Modelling strategies for particle aggregation in volcanic plumes

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Summary

- Empirical models:
  e.g., Carey and Sigurdsson (1982); Armienti et al. (1988);
  Cornell et al. (1983); Bonadonna et al. (2002)

- Computational models:
  e.g., Textor et al. (2006), Veicht and Wood (2001), Costa et al. (2010)

- Discussion on approximations and parameterizations

- Conclusion and open problems
Simplified approaches

Assumptions made to explain the secondary maximum at MSH 1980

All particles < 63 µm fall at 0.35 m/s  (Carey and Sigurdsson, 1982)
All particles < 63 µm fall at 0.55 m/s  (Armienti et al., 1988)

Wiesner et al. (1995) explained marine sediment trap data of Pinatubo 1991 eruption assuming 15-125 µm particles were made fall at 0.66 m s\(^{-1}\)
Empirical parameterizations

Cornell et al (1983)

first attempt to systematically quantify aggregation from field observation; significance of ash aggregation during Campanian Ignimbrite eruption

50% of particles between 44-63 μm +

75% of particles between 31 and 44 μm +

100% particles smaller that 31 μm

Fall as aggregates of 200 μm and density of 200 kg m⁻³
Empirical parameterizations

<table>
<thead>
<tr>
<th>Aggregate type</th>
<th>Model 1</th>
<th>Model 2</th>
<th>Model 3</th>
<th>Model 4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Not specified</td>
<td>Accretionary lapilli</td>
<td>Accretionary lapilli</td>
<td>Accretionary lapilli</td>
</tr>
<tr>
<td>Aggregate diameter (µm)</td>
<td>250</td>
<td>180–11 500*</td>
<td>180–11 500*</td>
<td>180–11 500*</td>
</tr>
<tr>
<td>Aggregate density (kg m⁻³)</td>
<td>2000</td>
<td>1840</td>
<td>1840</td>
<td>1840</td>
</tr>
</tbody>
</table>

Wt% of particles in aggregates:

<table>
<thead>
<tr>
<th>Size (µm)</th>
<th>Model 1</th>
<th>Model 2</th>
<th>Model 3</th>
<th>Model 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>125–63 µm</td>
<td>50</td>
<td>125–63 µm</td>
<td>100</td>
<td>91</td>
</tr>
<tr>
<td>63–31 µm</td>
<td>75</td>
<td>63–8 µm</td>
<td>100</td>
<td>95</td>
</tr>
<tr>
<td>&lt;31 µm</td>
<td>100</td>
<td>8–4 µm</td>
<td>100</td>
<td>91</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4–2 µm</td>
<td>100</td>
<td>63</td>
</tr>
</tbody>
</table>

Model 1 represents a slightly modified version of an aggregation model presented by Cornell et al. (1983). Models 2, 3 and 4 are based on observations made on Montserrat.

* Accretionary lapilli diameters are calculated using Gilbert & Lane (1994) theory, and computed for volcanic thermals with heights ranging from 2 to 15 km and temperatures ranging from 600 to 1100 K.

Bonadonna et al (2002) tested different models aimed to describe accretionary lapilli at SHV (including a model similar to Cornell et al., 1983).

Best models:

M3 for deposits originated by dome collapse;

\[ D = \frac{wEx}{2(\rho_P - \phi(\rho_P - \rho_\phi))} \]

(Gilbert and Lane, 1994)

M4 for vulcanian explosions.
Textor et al. (2006) describe the microphysics and parameterization of ash and hydrometeors. For aggregation they considered two processes only (both based on gravitational capture).

1- Accretion

\[
\frac{\partial N_s}{\partial t} \bigg|_{\text{acc}} = - \frac{\rho_e}{q_e} \pi E \int_0^\infty \int_0^\infty \pi (r_s + r_l)^2 \left| w_s(r_s) + w_l(r_l) \right| N_s(r_s) dr_s N_l(r_l) dr_l
\]

(19)

2- Autoconversion

\[
\frac{\partial N_s}{\partial t} \bigg|_{\text{aut}} = - \frac{\rho_e}{q_e} c_{\text{aut}} N_s
\]

\[c_{\text{aut}} = 3 \sqrt{\frac{\rho_{e0}}{\rho_e}} q_s E\]

**E** Collection efficiency

**q** Mass mixing ratio [kg kg\(^{-1}\)] in relation to total mass in the grid box

**w** Terminal fall velocity [m s\(^{-1}\)]

**N** Number concentration [number kg\(^{-1}\)] in relation to total mass in the grid box

**r** Particle radius [m]
**Smoluchowski (1917) equation**
(e.g. Veicht and Woods 2001; Costa et al. 2010)

\[
\frac{\partial n_v}{\partial t} = \frac{1}{2} \int_0^v \alpha(s, v-s)\beta(s, v-s)n_v(s)n_v(v-s)\,ds
\]
\[ \quad - \int_0^\infty \alpha(v, s)\beta(v, s)n_v(s)n_v(v)\,ds \]

\(\alpha = \text{sticking efficiency}\)

\(\beta = \text{collision frequency}\)

\(v = \text{particles volume}\)

\(n_v = \text{number of particles of volume } v\)

The first term on the right-hand side of the equation represents the rate of formation of aggregates with volume between \(v\) and \(v + dv\), whereas the second term denotes the rate of loss of aggregates of volume between \(v\) and \(v + dv\) to form larger aggregates.
Collision frequencies (well studied in aerosol science)

\[ \beta = \beta_B + \beta_S + \beta_T + \beta_G \]

\textbf{Brownian kernel:}

\[ \beta_B = \frac{2}{3} \frac{k_b T}{\mu} \frac{(d_i + d_j)^2}{d_i d_j} C_c \]

\textbf{Wind shear kernel:}

\[ \beta_S = \frac{1}{6} \Gamma_S (d_i + d_j)^3 \]

\textbf{Turbulent inertial kernel:}

\[ \beta_T \approx \frac{\pi}{4} \frac{\pi \epsilon^{3/4}}{\nu^{1/4}} \frac{\rho_p C_c}{18 \mu} (d_i + d_j)^2 \left| d_i^2 - d_j^2 \right| \]

\textbf{Gravitational kernel:}

\[ \beta_G = \frac{\pi}{4} \frac{(\rho_p - \rho_a) g}{18 \mu} \left| d_i^2 - d_j^2 \right| (d_i + d_j)^2 \]

\[ C_c = 1 + Kn \left( A_1 + A_2 \exp \left( \frac{-2A_3}{Kn} \right) \right) \]

\[ \Gamma_S = \frac{dU}{dz} \text{ in case of a laminar flow,} \]

\[ \Gamma_S = 0.1625 (\epsilon/\nu)^{1/2} \text{ in case of a turbulent flow} \]

\[ \epsilon \approx K_v \left[ \left( \frac{\partial U}{\partial z} \right)^2 - \frac{g}{T_p} \frac{\partial T_p}{\partial z} \right] \]
Sticking efficiency (not well constrained for volcanic ash)

After considerations from Veitch & Woods (2001) and fitting data from Gilbert and Lane (1994) for wet ash in presence of liquid water Costa et al. (2010) proposed:

\[
\alpha_{ij} = \frac{1}{1 + (St_{ij}/St_{cr})^q}
\]

whereas a constant value in presence of ice:

\[
\alpha_{ij} = 0.09
\]

where the Stokes number (e.g. Liu and Litster, 2002) is given by:

\[
St_{ij} = \frac{8 \rho_p \left| V_j - V_i \right|}{9 \mu_l} \frac{d_i d_j}{d_i + d_j}
\]

and the relative velocity can be expressed as:

\[
\left| V_i - V_j \right| \approx \left| V_{si} - V_{sj} \right| + \frac{\Gamma S}{6\pi} (d_i + d_j) + \frac{2}{3} \frac{k_b T}{\mu} \frac{1}{\pi d_i d_j}
\]

(or the max of the 3 terms)
Numerical solutions of the Smoluchowski equation

Costa et al. (2010)
Aggregate settling velocity

\[ V_{SA} = \frac{(\rho_p - \rho) g}{18 \mu} d_A^2 \psi_e \]

\[ \psi_e = (1 - \varphi)f \]

\[ \varphi = 1 - k_f \left( \frac{d_A}{d_p} \right)^{D_f-3} \]

Costa et al. (2010)
Simplified approach (e.g. Costa et al., 2010)

1- Consider decrease of the total number of particles

\[ \frac{dn_{\text{tot}}}{dt} = -\frac{1}{2} \int_0^\infty \int_0^\infty K(v_i, v_j)n(v_i, t)n(v_j, t)dv_i dv_j \]

2- Assume a fractal growth of aggregate:

\( v = \xi d^{1/D_f} \)

\( \xi = (6/\pi)^{1/3} \approx 1.24 \)

\[ N_j = k_f \left( \frac{d_A}{d_j} \right)^{D_f} \]

3- Assume a similarity solutions:

\[ n = \frac{\psi(z)n_{\text{tot}}^2}{\phi} \]

\[ \Delta n_{\text{tot}} = \alpha_m \left( A_B n_{\text{tot}}^2 + A_S \phi^{3/D_f} n_{\text{tot}}^{2-3/D_f} + A_{DS} \phi^{4/D_f} n_{\text{tot}}^{2-4/D_f} \right) \Delta t \]

4- Aggregates have the same effective diameter:

\[ \Delta n_i \approx \frac{\Delta n_{\text{tot}} N_i}{\sum_i N_i} \]

The model can be used to estimate aggregation within the eruption column (operational) or for long range ash transport (computationally expensive because coupling among particles).
Examples: MSH 1980 eruption

WITH AGGREGATION (Folch et al. 2010)

NO AGGREGATION
Aggregation in presence of charged particles
(Costa and Macedonio, in prep)

Smoluchowski equation in presence of charged particles:

\[ \frac{\partial n(m, q, t)}{\partial t} = \frac{1}{2} \int_{0}^{m} \int_{-\infty}^{\infty} K(m', q', m - m', q - q') n(m', q', t) n(m - m', q - q', t) dq' dm' \]

\[- n(m, q, t) \int_{0}^{\infty} \int_{-\infty}^{\infty} K(m', q', m, q) n(m', q', t) dq' dm' \]

\[ (26) \]

Simplifying assumption:

\[ K(m', q', m, q) = K_0(m', m) \gamma_{q', q} \]

For practical applications, the mean collision efficiency can be obtained by averaging over the charge distributions of the two particles

\[ \langle \gamma_{q'q} \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \gamma_{q'q} f'(q') f(q) dq' dq \quad (34) \]

where \( f(q) \) and \( f'(q') \) are the charge distributions of the particles.
Conclusion and open problems

Open problems concern quantification of:
- ash sticking efficiency under different conditions (from wet to dry conditions);
- aggregate settling velocity under different conditions (from wet to dry conditions)
- electrostatic charge effects on the coagulation kernel (mainly for dry conditions)

In order to develop quantitative models of ash aggregation we need to carry out further:

• Theoretical studies
• Field study and sampling
• Image analysis
• Lab experiments
• Remote sensing

European project

VERTIGO (FP7-PEOPLE-2013-ITN)
VOLCANIC ASH:
FIELD, EXPERIMENTAL AND NUMERICAL INVESTIGATIONS OF PROCESSES DURING ITS LIFECYCLE
See Poster above (U. Kueppers)

Loosely bonded aggregate
(from Sorem, 1983)

Accretionary pellets
(from Brown et al., 2012)
Thanks