We thank the Referees for their constructive comments. Please find the original Referee notes in bold, our responses in italics and modifications to the manuscript in blue, below.

### Author Response to Referee #1

The article presents an interpolation function to compute wet-bulb potential temperature as a function of pressure and temperature and its inverse, i.e. temperature as a function of pressure and wet-bulb potential temperature. The direct computation of wet-bulb potential temperature involves solving a nonlinear differential equation and therefore it can only be solved by iterative numerical methods. From this point of view, having a ready-made interpolant can be a valuable contribution within the scope of ACP for researchers and modellers. However, the manuscript can be improved by adding references and being more specific in the language used to present the mathematical description of the method. Perhaps more important is the definition of a set of 'true' adiabats that serve as reference to develop the interpolant. How accurate is this 'truth' itself? I think this deserves further discussion. I elaborate on these recommendations in the comments below.

Our responses below address the weaknesses of this technical note identified by the Referee.

## **Specific comments**

Table 1: How sensitive are the 'truth' adiabats to the values of the constants in Table 1? Also, what is the source of the constants' values? They do not always correspond to the values in e.g. Bolton (1980). Please, provide references.

For our proposed solution, we tried to use more recent estimates of constant values than those suggested in Bolton (1980), where available. However, to provide a quantitative response to the above concern, we have repeated our iterative calculation of the "truth" adiabats using the values in Bolton (1980). The MAE between the two sets of solutions is 0.004°C. The figure below shows the distribution of error throughout the modelled domain.



Notably, the accuracy of the method we propose in this technical note is largely unaffected by the choice of "truth". Any change merely results in an adjustment of the polynomial fitting coefficients. Should more precise constant values and/or thermodynamic relationships become established in the future, our method can be re-applied to produce updated parameters without loss of accuracy (within the limits of the specific

# polynomial optimizer used). We have added the following comment in the Evaluation section of the manuscript to address this:

The specific choice of thermodynamic constants and relationships undoubtedly effects the definition of "truth" used in this work, however, has little effect on the overall validity of the approach. Should more precise constant values and/or thermodynamic relationships become established in the future, the proposed method can be re-applied to generate updated fitting coefficients without loss of accuracy (within the limits of the specific polynomial optimization routine used).

# More textual changes:

- Table 1 is updated with references for the two constants that differed from Bolton (1980)
- We adjusted the value of  $C_p$  to include more significant figures to agree with Bolton (1980)
- Reference temperature typo was corrected
- All figures as well as coefficient values in the Supplement were regenerated to reflect the additional significant figures in  $C_p$  value. This resulted in alternative rounding for MAE values for  $T(P,\theta w)$ , which changed from 0.017°C to 0.016°C. We've adjusted this value throughout the manuscript.
- The following note was added in-text, at the beginning of Section 2.1:

The constants used to devise this solution are consistent with Bolton (1980), unless otherwise indicated in Table 1.

## P1L20: Include reference to Bolton (1980)

Added.

P2L21-L22: I don't see how normalizing the curves removes any inherent nonlinearity at all. Please explain further. Also give mathematical expressions for the operations you are doing here. I'm interpreting your division by a reference moist adiabat as  $T(P,\theta w)/Tref(P)$ , where  $Tref(P) = T(P,\theta ref)$  and  $\theta ref = -70$ °C is a constant. Is this interpretation correct?

We would first like to address the particular notation, to which the Referee points here and in later comments as well. Perhaps the source of confusion is the common meteorological convention, by which wetbulb potential temperature at standard pressure is used to label moist adiabats (see Ambaum 2010, p119; Stull 2017, p105 and p152-158). Such practice simplifies the use of thermodynamic diagrams, and is considered standard in applied meteorology. We, however, agree that some readers may be unfamiliar with such notation and it should be addressed explicitly. We've added the following brief statement in the beginning of Section 2.1:

Note, that throughout this technical note we will rely on a common meteorological convention, by which wet-bulb potential temperature at standard pressure is used to label moist adiabats. Such references, hence, represent curves, rather than constants and are bolded for clarity.

All references that rely on this notation in the manuscript have been changed to bold font to help differentiate them from constants.

# To address the remaining part of the comment:

The mathematical interpretation proposed by the Referee is correct - the operation is a simple division  $T(P,\theta_w)/T(P,\theta_{ref})$ . This, by the meteorological convection noted above, corresponds to  $\theta_w/\theta_{ref}$ , described in the first version of the manuscript on P2L22: "...we can normalize our curves by dividing each  $\theta_w$  by a reference moist adiabats  $\theta_{ref}$ ". In practice, however, this normalization is equivalent to fitting  $\theta_w$  as a function of  $\theta_{ref}$ . Overall, this is a purely technical trick employed to help the optimizer converge. As we are trying to capture all the moist adiabats with a single function, it helps to have the curves behave as similar as possible. Yet the moist adiabats represent a non-linear process, so there's no simple way (we tried!) to collapse them into a single shape, i.e. achieve some sort of similarity theory. Instead we fit one of the solutions ( $\theta_{ref}$ ), and then model the deviations from that fit.

### We've changed the beginning of Section 2.2 to describe this operation more precisely:

While the moist adiabatic curves  $\theta_w$  in Figure 1 look smooth and fairly similar, it is challenging for most common optimization routines to capture all of them with one analytical expression with high accuracy. Due to the inherently non-linear nature of the process, there is no simple way to collapse the curves into a single shape. However, to aid fitting, we can normalize our curves by modelling  $\theta_w$  as a function of a reference moist adiabat  $\theta_{ref}$ . That allows us to model only the deviations from a reference curve. For our example we used  $\theta_{ref} = -70^{\circ}$ C. This particular choice of  $\theta_{ref}$  implies no theoretical importance...

# P2L24: What does 'the resulting transformed adiabats shift around the θref unity line' mean? θref is not unity and is not even close to it.

This is fairly simple to visualize by comparing plots of transformed adiabats produced with  $\theta_{ref} = -70^{\circ}$ C vs.  $\theta_{ref} = +40^{\circ}$ C. The blue and red correspond to positive and negative values, respectively. Select adiabats are shown for clarity. The **transformed** curve corresponding to  $\theta_{ref}$  vs.  $\theta_{ref}$  is indeed a unity line.



P2L27: In what sense are polynomials are well-behaved and why is this behaviour convenient?

# We have added the following clarification to the manuscript to highlight the benefits of using polynomial functions:

We use polynomial fitting to describe T(P) for the fixed  $\theta_{ref}$ . This is convenient, since polynomials are generally well-behaved and are computationally easy to use. In particular, they are both continuous and smooth, while being able to capture a wide variety of shapes. Moreover, they have well understood properties and a simple form, allowing the model to be easily implemented in a basic spreadsheet.

Additional discussion on the particular properties of polynomial fitting important to our problem is provided as response to a later Referee comment on use of bi-exponential and arctan alternatives.

# P2L29: Chaotic behaviour is a property of dynamical systems and polynomials per se are not dynamical systems. So can you clarify what chaotic behaviour of high-degree polynomials are you referring to here? Please include references.

The term "chaotic behavior" indeed carries a much more specific mathematical meaning than we intended to imply. A more accurate description of the particular property of high-degree polynomials we wanted to address is their tendency to oscillate wildly. We updated the manuscript to remove the inaccurate use of the term and provide a brief clarification as follows:

...Since we are examining a fixed range of temperatures relevant to atmospheric applications, the potentially extreme oscillatory behavior of high-degree polynomials outside of the modelled domain is not a primary

concern. The fitted polynomials have no predictive value outside of the modelled range and serve purely as an interpolation function. While the large number of possible inflection points associated with high degree polynomials may be of a concern near the edges of the fitting interval, a problem known as Runge's phenomenon (Epperson, 1987), the current algorithm relies on least-squares method to minimize the effect and achieve a high quality fit. For this example, the aim was to ensure that the mean absolute error (MAE) is on the order of  $10^{-2}$  degrees C...

# P3L7: Discuss further the results that you get with bi-exponential and arctan to explain what the accuracy is insufficient. How different is this accuracy to that achieved by your chosen method?

Thank you for pointing out the lacking discussion of other fitting functions. In part, the evasive nature of our comment on alternative approaches is due to the difficultly in providing a true quantitative comparison of the different methods. While we were able to model the transformed curves with bi-exponential and arctan functions and achieve a visually-satisfactory fit with errors on the order of degrees, these fits do not constitute a complete solution. The remaining part of the problem is modelling the variable parameters k<sub>n</sub>. This is where the well-behaved nature of polynomials mentioned earlier plays a key role. Unlike polynomials, bi-exponential and arctan functions produce parameter curves, which are neither smooth, nor continuous. Most are asymptomatic, rendering them near-impossible to model with polynomials. Yet another set of alternative functions would be necessary to capture the parameter curves, which, combined with the errors already present from fitting the transformed adiabats would produce a complex and discontinuous error field. In essence, these alternative attempts are equivalent to trying to manually perform GEP, which was already [properly] done by Bakhshaii and Stull (2013). Their method resulted in errors, which were both discontinuous and larger than with our proposed approach.

Hence, while we are unable to provide a quantitative comparison of the different approaches to fitting, we hope that the following changes to the manuscripts address this point in a more clear and complete manner: For this work we tested bi-exponential, arctan, rational and polynomial functions. Generally, a reasonable (on the order of 1-2°C) fit can be achieved with both bi-exponential and arctan functions using as little as three variable parameters. While efficient, the results of such fit are unlikely to be sufficiently accurate to be useful for real-life modelling applications and, more importantly, only constitute a part of the solution. The bigger concern with these choices is that, unlike polynomials, they produce variable parameters that do not appear well-behaved. Discontinuity and asymptomatic behavior arising from error minimization for all transformed adiabats render the parameter curves very difficult to model. A variety of functions would be necessary to capture the parameter behavior, which in turn is likely to produce a complex and discontinuous error field, such as appeared in Bakhshaii and Stull (2013).

# Section 4: The notation in very confusing. For instance, step 2 of Section 4.1, in which the computation of $T(P,\theta w)$ is described, requires the computation of $\theta ref(P)$ .

However,  $\theta$  ref was assumed constant in Section 2.2!! I believe what you actually need to compute is Tref (P) = T (P,  $\theta$  ref ), where  $\theta$  ref is a constant. A similar notation problem is present in Section 4.2.

We hope that our earlier response on the use of meteorological notation has addressed the Referee's concern.

## Technical corrections Title: It should read 'noniterative'

Corrected, with much self-reproach.

# P1L20: It should read to 'To improve'

Corrected.

# P2L17: It should say θw (P, T).

Corrected.

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### Author Response to Referee # 2

This paper presents a technique for calculating temperature or wet bulb potential temperature along moist adiabats. Based on a high-order polynomial fit, the technique is considerably more accurate and less computationally burdensome than the iterative or look-up table procedures that are typically employed in most numerical weather prediction models. The high practical value of this work merits publication in ACP. The paper is well written and the methodology is clearly presented. I've provided a few minor suggestions for improvement below.

We thank the Referee's acknowledgement of the practical value of this note. We hope our responses below address the manuscript's shortcomings.

### Main comments:

1) There are more figures (seven in total) than necessary for a short technical note. Figures 2-5 provide no information beyond the demonstration that the polynomial fits are indistinguishable from the "truth". The authors could consider removing these figures.

We are happy to eliminate Figures 2-5, as per Referee's suggestion.

2) Some potentially useful context to add to the manuscript would be to address the question of whether errors associated with pre-existing methods are systematic or just noisy. Systematic errors in temperature would result in biased latent heating profiles, which could in turn have dynamical implications on the grid scale. If this were the case, then the improvements offered by the authors' methodology would be more substantial than a simple low-cost noise correction.

In our view, existing methods are likely to contain both random and systematic errors. We have added the following discussion to the manuscript to provide more detail:

While interpolating values from look-up tables generally results in random errors, iterative solutions with a coarse step could potentially suffer from a directional drift due to numerical integration errors, which may introduce a consistent bias into latent heating profiles. Moreover, near the top of the atmosphere, where each pressure step corresponds to a large temperature jump along the moist adiabats the numerical solutions tend to become unstable. Though both of these concerns are addressed with the proposed low-cost polynomial method, the broader challenge of our limited overall understanding of moist convection remains. Existing thermodynamic relationships are based on the assumption of either a reversible moist adiabatic or an irreversible pseudoadiabatic process. Real world atmospheric processes are likely to be a combination of both (Iribarne and Godson, 1981). The uncertainty introduced by our limited knowledge of the true state of saturated air is likely to remain the central obstacle in capturing moist convection.

### Other minor issues: P1.L20: Spelling error. "improve"

Corrected.

**P3.L7-8.** I don't understand why alternative function fits are "unlikely to be sufficiently accurate to be useful." Why not? What precisely does "well behaved parameters" mean here. The language used in this and the following paragraph is imprecise and the claims sound subjective.

We agree with the Referee that our approach to describing the alternative fitting functions is very vague. This point was also brought up by Referee #1. While we are unable to provide a precise quantitative answer, we hope that our response (copied below) will address this point in a clearer manner: Thank you for pointing out the lacking discussion of other fitting functions. In part, the evasive nature of our comment on alternative approaches is due to the difficultly in providing a true quantitative comparison of the different methods. While we were able to model the transformed curves with bi-exponential and arctan functions and achieve a visually-satisfactory fit with errors on the order of degrees, these fits do not constitute a complete solution. The remaining part of the problem is modelling the variable parameters k<sub>n</sub>. This is where the well-behaved nature of polynomials mentioned earlier plays a key role. Unlike polynomials, bi-exponential and arctan functions produce parameter curves, which are neither smooth, nor continuous. Most are asymptomatic, rendering them near-impossible to model with polynomials. Yet another set of alternative functions would be necessary to capture the parameter curves, which, combined with the errors already present from fitting the transformed adiabats would produce a complex and discontinuous error field. In essence, these alternative attempts are equivalent to trying to manually perform GEP, which was already [properly] done by Bakhshaii and Stull (2013). Their method resulted in errors, which were both discontinuous and larger than with our proposed approach.

Hence, while we are unable to provide a quantitative comparison of the different approaches to fitting, we hope that the following changes to the manuscripts address this point in a more clear and complete manner: For this work we tested bi-exponential, arctan, rational and polynomial functions. Generally, a reasonable (on the order of 1-2°C) fit can be achieved with both bi-exponential and arctan functions using as little as three variable parameters. While efficient, the results of such fit are unlikely to be sufficiently accurate to be useful for real-life modelling applications and, more importantly, only constitute a part of the solution. The bigger concern with these choices is that, unlike polynomials, they produce variable parameters that do not appear well-behaved. Discontinuity and asymptomatic behavior arising from error minimization for all transformed adiabats render the parameter curves very difficult to model. A variety of functions would be necessary to capture the parameter behavior, which in turn is likely to produce a complex and discontinuous error field, such as appeared in Bakhshaii and Stull (2013).

# P4.L21-22. How much accuracy is compromised if the Table values are used instead of the spreadsheet. Can you put some numbers to this claim. Is the Table even necessary if the authors are cautioning against the implementation of the numbers in the Table?

We were hesitant to provide the coefficient tables in-text form the start, and chose to include them for completeness only. We agree with the Referee that they are not particularly valuable, as most readers will use the spreadsheet for both: high accuracy and ease of data formatting. We, therefore, removed the tables from the manuscript.

# P6.L7-8 and L28-29 and elsewhere there are paragraphs comprised of single sentences. Can these sentences be merged with either the preceding or following paragraphs?

Line breaks were removed.

## REFERENCES

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# A noniteratiave noniterative approach to modelling moist thermodynamics

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Abstract. Formulation of noniterative mathematical expressions for moist thermodynamics presents a challenge for both numerical and theoretical modellers. This technical note offers a simple and efficient tool for approximating two common thermodynamic relationships: temperature T at a given pressure P along a saturated adiabat  $T(P,\theta_w)$ , as well as its corresponding inverse form  $\theta_w(P,T)$ , where  $\theta_w$  is wet-bulb potential temperature. Our method allows direct calculation of  $T(P,\theta_w)$  and  $\theta_w(P,T)$  on a thermodynamic domain bounded by  $-70 \le \theta_w < 40^{\circ}$ C, P > 1 kPa and  $-100 \le T < 40^{\circ}$ C, P > 1 kPa, respectively. The proposed parameterizations offer high accuracy (mean absolute errors of  $0.0170.016^{\circ}$ C and  $0.002^{\circ}$ C for  $T(P,\theta_w)$  and  $\theta_w(P,T)$ , respectively) on a notably larger thermodynamic region than previously studied. The paper includes a method summary, as well as a ready-to-use tool to aid atmospheric physicists in their practical applications.

#### 1 Introduction

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- 10 Saturated thermodynamics commonly present a challenge for theoretical studies because moist convective condensation, such as deep cumulus precipitation, often involves pseudoadiabtic (irreversible) processes. The latent heat released during water vapour condensation is important for estimating thunderstorm intensity and thickness, precipitation amount and phase, global climate and atmospheric general circulation (Stull, 2017). These processes are governed by nonlinear equations that require iteration to solve. Numerical weather prediction (NWP) models, hence, suffer from the added computational cost to their
- 15 cloud, precipitation, convection and turbulence schemes and parameterizations, because of the iterations required during each timestep of the NWP integration.

A common iterative approach, such as described by Caballero (2014), uses step-wise numerical integration along a saturated adiabat for any constant wet-bulb potential temperature  $\theta_w$ . The moist adiabatic lapse rate is derived from conservation of moist entropy as a function of temperature T and saturated mixing ratio  $r_s$ , which itself is a nonlinear function of T and

20 pressure *P*. To imporve improve efficiency Davies-Jones (2008) proposed a different iterative method, based on inverting Bolton's formula (Bolton, 1980) for equivalent potential temperature valid for the pressure range  $10 \le P \le 105$  kPa and wetbulb potential temperatures  $-20 < \theta_w < 40^{\circ}$ C. As a valuable noniterative alternative, Bakhshaii and Stull (2013) offer an approximate solution devised using gene-expression programming (GEP). They provide two separate sets of equations for determining  $T(P, \theta_w)$  and  $\theta_w(P, T)$ , for the domain bounded by  $-30 < \theta_w < 40^{\circ}$ C, P > 20 kPa and  $-60 < T < 40^{\circ}$ C. The complex nature of the problem required their splitting of the modelled region into sub-domains, resulting in error discontinuity. The method also produced fairly large errors (on the order of  $\frac{a \text{ degree} (1-2^{\circ} \text{C})}{a \text{ degree} (1-2^{\circ} \text{C})}$ ) in the upper atmosphere. Despite the limitations, to our knowledge Bakhshaii and Stull (2013) is the only existing noniterative solution to approximate saturated pseudoadiabats.

Our current study presents a different approach for directly calculating  $T(P,\theta_w)$  and  $\theta_w(P,T)$  offering improved accuracy

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for a larger thermodynamic domain. The method, described in Section 2, normalizes the raw data before fitting it with polynomials. The resultant approximation is evaluated against the "truth" (the iterated solution) and summarized in Sections 3 and 4, respectively. As Supplementary Material we offer the readers a ready-to-use spreadsheet implementing our methodology.

The goal of this paper is to provide a simple tool that can aid analytical modellers in their theoretical work as well as numerical modellers in reducing the computational cost of their simulations.

#### 10 2 Method Description

#### 2.1 Data

In order to obtain a set of "truth" curves for  $T(P, \theta_w)$  we have used an iterative approach to numerically integrate the equation for  $\frac{dT}{dP}$  (Tables 1 and 2) for values in the range of  $-100 \le \theta_w < 100^{\circ}$ C between  $105 \ge P > 1$  kPa. The constants used to devise this solution are consistent with Bolton (1980), unless otherwise indicated in Table 1. Note, that throughout this technical note

- 15 we will rely on a common meteorological convention, by which wet-bulb potential temperature at standard pressure of 100 kPa is used to label moist adiabats. Such references, hence, represent curves, rather than constants and are bolded for clarity. We found that numerical integration along a saturated adiabat  $\theta_w \theta_w$  from the bottom to the top of the domain required an increasingly refined pressure step, as all adiabats tend to absolute zero near the top of the atmosphere, and each consecutive pressure step corresponds to a larger temperature jump. For our numerical integration we used  $10^{-4}$  kPa step for  $105 \ge P > 10$
- 20 kPa,  $10^{-5}$  kPa step for  $10 \ge P > 2$  kPa and  $10^{-6}$  kPa step for  $2 \ge P > 1$  kPa. The resulting curves (shown on the thermo diagram in Figure 1) are taken as "truth", to which we fit our polynomial-based optimization. The non-iterative approximations for  $T(P, \theta_w)$  and  $\theta_w(T, \theta_w) \cdot \theta_w(P, T)$  described below are valid for thermodynamic ranges bounded by  $-70 \le \theta_w < 40^{\circ}$ C and  $-100 \le T < 40^{\circ}$ C, respectively.

#### 2.2 Approximating $T(P, \theta_w)$

- 25 While the moist adiabiatic curves  $\theta_w \quad \theta_w$  in Figure 1 look smooth and fairly similar, it is challenging for most common optimization routines to capture all of them with a single analytical expression. To remove some of the inherent nonlinearity in the data one analytical expression with high accuracy. Due to the inherently non-linear nature of the process, there is no simple way to collapse the curves into a single shape. However, to aid fitting, we can normalize our curves by dividing each  $\theta_w$  by a reference moist adiabat  $\theta_{ref}$ . modelling  $\theta_w$  as a function of a reference moist adiabat  $\theta_{ref}$ . That allows us to model
- 30 <u>only the deviations from a reference curve</u>. For our example we used  $\theta_{ref} = -70\theta_{ref} = -70^{\circ}$ C. This particular choice of  $\theta_{ref}$  $\theta_{ref}$  implies no theoretical importance. It is possible to choose any of the directly calculated normalized adiabats to represent

 $\theta_{ref}\theta_{ref}$ . Depending on the choice, the resulting transformed adiabats shift around the  $\theta_{ref}\theta_{ref}$  unity line. The single consideration for choosing a particular  $\theta_{ref}\theta_{ref}$  is the ease and accuracy with which it can be fit by a particular optimization tool.

We use polynomial fitting to describe T(P) for the fixed  $\theta_{ref} \theta_{ref}$ . This is convenient, since polynomials are generally well-

- 5 behaved and are computationally easy to use. In particular, they are both continuous and smooth, while being able to capture a wide variety of curve shapes. Moreover, they have well understood properties and a simple form, allowing the model to be easily implemented in a basic spreadsheet. The choice of the degree of polynomial depends on the desired precision level. Since we are examining a fixed range of temperatures relevant to atmospheric applications, the potentially ehaotic extreme oscillatory behavior of high-degree polynomials outside of the modelled domain is not a primary concern. The fitted polynomials have
- 10 no predictive value outside of the modelled range and serve purely as an interpolation function. While the large number of possible inflection points associated with high degree polynomials may be of a concern near the edges of the fitting interval, a problem known as Runge's phenomenon (Epperson, 1987), the current algorithm relies on least-squares method to minimize the effect and achieve a high quality fit. For this example, the aim was to ensure that the mean absolute error (MAE) is on the order of  $10^{-2}$  degrees °C, requiring a 20th degree polynomial to achieve such fit. The true and modelled  $\theta_{ref} = -70$ °C can be

15 seen in Fig. ?? with fit coefficients coefficients for this polynomial are provided in Table ?? II in Supplementary Material.

The next step is to choose a single functional form to represent the entire family of the transformed curves (i.e. the moist adiabat deviations from  $\theta_{ref}$ . Each given shape of a particular curve is then controlled by variable parameters of the same function. A number of simple functions exists that are able to model the above relationship. For this work we tested biexponential, arctan, rational and polynomial functions. Generally, a reasonable (on the order of 1-2°C) fit can be achieved

- 20 with both bi-exponential and arctan functions using as little as three variable parameters. While efficient, the results of such fit are unlikely to be sufficiently accurate to be useful for real-life modelling applications . Another and, more importantly, only constitute a part of the solution. The bigger concern with these choices is that the variable parameters are not , unlike polynomials, they produce variable parameters that do not appear well-behaved functions and are hence. Discontinuity and asymptomatic behavior arising from error minimization for all transformed adiabats renders the parameter curves very difficult
- 25 to model. A variety of functions would be necessary to capture the parameter behavior, which in turn is likely to produce a complex and discontinuous error field, such as appeared in Bakhshaii and Stull (2013).

Polynomial fitting doesn't appear to suffer from such issues. Moreover, the accuracy can be controlled by changing the degree of the polynomial and, hence, allowing a higher number of variable parameters. In this example, the curves were modelled using 10th degree polynomials, resulting in 11 variable parameters. Conveniently, and unlike other functional forms

30 mentioned above, these parameters are also well-behaved. They can, again, be modelled using high-degree polynomials to the desired level of accuracy. Results of parameter fitting for this given example were again produced using 20th degree polynomialsand can be see in Figure ??, with fit coefficients provided in Table ?? (Supplementary Material). The resulting modelled (non-iterative) moist adiabats can be seen in Figure 1, compared to the truth (iterated) values.

#### Approximating $\theta_w(P,T)$ 2.3

A similar approach can be used to produce a non-iterative approximation for  $\theta_w(P,T)$ . To obtain a new set of curves representing lines of constant temperature T in  $\theta_w$  domain, we have used our existing dataset for  $-100 \le \theta_w < 100^{\circ}$ C to extract isotherms on a 0.5°C and 0.1 kPa grid for  $-100 \le T \le 40$ °C and  $105 \ge P \ge 1$  kPa.

5 Similarly to our earlier approach, we select a single reference curve  $T_{ref} = T_{-100^{\circ}C} T_{ref} = -100^{\circ}C$  and use a high-order polynomial to model it as a function of pressure (Figure ??, Table ?? Table IV in Supplementary Material). We then produce a set of transformed curves by normalizing the isotherms with  $T_{ref}$  plotting the isotherms as a function of  $T_{ref}$ . We fit the transformed curves with 10th degree polynomials, obtaining a dataset for 11 variable parameters. Finally, we use polynomials to model the variable parameters (Figure ??, Table ?? Table III in Supplementary Material). The following section discusses

the results and accuracy of our optimization procedure. 10

#### **3** Evaluation

To test the accuracy of the proposed method, we compared our modelled curves for  $T(P, \theta_w)$  and  $\theta_w(P, T)$  with those obtained through direct calculation (the "truth" iterative solution). The results of the evaluation for  $T(P, \theta_w)$  are shown in Figure 2, indicating errors on the order of few hundredths of a degree throughout most of the domain. Warmer values near the top of

- the domain tend to be modelled least accurately. Mean absolute error (MAE) for the entire modelled thermodynamic region 15 is  $0.0170.016^{\circ}$ C. Error contours for  $\theta_w(P,T)$  are shown in Figure 3, with errors on the order of few thousandths of a degree throughout most of the domain and overall MAE =  $0.002^{\circ}$ C. Once again, values near the low-pressure limit tend to be least accurate. Notably, applying the above optimization on a slightly shallower pressure domain of P > 2 kPa, allows to improve improvement of the overall MAE for both approximations by an additional order of magnitude.
- 20 As mentioned earlier, improved accuracy may also be achieved with the use of even higher degrees of polynomials for parameter fits. However, such precision is unlikely to be necessary, as some of the thermodynamic relationships used in the "truth" iterative computations contain substantially larger errors, than those introduced by the above optimization procedure (Davies-Jones, 2009; Koutsoviannis, 2012). Moreover, conventional pseudoadiabatic diagrams, such as those used by U.S. Air Force (USAF), Environment Canada (EC) and Air Transport Association of America (ATAA), differ from each other by
- 25 nearly 1°C at the 20 kPa pressure level (Bakhshaii and Stull, 2013). The specific choice of thermodynamic constants and relationships undoubtedly effects the definition of "truth" used in this work, however, has little effect on the overall validity of the approach. Should more precise constant values and/or thermodynamic relationships become established in the future, the proposed method can be re-applied to generate updated fitting coefficients without loss of accuracy (within the limits of the specific polynomial optimization routine used).
- Though the upper 10 kPa of the atmosphere contains the largest errors with our proposed approach, this vertical subrange also 30 presents the most significant challenge for direct (iterative) numerical modelling. Accurate numerical computation requires an increasingly refined vertical step for the top part of the atmosphere. Hence, despite the errors, the proposed approximation offers

a more accurate solution than one would obtain with direct iterative approach using a somewhat coarse yet computationally demanding 0.001 kPa pressure step.

While common weather phenomena generally remain in the troposphere, the validity of the current method on a notably larger vertical domain is particularly useful in the lower latitudes. Deep vertical extent of tropical thunderstorms, hurricanes

5 and typhoons in combination with the high tropopause altitude in the tropics (10-15 kPa) (18 km or 8 kPa (WMO, 2017)) in the tropics contribute to large computational costs of modelling these potentially destructive events.

#### 4 Summary of approach

Individual steps to directly compute  $T(P, \theta_w)$  and  $\theta_w(P, T)$  are summarized below. This sample procedure, along with the required coefficient tables are provided in a ready-to-use form in the attached spreadsheet (Supplementary Material).

10 Note, that the same coefficients presented in Tables ?? - ?? are rounded to fewer significant digits to fit them and might, hence, offer lower accuracy, relative to the full significant digits in the suplementary spreadsheet.

#### 4.1 Computing $T(P, \theta_w)$

Let n = 0, ..., 10 correspond to the index of individual polynomial coefficients and m = 20 be the degree of polynomial fits for  $\theta_{ref}(P)$  and  $k_n(\theta_w)$ , respectively.

15 1) Compute coefficients  $k_n(\theta_w)$  using polynomial coefficients  $a_{20}, ..., a_0$  in Table I in Supplementary Material(and Table ?? here):

$$k_n(\theta_w) = \sum_{i=0}^m a_{(n,m-i)} \theta_w^{m-i} \tag{1}$$

for  $\theta_w$  in degrees °C.

2) Compute  $\theta_{ref}(P)$  using polynomial coefficients  $b_{20}, ..., b_0$  in Table II in Supplementary Material (and Table ?? here):

20 
$$\theta_{ref}(P) = \sum_{j=0}^{m} b_{(m-j)} P^{m-j}$$
 (2)

for P in kPa. Note, for users preferring older pressure units: 1 kPa = 10 mb = 10 hPa.

3) Compute  $T(\theta_{ref})$ :

$$T(P,\theta_w) = T(\theta_{ref}) = \sum_{h=0}^n k_h \theta_{ref}^{n-h}$$
(3)

where T and  $\theta_{ref}$  are in Kelvins, and values of  $k_{0,...,n}$  correspond to polynomial coefficients calculated in Step 1.

## 25 **4.2** Computing $\theta_w(P,T)$

Let n = 0, ..., 10 correspond to the index of individual polynomial coefficients and m = 20 be the degree of polynomial fits for  $T_{ref}(P)$  and  $\kappa_n(T)$ , respectively.

1) Compute coefficients  $\kappa_n(T)$  using polynomial coefficients  $\alpha_{20}, ..., \alpha_0$  in Table III in Supplementary Material (Table ??):

$$\kappa_n(T) = \sum_{i=0}^m \alpha_{(n,m-i)} T^{m-i}$$
(4)

for T in degrees °C.

2) Compute  $T_{ref}(P)$  using polynomial coefficients  $\beta_{20}, ..., \beta_0$  in Table IV in Supplementary Material (Table ??):

5 
$$T_{ref}(P) = \sum_{j=0}^{m} \beta_{(m-j)} P^{m-j}$$
 (5)

for P in kPa.

3) Compute  $\theta_w(T_{ref})$ :

$$\theta_w(P,T) = \theta_w(T_{ref}) = \sum_{h=0}^n \kappa_h T_{ref}^{n-h} \tag{6}$$

where  $\theta_w$  and  $T_{ref}$  are in degrees  $\mathcal{C}$ , and values of  $\kappa_{0,\dots,n}$  correspond to polynomial coefficients calculated in Step 1.

#### 10 5 Usage Example

Meteorologists typically use both  $\theta_w(P,T)$  and  $T(P,\theta_w)$  for moist convection such as thunderstorms, frontal clouds, mountainwave clouds, and many other phenomena where a saturated air parcel moves vertically. Cloud base of convective clouds marks the bottom of saturated ascent, and cloud top marks the top.

- For example, suppose that the forecast at some tropical weather station is P = 100 kPa,  $T = 32^{\circ}$ C with dewpoint  $T_d = 21^{\circ}$ C 15 (corresponding to a water vapor mixing ratio of approximately r = 16 g kg<sup>-1</sup>). Further suppose that a force (e.g., buoyancy, frontal uplift, or orographic uplift) causes an air parcel with these initial conditions to rise. Initially this air parcel is unsaturated (not cloudy), so we don't need to use the polynomial or iterative equations. Instead, simpler non-iterative equations apply for the thermodynamic state as the parcel rises dry adiabatically. Namely, its temperature cools at the dry adiabatic lapse rate (9.8°C km<sup>-1</sup>), and the mixing ratio and potential temperature are constant. This air parcel will become saturated (i.e., cloud
- 20 base) at the lifting condensation level (LCL). With this information, other thermodynamic equations (Stull, 2017) can be used to find conditions at the LCL:  $z_{LCL} = 1.375$  km,  $P_{LCL} = 85.4$  kPa, and  $T_{LCL} = 18.5$ °C.

Given this initial P and T at the LCL, we can use the polynomial equations provided in this paper to compute which moist adiabat the cloudy air parcel will follow:  $\theta_w(P,T) = 24.0^{\circ}$ C.

If this cloudy air parcel (still following the θ<sub>w</sub>(P,T) = 24.0°C adiabat) rises to an altitude where the pressure is P = 24.0
kPa, then we can use the second set of polynomial equations in this paper to find the final temperature of the air parcel at this new height: T(P,θ<sub>w</sub>) = -39.8°C.

#### 6 Discussion and Conclusions

The polynomial method proposed here is accurate, smooth, and computationally efficient. For example, given the cloud base and cloud top pressures of the previous example, the tally of computer operations to find both the initial and the final temperature are: 230 additions and subtractions, 2365 multiplies (where rational numbers to integer powers are counted as sequential

5 multiplies). Compare that to the computation tally for the "truth" iterative solution, requiring a total of 2,750,000 variable pressure steps, where each step has: 8 additions and subtractions, 17 multiplies (where rational numbers to integer powers are counted as sequential multiplies), 9 divides, and 2 math functions (e.g., log, exp, non-integer exponents), totalling to 988,200,000 operations from the bottom to the top of the domain.

Also, for comparison, some numerical weather prediction models use a look-up table to get the average saturated adiabatic

10 lapse rate  $\Delta \theta_w / \Delta P$  as a function of P and T. While this method is fairly fast, it is also less accurate, and approximates the saturated lapse rate as a series of short straight-line segments instead of a smooth curve. It also has discontinuous jumps of saturated lapse rate as T varies along an isobar.

Thus, the polynomial method While interpolating values from look-up tables generally results in random errors, iterative solutions with a coarse step could potentially suffer from a directional drift due to numerical integration errors, which may

- 15 introduce a consistent bias into latent heating profiles. Moreover, near the top of the atmosphere, where each pressure step corresponds to a large temperature jump along the moist adiabats the numerical solutions tend to become unstable. Though both of these concerns are addressed with the proposed low-cost polynomial method, the broader challenge of our limited overall understanding of moist convection remains. Existing thermodynamic relationships are based on the assumption of either a reversible moist adiabatic or an irreversible pseudoadiabatic process. Real world atmospheric processes are likely to
- 20 be a combination of both (Iribarne and Godson, 1981). The uncertainty introduced by our limited knowledge of the true state of saturated air is likely to remain the central obstacle in capturing moist convection.

The polynomial method proposed here provides a computation of high accuracy and smooth variation across the whole thermodynamic diagram range, at intermediate computation speed compared to the other methods. Moreover, it helps to model moist thermodynamics on a wider temperature range with roughly two orders of magnitude MAE improvement over the existing solution.

In addition to the reduced computational costs of obtaining solutions for  $T(P, \theta_w)$  and  $\theta_w(P, T)$  in numerical simulations and improving accuracy, we hope that our tool will aid analytical modellers in their theoretical work.

#### 7 Tables

#### Tables

25

Table 1. Table of constants

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Constant	Description [units]
$R_d = 287.058$	gas constant for dry air $[J K^{-1} kg^{-1}]$ (Burns, 2015)
$R_v = 461.5$	gas constant for water vapour [J K <sup>-1</sup> kg <sup>-1</sup> ]
$C_{pd} = 1005.7$	specific heat of dry air at constant pressure $[J K^{-1} kg^{-1}]$
$T_0 = 273.15$	reference temperature [K]
$P_0 = 100$	reference pressure [kPa]
$e_0 = 0.611657$	Clausius-Clayperon constant [kPa] (Koutsoyiannis, 2012)
$\varepsilon = \frac{R_d}{R_v} = 0.6220$	ratio of gas constants [kg kg <sup>-1</sup> ]

 Table 2. Variable definitions

Variable	Description [units]
Т	[K] ambient temperature
Р	[kPa] pressure
${m  heta}_w$	[K] saturated adiabat where the value of T defined at $P = P_0$ is defined as wet-bulb potential temperature
$e_s = e_0 exp \left[ 24.921 \left( 1 - \frac{T_0}{T} \right) \right] \left( \frac{T_0}{T} \right)^{5.06}$	[kPa] saturation vapour pressure
$L_v = 3.139 \times 10^6 - 2336 * T$	[K] latent heat of vapourization (Koutsoyiannis, 2012)
$r_s = \varepsilon \frac{e_s}{(P e_s)}$	[kg kg <sup>-1</sup> ] saturation mixing ratio
$\frac{dT}{dP} = \frac{\frac{\kappa_d}{C_{pd}} T + \frac{L_v}{C_{pd}} r_s}{\frac{L_v^2}{R_v C_{pd}} r_s}$	$[K kPa^{-1}]$ change of temperature with pressure along a saturated adiabat, which can be iterated to find T vs. P
$P(1 + \frac{r^{2}}{T^{2}})$	

#### 7 Figures

#### **Figures**



Figure 1. Emagram plot showing select "true" (solid black) and modelled (dashed red) moist adiabats  $\theta_w$  (difference not apparent at this scale). Temperature and pressure domains are restricted for clarity. An emagram (energy mass diagram) is a thermodynamic diagram with the log of pressure on the vertical axis, plotted with max and min values reversed, so that higher in the diagram corresponds to higher in the atmosphere, where pressures are lower. The non-iterative results presented in this paper can be plotted on any thermodynamic diagram, including tephigrams and skew-T diagrams.



Figure 2. Approximation error between iterated ("truth") and modelled T along moist adiabats  $\theta_w$ .



Figure 3. Approximation error between iterated ("truth") and modelled  $\theta_w$  along isotherms T.

Competing interests. No competing interests are present.

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