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Computationally efficient expressions for the collision efficiency between electrically charged aerosol particles and cloud droplets

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SUMMARY

A multiple factor parametrization is described to permit the efficient calculation of collision efficiency (E) between electrically charged aerosol particles and neutral cloud droplets in numerical models of cloud and climate. The four-parameter representation summarizes the results obtained from a detailed microphysical model of E, which accounts for the different forces acting on the aerosol in the path of falling cloud droplets. The parametrization's range of validity is for aerosol particle radii of 0.4 to 10 μm, aerosol particle densities of 1 to 2.0 g cm^{-3}, aerosol particle charges from neutral to 100 elementary charges and drop radii from 18.55 to 142 μm. The parametrization yields values of E well within an order of magnitude of the detailed model's values, from a dataset of 3978 E values. Of these values 95% have modelled to parametrized ratios between 0.5 and 1.5 for aerosol particle sizes ranging between 0.4 and 2.0 μm, and about 96% in the second size range. This parametrization speeds up the calculation of E by a factor of $\sim 10^3$ compared with the original microphysical model, permitting the inclusion of electric charge effects in numerical cloud and climate models.

KEYWORDS: Atmospheric electricity Cloud parametrization Solar–terrestrial physics

1. INTRODUCTION

Close encounters between aerosol particles and water droplets may ultimately lead to the incorporation of the aerosol into the droplet and the removal of the aerosol, depending on the relative sizes of the droplet and particle and their trajectories. Aerosol–droplet collisions are important in studies of the relationship between precipitation and atmospheric air pollution, and in engineering applications in which the removal of particles is required using a liquid spray. In the atmosphere, aerosol–droplet interactions are also important for cloud physics, because if a water droplet is supercooled and the colliding particle effective as an ice nucleus (in the contact mode), freezing of the droplet may result. Such a phase transition changes the radiative effect of a cloud and modifies the atmospheric energy balance.

Several theoretical studies have investigated the collision efficiency between aerosol and falling water droplets. Greenfield (1957) found that the probability of collision increased at the smaller and larger ends of the aerosol radii range 0.1–1.0 μm, due, to increased Brownian motion of the particle and increased particle inertia, respectively; both of these increase particle removal during streamwise flow around the droplet. The region between these two radii has the lowest collision efficiency, and has become known as the Greenfield Gap. Inclusion of an additional electrical (Coulomb) force, acting between droplet and particle, was considered by Grover and Beard (1975), who reported that the electrical force enhanced the collision efficiency. At small particle–droplet separations, however, an additional electrical image force acts, which is always attractive regardless of the relative polarities of the charges on the droplet and particle. Tinsley *et al.* (2000) extended the Grover–Beard theory to include the image force in calculating the collision efficiency. They found the electric image effect to be significant, even for moderately charged aerosols. With the image effect, the collision efficiency

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increased by up to factor of 30 for aerosols carrying a, relatively large, 50 charges, compared with that for phoretic and Brownian effects with relative humidity in the range 95–100%. From the work of Tinsley *et al.* (2001) the effect of the phoretic forces for 98% relative humidity is equivalent to a charge of ~20 e on the aerosol particle, and for 85% a charge of ~100 e.

Tripathi and Harrison (2001, 2002) formulated a similar model for aerosol particle and cloud droplet collision, which calculated the collision efficiency for prescribed aerosol particle radius, particle charge, particle density and droplet radius. This calculation is computationally expensive, which prevents the straightforward inclusion of collision efficiency effects in cloud and climate models.

Since atmospheric aerosol is almost always naturally charged from the effects of atmospheric electricity and cosmic rays (Harrison and Carslaw 2003), the representation of collision efficiency changes in a computationally efficient manner is necessary if electrical effects on cloud processes are to be represented in cloud and climate models. One application of such modelling is in quantifying the role of solar changes in climate, since solar modulation of galactic cosmic rays may cause changes in atmospheric aerosol electrification and, with them, cloud and climate changes (Carslaw *et al.* 2002).

Some efforts have been made in the past to parametrize the collision efficiency. Slinn (1983) proposed a representation of collision efficiency from a fit to experimental data. This relationship was obtained by dimensional analysis of the equation of motion for the particles, but it did not take into account the electric charges on aerosol particle, and was valid only for an aerosol particle density of 1.0 g cm^{-3}. In this work we present a much more extensive parametrization for collision efficiency using the microphysical model of Tripathi and Harrison (2001, 2002); this includes the functional dependence on aerosol particle density, particle radius, particle charge and cloud droplet radius. The electric charge on droplets does not appreciably affect the collision efficiency for droplets carrying charges up to 1000 e (Tinsley *et al.* 2000) as commonly found in weakly stratified clouds. For this reason, droplet charge is not included in the choice of parameters.

2. Electrified aerosol removal model

The Tripathi–Harrison electrified aerosol removal model provides the data for the comprehensive parametrization of collision efficiency, E, undertaken here. The model considers the frame of reference of a droplet, with the charged aerosol particle moving towards it. When the charged particle comes near to a droplet, it induces an image charge on the droplet, which is assumed to be initially neutral (e.g. Tinsley *et al.* 2000). This results in an attractive image force between aerosol particle and cloud droplet irrespective of the relative polarity of charge on the droplet and aerosol. The model incorporates the forces previously applied by Grover *et al.* (1977) (i.e. drag, gravitational, inertial and Coulomb forces) and the electrical image force given by Tinsley *et al.* (2000), assuming aerosol charges typical for atmospheric particles in non-thunderstorm conditions (Tripathi 2000). The model considers the flow field around the droplet to be governed by the Navier–Stokes equation rather than Stokes' law, as assumed by Tinsley *et al.* (2000). Drag forces are computed by solving the complete Navier–Stokes equation of motion for steady, incompressible flow past a rigid sphere, using a method originally developed by LeClair *et al.* (1970). The trajectory of the aerosol particle moving past the water drop is analysed, and the collision efficiency is calculated. Collision efficiencies are in excellent agreement with those calculated by Grover and Beard (1975) when only the long-range Coulomb force was included

TABLE 1. RANGE OF INPUT PARAMETERS IN THE COLLISION EFFICIENCY PARAMETRIZATION

Aerosol density ρ ($g\ cm^{-3}$)	1.0, 1.5, 2.0
Aerosol charge q (e)	0, 5, 10, 20, 50, 100
Aerosol radius a (μm)	First size range (0.2–2.0 μm) 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0 Second size range (2.0–10 μm) 2, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4, 3.6, 3.8, 4, 5, 6, 7, 8, 9, 10
Droplet radius A (μm)	18.55, 23.4, 26.77, 31.74, 41.5, 52.5, 62.1, 70, 76.89, 88.72, 100.7, 104, 142

(Tripathi and Harrison 2002). The collision efficiency using this model was given in Tripathi and Harrison (2002) for particle radii in the range 0.4–4.0 μm, particle densities of 1.0–2.0 g cm^{-3}, and particle charges from 0–100 e. The difference between the collision efficiencies calculated by Tripathi and Harrison (2002) and Tinsley *et al.* (2000) when image forces were considered, is attributed to the more explicit treatment of the inertial force. Collision efficiencies from the model were also used to calculate scavenging coefficients of radioactive aerosols (Tripathi and Harrison, 2001), which can acquire substantial electrical charges.

3. Parametrization of model results

The intention of this work is to parametrize the effects of electric charges on the collision efficiency between charged aerosols and neutral drops, in order to provide a computational method for use in cloud or climate models. To optimize the fit to the model, the parametrization has been divided into two aerosol particle ranges: 0.4 to 2 μm, where electric forces are dominant; and 2 to 10 μm, where the inertial force is dominant. There are a few cases, as can be seen in following section, where the two parametrizations do not agree with each other at 2.0 μm, but neither is likely to agree exactly with the data. Errors in the fitting for these radii where the collision efficiency is low is less important for application in cloud models than the errors of a factor of two or more in the electrical branch where the collection efficiencies are high.

The electrified-aerosol removal model was run for a range of input parameters selected to span conditions common in the atmosphere: drop radius 18.55–142 μm, particle radius ranges 0.4–2.0 μm and 2.0–10 μm, particle density 1.0–2.0 g cm^{-3}, and particle charge 0–100 e for atmospheric pressure 900 hPa and temperature 10 °C. In the aerosol particle range 0.001–0.4 μm the sizes of particles are sufficiently small for Brownian forces to become important, and the Tripathi and Harrison model is not applicable. This has restricted the range of aerosol radii used to 0.4–10 μm.

Using increments across the parameters as specified in Table 1, the final grid for parametrization contains a total of 3978 points for each range, although the data were filtered for efficiency with any value of E less than 10^{-4} deleted. The approach used in the parametrization was that of a multi-variable polynomial, consisting of the powers of independent variables (droplet radius, A; aerosol radius, a; cos ρ where ρ is the aerosol material density; exp q, where q is the aerosol charge), determined using the software package *Mathematica* (Modgil *et al.* 2005). A least-squares fit to the dataset, as a linear combination of functions of independent variables, was used to arrive at an initial parametrization of E. The basis function was chosen according to the nature of the individual curves of the functional dependence for each of the four independent variables.

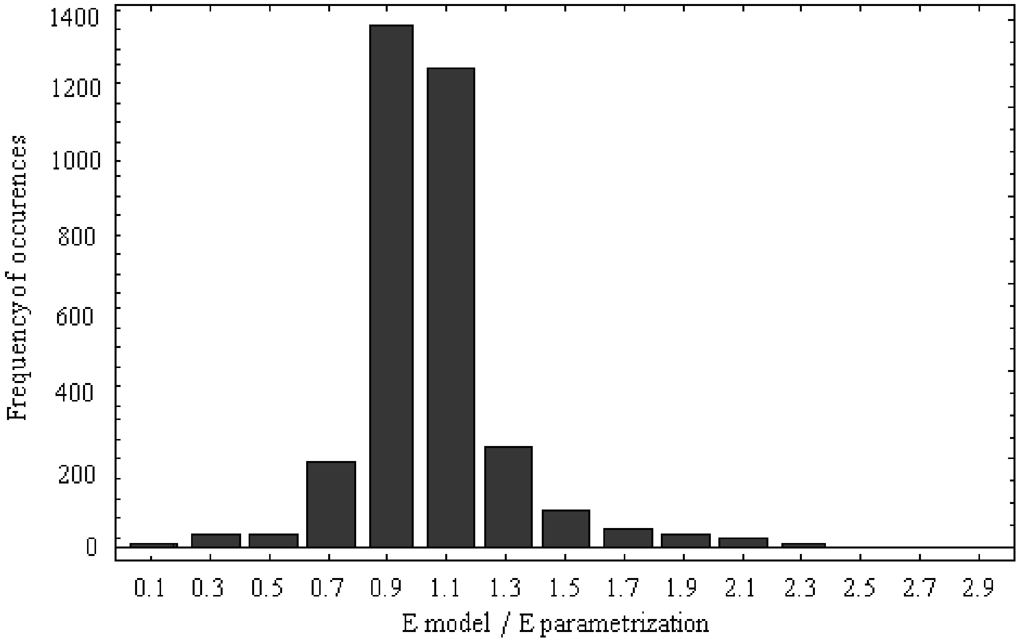

Figure 1. Histogram showing frequencies of occurrence of various ratios of modelled to parametrized collision efficiencies (E_m/E_p) for aerosol particle radii in the range 0.4 to 2 μm.

A better fit was found using the natural logarithms of a and E, which also circumvented a difficulty with *Mathematica* in fitting an exponential function in four variables. The new dataset was generated by transformation from the dataset obtained from the model, for fitting, by taking natural logarithm of a, and E. Finally the expression obtained from the parametrization is found to be a very good fit*.

4. Results and discussion

The expressions obtained from the parametrization give E values close to those from the microphysical model. For a comparison between the fitted and modelled values, a histogram of the frequency of occurrence of the ratio of model values, E_m, to parametrized values, E_p, is given in Figs. 1 and 2. Defining the fitting efficiency as the percentage of points where the ratio of model values to parametrized values falls between 0.5 and 2.0 for the condition $E > 10^{-4}$, the efficiency from the parametrization is ~95% and ~96% for the aerosol size ranges 0.4–2.0 μm and 2.0–10 μm, respectively.

A more illuminating comparison can be made on a point-to-point basis, by visually comparing the values of E obtained from the model with those from the parametrization. The values of E for all the drops were compared during the parametrization. Curves for several representative drop sizes are given here to provide visual confirmation of the parametrization's effectiveness.

For drop radius 18.55 μm: Figs. 3(a1) and (a2) each show that the parametrization function values (E_p, full lines) follow the same form as model values (E_m, dotted lines), for the two aerosol size ranges, respectively; they also show a change with aerosol

* The parametrization code in C Language is available from:
http://arxiv.org/abs/physics/0602007 (paper id: physics/0602007, PaperPassword: fzvg2).

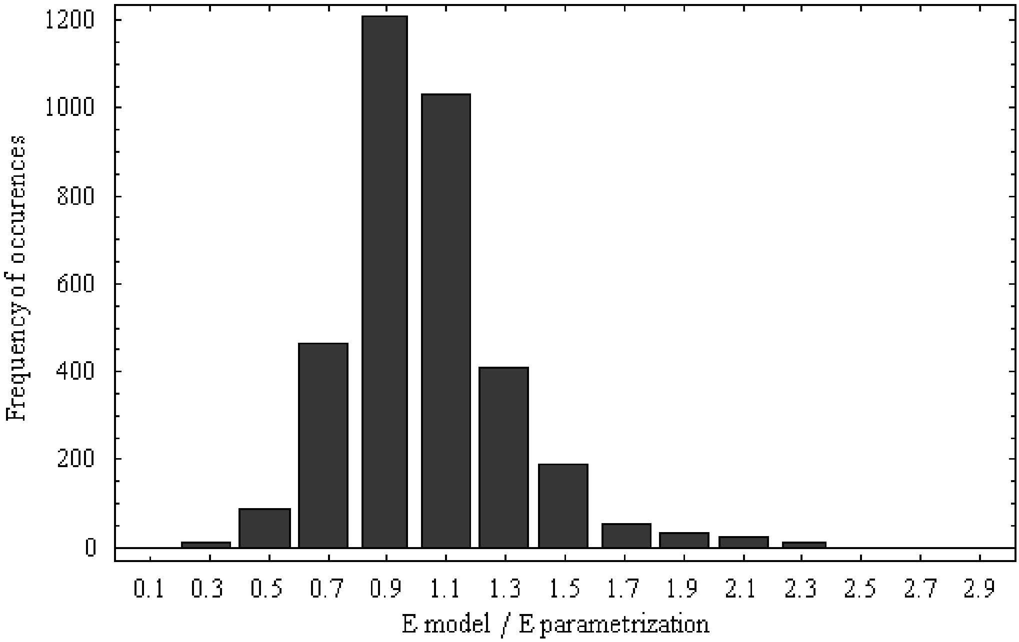

Figure 2. As Fig. 1 but for aerosol particle radii in the range 2 to 10 μm.

particle charge. The parametrized values are mostly very close to the model values. In Fig. 3(b1), for a larger density, ρ, the parametrized function remains sensitive to the aerosol charge, but somewhat overestimates E_m for aerosol charges 0 and 100 e for aerosol radii 0.5 to 1.5 μm, and conversely underestimates E_m for aerosol charges 10 and 20 e for particle radii from 0.5 to 1.5 μm. In Fig. 3(b2) the collision efficiency is less than 10^{-4} for aerosol particles greater than 2.5. In Fig. 3(c1) the E_p values conform with E_m values for most aerosol radii; but in Fig. 3(c2) no model values are shown since the collision efficiency is always less than 10^{-4} for all aerosol particle radii.

For drop radius 31.74 μm: in Fig. 4(a1) and (a2) the parametrization values follow a similar pattern to the model values for drop radius $A = 31.74$ μm and $\rho = 1.0$ g cm^{-3}. In Fig. 4(b1) the E_p and E_m values are very similar for all particle charges. In Fig. 4(b2) for the particle range 2.6–3.6 μm the parametrization overestimates the values in the Greenfield Gap region. In Figs. 4(c1) and (c2) the parametrized values are mostly very near to the model values. It is clear that as the aerosol particle radius increases the collision efficiency values overlap. The reason for this is that for large aerosol radii the inertial force become important and the effect of charge on collision efficiency is negligible.

For drop radius 41.5 μm: in Figs. 5(a1), (a2), (b1) and (c1) E_p follows the same trend as the model value, whereas in Figs. 5(b2) and (c2) for aerosol radii $4 < a < 8$ μm it deviates from the model, although only slightly in most of the cases.

For drop radius 52.5 μm: in Fig. 6(a1) E_p is similar to E_m both in trend and magnitude. In Figs. 6(b1) and (c1), for particle range 1–2 μm, the parametrized function underestimates the model values. In Fig. 6(a2) the E_p values are close to E_m whereas in Figs. 6(b2) and (c2), for $a > 4$ μm, the values differ but are well within 20%.

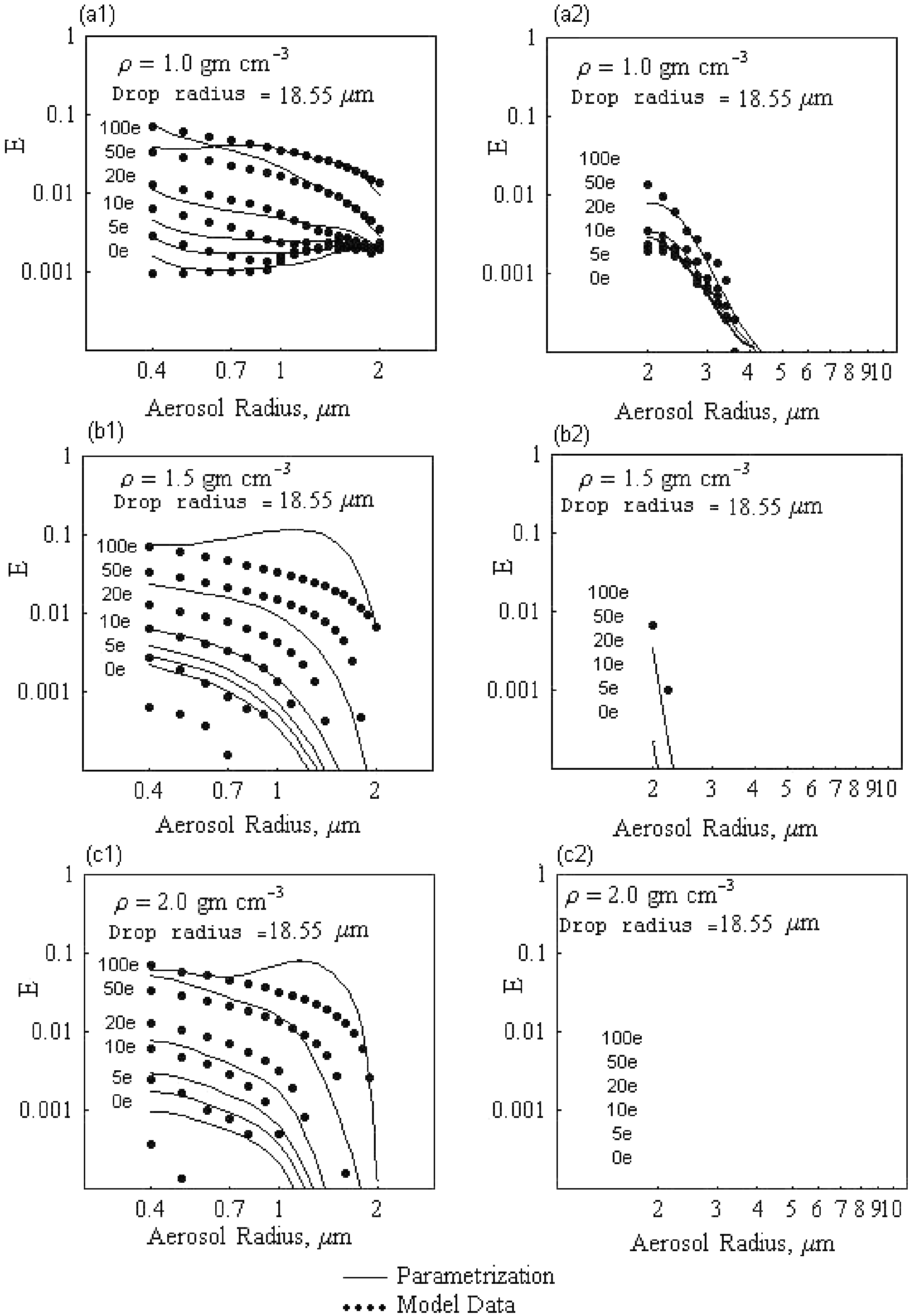

Figure 3. For drop radius 18.55 μm: (a1) collision efficiency, E, as a function of aerosol radius (μm) from the parametrization function and microphysical model aerosol charge 0–100 e, aerosol density 1 g cm^{-3}, and for aerosol radius 0.4–2 μm. (a2) Same as (a1) but for aerosol radius 2–10 μm; (b1) as (a1) but for aerosol density 1.5 g cm^{-3}; (b2) as (a2) but for aerosol density 1.5 g cm^{-3}; (c1) as (a1) but for aerosol density 2 g cm^{-3}; (c2) as (a2) but for aerosol density 2 g cm^{-3}.

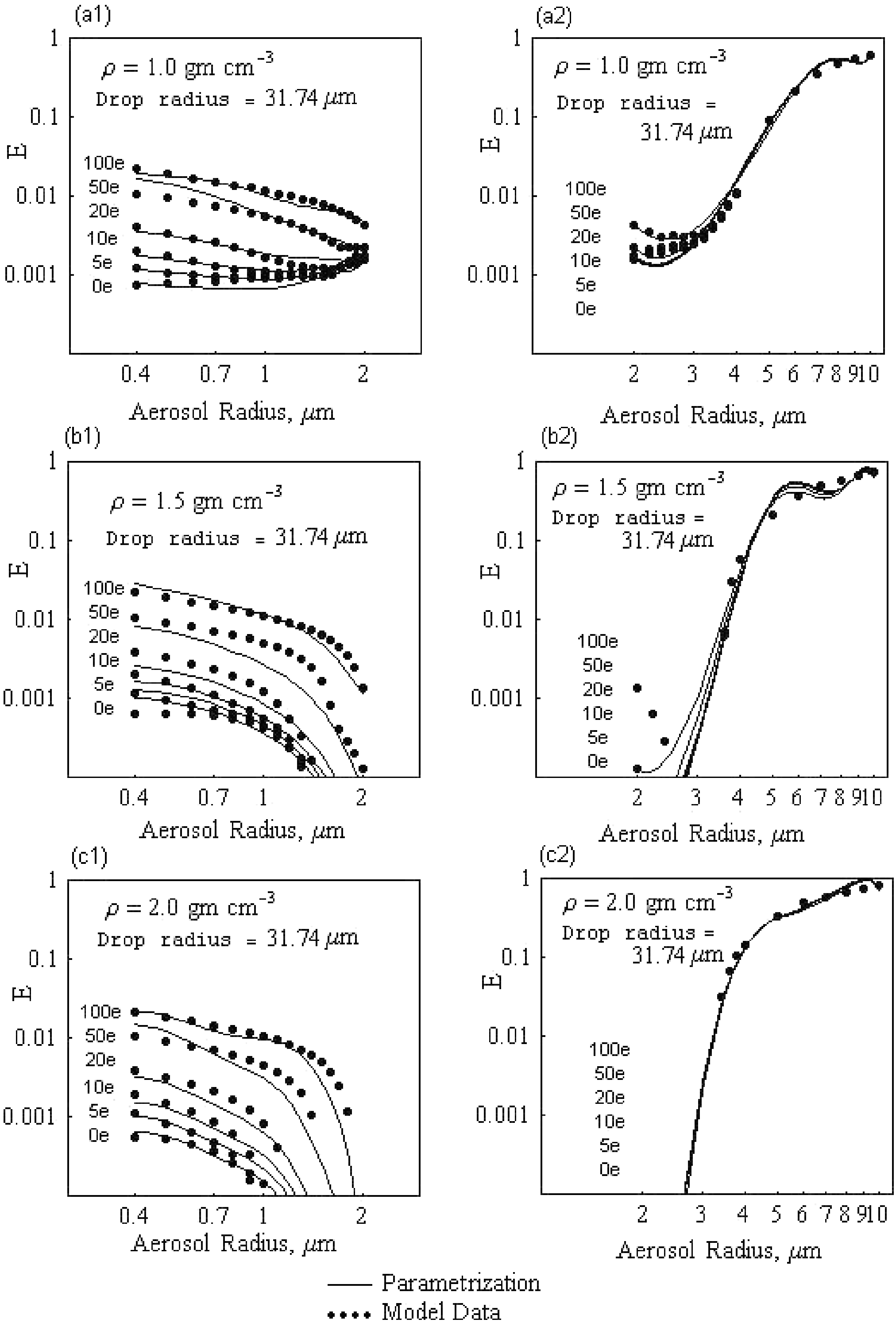

Figure 4. Same as Fig. 3 but for drop radius 31.74 μm.

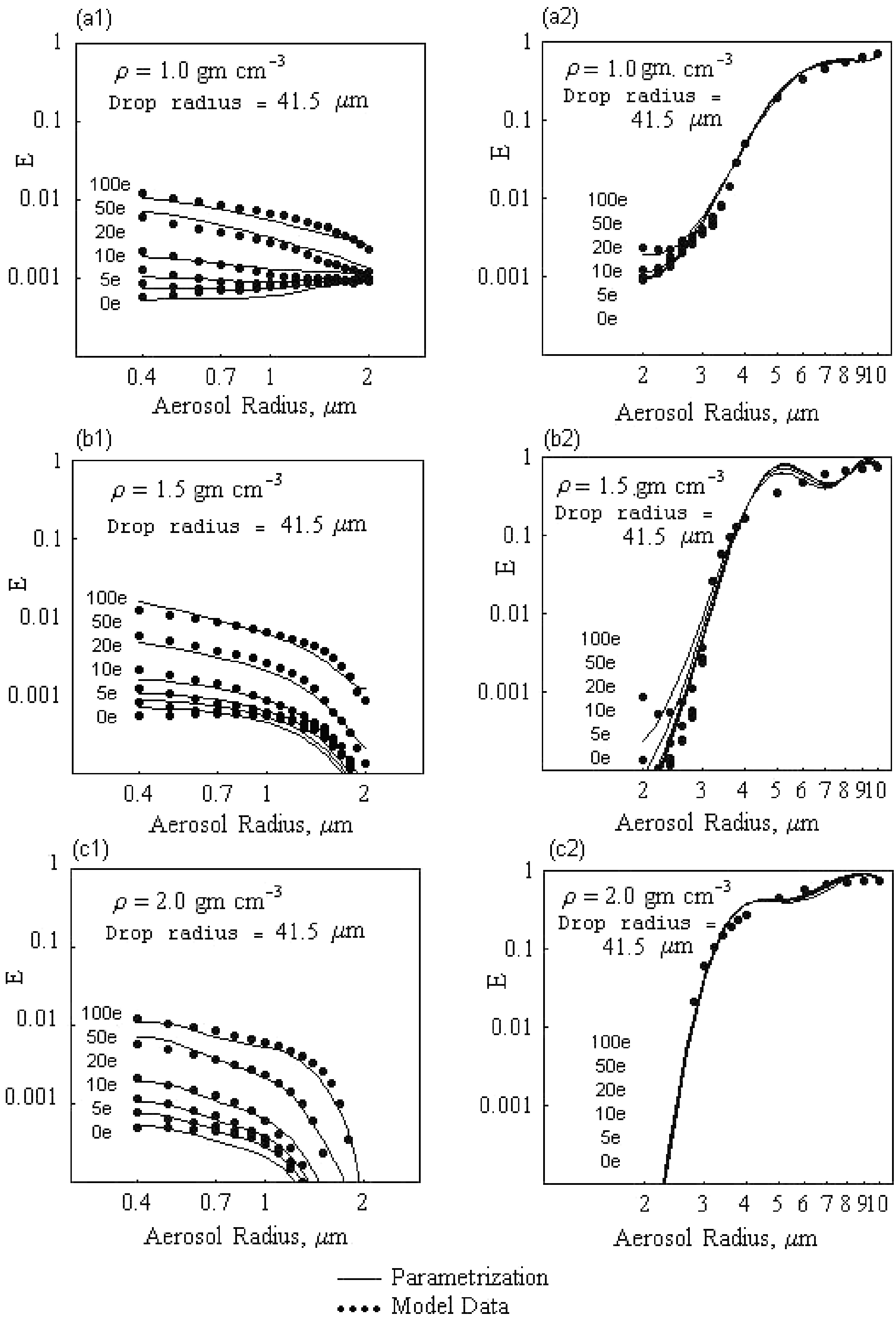

Figure 5. Same as Fig. 3 but for drop radius 41.5 μm.

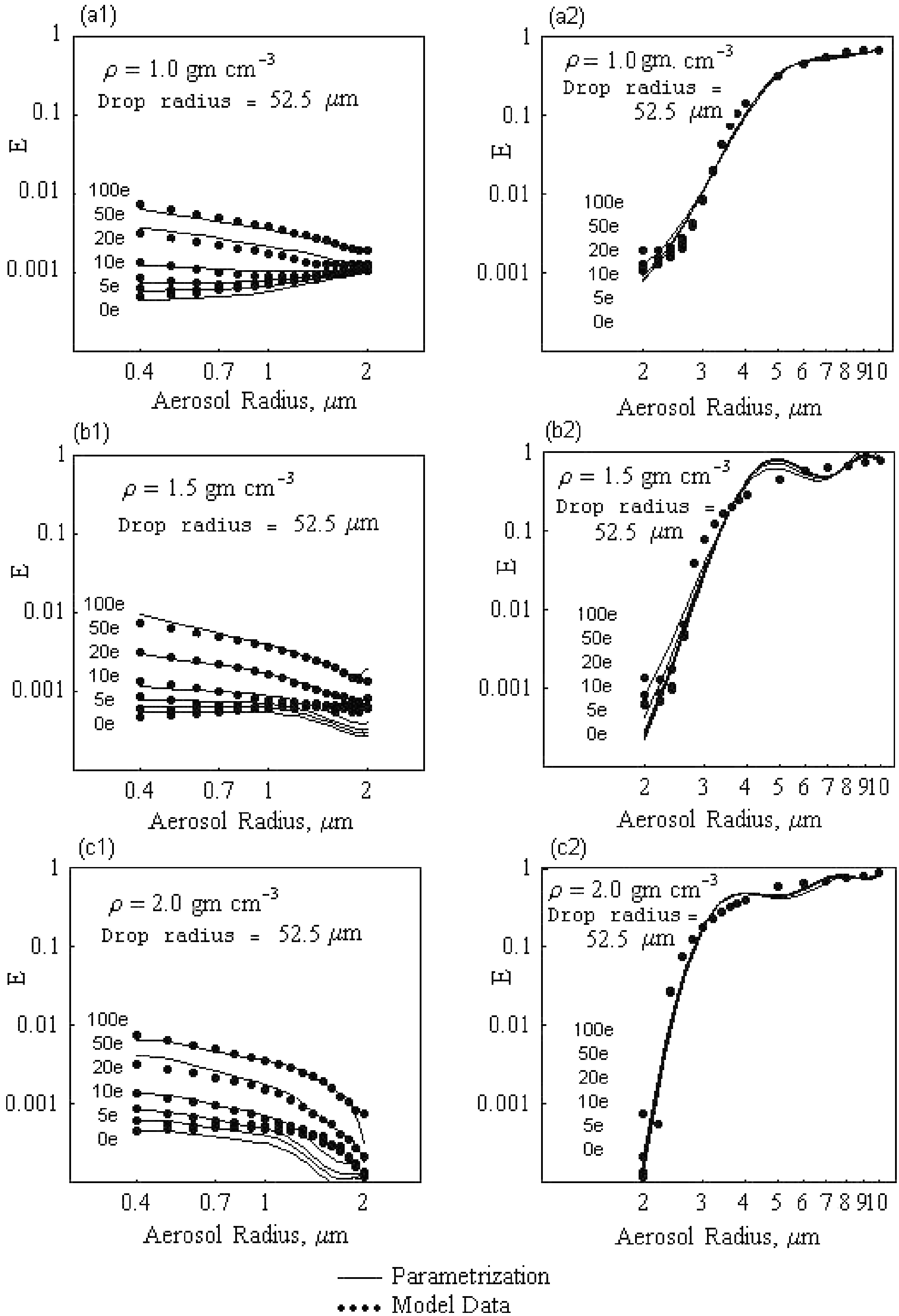

Figure 6. Same as Fig. 3 but for drop radius 52.5 μm.

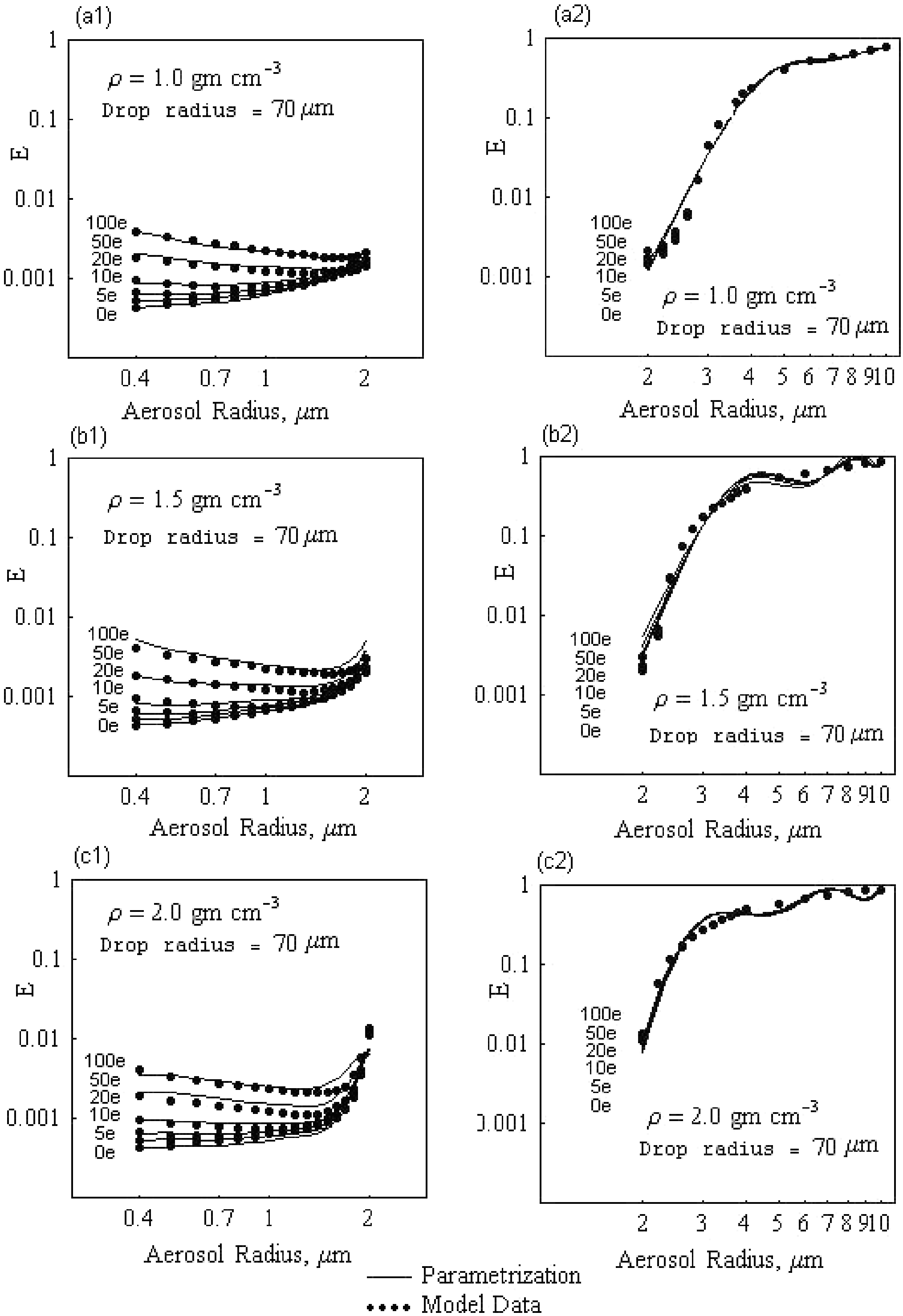

Figure 7. Same as Fig. 3 but for drop radius 70 μm.

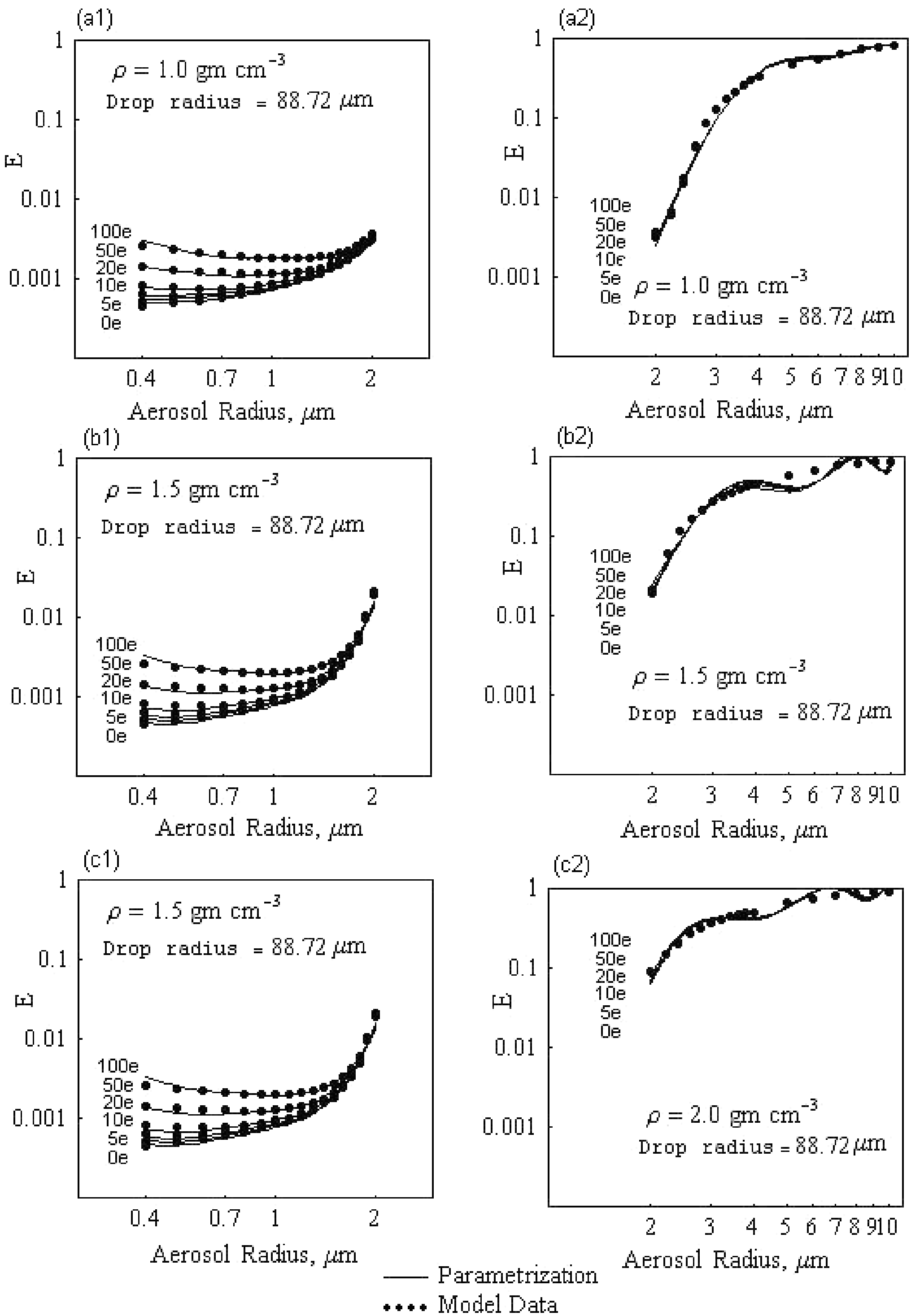

Figure 8. Same as Fig. 3 but for drop radius 88.72 μm.

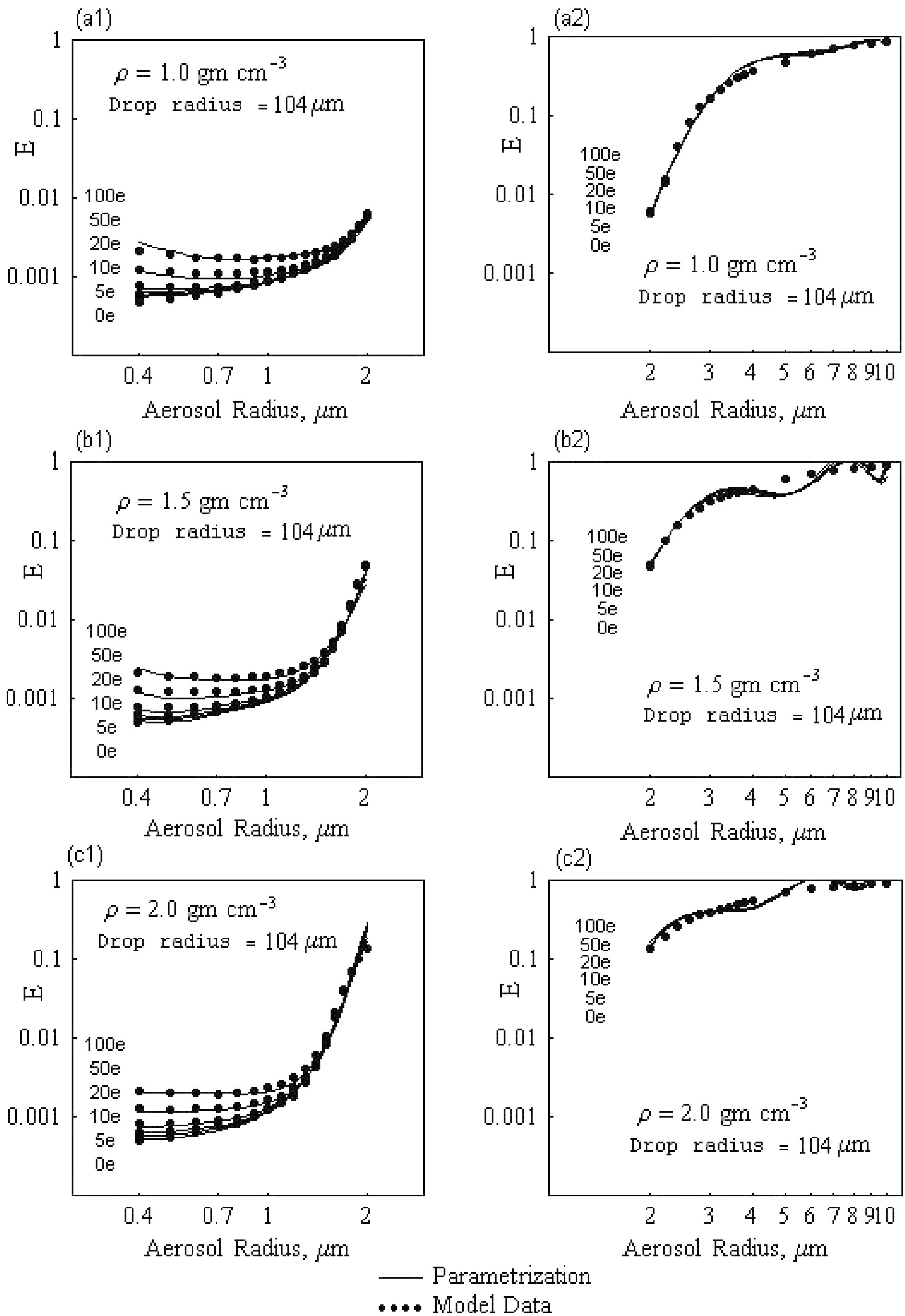

Figure 9. Same as Fig. 3 but for drop radius 104 μm.

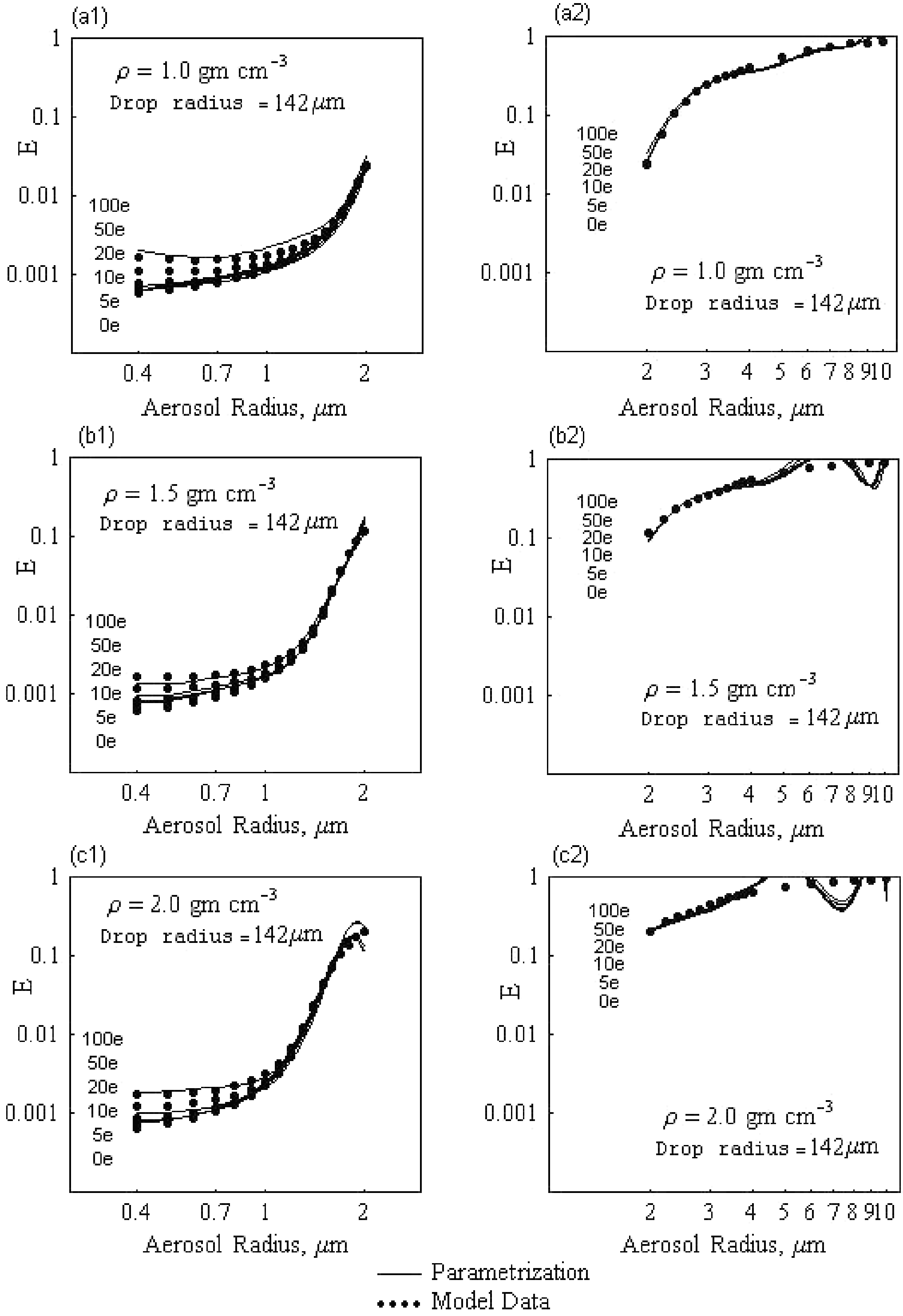

Figure 10. Same as Fig. 3 but for drop radius 142 μm.

For drop radius 70 μm, in Figs. 7(a1), (a2), (b1) and (c1) the parametrization functions follow similar patterns to those of model values, whereas in Figs. 7(b2) and (c2) the E_p values slightly deviate from E_m in the particle range $4 < a < 8$ μm.

For drop radius 88.72 μm: in Figs. 8(a1), (a2), (b1) and (c1) the parametrization function gives exactly the same values as those of the model for all particle charges. In Figs. 8(b2) and (c2) the parametrization function captures the form of the detailed model, except for a deviation between aerosol radius 4–10 μm (up to a maximum of 20%).

For drop radius 104 μm: in Fig. 9 the parametrization function gives very similar values to the model in almost all cases. The agreement between E_p and E_m is excellent except in Figs. 9(b2) and (c2) for the particle range 4–10 μm.

For drop radius 142 μm: in Fig. 10 for $a < 2$ μm the parametrization function is in good agreement with the model, but above 4 μm the values deviate $\pm$20% from the model. It should be emphasized that the parametrization always shows sensitivity to aerosol charge, no matter how small the values of charge.

5. Conclusion

The four-dimensional parametrization of collision efficiency between charged particles and neutral cloud water droplets is shown to represent the modelled values over a wide range of parameters. The parametrized values are, at worst, within a factor of four of modelled values, and 91.5% are within a factor of two. The time taken by the microphysical model to run on a 64 bit, 256 MB RAM PC is ~7.15 h, whereas the parametrization function, operating on the same computer, gives the results in 25 s. This factor of 10^3 increase in speed will permit the inclusion of charged aerosol–droplet collision efficiency calculations in a variety of cloud, pollution removal and radioactivity-dispersion models.

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