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BRIEF REPORT

REVISED The SquAd derivation: A Square Additive approach to the turbulent Prandtl number

[version 3; peer review: 1 approved, 3 approved with reservations, 1 not approved]

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Abstract

Liquid metals have been chosen as primary coolant of innovative nuclear systems under current development. They present a very high thermal conductivity and hence a very low molecular Prandtl number. This feature challenges the modeling of turbulent thermal flows applying the Reynolds analogy. This paper addresses this challenge. A new formula for the turbulent Prandtl number is derived in terms of local variables available from two-equations turbulence models. The derivation is a direct consequence of the expected square additivity of the molecular and flow parameters defining the effective viscosity and the effective conductivity. The formula does not degenerate and leads to a Kays like formulation if approximated. While constrained by the quality of the turbulent viscosity modeling, it has the potential to improve the numerical simulation of turbulent thermal flows.

Keywords

Prandtl, Kays, CFD, turbulence modelling

This article is included in the Euratom gateway.

Open Peer Review

Approval Status ✓ ✗ ? ? ?

	1	2	3	4	5
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version 1 07 Mar 2023	✓ view	✗ view			

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Any reports and responses or comments on the article can be found at the end of the article.

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Author roles: Moreau V: Conceptualization, Writing – Original Draft Preparation

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REVISED **Amendments from Version 2**

There is a strong divergence of opinion between some reviewers and the author with regard to the necessity of additional validation.

The difference between Kays correlation and the Squad formula for liquid metals is irrelevant. For this reason, validation of Kays correlation implies the validation of the Squad formula. And Kays correlation validation has already been done elsewhere.

However, for completeness I indicate in the Discussion part a recent paper in which the matter is extensively treated. This also allows to differentiate the use of the correlation together with direct numerical integration of universal profiles, in which the results are extremely good, from its use for CFD engineering application for which results cannot yet be so good. The text is the following:

"For low Pr_t, the difference between formula (13) and Kays correlation is irrelevant, making their validity strongly correlated. Kays correlation for low Pr_t is discussed, analyzed and validated in [7}. In this paper, a turbulent heat transfer model, giving excellent results, is proposed based on direct numerical integration using Kays correlation and universal profiles of velocity and eddy viscosity.

An issue remains for CFD engineering applications which are the original target of this work."

Except for few cosmetics, this is the only change/addition.

Any further responses from the reviewers can be found at the end of the article

Introduction

Low Prandtl number liquid metals serve as primary coolant for MYRRHA[1] and ALFRED[2], two Gen-IV reactors under development[1]. The low Prandtl number induces discrepancies in the modeling of the turbulent heat transfer when directly addressed according to the Reynolds analogy with a constant turbulent Prandtl number. The thermal boundary layer is considerably larger than the velocity one, up to the point that, while we can clearly define a bulk velocity, the temperature profile may not exhibit any almost constant bulk temperature plateau. The issue was investigated by several authors who reviewed the existing correlations and proposed their own one[2–4]. The correlations make use of adimensional numbers such as Reynolds and Peclet. Their functional form is mostly empirical with coefficients determined by best fit. The Reynolds number and the Peclet numbers are global parameters, only useful and well-defined for simple geometries. Their use in CFD[3] simulations of complex geometries is questionable. Among all correlations reviewed, Kays' correlation is the only one making exclusive use of local parameters. Variants of this correlation have been used with significant success. The variants share the same structure but feature different values for one numerical constant. In our previously published four page brief report[5], we showed that the correlations can be simply derived on a basic assumption with regards to the non-linear combination of stochastic effects and the variants then stem from different approximations of a mother formula. The objective of this former brief report was only to establish and keep trace of the probable relationship between the stochastic concept and the empirical correlation. It is in no way a bulletproof demonstration and there is no specific treatment of the viscosity. In particular, the definition of the asymptotic Prandtl number and its use are not completely consistent. Besides, from the purely numerical point of view, a defect of the mother formula, which is transferred to the variants, is that the turbulent Prandtl number becomes infinite at vanishing turbulence.

These considerations motivate to proceed further with the analysis which is the object of this current brief report. The key point resides in refining the concept that lies behind the formerly loosely determined asymptotic Prandtl number. What really needs to be done is to separate clearly what is from molecular origin and what is not. This is found to be more prolifically reformulated in terms of differentiating the properties of the fluid from the properties of the flow, being the flow either laminar or turbulent.

In order to proceed consistently with the flow versus fluid properties separation, it becomes necessary to apply the principle of square additivity not only to the thermal conductivity but also to the viscosity. This allows and brings us to define the "flow Prandtl number". Our driving hypothesis is that this number is a universal constant.

As previously, the principle of square additivity completely determines the turbulent Prandtl number. The new formula, while similar, is more articulated than the previous one presented in 5. Its first order approximation still has the functional shape of Kays' correlation and coincides with it for low Prandtl number fluids. Our formula however gives additional information on Kays' correlation range of validity. The new formula also correcly degenerates to the 0.85 traditional constant value commonly used for near unity Prandtl number fluids. Besides, as a good news for numerical implementation, the newly derived formula has the merit of not degenerating anymore at vanishing turbulence, which was not a feature of the previous formula.

Turbulent Prandtl number derivation

In the framework of thermal fluid dynamics of turbulent flows, the focus is concentrated on the determination and modeling of the effective viscosity and effective heat diffusion of the fluid. The viscosity and the heat diffusion both consist in the sum of two parts, one molecular and the other associated with turbulence.

With regard to the heat diffusion, both the molecular and the turbulent fluxes are oriented in the direction of the local temperature gradient and they are proportional to it. The intensity is also determined by the conductivity coefficients. The effective conductivity coefficient k_e can be expressed as

$$k_e = k + k_t \tag{1}$$

[1] Multi-purpose Hybrid Research Reactor for High-tech Applications

[2] Advanced Lead-cooled Fast Reactor European Demonstrator

[3] Computational Fluid Dynamics

denoting, respectively with k and k_t the molecular conductivity and the increment due to turbulence.

Indicating with ρ the fluid density and C_p its specific heat, this expression can be rewritten in terms of thermal diffusivity:

$$\alpha_e = \alpha + \alpha_t \tag{2}$$

in which $\alpha_e = k_e/(\rho C_p)$ stands for the effective diffusivity, $\alpha = k/(\rho C_p)$ is the molecular part and $\alpha_t = k_t/(\rho C_p)$ is the turbulent part.

Similarly, as far as the viscosity is concerned, the effective kinematic viscosity ν_e is the sum of the laminar contribution ν and the increment ν_t induced by turbulence:

$$\nu_e = \nu + \nu_t \tag{3}$$

The argument previously developed in 5 is the following. Conduction has a stochastic origin. The scale at which molecular conduction and the added conduction observed in turbulent flows operate are different and their mechanisms are unrelated. Molecular conduction is a molecular process and is a property of the fluid while the added conduction has a convective origin and is a property of the flow. The combination of their effects is better represented as a convolution rather than as a direct sum. Translated in formula, under this representation we expect to have:

$$\alpha_e = \sqrt{\alpha^2 + \alpha_0^2}, \tag{4}$$

where the diffusivity α_0 should be an intrinsic property of the flow rather than the fluid.

The same argument is extended to the viscous process and it states that the effective viscosity comes from two independent processes whose intensity should be square additive:

$$\nu_e = \sqrt{\nu^2 + \nu_0^2}. \tag{5}$$

By simple substitution, we have just defined two new quantities: the flow viscosity ν_0

$$\nu_0 = \nu_t \sqrt{1 + \frac{2\nu}{\nu_t}} \tag{6}$$

and the flow diffusivity α_0

$$\alpha_0 = \alpha_t \sqrt{1 + \frac{2\alpha}{\alpha_t}}. \tag{7}$$

We can also redefine ν_t and α_t in terms of ν_0 and α_0:

$$\nu_t = \sqrt{\nu^2 + \nu_0^2} - \nu \tag{8}$$

$$\alpha_t = \sqrt{\alpha^2 + \alpha_0^2} - \alpha \tag{9}$$

Therefore, the representations with (ν_t, α_t) and with (ν_0, α_0) are completely equivalent and interchangeable.

We now introduce the known Prandlt number $Pr = \frac{\nu}{\alpha}$ and turbulent Prandtl number $Pr_t = \frac{\nu_t}{\alpha_t}$. Besides, we can now also define the flow Prandtl number $Pr_0 = \frac{\nu_0}{\alpha_0}$ and look at how these numbers are related.

Noting that $\frac{\alpha}{\alpha_0} = \frac{Pr_0 \nu}{Pr \nu_0}$, by combining the former equations, we obtain:

$$Pr_t = \frac{Pr_0^2}{Pr} \frac{\sqrt{1 + \left(\frac{Pr \nu_0}{Pr_0 \nu}\right)^2} + 1}{\sqrt{1 + \left(\frac{\nu_0}{\nu}\right)^2} + 1}. \tag{10}$$

This specific form is chosen to show that it cannot degenerate to zero or infinity. In effect, because ν_0 goes to zero if ν_t does, then Pr_t tends to $\frac{Pr_0^2}{Pr}$ while for large turbulence, Pr_t tends to Pr_0.

Expression 10 can be rewritten in terms of ν/ν_0.

$$Pr_t = Pr_0 \frac{\sqrt{1 + \left(\frac{Pr_0 \nu}{Pr \nu_0}\right)^2} + \frac{Pr_0 \nu}{Pr \nu_0}}{\sqrt{1 + \left(\frac{\nu}{\nu_0}\right)^2} + \frac{\nu}{\nu_0}}. \tag{11}$$

This formula is quite complicated and not easy to interpret at first glance, but considering ν/ν_0 as a small parameter, a brutal simplification of 11 at first order in this parameter gives:

$$Pr_t \simeq Pr_0 [1 + (\frac{Pr_0}{Pr} - 1) \frac{\nu}{\nu_0}] \tag{12}$$

This formulation is practical only if ν_0 is readily available. This would be the case if we had a transport equation for ν_0 or a related variable similarly to what is done with the usual 2-equations turbulence models. Exploring the potential of this possibility is beyond the scope of the current discussion and we need to express Pr_t in terms of known parameters.

Thus, expressing Pr_t in terms of ν_t instead of ν_0, formula 10 becomes:

$$Pr_t = \frac{Pr_0^2}{Pr} \frac{\sqrt{1 + \left(\frac{Pr}{Pr_0}\right)^2 \frac{\nu_t}{\nu}\left(\frac{\nu_t}{\nu} + 2\right)} + 1}{2 + \frac{\nu_t}{\nu}}, \tag{13}$$

this form being useful for interpretation at vanishing turbulent viscosity.

Dividing this last formula by Pr_0, we have a relation between the three dimensionless groups $\frac{Pr_t}{Pr_0}$, $\frac{Pr}{Pr_0}$ and $\frac{\nu_t}{\nu}$ in the form:

$$\frac{Pr_t}{Pr_0} = f(\frac{Pr}{Pr_0}, \frac{\nu_t}{\nu}). \tag{14}$$

In view of a development in ν/ν_t, formula 13 becomes:

$$Pr_t = Pr_0 \frac{\sqrt{1+\frac{2\nu}{\nu_t}+\left(\frac{Pr_0\nu}{Pr\nu_t}\right)^2}+\frac{Pr_0\nu}{Pr\nu_t}}{1+\frac{2\nu}{\nu_t}} \quad (15)$$

Here again, a brutal first order development in terms of ν/ν_t, valid only when both ν_t/ν and $Pr\nu_t/Pr_0\nu$ are large, gives the following approximation for Pr_t:

$$Pr_t \simeq Pr_0[1+(\frac{Pr_0}{Pr}-1)\frac{\nu}{\nu_t}], \quad (16)$$

meaning that changing from ν_0 to ν_t brings only second order terms approximation. In particular, this last expression has the same form as the Kays correlation[2].

Discussion

Our driving hypothesis is that the flow Prandtl number Pr_0 is constant. Therefore, it must coincide with the value used for highly turbulent flow and near unit Pr. That is, $Pr_0 = 0.85$.

For $Pr \simeq 0.025$, a typical value for heavy liquid metals, formula 16 becomes almost exactly the first Kays correlation:

$$Pr_t \simeq 0.85 + \frac{0.70}{Pr\frac{\nu_t}{\nu}} \quad (17)$$

For the second coefficient (here 0.7), Kays indicated two values, 0.7 and 2, discussing without reaching a conclusion in favor of one or the other value. However, a less brutal approximation could lead to a different coefficient. For example, in 6, 1.46 is obtained from direct analytical integration and best fit of heat transfer in a tube. Moreover, our newly derived formula is not much different than the one derived previously in 5 and a more precise approximation, while more complex to derive, would most probably also lead to an increased second coefficient about 1.45.

A particular case is when $Pr = Pr_0$. Then $Pr_t = Pr_0$ too. For medium and high Pr, we observe that Pr_t in formula (11) does not significantly departs from Pr_0, except for strongly vanishing ν_t/ν.

With a little algebra, we found that Pr_t is a decreasing function of ν_t for $Pr \leq Pr_0$ and increasing function of ν_t for $Pr \geq Pr_0$, with values spanning the interval $[Pr_0;\ Pr_0^2/Pr]$ and $[Pr_0^2/Pr;\ Pr_0]$. The approximation in 16, while with the same monotonicity, fails to meet the correct bound for vanishing viscosity, for which it degenerates. Interestingly, we can see that the second coefficient depends critically on the Prandtl number, to the point that it vanishes for $Pr_t = Pr_0$ and changes sign afterwards, like for the complete expression. This is a clear indication that the Kays correlation should be used as such only for low Prandtl number (say < 0.1) fluids.

For low Pr_t, the difference between formula 13 and Kays correlation is irrelevant, making their validity strongly correlated. Kays correlation for low Pr_t is discussed, analyzed and validated in 7. In this paper, a turbulent heat transfer model, giving excellent results, is proposed based on direct numerical integration using Kays correlation and universal profiles of velocity and eddy viscosity. An issue remains for CFD engineering applications which are the original target of this work. The derived formula is ought to be used within a CFD turbulence model. It would make sense only if the turbulence model correctly predicted the turbulent viscosity. This has to be true not only in the viscous boundary layer but also and principally in the bulk, in which the thermal boundary layer could still be in development. The problem is that the turbulence models mainly focus on the correct near-wall boundary layer turbulent viscosity profile, as it is the place where almost all the pressure drop is built, with the main aim to capture the correct wall shear stress. The turbulent viscosity profile in the bulk is normally of no practical importance, except for thermal flows of low Prandtl number fluids.

Looking at the profile of ν_t compared with direct numerical simulation data even in the simplest 2D channel flow, see figure 5 in 8, we can see that the turbulence models fail to give a correct profile for a wall Y+ value above 30. In particular, ν_t is underpredicted below Y+ up to 100–150 and over predicted afterward. The difference between the simply additive and the square additive approaches is mainly concentrated and felt around the values where both contributions are of similar intensity: $\nu/Pr \sim \nu_t/Pr_0$ or equivalently $\nu_t/\nu \sim Pr_0/Pr$. For a low Prandtl number fluid with $Pr = 0.025$ we have $Pr_0/Pr = 34$, so all the region where ν_t/ν lies between say 10 and 100 is concerned, that is precisely for Y+ above 30 for the case analyzed in 8. The balance between the thermal effects of both Y+ regions is shifted towards an artificially increased diffusion. To counteract this effect, the turbulent Prandtl number can be increased artificially for a better fit. This could be an explanation for the use of an augmented second coefficient in the Kays correlation as indicated previously.

The main effect of applying the square additivity to the effective viscosity is that it removes the degeneration of the Pr_t formula for vanishing viscosity that was still present in 5. It is not clear nor sure that it is of practical importance anywhere else. It seems that, within the level of approximation given by the 2-equations turbulence models, ν_t and ν_0 can be used indifferently in the formula. In other words, the square additivity could be used solely for the energy equation.

Conclusions

We consider that the effective viscosity takes origin from two independent stochastic processes whose intensity is square additive. The same consideration is extended to the effective conductivity. We have defined a flow Prandtl number which is expected to be a universal property of the flow and to be in fact a constant under the square additive approach. The turbulent Prandtl number is then determined by a formula reproducing the first variant of Kays' correlation when approximated at the first order. The derivation sheds light on the Kays correlation and indicates that the second coefficient depends critically on the Prandtl number to the point that it vanishes when $Pr = 0.85$. Under the condition that the classical 2-equations

turbulence models become able to capture correctly the turbulent viscosity profile, we expect that the turbulent Prandtl number formula can give improved thermal results independently of the Prandtl number and particularly for the low Prandtl liquid Lead and Lead alloys.

The Reynolds analogy could have a much wider domain of validity by combining it with the SquAd (Square Additive) derivation.

Data availability

No data are associated with this article.

Acknowledgments

A previous (non-peer reviewed) version of this article is available on preprints.org (https://www.preprints.org/manuscript/202212.0160/v1) and the publications.crs4.it repository (http://publications.crs4.it/pubdocs/2022/Mor22/).

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Open Peer Review

Current Peer Review Status: ✔ ✘ ? ? ?

Version 3

Reviewer Report 26 February 2024

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✘

Davide Modesti
Delft University of Technology, Mekelweg, Delft, The Netherlands

The major issues that I pointed out from the first revision have not been addressed, therefore I cannot recommend the manuscript for indexing. I summarize again the main issues. The author proposes a new definition of effective viscosity and effective thermal diffusivity, namely \alpha_e = sqrt(\alpha^2 + \alpha_0^2), where \alpha_0 is a property of the fluid. This new definition is used to derive a new formula for the turbulent Prandtl number

Major issues: 1) The new definitions (equations 4 and 5) don't have a clear theoretical fundation, or if they do it is not clear. The canonical definition of effective thermal diffusivity stems from the mean thermal balance, when using \overline{T'v'} = \alpha_T dT/dy. What is instead the reasoning behind equations (4) and (5). For instance, why using this definition and not \alpha_e = (\alpha^4 + \alpha_0^4)^(1/4), or any other exponent? Why not another function f(alpha,alpha_0)? 2) The author did not validate his hypothesis with experimental or numerical data, therefore I cannot comment on the accuracy of the validity of the hypothesis, as the paper does not contain any figure. I would like to see a comparison of the proposed turbulent Prandtl number with the Prandtl number computed from available DNS or experiments. DNS data at low Prandtl number are available, see for instance the work by Pirozzoli, Sergio. "An explicit representation for mean profiles and fluxes in forced passive scalar convection." Journal of Fluid Mechanics 968 (2023): R1. In the previous paper by Pirozzoli, the eddy diffusivity is found to be nearly independent from the Prandtl number, which seems to contradict the main point of the author.

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Wall turbulence; turbulent flows; compressible flows; forced thermal convection; heat transfer

I confirm that I have read this submission and believe that I have an appropriate level of expertise to state that I do not consider it to be of an acceptable scientific standard, for reasons outlined above.

Reviewer Report 16 February 2024

https://doi.org/10.21956/openreseurope.17933.r37496

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Agustín Villa Ortiz
Universidad Rey Juan Carlos, Madrid, Spain

This work is a nice derivation of a Prt formula that could be used later in thermal flows.

I have a comment on the introduction of the turbulent Prandtl number, Reynolds analogy... The Simple Gradient Diffusion Hypothesis (SGDH) should be mentioned anywhere before the text: *"With regard to the heat diffusion, both the molecular and the turbulent fluxes are oriented in the direction of the local temperature gradient and they are proportional to it. The intensity is also determined by the conductivity coefficients."*
In the case of turbulent heat fluxes (THF) it is not possible to assume that in general both THF and temperature gradient vectors are proportional (please check natural convection cases). If you assume the SGDH and therefore use the Reynolds Analogy you can for sure affirm your comment.

A few figures -where you show the similarities between SquAd and Kays, or the range of validity your simplifications (formulas 10 to 11 and 15 to 16) on the ν/ν_0 ν/ν_t... ratios- might help to validate your approach. Even the comparison of SquAd and Kays for a simple 2D flow at different Prandtl numbers should demonstrate the SquAd effectiveness and preference over Reynolds Analogy.

Is the work clearly and accurately presented and does it cite the current literature?
Yes

Is the study design appropriate and does the work have academic merit?
Yes

Are sufficient details of methods and analysis provided to allow replication by others?
Partly

If applicable, is the statistical analysis and its interpretation appropriate?
Not applicable

Are all the source data underlying the results available to ensure full reproducibility?
No source data required

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Liquid metals, RANS themal turbulence modeling

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Reviewer Report 16 February 2024

https://doi.org/10.21956/openreseurope.17933.r37511

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?

Andrea Pucciarelli
University of Pisa, Pisa, Tuscany, Italy

The contribution proposes an interesting approach for the calculation of the effective viscosity (and diffusivity) by means of a square additive approach.
The hypothesis leads to a formulation of a relation allowing the calculation of the Prtur which is qualitatively similar to Kays relation.

In this regard, in the Kays equation at the denominator there is a Peclet number. In Equation 17 the role of the Reynolds number is made by Nit/Ni. While I understand that the higher the Reynolds the higher (probably) the turbulent viscosity, it would be nice understanding or commenting how these two quantities scale and if there is any limitation in this sense to its application.

Concerning the approval of this contribution, it depends on the spirit of this repository.

As a CFD user I would like to have an idea of the applicability of the present approach to calculations; it is also to be understood how it copes with the eddy viscosity field relations proposed in literature. A validation in this sense would be required for indexing. I do understand it is not the aim of this report, which clearly states that "It is not clear nor sure that it is of practical importance anywhere else" except for the present application.

Nevertheless, I do believe it is worth sharing this idea, the obtained similarity is for sure fascinating, it got my curiosity and I think I could give it a try in some calculations of ours.

Thank you for sharing the contribution.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?

Partly

Are sufficient details of methods and analysis provided to allow replication by others?
Partly

If applicable, is the statistical analysis and its interpretation appropriate?
Not applicable

Are all the source data underlying the results available to ensure full reproducibility?
No source data required

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Computational Fluid Dynamics

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Version 2

Reviewer Report 22 August 2023

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?

Iztok Tiselj
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I share the opinion of the other reviewers:

1. This is an interesting approach to modelling of turbulent Prandtl number. However, it is not completely clear why replacement of one type of flow-dependent and material-independent variables (turbulent viscosity and turbulent diffusivity) with another pair of similar variables is really beneficial.

2. The main concern: the advantage of a new approach should be validated with available numerical data and experiments. The future and further applications of the proposed approach will show, whether the added value is relevant.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Partly

Are sufficient details of methods and analysis provided to allow replication by others?
Yes

If applicable, is the statistical analysis and its interpretation appropriate?
Not applicable

Are all the source data underlying the results available to ensure full reproducibility?
No source data required

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: References relevant for the present review: DNS simulations of channel flow heat transfer with and without conjugate heat transfer at low Prandtl numbers.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 06 Sep 2023

Vincent MOREAU

The reviewer text is indicated in slanted. *I share the opinion of the other reviewers:*
This is an interesting approach to modelling of turbulent Prandtl number. However, it is not completely clear why replacement of one type of flow-dependent and material-independent variables (turbulent viscosity and turbulent diffusivity) with another pair of similar variables is really beneficial. I think that this paper is bringing undue expectations.
No replacement is required. Enforcing the equivalence of two different approaches to the same phenomena had the result to produce automatically a formula for the turbulent Prandtl number. The formula is substantially equivalent to Kays correlation for liquid metals and revert to the classical constant value for near unit Prandtl fluids. That is all, but it is already in my opinion a worthwhile result.
While the concept was already presented in a previous paper, it was done in an unfinished way and with a confusing terminology. It took me more than a year to realize that there was room for improvement. Systemization of the approach led to the present formula. For this, I had to give first letters then names to things. I understand that giving names to things is quite presumptuous but is has been raised necessary for clarity.

The main concern: the advantage of a new approach should be validated with available numerical data and experiments. I strongly disagree with this. The advantage of the new approach is only to give a possible interpretation to Kays correlation and, if one wants, to use a non-degenerating equivalent formula without empirical constant. This is the over-expectation issue. It is not the aim of this paper to validate the Kays correlation with experiments. I chose to make a brief report also to avoid this kind of undue request. Validating Kays correlation is far beyond my competence, budget, time availability and has already been done elsewhere. However, for completeness, and as a compromise, I an adding in the report a more recent publication (ref. 7, 2020) in which Kays correlation is discussed and validated. *The future and further applications of the proposed approach will show, whether the added value is relevant.* For me, re-interpreting an efficient correlation as a formula without empirical constant is already an extremely relevant result. Maybe this is a deformation due to my original formation as a mathematician. I understand though that for most people working in the field, this feature is almost totally irrelevant. I wanted to publish this result for the few others, who can also read simple formulas, if I am let do it. Another point I wanted to stress is the need of a turbulence model giving decent effective viscosity profiles. I have no competency in that matter, so my contribution in any case ends here.

Competing Interests: No competing interests were disclosed.

Reviewer Report 10 August 2023

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The manuscript has only slightly changed compared to the original version, and I still have major concerns regarding the validation. For this reason I cannot recommend the article for indexing.

1. Validation cannot be done only with Kays formula. This formula is for Prandtl numbers close to unity and not for low Prandtl numbers. Data from experiments or simulations should be used and figures should be added to the manuscript to support the hypotheses and the results.

2. I still miss how the effective diffusivity can satisfy the mean temperature balance.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Partly

Are sufficient details of methods and analysis provided to allow replication by others?
Partly

If applicable, is the statistical analysis and its interpretation appropriate?
Partly

Are all the source data underlying the results available to ensure full reproducibility?
Partly

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Wall turbulence; turbulent flows; compressible flows; forced thermal convection; heat transfer

I confirm that I have read this submission and believe that I have an appropriate level of expertise to state that I do not consider it to be of an acceptable scientific standard, for reasons outlined above.

Author Response 06 Sep 2023

Vincent MOREAU

The reviewer text is indicated in slanted. *The manuscript has only slightly changed compared to the original version, and I still have major concerns regarding the validation. For this reason I cannot recommend the article for indexing.* The manuscript has been modified in order to take into account the constructive and relevant indications of the first reviewers. It seems to me that your review is mainly based on misunderstanding. This led me to try to improve the paper clarity.
One nice thing about the transparency politics of Open-Research-Europe is that in case of disagreement between author and reviewer, an interested reader can make its own informed opinion. *Validation cannot be done only with Kays formula. This formula is for Prandtl numbers close to unity and not for low Prandtl numbers.* First you suggest to use validation from Kays old work and when I stress that this is already done with a much more recent one with all the improvement a researcher can do in 14 years, then you pretend that it is no more valid. This is quite confusing. The affirmation in the second sentence is extremely surprising and I really wonder where it does come from. If you read Kays reference (1994), you will see that this is clearly not the case. Same thing with the more recent reference (2016) from Taler. Maybe you made confusion with eq.21 (Kays and Crawford) in Kays paper related to Prt for air. What is referred as Kays correlation is eq.17 in his 1994 paper (and sometimes also eq.18). *Data from experiments or simulations should be used and figures should be added to the manuscript to support the hypotheses and the results.* I strongly

disagree. Kays correlation does not need any more validation. A discussion on this point can be found in a more recent paper:
Zhang R, Wang Z, Wang Z, Ren T and Shi J (2020) Theoretical Investigation on the Fully Developed Turbulent Heat Transfer Characteristics of Liquid Sodium. Front. Energy Res. 8:10. doi: 10.3389/fenrg.2020.00010
For completeness, I refer to this paper in the Discussion section and add it in the references.
To quote Kays paper: "During the past 40 years dozens of solutions for Prt based on a variety of analytic models have appeared in literature.(...) but virtually all [analyses] contain free constants, which must be evaluated by comparison with the available experimental data."
My finding is that Kays correlation, which also seems to contain a "free" constant, in fact does not, once you interpret it in the framework of stochastic process.
In other words, my work is a theoretical validation of Kays correlation and if Kays correlation is wrong or is of very limited range of validity, then the "theory" is also wrong. There is no room and no need in this context for figures. The paper is intended for people who can read simple formulas.
I still miss how the effective diffusivity can satisfy the mean temperature balance. I do not understand what you mean. I do not understand at what level I should state my answer. Is what you miss present only for my effective diffusivity coefficient formula or is it already present with Kays correlation? I do not propose any structural change in the diffusive term of the energy equation so I do not understand where or how there could be an issue that would not be pre-existing.

Competing Interests: No competing interests were disclosed.

Version 1

Reviewer Report 08 June 2023

https://doi.org/10.21956/openreseurope.16612.r32061

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The manuscript introduces the concept of "flow Prandtl number", namely a universal constant that does not depend on the fluid. This concept is introduced theoretically but then it is not verified using available experimental or numerical data, which is a major shortcoming of this work.

I believe that the manuscript has the following shortcomings:

1. I don't understand why we need to introduce a flow Prandtl number. Isn't it enough to say that the turbulent Prandtl number is independent from the molecular Pr?

2. My main concern is that conclusions are not supported by results. After the derivation of the expression for the flow Prandtl number, I would have expected a validation of the theory using available numerical data. There are many data on this topic. For instance, we have recently generated a comprehensive dataset of turbulent plane channel flow spanning Prandtl numbers between 0.0025-4, which also covers the low Prandtl number regime of this manuscript. The manuscript is available on JFM (Pirozzoli and Modesti, 2023[1]) and the data are also available online at http://newton.dma.uniroma1.it/.

3. The other major concern that I have is on the effective diffusivity in equation (4). The canonical definition of thermal diffusivity (equation 2) is not arbitrary, but it stems from the mean temperature equation upon introducing the eddy diffusivity hypothesis. How does equation (4) comply with the mean temperature balance?

4. The new formulation should be validated against reference numerical data and other state of the art formulas for the turbulent Prandtl number, such as the one by Cebeci (1973[2]), or the variant proposed by Na and Habib (1973[3]), or the formula by Kays *et al.* (1980[4]).

5. In the text of the manuscript I see reference to figures, but I cannot visualize any figure.

References

1. Pirozzoli S, Modesti D: Direct numerical simulation of one-sided forced thermal convection in plane channels. *Journal of Fluid Mechanics*. 2023; **957**. Publisher Full Text
2. Cebeci T: A Model for Eddy Conductivity and Turbulent Prandtl Number. *Journal of Heat Transfer*. 1973; **95** (2): 227-234 Publisher Full Text
3. Na T, Habib I: Heat transfer in turbulent pipe flow based on a new mixing length model. *Applied Scientific Research*. 1973; **28** (1): 302-314 Publisher Full Text
4. Kays W, Crawford M, Weigand B: Convective Heat and Mass Transfer. *McGraw-Hill, New York*. 1980.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Partly

Are sufficient details of methods and analysis provided to allow replication by others?
Yes

If applicable, is the statistical analysis and its interpretation appropriate?
Not applicable

Are all the source data underlying the results available to ensure full reproducibility?
No source data required

Are the conclusions drawn adequately supported by the results?
No

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: wall turbulence; turbulent flows; compressible flows; forced thermal convection; heat transfer

I confirm that I have read this submission and believe that I have an appropriate level of expertise to state that I do not consider it to be of an acceptable scientific standard, for reasons outlined above.

Author Response 21 Jun 2023

Vincent MOREAU

The reviewer text is indicated in italics.

The manuscript introduces the concept of "flow Prandtl number", namely a universal constant that does not depend on the fluid.

That is correct.

This concept is introduced theoretically but then it is not verified using available experimental or numerical data, which is a major shortcoming of this work.

The concept is indeed first introduced theoretically together with the necessary notation. The notation has been clarified giving proper names to α_0 and ν_0. The subscript 0 is not very satisfying but is raised necessary for consistency with the definition of Pr_0 for which it makes sense. For a comparison with published data it is necessary to look at the consequences of the hypothesis on Pr_t expressed in terms of the eddy viscosity, eq. 13 which is the most practical form for numerical implementation but not for further understanding of its meaning. Before proceeding with the validation, eq. 13 is rewritten as eq. 15 to make appear clearly the near constant aspect perturbed by the “natural” small parameter nu/nu_t.

The concept is verified from experimental data at the very beginning of the Discussion section. In effect, eq.17 (first Kays correlation in ref.2) is retrieved by substantiation of eq.16 for Pr=0.025. As in turn eq. 16 is a first order approximation of eq. 15, put in this form for this purpose. From what I have extensively seen and read, for liquid metals, Kays’ correlation is the ultimate comparison to overcome for more elaborated turbulence thermal models, such as 3 or 4 eq. models.

So, I see that my formula is substantially identical, up to a second order term to Kays’ correlation and I sincerely think that it is more than enough for a validation when dealing with liquid metals which is the main focus of this brief report. Besides, my derivation gives better insight on the range of validity of the Kays correlation. This can help users avoid

using it for about unit Pr_t. As easily seen from formula 13 or 15, when Pr=Pr_0 then Pr_t becomes constant which is the choice made by the main CFD code providers with their extensive suite of validation. I have seen the constant taken either at 0.85 or 0.9. It means that there is already there a non negligible uncertainty. This is also why I do not think that going above the first order approximation for validation makes sense.

I believe that the manuscript has the following shortcomings:

I don't understand why we need to introduce a flow Prandtl number. Isn't it enough to say that the turbulent Prandtl number is independent from the molecular Pr?

This is all the point of this brief report. While the hypothesis you state is usually sufficient for engineering application it is no more when dealing with liquid metals. In this case, the region where nu and nu_t are of similar order is much wider that usual and simple summation leads to an overestimation of the effective heat transfer. Would it have been an underestimation, things would have been easier because a constant Pr_t would have provided a slightly conservative solution. Modifying the constant value can be done a posteriori but is not satisfying for prediction capabilities. Besides, we commercial CFD users have the pretention not only to give one or two global parameters but also to give better global fields description. So, it is necessary at least, and still waiting for better, to use Kays' correlation. Problem is that there are two such correlations and authors have also interpolated between them. We are still stuck with the difficulty to reach predictability of the results.

By giving a theoretical foundation to the Kays correlation which address the issue of the dependence of Pr_t on Pr, I believe this brief node can give a useful contribution.

My main concern is that conclusions are not supported by results. After the derivation of the expression for the flow Prandtl number, I would have expected a validation of the theory using available numerical data. There are many data on this topic. For instance, we have recently generated a comprehensive dataset of turbulent plane channel flow spanning Prandtl numbers between 0.0025-4, which also covers the low Prandtl number regime of this manuscript. The manuscript is available on JFM (Pirozzoli and Modesti, 20231) and the data are also available online at http://newton.dma.uniroma1.it/.

This point has been abundantly answered before. The validation comes directly from the extensively validated Kays' correlation from the one hand and from the constant value when Pr=Pr_0 fro the other hand.

The other major concern that I have is on the effective diffusivity in equation (4). The canonical definition of thermal diffusivity (equation 2) is not arbitrary, but it stems from the mean temperature equation upon introducing the eddy diffusivity hypothesis. How does equation (4) comply with the mean temperature balance?

I have named α_0 and ν_0 to clarify the procedure. The description with (α_0, ν_0) and (α_t, ν_t) are completely equivalent and can be retrieved one another. The first couple comes from physical/stochastic consideration and the second couple from the averaging procedure of

the NS equations. They describe the same thing with a different couple of variables. It is only a reversible change of variable from eq. 4 to eq. 9. You can also see (alpha_0, nu_0) as intermediate variables aimed at a simple definition of Pr_0, somewhat like imaginary numbers have been used for so many years as a trick to factorize 3dt and 4^{th} order polynomials.

The new formulation should be validated against reference numerical data and other state of the art formulas for the turbulent Prandtl number, such as the one by Cebeci (19732), or the variant proposed by Na and Habib (19733), or the formula by Kays et al. (19804).

The new validation is indeed validated against the formula by Kays but taking his much more recent, even if already quite old, comprehensive paper of 1994, see. Ref. 2, which is precisely the core of the validation.

In the text of the manuscript I see reference to figures, but I cannot visualize any figure.

The reference to a figure is given in the penultimate paragraph of the Discussion section. It is written “see figure 5 in 7” where 7 is the number for the reference and in effect the figure is not in the brief report. There is a very large number of figures in the referenced document and I thought it would ease the reader who would like to look at the source and not only rely on the description following the reference.

This reference is particularly important because before its publication I could not find, probably my bad, any ν_t profile usable for interpretation and/or reference. I indeed postponed the submission of this brief report until the reference 7 is at least theoretically publicly available.
My first brief report submission was much more concise, but at the editorial level I was asked to develop some arguments and then new requests arise about the new development in something that looked like and endless loop. Most of the Discussion section arises from this interaction. I had to put a stop to it, because I want this brief report to remain a brief report. It is also why I do not want to add any graph or picture. That would restart the endless loop without adding substance. If one point must be kept after the validation part, it is that it would be very easy to discard my finding, independently of its validity, by testing it against some of the popular 2-eq models, just because my formula relies on the ν_t profile and this ν_t profile is very badly reproduced, as shown in ref.7. Unfortunately, even if valid, the new formula do not lead directly to much simulation result improvement. However, it suggests to work on the existing 2-equations turbulence models so that they can procure valid ν_t profiles and not only the correct pressure loss.

As a final word, please also look at the “Amendment from Version 1”. Looking at the brief report after a few month, let’s say with refreshed eyes, I could see and correct many imprecisions and/or incorrect wording. I hope the version 2 of the document is now more clear and easier to understand.

Competing Interests: No competing interests were disclosed.

Reviewer Report 30 May 2023

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The present article deals with the analysis of an explicit formula for the turbulent Prandtl number (Pr_t) evaluation. The use of a square additivity approach leads to a new formulation that is coherent with other well-known expressions from turbulence modeling literature. The author extends a previous result, improving upon it by avoiding the degeneration of Pr_t to zero or infinity. Moreover, the author's formula can be related to the Kays correlation by considering a first-order development of the full new expression.

Overall, this work is interesting for thermal turbulence modeling, and the manuscript is well-organized. However, there are a few issues that need clarification:

- Since the meaning of Pr_0 can be seen as the asymptotic value of Pr_t, it is suggested to underline the meaning of α_0 and ν_0. It should be noted that these properties are introduced with the same description as α_t and ν_t, representing properties of the flow rather than the fluid.

- In formula 15 a bracket is missing.

- It is recommended, if possible, to include a plot depicting the behavior of the new formulation of Pr_t. The plot should consider a comparison with the Kays formula and highlight the different situations described in the first paragraphs of the Discussion section.

Is the work clearly and accurately presented and does it cite the current literature?
Yes

Is the study design appropriate and does the work have academic merit?
Yes

Are sufficient details of methods and analysis provided to allow replication by others?
Yes

If applicable, is the statistical analysis and its interpretation appropriate?

Not applicable

Are all the source data underlying the results available to ensure full reproducibility?
No source data required

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Turbulence modeling of low Prandtl number fluid. Finite element implementation of thermal turbulence models for liquid metal.

We confirm that we have read this submission and believe that we have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Author Response 06 Jun 2023

Vincent MOREAU

Thank you very much for your fast and accurate review. About the 3 issues raised:

1. You are totally right. I struggled a lot to make things clear without so much success. What I intend to do for improvement is to names the quantities more accurately:
    - remove "turbulent" after eq. 4
    - add "the flow viscosity nu_0" before eq. 6
    - add "the flow diffusivity alpha_0" before eq. 7
2. In formula 15, the last bracked must indeed be removed
3. I would definitively prefer not to add a plot. This is a brief report and is already too much extended for my taste, as I had to compose with the editorial team. What you recommend, while surely of interest, would bring this brief report outside of its domain of definition.

I will wait for another review before making an update. Thank you again.

Competing Interests: No competing interests were disclosed.