

Using enthalpy as a prognostic variable in atmospheric modelling with variable composition[†]

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ABSTRACT: Specific enthalpy emerges from a general form of the internal energy equation as a convenient prognostic thermodynamic variable for atmospheric modelling with variable composition, including models of moist air. This choice presents a general and flexible alternative to the common formalism of virtual temperature employed in most numerical weather prediction and climate models to account for the presence of water vapour and other constituents. The new approach eliminates the need for additional terms in the energy equation, resulting from composition variations along the air-parcel trajectories and routinely neglected in models. This note presents a derivation of relevant equations from first principles and outlines the changes to existing model codes necessary to accommodate the new formulation. Published in 2008 by John Wiley & Sons, Ltd.

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1. Introduction

The gas constant, R , of a mixture of gases is inversely proportional to the mean molecular mass. The mixture's specific heat capacities additionally depend on the number of internal degrees of freedom of individual molecules, which may be different for different constituents. These thermodynamic parameters therefore generally vary in space and time and along air-parcel trajectories depending on sources, sinks, and fluxes of individual tracers. Specific enthalpy,

$$h = c_p T, \quad (1)$$

where c_p is the specific heat capacity at constant pressure and T is temperature, has long been used as a convenient thermodynamic variable in some numerical models with variable composition such as in the thermosphere (e.g. Richmond and Matsushita, 1975; Fuller-Rowell and Rees, 1980). Most lower-atmospheric weather prediction and climate models still rely on an alternative formalism of virtual temperature T_v to account for the presence of water vapour and other constituents in the air (e.g. Benjamin *et al.*, 2004; Untch and Hortal, 2004; Davies *et al.*, 2005).

The purpose of this note is to revisit from first principles the derivation of the internal energy equation (IEE),

also commonly referred to in meteorological literature as the thermodynamic energy equation (section 2), and to examine the applicability of the traditional approach to arbitrary gas mixtures. This analysis reveals, somewhat surprisingly, that in models using T_v or T as prognostic thermodynamic variables, additional correction terms resulting from composition variations are required in the IEE, which are routinely neglected apparently with no justification of this approximation (section 3). The number of the additional terms scales as the number of tracers n and their size is comparable to the correction sought by the introduction of T_v in the first place.

It then becomes clear that specific enthalpy provides a viable alternative to account for the effects of compositional changes on thermodynamics and, consequently, on dynamics, including in the moist atmosphere. No additional terms appear in the IEE written for enthalpy thus resulting in a general, flexible, and compact formulation, which requires minimal changes in existing numerical schemes and model codes (section 4). In models using isentropic or related vertical coordinates (e.g. Benjamin *et al.*, 2004), potential temperature may be replaced by potential enthalpy.

Numerical experiments (to be described in detail elsewhere) with the US National Centers for Environmental Prediction operational Global Forecast System (GFS) model have shown certain advantages of the new approach, which is currently planned to be implemented into operations. The enthalpy-based IEE is also employed in the Whole Atmosphere Model (WAM), a version of GFS extended upward to cover the atmosphere from the

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surface to approximately 600 km (Akmaev *et al.*, 2008; Fuller-Rowell *et al.*, 2008).

2. Internal energy equation

A sufficiently general form of the IEE for a mixture of chemically reacting gases may be derived from the Boltzmann kinetic equation (de Groot and Mazur, 1962; Hirschfelder *et al.*, 1964; Zdunkowski and Bott, 2004):

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot \rho e \mathbf{v} + p \nabla \cdot \mathbf{v} = \rho Q. \quad (2)$$

Here $\mathbf{v}$ is the mass-weighted average velocity; the mixture's mass density ρ and pressure p are sums of partial densities ρ_i and pressures p_i of the constituent gases. Internal energy per unit mass e is a mass-weighted average of the internal energies of the constituents,

$$e = \sum_i e_i q_i, \quad (3)$$

where tracer mass mixing ratios $q_i = \rho_i / \rho$. (This definition differs from the one commonly used in meteorological literature, where partial densities are normalized by the density of dry air.) On the right-hand side of Equation (2), Q represents non-adiabatic contributions to internal energy per unit mass (heating rates) by such processes as radiative and chemical heating, phase transitions, eddy or molecular thermal conduction, and dissipation of kinetic energy into heat by viscous forces. It is also assumed that external forces acting on a molecule are proportional to its mass, m_i , as is the case with the gravity or Coriolis forces, which eliminates certain additional non-adiabatic terms.

Equation (2) may be rewritten in a more familiar form using the continuity equation,

$$\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0,$$

also following from the Boltzmann equation, where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$$

is the material time derivative along the air-parcel trajectories, and the equation of state

$$p = \sum_i p_i = \sum_i \rho_i R_i T = \rho R T. \quad (4)$$

Here $R_i = k_B / m_i$ are individual gas constants for each species and k_B is the Boltzmann constant. The IEE (2) may now be compactly written in the familiar 'advective' form

$$\frac{dh}{dt} - \frac{\omega}{\rho} = Q, \quad (5)$$

where $\omega = dp/dt$ and specific enthalpy is generally defined as

$$h = e + \frac{p}{\rho} \quad (6)$$

(de Groot and Mazur, 1962; Hirschfelder *et al.*, 1964; Zdunkowski and Bott, 2004). It follows from (3) and (4) that specific enthalpy of the mixture is also a weighted sum of partial enthalpies

$$h = \sum_i h_i q_i,$$

where $h_i = e_i + p_i / \rho_i$.

According to the principle of energy equipartition (Hirschfelder *et al.*, 1964; Landau and Lifshitz, 1980), every molecular degree of freedom excited thermally contributes $R_i/2$ to the specific heat capacity at constant volume c_{vi} . In addition to the three translational degrees of freedom, at atmospheric temperatures every linear (e.g. diatomic) molecule has two rotational degrees, and every polyatomic nonlinear molecule has three rotational degrees available (Landau and Lifshitz, 1980). Although thermal excitation of vibrational levels of some molecules is important in the radiative balance of the atmosphere, their relative populations are so low that their contribution to the heat capacity may be neglected (Landau and Lifshitz, 1980). This means that the individual heat capacities c_{vi} may be assumed to be independent of temperature everywhere in the atmosphere and the internal energy written in the form

$$e = c_v T,$$

where, according to Equation (3), the specific heat at constant volume for the mixture is a mass-weighted average of specific heats for individual species

$$c_v = \sum_i c_{vi} q_i. \quad (7)$$

Introducing specific heats at constant pressure for each species, $c_{pi} = c_{vi} + R_i$, and using the relation

$$R = \sum_i R_i q_i, \quad (8)$$

following from Equation (4), the specific heat at constant pressure for the mixture becomes

$$c_p = \sum_i c_{pi} q_i = c_v + R. \quad (9)$$

Relation (1) then immediately follows from Equations (4), (6), and (9). Although heat capacities and gas constants of individual tracers may be assumed constant in the atmosphere, the heat capacities for the mixture c_v and c_p , as well as R , generally vary in space and time depending on the composition via Equations (7)–(9).

3. Discussion

It is instructive to compare Equation (5) with forms commonly employed in atmospheric models. Using Equations (1) and (4), it may be written as

$$\frac{dc_p T}{dt} - \frac{RT}{p} \omega = Q. \quad (10)$$

What is often referred to in meteorological literature as the thermodynamic energy equation is commonly written as

$$c_p \frac{dT}{dt} - \frac{RT}{p} \omega = Q \quad (11)$$

(e.g. Holton, 1992). Comparing with Equation (10), it is clear that Equation (11) is valid only if c_p is constant. In some models c_p is explicitly set to the heat capacity of uniformly mixed dry air $c_p = c_{pd}$ (e.g. Davies *et al.*, 2005), which is of course an approximation.

If, on the other hand, c_p is allowed to vary according to Equation (9) (e.g. Untch and Hortal, 2004), then clearly Equation (11) is only an approximation and its exact form should contain additional terms depending on individual tracer tendencies dq_i/dt via Equation (9). These tendencies depend on chemical or phase-transition production and loss processes and diffusive fluxes. The total number of such production and flux terms scales as the number of tracers n . (cf. Equation (7.6–9) of Hirschfelder *et al.* (1964) or Equation (3.52) of Zdunkowski and Bott (2004)). No such correction terms are usually accounted for in atmospheric models and no justification or even acknowledgment of this approximation is given.

Many models of the moist atmosphere use virtual temperature defined to satisfy the equality

$$R_d T_v = RT, \quad (12)$$

where R_d is the gas constant for dry air. T_v is a measure of relative humidity and is introduced into Equation (11) to account for the effects of water vapour on the gas constant R and, consequently, on the relation between the mass, pressure, and temperature fields via the equation of state (4). The use of virtual temperature in Equation (11) implies that the gas constant is variable according to Equation (8). This is inconsistent with an implicit assumption that c_p is constant, necessary for Equation (11) to be correct or even derivable.

The advantage of using T_v in numerical models remains questionable even regardless of whether Equation (11) is correct. Dividing by c_p and substituting definition (12) into the second term of Equation (11) results in a prognostic equation containing two different thermodynamic variables T and T_v (cf. Untch and Hortal, 2004):

$$\frac{dT}{dt} - \frac{R_d T_v}{c_p p} \omega = \frac{Q}{c_p}. \quad (13)$$

Substituting T_v also into the tendency term of Equation (13) will again require additional correction terms

resulting from the variation of R and depending on the tendencies dq_i/dt via Equation (8) (J. Sela, personal communication, 2005). These terms are also routinely neglected in models.

In models with a limited number of gaseous tracers, such as in the standard approximation of the lower atmosphere as consisting of uniform dry air and water vapour, it may not be too difficult to properly account for the additional terms in Equations (11) or (13). The number of tracers to be accounted for may increase if other phases of water are included (e.g. Benjamin *et al.*, 2004; Davies *et al.*, 2005). It may become a serious concern in the presently emerging ‘whole-atmosphere’ models commonly built by extending upward lower-atmospheric general circulation models and including additional species ranging from ozone in the stratosphere to atomic oxygen in the thermosphere (Fomichev *et al.*, 2002; Miyoshi and Fujiwara, 2003; Sassi *et al.*, 2004; Schmidt *et al.*, 2006; Akmaev *et al.*, 2008). In this case even bookkeeping of all the additional terms in Equations (11) or (13) may become unnecessarily cumbersome.

The compact Equation (5) is applicable to an arbitrary number of tracers n and requires no additional terms. This coordinate-invariant equation may be used in both hydrostatic and non-hydrostatic models (cf. Davies *et al.*, 2005).

Although an exhaustive overview of all possible approaches is outside the scope of this note, it should be mentioned that compact formulations are possible using other thermodynamic potentials (Zdunkowski and Bott, 2004) as prognostic variables. For example, the IEE (2) written for internal energy e also contains no additional terms depending on tracer tendencies (Zdunkowski and Bott, 2004). However its use in atmospheric models may require more substantial changes in numerical schemes since its adiabatic part contains terms that differ from the so-called energy-exchange term (second term on the left-hand side) in Equation (5). The finite-difference schemes in existing atmospheric models have been historically designed to provide a consistent treatment of this term in both the IEE and the momentum equations to ensure energy conservation (e.g. Arakawa and Lamb, 1977).

Interestingly, in the hydrostatic models of Richmond and Matsushita (1975) and Fuller-Rowell and Rees (1980) a prognostic equation for the sum of enthalpy and kinetic energy of horizontal motion is solved. This eliminates the energy-exchange term and automatically guarantees energy conservation. However, generalization of this approach to non-hydrostatic models may not be trivial. Diagnostics of temperature from the total energy is somewhat cumbersome as well.

Specific entropy has also been suggested as a thermodynamic variable (e.g. Schumann *et al.*, 1987). As noted by Hauf and Höller (1987) however, entropy is conserved and so may have special advantages only in models of reversible rather than simply adiabatic processes, as often assumed. The stricter former condition implies the absence of irreversible composition changes due to phase transitions, chemical production, or mixing. This

follows from the entropy balance equation, which contains entropy production and flux terms related to tracer tendencies dq_i/dt (de Groot and Mazur, 1962; Hauf and Höller, 1987; Zdunkowski and Bott, 2004).

The physical reason for this is not just the compositional dependence of the gas constant or heat capacities via Equations (7)–(9), but also the fundamental fact that partial entropy of mixture components is greater than entropy of individual pure tracers as formally represented by the so-called mixing terms (de Groot and Mazur, 1962; Hauf and Höller, 1987; Zdunkowski and Bott, 2004). In addition to a complicated balance equation, the mixing terms make the diagnostics of temperature from entropy cumbersome. This may explain why models using entropy as a prognostic variable (e.g. Schumann *et al.*, 1987) have not become widely used in atmospheric modelling with variable composition.

4. Implementation into existing models

The form of Equation (5) is very similar to those commonly used in atmospheric models but with h substituted for T or T_v . This substitution requires no major changes in existing model codes or their integration cycles. Some of these changes are briefly outlined below.

Equation (5) may be written as

$$\frac{dh}{dt} - \frac{\kappa h}{p} \omega = Q, \quad (14)$$

where $\kappa = R/c_p$ is generally variable. This equation is very similar to Equations (11) or (13). Rewriting the static equation with h in hydrostatic models is also straightforward. In models using the semi-implicit time integration scheme (Robert *et al.*, 1972) the IEE is linearized with respect to a globally uniform background temperature or virtual temperature profile T_0 , possibly depending on the vertical coordinate (Simmons *et al.*, 1978). Equation (14) is readily linearized with respect to a prescribed vertical profile of enthalpy h_0 in a similar fashion.

Temperature T is needed on model grids for radiative and other physics parametrizations. In models using virtual temperature, T is calculated from T_v and tracer mixing ratios using Equations (12) and (8). Temperature is easily recovered from h using Equations (1) and (9) in a similar fashion. It is relevant to note here that the diabatic heating terms on the right-hand side of Equation (14) need not be calculated as temperature tendencies, but rather as tendencies of energy inputs per unit mass, e.g. in units of W kg^{-1} . This means that physical parametrizations contributing to Q need not assume any particular distribution of c_p . If non-gaseous phases of water are explicitly treated as tracers, their contribution to c_p should be included in Equation (9) but there is no contribution to the gas constant R in Equation (8) (cf. Davies *et al.*, 2005).

In models using isentropic vertical coordinates, potential temperature θ or virtual potential temperature θ_v

has to be defined (e.g. Benjamin *et al.*, 2004). Potential enthalpy may be defined and used in a similar way:

$$\chi = \frac{h}{(p/p_0)^\kappa},$$

where p_0 is some reference pressure. Depending on the particular application, κ may be assumed here to be variable or constant, e.g. set to R_d/c_{pd} . It is worth noticing again that, with any choice of κ , none of the variables θ , θ_v , χ , or any other variable related to entropy satisfies the respective adiabatic ($Q = 0$) Equations (11), (13), or (14) unless the composition is uniformly constant (Hauf and Höller, 1987).

5. Conclusion

A general form of the internal energy equation (2) naturally suggests using specific enthalpy as a prognostic thermodynamic variable in numerical models seeking to account for the effects of variable composition on the thermodynamics and dynamics of the atmosphere. This approach offers a general and flexible alternative to the standard formalism of virtual temperature. Although other compact formulations are possible and may be worth pursuing, the use of enthalpy requires minimal changes in existing model codes, which are briefly outlined here as well.

Further analysis reveals that the thermodynamic energy equation used in many models is only an approximation of the general Equation (2), and that the use of virtual temperature apparently offers no benefits for atmospheric modelling with variable composition.

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