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Interactive comment on "Conceptual study on nucleation burst evolution in the convective boundary layer – Part I: Modelling approach" *by* O. Hellmuth

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RC1: Description of "all tests carried out for this model"

AC: A new section on numerical question has been added (see below)

4 Numerical realisation and basic tests

The partial differential equations (PDEs) of the present model represent a mixed class of two types of initial value problems. The advective terms in the gouverning equations

belong to the class of *flux-conservative initial value problems* (Press et al., 1996, p. 824-838, chapter 19.1, Eq. (19.1.6)), and the diffusive terms in the parabolic parts of the gouverning equations belong to the class of *diffusive initial value problems* (Press et al. 1996, p. 838-844, chapter 19.2, Eq. (19.2.1)). The PDEs can be numerically solved simplest by means of the *Forward Time Centered Space* (FTCS) representation (Press et al., 1996, p. 825-827, Eqs. (19.1.1), (19.1.11)). Thereafter, the time-derivative term is numerically represented by the *forward Euler* differencing [1], which is only first-order accurate in Δt (Press et al., 1996, p. 826, Eq. (19.1.9)). For the space derivative a *centered space* differencing [2] of second-order accuracy in Δz is applied (Press et al., 1996, p. 827, Eq. (19.1.10)). The FTCS scheme is an *explicit* scheme [3]. Regarding the requirements of a numerical scheme Press et al. (1996, p. 830)) argued, that *"the* (numerical) *inaccuracy is of a tolerable character when the scheme is stable."* Later on the authors added an argument, *"that annoys the mathematicans: The goal of numerical simulation is not always 'accuracy' in a strictly mathematical sense, but sometimes 'fidelity' to the underlying physics in a sense that is looser and more pragmatic. In such contexts, some kinds of error are much more tolerable than other"* (Press et al., 1996, p. 832). The numerical realisation of the model closely follows pragmatic arguments as well as the recommendations given in the basic papers of Andre et al. (1976a, 1976b, 1978, 1981, 1985), Bougeault et al. (1981a, 1981b, 1985, 1986, 1989), Moeng et al. (1984a), Verver et al. (1997), Wichmann et al. (1985, 1986). However, there was no *a priori* guarantee, that the underlying PDEs are *physically stable*. In cases they would not, the search for a stable differencing scheme must fail. To ensure the stability and to evaluate the accuracy of the numerical scheme a number of tests have been carried

[1]The *forward Euler* time scheme has the advantage, that the quantities at timestep $n+1$ can be calculated in terms of only quantities known at timestep n.

[2]The *centered space* differencing also uses quantities known at timestep n only.

[3]*Explicite* scheme means, that the quantities at the time step $n+1$ at each level can be calculated explicitely from the quantities that are already known. The FTCS approach is also classified as a *single-level* scheme, since only values at time level n have to be stored to find values at time level $n+1$.

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out, which are described below. An important result of the present approach is the objective evidence, that the considered modelling concept is *conditionally stable* [4] with respect to the treatment of the physico-chemical processes.

4.1 Amplitude error

The satisfaction of the *Courant-Friedrichs-Lewy stability criterion* (CFL) (Press et al., 1996, p. 829) was ensured by empirical adjustment of the time integration step according to the prescribed vertical grid resolution. To investigate the sensitivity of the model results against the time integration scheme, the first-order *forward Euler* time differencing scheme was compared with the third-order Adams-Bashforth time differencing scheme [5], which is known to have attractive stability characteristics (Durran, 1999, p. 65-72, Table 2.1). The differences were visually inspected and found to be small, and hence, being not relevant for the question of interest. This agrees with the findings of Durran (1999, p. 65), who argued: *"... A major reason for the lack of interest in higher-order time differencing is that in many applications the errors in the numerical representation of the spatial derivatives dominate the time-discretization error, and as a consequence it might appear unlikely that the accuracy of the solution could be improved through the use of higher-order time difference."* The studies presented in part II and III were carried out using the third-order Adams-Bashforth scheme.

[4] To ensure physical stability, the third-order moment PDEs for the physico-chemical variables must be modified. See part III.

[5] There exists a second-order version of this scheme too.

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4.2 Transport error

The large-scale subsidence is considered by additional vertical-advection terms in the gouverning PDEs. The discretisation of these terms can cause *transport errors* (Press et al., 1996, p. 831). It was found, that the application of centered differencing scheme does work well for meteorological advection, but not for advection of physico-chemical properties, where at very low mean concentrations first-order moments can become negative. To avoid this effect, an *upwind differencing* is generally used for the advection terms (Press et al., 1996, p. 832, Eq. (19.1.27)). This scheme is only first-order accurate in the calculation of the spatial derivatives, but it was found to be appropropriate for the discretisation of advection terms.

4.3 Phase error and nonlinear instability

(a) Inspection of clipping approximation
The clipping approximation was found to be a *necessary and sufficient condition* to ensure the stability of the meteorological model. This is fully in accordance with Andre et al. (1978, p.1881, see conclusions), who concluded, that the realisability inequalities are absolutely necessary *"since if one ceases to enforce them at any time the model blows up very rapidly."* In opposite to this, in the physico-chemical part the clipping approximation alone was found to be *necessary but insufficient* to stabilise the model (see below).
(b) Inspection of spurious oscillations
Moeng et al. (1984a) demonstrated, that the third-order equations proposed by Andre et al. (1978) are of hyperbolic type (*"wave equation"*). The solution of these equations exhibits oscillations, which arise from the mean-gradient and buoyancy terms of the triple-moment equations. In the present approach, the author followed the attempt of Moeng et al. (1984, Eq.(3.5)) to damp these oscillations by introducing artificial diffu-

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sion terms into the triple-moment equations. With a reasonable choice of the diffusion coefficient, these oscillations can be additionally damped in the dry-cloud case such as considered here. This is fully in accordance with Moeng et al (1984a). It was found, that the numerical stability of the scheme is a prerequisite to damp spurious oscillations, not vice versa. When the numerical scheme is not stable, stability can not be achieved by considering artificial diffusion terms. From a visual inspection of the triple moments it was found, that the amplitude of the spurious oscillations can be effectively damped, but not be prevented. It should be noted, that spurious oscillations - even being nonphysically - are a mathematical part of the solution of the underlying hyperbolic PDEs. These parts of the solution can be traced back to an insufficient physical parameterization of quadruple correlations. The spurious oscillations occuring in the meteorological part of the third-order moment PDEs could be succesfully damped by the recommendations given by Moeng et al (1984a). In contrary to this, the damping of these spurious oscillations is exceptionally difficult in the physico-chemical part. Apart from simulating passive tracers, these oscillations were found to amplify themselves causing instability of the physico-chemical part [6]. Hence, the introduction of artificial diffusion terms damps physico-chemical oscillations *effectively but not sufficiently*.

(c) Inspection of space differencing

Performing a third-order modelling study of a marine stratocumulus layer Bougeault (1985) pointed out, that a modification of the vertical finite differencing scheme is required to handle the strong gradients in the temperature and moisture profile at the inversion level. During the simulation of stratocumulus a very sharp inversion can develop, featuring a strong change over one grid length with negligible gradients immediately above and below. The vertical derivatives of the first-order moments appear both in second- and third-order equations. The authors argued, that owing to the

[6]Remember, that the same numerical model and subroutines are used in both the meteorological and the physico-chemical model. Self-amplifying oscillations can hardly be called "spurious". However, it seems that the amplification directly originate from spurious oscillations, or at least are strongly related to them.

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staggered structure of the grid [7] the derivatives evaluated by the centered finite difference scheme at the half levels can differ by a factor 2. This creates problems in the third-order equations, leading to the appearance of negative values of the variances at the half level just below the inversion. The ultimate way to solve this problem is a variable grid spacing with higher resolution near the inversion. To bypass a variable grid, the authors proposed a more empirical solution. The centered differencing of the derivatives of the first-moment variables in the third-order equations are replaced with a *"geometric approximation"*, while all other derivatives are still evaluated by centered finite differencing Bougeault (1985, p. 2827-2828, Fig. 1, Eqs. (2)-(3)). In the present study it was found, that the revised finite differencing scheme for the mean variables in the third-moment equations - originally designed to be applied near a stratocumulus top - is not necessary for the simulation of the meteorological conditions during the clear-sky case. This is plausible, as near the cloud-free PBL top such large gradients of temperature and humidity as observed near stratocumulus cloud tops are unlikely. Anyway, for physico-chemical properties the situation is completely different: Here, for both the cloudy and the clear-sky case much higher vertical gradients can be expected compared to that appearing in meteorological profiles. Consequently, the revised finite differencing scheme was applied. It was found, that the stability of the model could effectively be enhanced. To be consistently, the approach proposed by Bougeault (1985) is used both in the meteorological and in the physico-chemical model. As for artificial diffusion, the stability of the scheme is a prerequisite for the stabilising effect of the revised differencing scheme, not vice versa. When the model is unstable, instability can be damped, but stability not be be achieved by the proposed alteration of the differencing scheme.

(d) Effect of artificial retardation terms

To prevent the amplifying oscillations of physico-chemical third-order moments several attempts have been made to consider additional empirical retardation terms in the

[7] In a staggered grid, first and third-order moments are calculated at the main levels, and second-order ones are calculated at the half levels.

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corresponding PDEs. Such terms secure an evolutionary tendency of the predicted fields toward some prescribed values, such as realised in the classical nudging concept. Runs were performed, e. g., with different retardation time scales. It was found, that such terms can prolongate the "characteristic runtime" of an executable exhibiting amplifying oscillations, but it was not possible to prevent the amplification of such oscillations at all.

(e) Conclusion and open problems

To prevent the amplification of oszillations, which destabilise the model, physical arguments must be considered for the modification of the third-order moment equations of the physico-chemical model. This is explained in detail in part III. Finite-difference schemes for hyperbolic equations can exhibit purely numerical dispersion (*phase errors*) and *nonlinear instability* as well (Press et al., 1996, p. 831). The question, inhowfar numerical phase errors and nonlinear instability can be separated from spurious oscillations or how they interact, could not be answered for the time being. This issue deserves a special evaluation in a separate work.

4.4 Mass conservation

The mass conservations was investigated in connection with the prevention of amplifying oscillations in the physico-chemical part. Three tests using a passive tracer have been performed. Firstly, a scenario with zero-background tracer concentration and a source with a time-independent unit strength located at the ground was considered. Sinks were excluded. In the course of the day, the source continously replenished the mixing layer with the tracer. The result was a tracer profile exponentially decreasing with height. The tracer concentration near the ground increased when the mixing layer height collapsed in the late afternoon. Secondly, a number of runs were performed with different height-dependent initial profiles without a ground source. In each case, the tracer concentration became stationary and height-independent after a couple of

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model hours, i. e., the tracer was fully diluted throughout the boundary layer. Thirdly, runs were performed with a height-independent initial profile. This profile was found to remain nearly constant during the runs, i. e., the fluctuations around the initial profile were found to be negligibly small with respect to the question of interest. Such kinds of tests were performed several times, e. g., when numerically relevant revisions were conducted (replacement of the time integration scheme and the vertical discretisation scheme, modification of the clipping approximation, alteration of prescribed fine-tuning parameters etc.). A detailed reevaluation of this issue is intented to be performed in the context of skipping the clipping approximation at all, e. g., by persecuting a state-of-the-art parameterisation of third-order moments recently proposed in the literature.

4.5 Sensitivity against changes in the turbulence parameterisation

(a) Extension of PDE numbers
The model equations originally proposed by Andre et al (1978) are based on a number of simplifications, e. g., the gouverning equations for the kinematic humidity fluxes inclusive the corresponding equations of the related triple correlations are neglected therein. In the present model version, these simplifications were omitted to generalise the approach. Although the consideration of the additional equations is numerically more expensive compared to the base case, the model was found to behave "well-tempered" against that important extension of the number of equations, i. e., stability remains ensured and the results are qualitatively similar.
(b) Fine-tuning turbulence parameters
The fine-tuning parameters recommended to use by Andre et al. (1978) should be not changed without reasonable care, especially without a physically motivated revision of the underlying parameterisation. The model was found to be noticeably sensitive against changes of these parameters, whereas corresponding tests were not systematically performed and are only ill-motivated at the present stage of work. It should be

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pointed out, that the pioneering work of André and his co-workers is the *sine qua none* for the approach presented here.

(c) Length-scale parameterisation

The mixing length effectively affects the dissipation rate. As already stated by Moeng et al. (1984a), there exists no proper way to determine the length scale. The existing formulations are more or less arbitrary or their validity is restricted to special conditions, such as certain ranges of atmospheric stability, respectively. Tests using several commonly accepted parameterizations of the mixing length scale and the mixing layer height (used as scaling property) were carried out. In present case, the mixing-length parameterisation was extensively evaluated in the context of the treatment of spurious oscillations. Bougeault et al. (1986) argued, that the mixing-length formulation of Mellor et al (1974) is known to grossly overestimate the mixing length near the inversion, and leads therefore to a gross underestimation of the dissipation rate. From a linear stability analysis the authors concluded, that oscillations can only develop in a region of unstable stratification, and that in this case, they can be efficiently controlled by decreasing the mixing length. These findings are very important, especially for the cloud-topped PBL, but perhaps even though for physico-chemical processes near the cloudless PBL top. Sensitivity tests performed show, that the mixing-length parameterisation used in Andre et al (1978) is appropriate to simulate the meteorological evolution of the non-cloudy PBL. But owing to the more sophisticated adjustment of their length-scale parameterisation to buoyancy-induced instabilities, the approach of Bougeault et al (1986) was evaluated as well. With respect to the meteorological model the results using different schemes were found to be qualitatively very similar, but to differ quantitatively. Without a more detailed PBL verification study, no scheme could be *ad hoc* favoured over the other one. Considering the physico-chemical model it appeared, that the revised approach proposed by Bougeault et al. (1986) enhanced the model stability. However, as previously discussed, when the model was not stable, than stability could also not be achieved by alteration of the mixing-length parameterisation. The observed sensitivity of the model results against the length-scale parameterisation

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shows, that its evaluation in a model like the present one remains an important task, even after years of great efforts on this subject.

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