitable for the modelling. We overcome this issue by solving the transport equation of \( \varepsilon \) (see Eq. (12)) with \( c_{\varepsilon} = 1.44, c_{2\varepsilon} = 1.92, \sigma_\varepsilon = 1.3 \), where all the other quantities, such as \( \overline{v\theta}, U, \Theta, k \), are extracted from DNS

\[
-\varepsilon [c_{\varepsilon} (P + G) - c_{2\varepsilon} \varepsilon] = \frac{d}{dy} \left((\nu + \frac{\nu_t}{\sigma_\varepsilon}) \frac{d\varepsilon}{dy}\right) \tag{12}
\]

and \( P = -\overline{v\theta} dU/dy, G = g\beta \overline{v\theta} \). Another step is the way to approximate \( \nu_t \) (the infinity issue discussed in §2.3), which is delineated in §3.2.

### Algorithm 1: \textit{frozen} training

1. Get \( \overline{v\theta}, U, \Theta, k \) from DNS data.
2. if do not have suitable DNS-based \( \varepsilon \) then
3.  Solve transport equation of \( \varepsilon \) (Eq. (12)) with DNS-based \( \overline{v\theta}, U, \Theta, k \) as input
4. end
5. Calculate positive smoothed \( \nu_t^{mod} = f_\mu c_\mu k^2/\varepsilon \) for VMC, Eq. (15) for VNC
6. for each generation step \( i = 1, 2, ..., N \) do
7.  randomly generate population in the environment
8.  for each population step \( j = 1, 2, ..., M \) do
9.    genetic evolution to find the best candidate models based on the minimum fitness \( J(\overline{v\theta}) \) for the \( i^{th} \) generation
10. end
11. end
12. Solve RANS scalar equation with new model to obtain \( \Theta, Nu \)

### 3.1.2 CFD-driven training

The resulting data-driven models via \textit{frozen} training can improve the performance of \( \overline{v\theta} \), but sometimes the improvement fails to be shown in the mean flow field \( \Theta \) and Nusselt number \( Nu \). To find better turbulent heat flux models, we implement a loop algorithm that integrates GEP and a RANS solver, referred to as \textit{CFD-driven} training [Zhao et al., 2020](#) (see Algorithm 2). The major modification compared with \textit{frozen} training is solving the RANS scalar equation for each candidate model and then obtaining the RANS-based \( \Theta, d\Theta/dy \) and \( Nu \) to calculate the cost function (see Eq. (13)) in terms of quantities of interest. For example, the cost function can be the error of mean temperature \( J(\Theta) \) (Eq. (11)) where \( \varphi = \Theta \). We can also use the absolute error of \( Nu \) (\( J(Nu) \) in Eq. (13a)) or the combination of errors, such as \( J(cNu) \) in Eq. (13b) and \( J(cdc) \) in Eq. (13c).
Algorithm 2: CFD-driven training

1. Get $\overline{v}$, $U$, $\Theta$, $k$ from DNS data, calculate $\varepsilon$, $\nu_t$ (same as frozen training)
2. for each generation step $i = 1, 2, ..., N$ do
   3. randomly generate population in the environment
   4. for each population step $j = 1, 2, ..., M$ do
      5. feed $f(I, J)$ into RANS scalar equation for $\alpha_t$
      6. solve the RANS scalar equation for each candidate model for the $i^{th}$ generation and obtain $\Theta, Nu$
      7. find best candidate models constrained by customized cost $J(\varphi)$ based on $\Theta$ or $d\Theta/dy$ for the $i^{th}$ generation
   8. end
   9. end

$J(Nu) = \frac{|Nu^{dns} - Nu^{grp}|}{Nu^{dns}} \times 100\%$, \hspace{1cm} (13a)

$J(cNu) = J(\Theta) + \lambda J(Nu)$, \hspace{1cm} (13b)

$J(cdc) = J(\Theta) + \lambda J(d\Theta/dy)$. \hspace{1cm} (13c)

3.2 Data preparation of DNS-based input quantities

In §2.3, a close inspection of the flow features at different regions allows us to identify some issues with the linear gradient-based assumption and the validity of LEVM, especially the near-wall region for VNC. In practice, as the mean velocity gradient $dU/dy \to 0$ at $y_2$, that is, $\nu_t^{dns}$ could be a non-physical value in the vicinity of the wall region as it tends to $\nu_t^{dns} \to \pm \infty$

$$\nu_t^{dns} = \frac{-\overline{uv}}{dU/dy}$$ \hspace{1cm} (14)

Here, by assuming a smooth and positive $\nu_t$ [Xu et al., 1998], for VNC, we devise a limiter function (see Eq. 15) under the condition $\gamma$, where $\gamma = |dU/dy| \leq 1.2$ if $y_w/H < 0.12$ to remove the singularity for the region of the infinity anomaly. The empirical constants in Eq.15 are obtained according to DNS data, which can be seen in Fig. 2 (b). More specifically, $y_w/H < 0.12$ gives the upper bound of the near-wall region for the smoothing operation and $|dU/dy| \leq 1.2$ provides a good estimate for the infinity anomaly region for all $Ra$ from $10^5$ to $10^9$. Fig. 6 illustrates the performance of Eq. 15 at $Ra = 5.4 \times 10^5$ and $Ra = 1.0 \times 10^6$. It is clear that this limiter function can successfully remove the singularity and smoothly link the near-wall laminar and the bulk turbulent regions.

$$\nu_t^{mod} = \begin{cases} \frac{|\overline{uv}|}{max(|dU/dy|, 1.2)} & \text{if condition } \gamma \\ \frac{|\overline{uv}|}{|dU/dy|} & \text{else} \end{cases}$$ \hspace{1cm} (15)

![Figure 6: The smoothed turbulent eddy viscosity $\nu_t^{+} = \nu_t/(HU)_f$ for VNC: (a), $Ra = 5.4 \times 10^5$; (b), $Ra = 2.0 \times 10^7$; (c), $Ra = 1.0 \times 10^9$, where $\circ$ indicates DNS-based $\nu_t^{dns}$ (see Eq. 14); $_{-}$ indicates $\nu_t^{mod}$ based on Eq. 15](image)

A treatment of the eddy viscosity is also needed in VMC. Unlike the anti-symmetric mean profile in VNC, the asymmetry increases the complexity of identifying the position of $y_2$ (see Fig. 4) at different $Rt_b$. Hence, we use a
damping function $f_\mu$, based on the low Reynolds number modelling approach instead of the limiter function in VNC. The damping function $f_\mu$ [Myong and Kasagi, 1990] is

$$f_\mu = 1 + 3.45/\sqrt{Re_t \left[ 1 - \exp(-y^+ / 70) \right]^2}, \quad (16)$$

where local Reynolds number $Re_t = k^2/(\nu \varepsilon)$, the viscous length scale $y^+ = y_w U_\tau/\nu$. Eq. 16 is compared to DNS-based $f_\mu^{dns}$ for the $Ri_0$ case (forced convection) in Fig. 7 (a), in which we can see that the near-wall (within $y^+ < 10$) prediction is fairly good. Hence, $\nu_t^{mod} = f_\mu c_\mu k^2/\varepsilon$ can be estimated quite well (Fig. 7). The damping function is further tested in the VMC case. Fig. 8 shows that $f_\mu$ finds the best approximation with respect to several other damping functions [see Rodi and Mansour, 1993, for a review on the low Reynolds number modelling approach]. Note that the friction velocity at the hot and cold wall is different. Hence, Figs. 8 (b) and (c) give the comparison at both walls in wall units.

![Figure 7: The turbulent eddy viscosity $\nu_t^+ = \nu_t/U_\tau h$ for forced convection. (a) distribution of the damping function, Eq. 16 -----; $f_\mu^{dns} = 1/c_\mu \exp(-y^+/k)$, ○. The approximated $\nu_t^{mod} = f_\mu c_\mu k^2/\varepsilon$ is -----; DNS-based $\nu_t^{dns}$ is ○ in wall units in (b) and in global coordinates in (c).](image)

![Figure 8: The turbulent eddy viscosity $\nu_t^+ = \nu_t/U_\tau h$ for VMC at $Ri_b = 0.050$, approximated by Eq. 16 where $\nu_t^{mod} = f_\mu c_\mu k^2/\varepsilon$ is indicated by ----- and DNS-based $\nu_t^{dns}$ is indicated by ○. The other damping functions are the standard $k - \varepsilon$ model where $f_\mu = 1, -$-$-$; and the Lam-Bremhorst model where $f_\mu = \left[ 1 - \exp(-0.0165\sqrt{ky_w}/\nu) \right]^2 (1 + 20.3/Re_t)$, $-$-$-$. (a) in global coordinates; (b) in viscous wall units at the hotter wall $y_h^+ = y_w U_{\tau,h}/\nu$; (c) in viscous wall units at the colder wall $y_c^+ = y_w U_{\tau,c}/\nu$.](image)
4 Results

In this section, the machine learnt models are first presented. Then, we appraise the performance of the models resulting from various training datasets and approaches by comparisons with the DNS database. Last, an *a priori* test on the turbulent Prandtl number and an *a posteriori* assessment for quantities of interest are shown.

4.1 Machine learnt models

The GEP training approaches (Algorithms 1 and 2) are applied the dataset in Table 1. Here, we delineate the detailed information of a machine learning case for VNC at $Ra = 2.0 \times 10^7$. Fig. 9 shows the normalized error metric (in this case, $J(v\theta)$ via frozen training) in the training process. The population mean error dramatically decays until the 100th generation during the GEP evolution process. After the 100th generation, the population mean error fluctuates around a fixed value, and the population minimum stays at a relatively small value. Thus, the 100th generation candidate model is chosen, which is

$$f(I, J) = 1.116 + (0.205 I - 12J).$$  \hspace{1cm} (17)

For CFD-driven machine learning, the computer costs are augmented by solving a RANS scalar equation for the candidate models in each generation. For a personal computer (4 cores, Intel core i7–7500U), the training procedure, involving around $2 \times 10^4$ RANS calculations (100 generations and 200 population size), takes approximately 27 hours. (Each RANS calculation takes around 20 seconds on one core to converge with the baseline results as initial condition). Besides, the resulting models are more compact than the frozen approach, as indicated by Zhao et al. [2020], and have the form of $f(I, J) = 0.969 + 2J$, for instance, in case of ncgrad.

For RANS model development in turbulent wall-bounded flow, a long-standing struggle is to satisfy the wall asymptotic behaviour. Due to the no-slip condition for velocity terms, the isothermal condition at both walls, and the continuity equation, we can derive that $v \propto O(y^3)$, $u, w, \theta \propto O(y^4)$, where $\propto O(y^n)$ indicates a quantity is proportional to the nth order of the wall-normal coordinate. Then, it directly suggests $v\theta \propto O(y^5)$, $\frac{\partial v}{\partial y} \propto O(y^5)$. For our model target, $\nu_t \propto O(y^3), \alpha_t \propto O(y^3), Pr_t \propto O(y^3)$; hence, $f(I, J) \propto O(y^3)$. In Eq. [17], Table 3 and Table 4, the GEP resulting models always have a constant term and thus satisfy $O(y^3)$. The other terms consist of invariants $I \propto O(y^4)$ and $J \propto O(y^6)$, which means the $I$ and $J$ terms do not affect the near-wall asymptotic behaviour. Overall, comparing $f(I, J) \propto O(y^3)$, it indicates that the GEP approach can ensure the correct wall-limiting behaviour. All the *a priori* and *a posteriori* assessments for these models are described in the following text.

4.2 Sensitivity study on training datasets and training approaches

Following the same numerical treatment, we obtain a series of resulting GEP models via frozen and CFD-driven training. Table 3 lists the models for the VNC cases, which are trained on $Ra = 2.0 \times 10^7$. For the VMC cases, Table 4 shows...
Table 3: GEP models for VNC based on $Ra = 2.0 \times 10^7$ via GEP in form of $f(I, J)$.

| Label  | Training approach | Cost function             | Heat flux models $f(I, J)$ |
|--------|-------------------|---------------------------|---------------------------|
| base   | -                 | $\lambda$ (Θ) + $\mu$ $\nu$ (Θ) | 1.111 $(Pr_f = 0.90)$      |
| ncfux  | frozen            | $J(\nu \theta)$          | 1.116 + 0.205$I - 12J$   |
| mcmean | CFD-driven        | $J(\nu u)$               | 1.195 - $I + J$           |
| mcnu   | CFD-driven        | $J(\nu u)$               | 1.031 - $I$               |
| mcgrad | CFD-driven        | $J(\nu u)$               | 0.969 + 2$I$             |

Table 4: GEP models for VMC based on $Ri_b = 0.050$ via GEP in the form of $f(I, J)$. The combination factor $\lambda$ is used to ensure the error metric at the same magnitude, where $\lambda_1 = 0.1$, $\lambda_2 = 20$.

| Label  | Training approach | Cost function             | Heat flux models $f(I, J)$ |
|--------|-------------------|---------------------------|---------------------------|
| base   | -                 | $\lambda$ (Θ) + $\mu$ $\nu$ (Θ) | 1.111 $(Pr_f = 0.90)$      |
| mcfux  | frozen            | $J(\nu \theta)$          | 1.057 - 0.56$I - 0.188J$ |
| mcmean | CFD-driven        | $J(\nu u)$               | 1.000 + 0.86$I(-0.21 + I - 0.5J)$ |
| mcgrad | CFD-driven        | $J(\nu u)$               | 1.099 + $I(-1.180 - 0.900J)$ |
| mcnuc  | CFD-driven        | $J(\nu u)$               | 0.970 - 0.30$I^2$         |
| mcncf  | CFD-driven        | $J(\nu u)$               | 1.090 - $I$               |

the models that are trained on $Ri_b = 0.05$. In this section, the dependence on the training datasets and cost functions are presented to seek the best model in an \textit{a posteriori} sense.

4.2.1 Dependence on training datasets

Since the data-driven approach can depend on the training case, it is essential to cross-validate each model. We adopt a holdout training and testing approach, where a $Ra$ or $Ri_b$ case is selected to train a model and other cases are used to test the performance of this model. The dependence on training datasets (or cases) is studied for both VNC and VMC. Fig. [10] and Fig. [11] lay out the error of $\nu u$ and $\Theta$, respectively, with comparison of the \textit{a posteriori} performance across $Ra$ for VMC. Note that we omit the other GEP models for cross-validation.

Fig. [10] \textit{a} presents the correlation map depicting the performance of trained models for $\nu u$ in an \textit{a posteriori} sense via the frozen approach with cost function $J(\nu \theta)$. The legend is scaled by the absolute percentage error $J(\nu u)$ of the baseline model, which is 28.7% for the $Ra80$ case. The maximum GEP-based $J(\nu u)$ for all testing cases is 9.5%, which shows the significant improvement achieved by GEP training. Moreover, the performance of the models trained on each $Ra$ is generally better than the performance for the other cases; see the diagonal component in Fig. [10] \textit{a}, and interestingly, there are exceptional cases such as $Ra90$, where $J(\nu u)$ is the largest for itself (6.7%). Nevertheless, the best model via the \textit{frozen} approach resulting from the $Ra63$ case can reduce $J(\nu u)$ to 3.5% for all the VNC cases. Similarly, Fig. [11] \textit{a} shows the performance of trained models with cost function $J(\nu \theta)$ for $\Theta$ in an \textit{a posteriori} sense. The legend is scaled by the square root error $J(\nu u)$ of the baseline model, which is 11.5 $\times 10^{-3}$ for the $Ra80$ case. In contrast to the universal and significant improvement seen for $J(\nu u)$, the error reduction on $J(\nu u)$ is relatively small across different $Ra$ cases. The reduction of predictive error is 6.1% with respect to the maximum baseline error for $Ra80$ by the frozen trained models at $Ra50$. However, we can obtain a generalized GEP model. The best model via the \textit{frozen} approach results from the $Ra73$ case, which can reduce $J(\nu u)$ to 5.6 $\times 10^{-3}$ for all the VNC cases, achieving approximately 90% improvement. In brief, the machine learnt models are independent of $Ra$ for VNC cases, and the GEP models via the \textit{frozen} approach generally perform better than baseline models, especially at the higher $Ra$ range.

Fig. [12] illustrates the performance of GEP models trained on $Ri_{18}, R50$, and $Ri_{94}$ cases via \textit{frozen} training. The baseline model perfectly captures $\nu u$ for forced convection $Ri_b = 0$. However, the prediction errors of both $\nu u$ and $\nu \theta$ linearly increase with the growth of the buoyancy effect (see Fig. [12] \textit{a}, \textit{c}). Conversely, the error reductions of GEP models trained on the $Ri_{94}$ case nearly linearly increase with the decrease in the buoyancy factor. The resulting models trained on $Ra50$ significantly reduce the error of $\nu u$ to 5%. Moreover, all the GEP models can reduce the prediction error of $\nu \theta$. Surprisingly, for the mean temperature, the baseline model is better than all the GEP modes trained on different $Ri_b$ cases via \textit{frozen} training except the largest $Ri_b$. To summarize, the GEP models depend on different $Ri_b$ cases, where the middle range case $Ri_{50}$ shows the best performance for $\nu u$ if we regard the $Ri_{00}$ case as an exception. This result further suggests the limitation of the \textit{frozen} training approach.
The comparison of training approaches is the assessment on cost functions for the data-driven method. When we select $J(N_u)$ as the cost function, i.e. we use the CFD-driven approach, the performance of GEP models on the prediction of $N_u$ is generally better than that of using other cost functions. For instance, for VNC, Fig. 10(b) depicts the a posteriori correlation error of $N_u$ trained by $J(N_u)$ via the CFD-driven approach and shows the diagonal component, which means training and testing for the same case, is smaller than that of Fig. 10(a) (trained by $J(\mathbf{v}\theta)$) via the frozen approach, i.e. without involving CFD while training. This is also true for the a posteriori predication of $J(\Theta)$, when the models are trained on $J(\Theta)$ (using the CFD-driven approach), see Fig. 11(b), rather than when using training based on $J(\mathbf{v}\theta)$ via the frozen approach (Fig. 11(a)). Accordingly, when we select $J(N_u)$ as the cost function, it can undermine the performance on $\Theta$ of the resulting GEP models and vice versa. The maximum a posteriori error of $J(N_u)$ trained by cost function $J(\Theta)$ is 18.3%, which is worse than training by $J(N_u)$. However, the performance of GEP models constrained by $J(d\Theta/d\mathbf{y})$ (Fig. 10(c) and Fig. 11(c)) is slightly better than that of $J(\mathbf{v}\theta)$. Overall, the model trained on Ra73 by $J(d\Theta/d\mathbf{y})$ (mcgrad in Table 3) seems to be the best model for VNC.

For VMC, as stated in 4.2.1, the frozen approach can reduce the error of $N_u$, but the performance on $\Theta$ is even worse than when using the baseline. Fig. 13 shows the effect of various cost functions (see Table 4) based on Ra50. All the CFD-driven-based results can achieve a better prediction than the frozen approach for both $N_u$ and $\mathbf{v}\theta$. Interestingly, the models developed with $J(\Theta)$ in the cases mcmean and mcenu (see Table 4) perform better than the frozen approach but worse than the baseline model. In contrast, they can reduce the error in $\Theta$ (see Fig. 13(b)) at the low $Ri_b$ regime for the cost function with the inclusion of $d\Theta/d\mathbf{y}$ (cases mncgrad and mcde). Moreover, when we investigate the
Figure 12: Error metric with the baseline or GEP models, (a) error of Nusselt number \( J(Nu) \) (see Eq.13a); (b) error of mean temperature (see Eq.[11] where \( \varphi = \Theta \)); (c) error of wall-normal heat flux (see Eq.[11] where \( \varphi = v\theta \)). At each \( Ri_b \), ×, base; △, mcflux, trained on \( Ri_b = 0.018 \); ○, trained on \( Ri_b = 0.094 \), \( f(I, J) = 0.966 - I - 2(-0.43 + J)(I - 0.089J)J \), mcgrad. For each model, we plot a fitting curve to show the trend at different \( Ri_b \) cases, ×, base; △, mcflux; □, mcgrad. For each model, we plot a fitting curve to show the trend at different \( Ri_b \) cases, from light to heavy, mcmean, nccnu, mcdc, mcgrad, the heaviest (black) solid line, mcgrad.

combination of quantities of interest, the mcdc case is the best model for the VMC cases. To summarize, the influence of training approaches for VMC cases is more significant than that for VNC cases. With the precondition of training on the middle range \( Ri_b \) case, we finally find a machine learnt model via the CFD-driven approach with the cost function \( J(\Theta) + \lambda_2 J(\partial \Theta / \partial y) \) that performs well for all the considered \( Ri_b \) cases.

Figure 13: Error metric with baseline or GEP models, (a) error of the Nusselt number \( J(Nu) \) (see Eq.13a); (b) error of the mean temperature (see Eq.[11] where \( \varphi = \Theta \)); (c) error of wall-normal heat flux (see Eq.[11] where \( \varphi = v\theta \)). At each \( Ri_b \), ×, base; △, mcflux; □, mcgrad; CFD-driven, -----, from light to heavy, mcmean, nccnu, mcdc, mcgrad, the heaviest (black) solid line, mcgrad.

4.3 A priori test on the turbulent Prandtl number

The predicted turbulent Prandtl number for VNC is shown in Fig.[14] where the DNS results [Ng et al., 2015] and baseline calculate with a constant \( Pr_t = 0.90 \) are included, with \( Ra \) spanning four decades from \( 10^5 \) to \( 10^9 \). The \( Pr_t \) has the same feature. In the turbulent layer region \( (y < y_w < h) \), \( Pr_t^{dn} \) remains at a constant value, which stays in the range of \( 0.85 \sim 1.0 \) across different \( Ra \) numbers. Therefore, constant \( Pr_t \) may turn out to be a good approximation as \( Ra \rightarrow \infty \) and the region of infinity anomaly diminishes. Conversely, it shows that the machine learnt model provides spatially varying \( Pr_t \) in the near-wall region. It is essential that the resulting GEP model can identify the adjustment
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region \((y_1 < y < y_2)\) and bridge the infinity region of \(Pr_t\) with a finite value, without any user intervention, due to the self-adapting feature of dimensionless frame invariants.

In Fig. 15, the GEP generated \(Pr_t\) for VMC (Table [mcgrad]) is compared against the DNS-based \(Pr_t\) [Sutherland et al., 2015] and a constant \(Pr_t = 0.90\) for different \(Ri_b\). In the very near-wall region, \(I\) and \(J\) are near zero (owing to \(k = 0\) at the hotter \((y/h = 0)\) and colder \((y/h = 2)\) walls); hence, \(Pr_t = 1/f(I, J) = 0.91\), which is smaller than the DNS near-wall results. Away from each wall, the \(Pr_t^{\text{grd}}\) quickly reaches a maximum (at approximately 1.4) near \(y^+ = 10\), while the maxima of \(Pr_t^{\text{dns}}\) (see Fig. 5) are close to each wall. However, they both decrease to 0.90 before entering the infinity region (near \(y_2\)). Moreover, the agreement between GEP and DNS results is not as good compared with VNC case. One possible reason could be the discrepancy of the approximated eddy viscosity \(\nu_{\text{mod}}\) with DNS-based eddy viscosity . Nevertheless, the \textit{a priori} assessment shows GEP explicitly returns a variable \(Pr_t\), and the infinity regions are approximated by values of nearly 0.90 across the different \(Ri_b\) cases.

4.4 \textit{A posteriori} performance for quantities of interest

Fig. 16(a) shows the comparison of \(Nu\) resulting from the baseline and GEP models with DNS data at different \(Ra\) numbers. The baseline model significantly underpredicts the \(Nu\), especially at higher \(Ra\), with an absolute percentage error over 25%. Conversely, the GEP models can successfully predict the classical heat-transfer relationship \(Nu \sim Ra^{1/3}\). Fig. 16(b) illustrates \(Nu\) versus \(Ri_b\) for VMC. Interestingly, as we showed earlier, the baseline can nearly perfectly predict \(Nu\) in the forced convection case but considerably overpredicts \(Nu\) with at least 10% absolute percentage error for higher \(Ri_b\) values. The performance of the GEP models reduces the error to less than 5%.
Figure 16: A posteriori assessment of the Nusselt number, ○, DNS; ■, GEP; ×, base; (a) $Nu$ versus $Ra$ for VNC, on a log-log scale, · · ·, $Nu = 0.071(RaPr)^{1/3}$ by Versteegh and Nieuwstadt [1999]; (b) $Nu$ versus $Ri_b$ for VMC.

Figure 17: A posteriori assessment of (a ∼ c) mean temperature profile, (d ∼ f) wall-normal heat flux for VNC; here, inner scaling [George Jr and Capp, 1979, Ng et al., 2013] is used. —— GEP, · · · DNS, - - - baseline.

Further results for the mean profile and wall-normal heat flux are shown in Fig. [17] for VNC and Fig. [18] for VMC. In Fig. [17] (a ∼ f) are plotted with an inner layer scaling [George Jr and Capp, 1979, Ng et al., 2013], where the inner temperature scales $[|f_w|^3/(gβκ)]^{1/4}$ and the inner length scale $[κ^3/(gβ|f_w|)]^{1/4}$, in order to show the near-wall results. Due to the asymmetry profiles, here, we only show the half channel from the hotter wall. It is clear that the GEP model is better than the baseline for $Θ$ and $vθ$ at the bulk region. In total, GEP-based models are fairly good, and the
improvement holds for the whole field for VNC. Moreover, for VMC, Fig. 18 (a ∼ c) shows the mean temperature Θ profile along the hotter and colder wall, respectively, and Fig. 18 (d ∼ f) depicts the wall-normal heat flux $v\theta$ in the global coordinates. Compared with the VNC case, the performance of baseline models is better, yet there is still room to improve. Although the baseline model correctly predicts the $Nu$ in the forced convection case, surprisingly, the improvement of GEP models on Θ and $v\theta$ is consistently better than the baseline at different $Ri_b$ ($0 \leq Ri_b \leq 0.094$).

5 Concluding remarks

As the angle between the gravitation direction and temperature gradient reaches $90^\circ$, the turbulent Prandtl number $Pr_t$ and eddy viscosity $\nu_t$ tend to infinity in a thin adjustment region between the near-wall laminar-viscosity layer and the bulk turbulent region for vertical natural convection (VNC) in a range of Rayleigh numbers ($10^5 \sim 10^9$). Whereas recent studies on VNC adopt an inner-outer two-layer structure [George Jr and Capp, 1979; Hölting and Herwig, 2005; Ng et al., 2013, 2015], we argue that this extra adjustment region can be identified by the zero point of Reynolds shear stress and the mean velocity gradient. Meanwhile, for vertical mixed convection (VMC) it also exists singular points of $Pr_t$ and $\nu_t$. They vary with increase of the buoyancy force, as the mean velocity maximum shift from the centreline to the hotter wall. This finding indicates that the primary effect of buoyancy on the mean profile for VMC is the break of symmetry, even for the flow in the shear-dominated regime ($0 < Ri_b < 0.1$).

To approximate the essential thermal quantities, including Nusselt number, mean temperature and wall-normal heat flux, we implement the machine learning framework via gene expression programming (GEP) to develop new turbulent heat flux models by using the DNS-based velocity fields as input for turbulent natural and mixed convection in a vertical channel. Furthermore, a sensitivity study on the training dataset and cost functions via both frozen and CFD-driven concepts are implemented to find the best prediction of the Nusselt number, mean temperature, and wall-normal heat flux. Comparing the a posteriori performance on $Nu$, Θ, and $v\theta$, we discover that the error of the baseline (a constant $Pr_t = 0.90$) model for VNC case is larger than for the VMC case, and it is relatively easy to find effective GEP models for VNC. The data-driven method in this study is almost independent of the training dataset and cost function for the VNC case. In contrast, the VMC cases needs a strict selection of both the training dataset and cost functions. We
discover that the inclusion of the mean gradient, which acts as a bridge between first- and second-order statistics, in the cost function shows significant advantages in finding a better GEP model. This is also true for the VNC cases. In general, using cost functions that include the mean temperature gradient based on the middle range of the DNS dataset across the parameter space for both VNC and VMC can obtain a better model.

The best performing GEP models can predict $Nu$ within a 5% absolute percentage error for the VNC case across four decades of $Ra$ ($10^5 \sim 10^9$) and for VMC in the entire range of $0 < Ri_b < 0.1$ at a mean friction Reynolds number of 395, even though the training is carried out for a specific DNS dataset case. The reduction of error by GEP models is achieved across the current parameter space and cover all of the domain without any regional treatment. It is also important that the data-driven method overcomes the singularity issues of linear gradient-based models with a spatially varying $Pr_t$.

The RANS model development is an odyssey when the pursuit is generality and universality. Nevertheless, we can show the robustness and accuracy of the current GEP models for the turbulent Prandtl number. We capture the correct physics of the turbulent Prandtl number, but concede that the result of full RANS-based CFD for VNC and VMC would still benefit from further improvement. One avenue to pursue in future work is addressing the fact that the time and length scale calculated by $k$ and $\varepsilon$ (or $\omega$) in RANS have a large discrepancy with the DNS dataset in the near-wall region, which undermines the suitability of the dimensionless velocity and temperature invariants.

Declaration of Competing Interest

We wish to confirm that there are no known conflicts of interest associated with this publication.

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Appendix A, DNS on vertical mixed convection

The cited turbulent mixed convection cases are conducted by [Sutherland et al., 2015]. As the reference is an abstract for the American Physical Society (APS) conference, it lacks computational details. Therefore, after private communication, we can provide the simulation setup and governing equations. As previously mentioned, some flow parameters are held constant for all simulations. $Pr = 0.709$, $\Delta \Theta = 1$, and $g_1 \beta = (-1, 0, 0)$. All simulations are carried out with computational domain size $(L_x, L_y, L_z) = (16h, 2h, 8h)$. The present grid spacing is uniform in the $x$- and $z$-directions and is stretched by a non-uniform Chebyshev grid $y_j = L_y \cos(\pi j/Ny)/2$ in the $y$-direction to resolve the steep, near-wall gradients. The number of grid points $N_x$, $N_y$, and $N_z$ are chosen following [Kim et al., 1987], so that $\Delta x^+ \approx 10$, $\Delta y^+ \approx 0.05$ and $\Delta z^+ \approx 5$ and to maintain an aspect ratio of approximately one in the centre of the channel. The time step is chosen to satisfy the CFL condition.

\[
\begin{align*}
\frac{\partial u_i}{\partial x_i} &= 0, \\
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} &= -\frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + \delta_{i1} g_1 \beta \Theta + \nu \frac{\partial^2 u_i}{\partial x_j^2}, \\
\frac{\partial \Theta}{\partial t} + u_j \frac{\partial \Theta}{\partial x_j} &= \kappa \frac{\partial^2 \Theta}{\partial x_j^2}.
\end{align*}
\]

The numerical scheme used is a fully conservative fourth-order finite difference method on a staggered grid for the velocities following [Morinishi et al., 1998], and the temperature field is advected using the QUICK scheme [Leonard, 1979]. Time-stepping is accomplished by a low-storage third-order Runge-Kutta scheme due to [Spalart et al., 1991]. The continuity equation is enforced using the time-splitting method [Kim and Moin, 1985]. The solver has been successfully used for some recent studies, for example, [Chung and Matheou, 2012] and [Ng et al., 2015].

References

Batchelor, G., 1954. Heat transfer by free convection across a closed cavity between vertical boundaries at different temperatures. Q. Appl. Math. 12, 209–233.
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| label  | Flow case    | \(Re_b\) | \(Ra\)  | \(Re_{\tau}^a\) | \(Re_{\tau}^b\) | \(Re_{\tau}^c\) | \(Nu\)  | \(N_x\) | \(N_y\) | \(N_z\) |
|--------|--------------|-----------|---------|-----------------|-----------------|-----------------|--------|--------|--------|--------|
| R100   | Ra0.3_Re4.1  | 13846     | 0       | 0               | 395.33          | 395.37          | 395.28 | 12.75  | 512    | 256    | 256    |
| R113   | Ra6.3_Re4.2  | 14239     | 1.9 \times 10^6 | 0.013          | 405.33          | 418.86          | 391.80 | 12.79  | 512    | 256    | 256    |
| R118   | Ra6.3_Re4.1  | 12963     | 2.2 \times 10^6 | 0.018          | 375.19          | 391.45          | 358.94 | 12.32  | 512    | 256    | 256    |
| R23    | Ra6.5_Re4.2  | 14710     | 3.6 \times 10^6 | 0.023          | 419.81          | 440.46          | 399.16 | 13.57  | 512    | 384    | 256    |
| R35    | Ra6.6_Re4.1  | 12696     | 4.0 \times 10^6 | 0.035          | 370.92          | 396.04          | 345.79 | 12.86  | 512    | 384    | 256    |
| R50    | Ra6.9_Re4.2  | 15232     | 8.3 \times 10^6 | 0.050          | 438.10          | 484.09          | 392.11 | 14.88  | 512    | 384    | 256    |
| R94    | Ra7.0_Re4.1  | 11825     | 9.3 \times 10^6 | 0.094          | 356.11          | 398.27          | 313.95 | 13.54  | 512    | 384    | 256    |

Table 5: List of parameters for a vertical buoyant turbulent channel. \(Re_b = 2hU_b/\nu\) is the bulk Reynolds number, \(Re_\tau^a = hU_\tau/\nu\) is the friction Reynolds number, \(Re_\tau^b = 2\beta g \Delta \Theta h / U_\tau^2\) is the bulk Richardson number, \(Ra = \beta g \Delta \Theta (2h)^{3/2} \alpha / (\alpha \nu)\) is the Rayleigh number, \(Nu = (2h / \Delta \Theta) |d\Theta/dy|_w\) is the Nusselt number. \(N_x, N_y, N_z\) are the number of grid points in the streamwise, wall-normal, and spanwise directions, respectively. The grid is stretched using a Chebyshev grid.

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