Application of the Volume-of-Fluid Method to the Advection–Condensation Problem

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ABSTRACT

The authors demonstrate the application of the volume of fluid (VOF) method, a specialized grid refinement technique, to the numerical simulation of clouds. In particular, it is shown that VOF eliminates most of the well-recognized numerical difficulties (spurious oscillations and/or diffusion in vicinity of a cloud–environment interface) associated with finite-difference Eulerian advection of cloud boundaries. In essence, VOF is a subgrid-scale advection parameterization that accounts for the transport of material interfaces. VOF is an Eulerian approach, as it does not track explicitly material interfaces. Instead, it reconstructs such interfaces using auxiliary dependent variables—the partial volume fractions of immiscible materials within computational cells. A feature of VOF particularly important for cloud modeling is its ability to identify cells with a subgrid-scale cloud–environment interface. Consequently, relevant parameterizations of microphysical processes can be applied consistently in “clear” and “cloudy” regions. In this study, the authors first demonstrate the advantages of VOF using the elementary advection–condensation problem with a known analytic solution. The results of this exercise document that simulations employing VOF are significantly more accurate; to achieve equivalent accuracy, they require almost one order of magnitude less spatial resolution. Next, the method is applied to simulations of both dry and moist thermals. These calculations demonstrate the importance of minimizing numerical diffusion at the cloud–environment interface to accurately capture small-scale flow features evolving in the vicinity of the cloud boundary.

1. Introduction

In this paper we demonstrate how state-of-the-art techniques for interface reconstruction can be used to improve the accuracy of numerical models that simulate the evolution of clouds. Such models must treat the advection of the thermodynamic variables, as well as the processes of condensation and evaporation. These coupled processes usually result in a sharp transition region between the cloudy and the clear-air region. A major difficulty in numerical simulations of clouds is to preserve the sharpness of this transition region.

In an Eulerian framework, the difficulties encountered while advecting fields with sharp gradients or discontinuities (i.e., sharp gradients not resolved on the computational mesh) using finite-differencing techniques are well recognized. Low-order linear methods smear the regions of rapid change, while higher-order techniques introduce spurious oscillations. Nonlinear (nonoscillatory) techniques, such as flux-corrected transport (FCT; Boris and Book 1973) or total variation diminishing (TVD) schemes (Sweby 1984), can maintain steep gradients without introducing oscillations in simple advective problems. But in problems where the advected field also appears in forcing terms on the right-hand side of the equation, the feedback between advection and forcing can lead to oscillations in the vicinity of steep gradients, even when nonoscillatory advective techniques are employed. As noted in previous studies (Klaassen and Clark 1985; MacVean and Nicholls 1988; Grabowski 1989), the coupled processes of advection and condensation occurring in clouds are a particular example of such a problem.

Grabowski and Smolarkiewicz (1990, hereafter GS) constructed FCT algorithms that directly incorporate information regarding the phase changes and were able to eliminate most of the spurious oscillations at the cloud boundary. However, the FCT approach itself leads to additional smearing of steep gradients. Also, the resultant algorithms are relatively complex. Furthermore,
FCT algorithms are designed to identify spurious oscillations by comparing a high-order and a low-order solution. No oscillations found in the low-order approximation can be corrected by an FCT scheme. Recently, Pellerin et al. (1995) discussed a similar (conceptually) approach in the context of semi-Lagrangian integration methods.

An alternative suggested by GS is to track the actual position of the cloud boundary within a grid box. In principle, any Lagrangian method (such as interface tracking, MAC, PIC, etc.) could be used for this purpose. However, strong convolution of the cloud boundaries makes such techniques computationally inefficient due to the associated distortions of the Lagrangian mesh. An alternative approach is interface reconstruction (Hirt and Nichols 1981), where partial volumes of two materials separated by an interface become grid-cell variables advected with the fluid. Local differentials of such volume-of-fluid (VOF) variables are then used to reconstruct the interface. This approach is easier to implement, more accurate, and less computationally intensive than particle methods (Ashgriz and Poo 1991; Rider and Kothe 1995). The efficacy of VOF is due to its local nature: VOF needs to be applied only in grid cells in vicinity of a cloud boundary.

Although the notion of VOF is fairly simple (see the following section), VOF computer programs can be tedious (especially in 3D). The latter is related to a substantial logic component associated with the geometry of the problem. In essence, VOF reduces to (a) locating the position and orientation of the interface within the cell and (b) evaluating volumes (areas in 2D) of material advected through cell boundaries. The overall accuracy and technical complexity of the approach strongly depend on both the assumed shape of the interface as well as numerical details of its reconstruction. Early VOF algorithms (Hirt and Nichols 1981) assumed interfaces parallel to the cell walls (Fig. 1b); more recent schemes such as the Youngs method (Youngs 1984; Parker and Youngs 1992), PLIC (Rider and Kothe 1995), and FLAIR (Ashgriz and Poo 1991) assume piecewise-linear interfaces (Figs. 1c and 1d). Consequently, the latter schemes are more complex but preserve the shapes of advected fields more accurately than the early algorithms. In this paper we follow the Youngs approach, primarily for its relative simplicity. In particular, all the VOF solutions presented in this paper were obtained with our implementation of the Youngs method.

The reconstruction of the interface is a unique aspect of VOF; but additional elements are required to complete the algorithm. In the next section, we outline the individual steps of the basic VOF approach, while in section 3 we discuss some special issues associated with applying VOF to the advection–condensation problem. We illustrate the theoretical discussions of sections 2 and 3 with idealized tests and simulations of dry and moist thermals in section 4. We conclude the paper in section 5.

![Fig. 1. Schematic of representing material interface (a) by different types of VOF reconstruction approaches (b)–(d).](image)
immiscible materials, (1) can be reformulated as two auxiliary, conjugate equations:

\[
\frac{\partial \Lambda \psi}{\partial t} + \nabla \cdot \tilde{\nabla} \psi = 0, \tag{2a}
\]

\[
\frac{\partial \Lambda' \psi'}{\partial t} + \nabla \cdot \tilde{\nabla}' \psi' = 0, \tag{2b}
\]

where \( \psi = \Lambda \phi, \psi' = \Lambda' \phi, \tilde{\nabla} = \Lambda \nabla, \tilde{\nabla}' = \Lambda' \nabla, \Lambda' = (1 - \Lambda), \) and \( \Lambda(t, x) \) is the characteristic function of one of the materials equal either 1 or 0 depending on whether \( x \) belongs in the material or not; by design,

\[
\frac{DA}{Dt} = 0. \tag{3}
\]

Such a reformulation is possible because the definition of \( \Lambda \) implies the identities \( \Lambda \Lambda = \Lambda, \Lambda' \Lambda' = \Lambda', \Lambda' = 0, \) and

\[
\phi = \psi + \psi' = \Lambda \phi + \Lambda' \psi', \tag{4}
\]

which together with (3) lead from (1) to (2).\(^1\)

Any flux-form finite-difference scheme for, say, (2a) can be always interpreted as some particular approximation to the formal integral of (2a) over time step \( \Delta t \) and a volume element \( \Delta V \) of a discrete grid:

\[
\frac{1}{\Delta V} \int_{\Delta V} (\Lambda \psi)^{n+1} \, d^3x = \frac{1}{\Delta V} \int_{\Delta V} (\Lambda \psi)^{n} \, d^3x - \frac{1}{\Delta V} \int_{\Delta V} \nabla \cdot \tilde{\nabla} \psi \, dt \, d\sigma, \tag{5}
\]

where all undefined symbols have their usual meaning. Finite-difference approximations to (5) can be symbolically written as

\[
\tilde{\theta}_{I}^{n+1} \psi_{I}^{n+1} = \tilde{\theta}_{I}^{n} \psi_{I}^{n} - \sum_{I=1}^{3} (\tilde{\alpha}_{I+1/2e}^{I} \psi_{I+1/2e}^{I} - \tilde{\alpha}_{I-1/2e}^{I} \psi_{I-1/2e}^{I}), \tag{6}
\]

where \( I \) labels the spatial directions, \( I \) denotes position on the grid, \( \epsilon_{I} \) is the unit vector in the \( I \)th direction, and products of the effective local Courant numbers \( \tilde{\alpha}_{I} \) and the effective transported field \( \psi^{*} \) are the effective fluxes of \( \psi \) through the cell walls. The auxiliary dependent variable \( \tilde{\theta} \) appearing in (6) has the sense of a grid-volume average of the characteristic function

\[
\tilde{\theta}_{I} \in [0, 1] = \frac{1}{\Delta V} \int_{x_{I-1/2e}^{xI+1/2e}} \Lambda(p, \ x') \, d^3x' \tag{7}
\]

and is usually referred to as the “partial volume fraction” (PVF) of one of the materials within a cell \( \Delta V \). Note that for a single material problem in (1) \( (\Lambda = 1) \Rightarrow (\tilde{\theta} = 1, \ \psi = \phi, \ \psi^{*} = \phi^{*}) \). Then, (6) is merely a symbolic form for a standard flux-form Eulerian transport scheme, where (in general) both \( \tilde{\alpha} \) and \( \psi^{*} \) may be complicated functions of velocity components and transported field defined at temporal and spatial locations surrounding \( (n, i) \). Particular choices for these functions define a particular transport scheme. It is apparent, therefore, that the generalized transport algorithm (6) need only be considered in the vicinity of “mixed” cells where \( 0 < \tilde{\theta} < 1 \). From here on, we reserve the term “mixed” for the cells containing two materials and, when necessary, will explicitly identify viscous mixing.

The algorithm in (6) provides a general framework for incorporating subgrid-scale information (on material interfaces) into the Eulerian transport problem, but it offers no specific recipes for approximating \( \tilde{\theta} \) or \( \tilde{\alpha} \) in mixed cells. The uniqueness of VOF is in such approximations. What essentially distinguishes VOF from either particle or interface-tracking methods is that VOF never makes explicit use of \( \Lambda \) (or any other Lagrangian marker) and (7), but it rather relies on the auxiliary dependent variable \( \tilde{\theta} \) to reconstruct an approximate material interface within mixed cells at each time step of computations. After assigning an initial condition \( \tilde{\theta}_{I}^{0} \), the evolution of PVF is approximated (as is any other transported variable) by Eq. (6) for \( \tilde{\theta}_{I}^{t+1} = \tilde{\theta}_{I}^{t} - \sum_{I=1}^{3} (\tilde{\alpha}_{I+1/2e}^{I} \tilde{\theta}_{I+1/2e}^{I} - \tilde{\alpha}_{I-1/2e}^{I} \tilde{\theta}_{I-1/2e}^{I}) \),

\[
\tilde{\theta}_{I}^{t+1} = \tilde{\theta}_{I}^{t} - \sum_{I=1}^{3} (\tilde{\alpha}_{I+1/2e}^{I} \tilde{\theta}_{I+1/2e}^{I} - \tilde{\alpha}_{I-1/2e}^{I} \tilde{\theta}_{I-1/2e}^{I}), \tag{8}
\]

whereupon providing the proper \( \tilde{\alpha} \) becomes the central issue of the VOF approach. Here, we emphasize that to arrive at (8) and/or (8) from (1) through (5) necessarily requires the assumption of flow incompressibility; we shall return to this point later in this paper.

Choosing \( \psi = 1 \) in (5) and (6) implies

\[
\tilde{\alpha}_{I+1/2e}^{I} = \frac{1}{\Delta V} \int_{x_{I}^{xW}} \int_{\Delta \sigma} \tilde{\nabla} \, dt \, d\sigma, \tag{9}
\]

where subscript \( W \) refers to the \( I + 1/2e \) location, surface integration is over a cell wall normal to \( \nu^{I} \), \( d\sigma \) is a length element parallel to \( \nu^{I} \), and \( \tilde{\nabla} = (\Delta t)^{-1} \int_{\Delta \sigma} \tilde{\nabla} \, dt \). In “full” cells where \( \tilde{\theta} = \Lambda = 1, 2 \) (9) recovers the standard meaning of a local Courant number. In mixed cells, however, \( \tilde{\alpha} \) acquires a sense of the normal flux of PVF through a cell wall (see Fig. 2). Having an approximation to \( \Lambda \) within a cell (and an approximation to \( \tilde{\nabla} \), discussed later in this section) the evaluation of

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\(^1\) Note that due to the inherent discontinuity of the problem, \( \phi \) and \( \Lambda \) are not differentiable across the interface and, formally, Eqs. (1)–(4) should be viewed in the weak sense (cf. section 12.14 in Richtmyer and Morton 1967).

\(^2\) We do not discuss “empty” cells with \( \tilde{\theta} = \Lambda = 0 \), as those are full cells for \( \Lambda' = 1 \) in Eq. (2b).
\[ \partial z = (\partial_{x_{i,j-1}} + 2\partial_{y_{i,j-1}} + \partial_{y_{i,j-1}})/4, \]
\[ \partial_{x_{i,j}} = (\partial_{x_{i-1,j}} + 2\partial_{y_{i-1,j}} + \partial_{y_{i-1,j}})/4, \]
\[ \partial_{y_{i+1,j}} = (\partial_{x_{i,j-1}} + 2\partial_{y_{i,j-1}} + \partial_{y_{i,j-1}})/4, \]
\[ \partial_{y_{i,j-1}} = (\partial_{x_{i,j-1}} + 2\partial_{y_{i,j-1}} + \partial_{y_{i,j-1}})/4. \]

Having some finite-difference analogs to (10) and/or (11), the intercept of the linear equation for the interface can be found by requiring that the two partial volumes (areas in 2D) reproduce the known values of \( \partial \) and \( \partial' \) [see (7)]. [Note that (12) may not always preserve planar fronts even on a regular grid and with “exact” advection (D. B. Kothe 1996, personal communication).] In this paper, we use an iterative bisection process to find the location of the interface; that is, take an initial guess for the location of the interface within a cell and compute the area underneath the interface; if the area is larger/smaller than the actual value of \( \partial \), move the interface down/up by half of the initial distance from the bottom of a cell, etc.

In summary, given the initial condition of the auxiliary fields \( \partial, \partial', \psi, \text{ and } \psi' \), in each time step of integration, a VOF algorithm consists of four distinct steps (note the reversed order compared to that in the presentation above): (a) reconstruction of the interface based upon knowledge of \( \partial \), (b) evaluation of \( \psi \), which is consistent with the advection scheme employed (discussed below). Step (c), as given by (8), may require additional time step restrictions or flux limiting to prevent unphysical values \( \partial < 0 \) or \( \partial > 1 \). This issue may be avoided if an alternate-direction split version of (8) is used; however, the resulting splitting errors may be unacceptable large. In this paper, we have chosen the unsplit form (8) and used a simple flux limiting scheme that modifies each of the outgoing fluxes that contribute to unphysical values of \( \partial \) within a cell. If the provisional value of \( \partial \) in (1) need not be updated nor stored but may be reconstructed from (4) whenever required (e.g., for display). The approach above allows for a number of different implementations. For instance, in step (a), one may consider alternate finite-difference approximations to (11), as well as various methods (based on either analytic formulas or iterative approaches) for locating the interface within the mixed cell. In step (b), a variety of approximations for the mean velocity \( \bar{v}' \) may be used; in this paper, we assume \( \bar{v}' = \bar{u}' 1 + 2/4 \), which is consistent with the advection scheme employed (discussed below). Step (c), as given by (8), may require additional time step restrictions or flux limiting to prevent unphysical values \( \partial < 0 \) or \( \partial > 1 \). This issue may be avoided if an alternate-direction split version of (8) is used; however, the resulting splitting errors may be unacceptable large. In this paper, we have chosen the unsplit form (8) and used a simple flux limiting scheme that modifies each of the outgoing fluxes that contribute to unphysical values of \( \partial \) within a cell. If the provisional value of \( \partial \) in (1) exceeds unity (is negative), then we increase (decrease) the magnitude of each of the outgoing fluxes in proportion to the excess (deficit) and to the ratio of the individual and total outgoing flux. This leads to a new set of provisional values, which are examined again and modified if necessary. This procedure produces a realizable solution in a few iterations. Step (d) of the VOF procedure admits an arbitrary trans-
port algorithm in (6). Here, we use a second-order, sign-preserving, conservative MPDATA scheme [broadly documented in Smolarkiewicz (1984), Smolarkiewicz and Clark (1986), and Smolarkiewicz and Grabowski (1990)]. MPDATA consists of a few iterations of the donor-cell (upwind) flux-form advection scheme. The first iteration is a first-order-accurate advection of a scalar field in a given flow. Subsequent iterations reduce the truncation error of the first iteration. As in traditional VOF schemes, we use the classic (uniterated) donor-cell fluxes at the walls of the mixed cells. This is in the spirit of the FCT methods that reduce the local accuracy of approximation to first order in vicinity of steep gradients.

Before we close this section, we draw the reader’s attention to an important physical assumption underlying the VOF approach. The theory of VOF relies on the incompressibility assumption will lead to is only valid for incompressible flows. In general, the assumption underlies the VOF approach. The theory of VOF relies on attention to an important physical assumption underlying the VOF approach.

3. Application of VOF to the advection–condensation problem

The discussion so far has addressed the simplest case, where the interface marks the boundary between two materials, or between a material and a vacuum. Such an interface moves with the local fluid velocity and is a Lagrangian surface governed by (3). VOF may be applied in more general circumstances when the distinction between the two materials changes in time, that is, when (3) includes a source term on the rhs. This is the case in modeling clouds, where the cloud boundary marks the region of rapid change of phase of a single material. The motion of the cloud boundary is nearly, but not exactly, Lagrangian; the cloud boundary moves not only because of the local fluid velocity, but also due to the thermodynamic processes of evaporation and condensation. To represent clouds, therefore, we add one additional step. After the advection calculations are completed, the partial volume fractions in (8) are adjusted to take into account thermodynamic processes. This sequential treatment of concurrent processes is in the spirit of standard fractional-time-step advection–condensation algorithms (cf. section 3a in GS and section 4a in Grabowski and Smolarkiewicz 1996).

In this paper, we employ the anelastic advection–condensation model of GS for a Boussinesq fluid. The governing equations are

$$\frac{\partial \rho_\theta}{\partial t} + \nabla \cdot (\rho_\theta \mathbf{u}) = \rho_\theta \frac{\hat{\theta}}{C_p} C_{d} \tag{13a}$$
$$\frac{\partial \rho_\omega}{\partial t} + \nabla \cdot (\rho_\omega \mathbf{u}) = -\rho_\omega C_{d} \tag{13b}$$
$$\frac{\partial \rho_\omega}{\partial t} + \nabla \cdot (\rho_\omega \mathbf{u}) = \rho_\omega C_{\omega} \tag{13c}$$

where $\theta$ is the potential temperature, $\omega$ and $q_\omega$ are the water vapor and cloud water mixing ratios, and $T$ and $\hat{\theta}$ are temperature and potential temperature of the environment such that $T/\theta = \text{const}$. $L$ is the latent heat of condensation, and $\rho_\omega = \text{const}$ is the density of the reference state. The condensation rate $C_{\omega}$ is uniquely determined by the constraint of zero supersaturation for cloudy regions [see (3)–(7) in GS].

We solve (13) by adapting the forward-in-time approach of Smolarkiewicz and Margolin (1993) for the transport problem (1) with a forcing term, $F_i$, on the rhs. For such a problem, any algorithm in the form

$$\phi_i^{n+1} = \mathcal{A}(\phi_i + 0.5\Delta t F_i^n) + 0.5 \Delta t F_i^{n+1} \tag{14}$$

assures (for smooth initial data) second-order-accurate solutions given a second-order-accurate, forward-in-time (Crowley type) advection scheme $\mathcal{A}$ and at least $O(\Delta t^2)$-accurate approximation to $F_i$ on the rhs. When applied to (13), $\phi_i$ and $F_i$ refer, respectively, to any of $\theta$, $q_\omega$, or $q_v$ variables and their associated forcings on the rhs of the equations. The solution of (14) is accomplished in two steps. In the first step, auxiliary fields $\hat{\phi} = \phi + 0.5 \Delta t F_i^n$ are advected using the VOF approach discussed in the preceding section. The characteristic function $\Lambda$ in (3) is one in clouds and zero elsewhere. In the second step the conjugate auxiliary fields $\psi$ and $\psi'$ in (2a) and (2b) for $\hat{\theta}$, $\hat{q}_v$, and $\hat{q}_\omega$ are updated individually in mixed cells. This update procedure is identical to that used in unmixed cells (i.e., inverting the relations describing thermodynamic equilibrium for the condensation rate; see section 3a in GS for details). Note that the VOF approach allows us to treat both advection and thermodynamic processes on the subgrid scale, which is essential for accurate representation of a cloud boundary in Eulerian models (Stevens et al. 1996).

After solving (14), $\hat{\phi}$ and $\hat{\phi}'$ are adjusted to account for the phase-change processes on the subgrid scale. In unmixed cells, $\hat{\theta}$ is redefined when the status of the cell changes from cloudy to clear or vice versa. In mixed cells, if the clear fraction becomes cloudy (implying $q_v' > 0$), then $q_v$, $q_\omega$, and $\theta$ are mixed according to the finite-difference approximation of (4),

$$\phi_i = \hat{\phi}_i + (1 - \hat{\theta}_i) \psi'.$$  \tag{15}  

Note that $\hat{q}_v = 0$ and need not be stored.
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and then $\theta$ is set to 1. Alternately, if the cloudy fraction becomes clear, then the thermodynamic variables are mixed and $\theta$ is set to zero. In the unlikely case that both regions change phase, $\theta$ is replaced by $(1 - \theta)$ and the cell remains mixed. When the mixed-cell becomes unmixed, and the conjugate variables are combined as in (15), then the cell variables may no longer be in thermodynamic equilibrium. One may ignore this inconsistency, which will be rectified in the next time step (a default option of the model). Alternately, one may recompute or adjust the thermodynamic equilibrium. We have found experimentally that this extra step leads to no noticeable improvement.

4. Computational examples

a. Idealized tests

We first apply our VOF method to the advection–condensation problem described in section 5 of GS. The square wave perturbations of potential temperature and water substance rise with constant vertical velocity in an environment characterized by constant values of stability and relative humidity. The evolution of the perturbations is governed by (13). The problem setup is essentially the same as that in section 5 of GS; that is, the environmental stability and humidity are 0 and 30%, respectively; the domain of integration is 600 m deep; a 160-m-deep initial perturbation, placed near the bottom of the layer, has 0.1-K potential temperature excess over the environment, 100% relative humidity, and 0.2 g kg$^{-1}$ of cloud water; the spatial resolution is 4 m, and the vertical velocity is 2 m s$^{-1}$; the time step is 2/3 s, and the results are shown after 150 s. Figure 3a shows the exact solution for $\theta$. Figure 3b shows the corresponding numerical solution generated with a monotone MPDATA transport scheme. Although the advection procedure is nonoscillatory, spurious oscillations arise in the solution, with the undershoots at the cloud edges being especially obvious. Figure 3c shows the solution equivalent to that in Fig. 2b but employing our VOF technique augmenting basic MPDATA. The dramatic improvement of the computational results is apparent. This solution is clearly superior to that shown in Fig. 8 of GS, which employs a custom-designed FCT advection–condensation MPDATA scheme; also, it is comparable to that in Fig. 5 of Pellerin et al. (1995) based on a custom-designed semi-Lagrangian scheme. The other thermodynamic fields (not shown) exhibit similar improvement.

To quantify the accuracy of the method, we compute the $L_2$ norm of the error relative to the exact solution [Eq. (21) in section 4 of Smolarkiewicz and Grabowski 1990] for both the VOF and non-VOF simulations at varying resolution. Figure 4 compares the error convergence for the two series of simulations. At low resolutions of $O(10)$ grid points, the error of the simulations employing VOF is at least one order of magnitude smaller than that for simulations without VOF. Furthermore, the convergence rate of the VOF simulations is about one order of magnitude faster than that of the simulations without VOF. Neither scheme exhibits a second-order convergence rate even though MPDATA is at least second-order accurate for advection (with smooth initial data). In the combined problem of advection and condensation in Fig. 3, the VOF scheme is first-order accurate and the convergence rate of the non-VOF scheme

**Fig. 3.** Potential temperature fields at the initial (dashed lines) and final states (solid lines) for the idealized advection–condensation problem: (a) the exact solution, (b) the non-VOF solution, and (c) the VOF solution.
is even slower. Here, errors due to the presence of discontinuities dominate the overall accuracy of the solutions. This makes standard arguments about the order of the truncation error, based on the Taylor series expansion of finite differences, simply inapplicable and the mere statement of the convergence encouraging (cf. the discussion on p. 3321 of Pellerin et al. 1995). The same test redesigned for smooth (Gaussian) initial data makes the VOF approach irrelevant but does exhibit a nearly second-order convergence for the non-VOF solutions (W. Grabowski 1996, personal communication).

b. Application to cloud dynamics

The VOF algorithm described in sections 2 and 3 has been implemented in the nonhydrostatic model described in Smolarkiewicz and Margolin (1996) and Grabowski and Smolarkiewicz (1996). The advection in this model can be approximated with either semi-Lagrangian or Eulerian difference schemes. Here, we select the Eulerian option using second-order-accurate MPDATA (optionally monotone) for all prognostic variables.

We start by demonstrating the application of VOF to modeling the evolution of a dry buoyant bubble [i.e., without thermodynamic source terms in (13)] rising in a Boussinesq fluid. The model domain consists of 361 × 241 grid points with ΔX = ΔZ = 10 m. The bubble is initially circular, is centered at x = 0 m and z = 800 m, and has a radius of 500 m. It has a temperature excess of 0.5 K over the constant background. The model was integrated for a total of 8 min of simulated time with Δt = 1 s. Figure 5 shows the comparison of two simulations: one using VOF (for the transport of \( \theta \)) and one using standard nonoscillatory MPDATA. Taking into account the nonlinearity of the evolution of the thermal's boundary and the sensitivity of the problem to the details of numerical schemes (cf. section 5.1 in Smolarkiewicz and Grabowski 1990). However, the VOF solution (Fig. 5a) remains nearly inviscid,\(^4\) while the interface’s dilution due to the implicit viscosity is apparent in the standard nonoscillatory solution (Fig. 5b).

The differences between the VOF and non-VOF solutions are enhanced dramatically when the phase-change processes are included. To demonstrate this, we simulate the development of a moist thermal in a shear-free environment. The spatial and temporal domain and resolution and the geometry of the initial perturbation are the same as in the dry bubble simulation discussed above. The background state is described in Grabowski and Clark (1991): it has constant stability 1.3 \( \times 10^{-5} \) m\(^{-1}\) and constant relative humidity of 20%, with surface temperature and pressure of 283 K and 850 hPa, re-

\( ^4 \) Multiple connectivity of the isentropes evidences some residual, time-irreversible truncation error.
The development of the thermal is driven by an initial buoyancy due to the saturation of the bubble. Figure 6 shows the fields of liquid water content for the VOF and standard nonoscillatory MPDATA solutions after 8 min of simulated time. The two solutions agree well insofar as the overall shape and position of the thermal are concerned. However, in contrast to the dry case, they differ significantly in gross features of the convoluted boundary. The VOF solution exhibits the enhanced development of large thermal eddies, consistent with the results generated using sophisticated FCT schemes custom designed for the advection–condensation problem (section 6 in GS). We attribute the improved results in the VOF solution to the suppression of enhanced evaporation and spurious buoyancy undershoots generated in the traditional (no VOF) model (cf. Fig. 3). These issues are absent from the dry thermal simulations.

5. Concluding remarks

High-resolution numerical simulations are an effective tool to study the dynamics of clouds. It is well recognized that basic numerical schemes suffer from errors that may alter physical processes, especially at the cloud boundary. It is the inherent discontinuities in the problem combined with the nonlinear thermodynamic feedback that cause serious difficulties in the numerical approximations. Several customized advection–condensation finite-difference schemes have been proposed in the literature. These schemes exploit the physical properties of evaporation–condensation processes and their range of applicability is limited.

The problem of representing material interfaces on a discrete mesh has a long tradition in computational fluid dynamics. One technique that addresses such problems is the volume of fluid (VOF), which has been successfully used in a variety of applications ranging from low-speed industrial flows to high-speed flows in plasma physics and astrophysics. The theory of VOF (section 2) relies on the assumption that the interface is a Lagrangian surface. Nonetheless, VOF is an Eulerian approach as it reconstructs the material interface using auxiliary Eulerian fields rather than tracking the interface explicitly using Lagrangian markers. Inasmuch as a cloud boundary is not strictly Lagrangian (it propagates in part due to phase changes), applying VOF to the advection–condensation problem is not necessarily straightforward (section 3).
weakly viscous, 3D anelastic transport with phase-change processes relevant to deep convection problems.

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