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AN IMPROVED METHOD FOR CALCULATION OF THE WET PARTICLE DIAMETER AND THE KAPPA PARAMETER FROM THE CCN DATA

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INTRODUCTION

The study of particle size distribution and hygroscopic growth is important for several reasons. Particle diameter is available experimentally, but the relationship of hygroscopic growth to cloud condensation nuclei (CCN) and AMS data can be modeled mathematically. In this paper, we present an improved algorithm for calculating the wet particle diameter and the κ parameter that is faster, more accurate, and more reliable than the algorithm used by other authors.

MATHEMATICAL METHOD

The basis for calculation is Köhler's theory. Petters and Kredenweis (2007) showed that water vapour saturation ratio s over an aqueous droplet is expressed by

$$s = \frac{D_{\mathrm{wet}}^3 - D_c^3}{D_{\mathrm{wet}}^3 - D_c^3(1-\kappa)} \exp\left(\frac{4\sigma_w M_w}{RT\rho_w D_{\mathrm{wet}}}\right) \tag{1}$$

where D_{wet} is the wet particle diameter, D_c is the critical diameter of the dry particle, σ_w, ρ_w, M_w are the surface tension, density, and molar weight of water, and κ is a single parameter combining specific properties of aerosols such as molar weight, density, and van't Hoff factor. For given $s = 1 + S/100\%$, where S is a selected supersaturation, and D_c, it yields a single equation for two unknowns, namely D_{wet} and κ and has thus infinite number of solutions. Thus it is necessary to find D_{wet} that maximizes the saturation ratio while matching the selected supersaturation (Rose *et al.* 2010). To solve the problem they use nested minimization of $(-s)$ and $|s - 1 + S/100|$ by double application of the *fminsearch* function from Matlab. This approach has a serious drawback. The *fminsearch* function is an implementation of a Nelder-Mead algorithm designed for multidimensional optimization but used here in a single dimension. Since an absolute value is minimized, the method can find a false solution satisfying the minimization criterion but equation (1) is not satisfied.

When we examine the problem, we find that it is indeed a constrained optimization where the same equation plays both roles, it is both the criterion function and the constraint. The necessary condition for a local maximum is obtained by differentiation:

$$\frac{\partial s}{\partial D_{\mathrm{wet}}} = \frac{1}{D_{\mathrm{wet}}^3 - D_c^3(1-\kappa)} \left[\frac{3D_{\mathrm{wet}}^2 D_c^3 \kappa}{D_{\mathrm{wet}}^3 - D_c^3(1-\kappa)} - (D_{\mathrm{wet}}^3 - D_c^3)\frac{4\sigma_w M_w}{RT\rho_w D_{\mathrm{wet}}^2}\right] exp\left(\frac{4\sigma_w M_w}{RT\rho_w D_{\mathrm{wet}}}\right) = 0 \tag{2}$$

Fig. 1 shows the values of the partial derivative of the saturation ratio with respect to the wet diameter for different values of supersaturation. For values slightly above the diameter of the dry particle, the derivative is a decreasing function that reaches a minimum and then asymptotically approaches zero. The root of Eq. (2) can therefore be easily bracketed. D_{wet} and κ are then computed by nested solution of both equations using an algorithm we have implemented in GNU Octave that is always convergent.

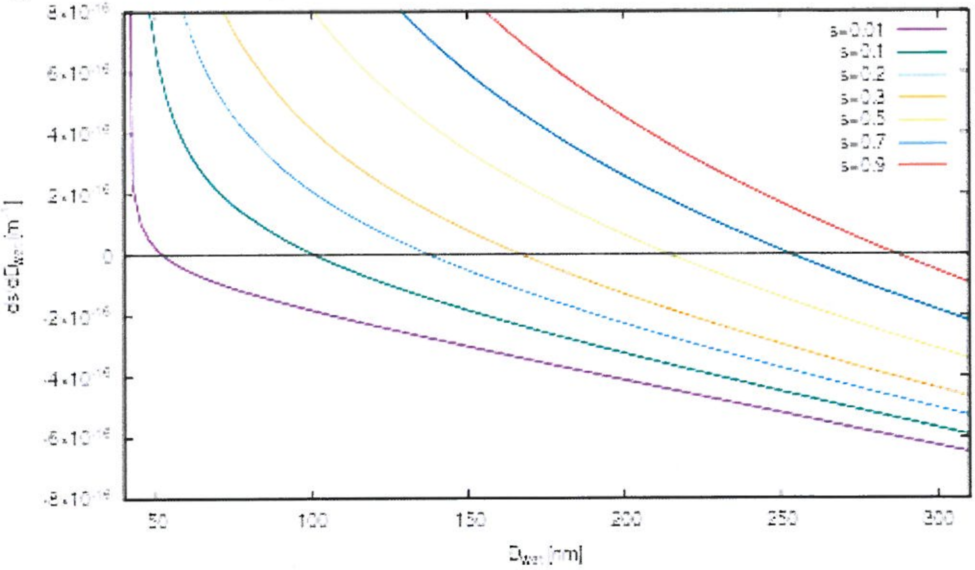

Fig 1: Dependence of partial derivative of saturation ratio with respect to the wet particle diameter for D_c = 40 nm and several values of supersaturation

CONCLUSIONS

The algorithm proposed here is based on a rigorous mathematical derivation and is implemented in GNU Octave. The procedure for solving a real equation with a single real variable is a combination of several algorithms that ensures that the iteration operator contracts in Banach space, i.e., the algorithm is always convergent provided that the root of the equation has odd multiplicity and can be bracketed. The method converges quickly and reliably even if the root is a turning point. The algorithm does not fall into a false solution at a very low supersaturation which is another advantage over using the *fminsearch* function, in addition to speed and precision.

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