A probabilistic view of the distribution of bubble volumes involving coalescence

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These notes were inspired by conversations with Prof. Kristen Fauria and her PhD student Sarah Ward. The problem pertains to bubbles in magmas.

Let $f_{V_\mathrm{b}}(V_\mathrm{b}, t)$ [L^{-3}] denote the probability density function of bubble volumes V_b, which may vary with time t. In turn let N denote a Gibbs great number such that we may define the number density function as $n_{V_\mathrm{b}}(V_\mathrm{b}, t) = N f_{V_\mathrm{b}}(V_\mathrm{b}, t)$ [L^{-3}]. Note that "number density" is in reference to the volume domain; it should not be confused with the number of bubbles per unit rock volume, despite having the same dimensions. That is, $n_{V_\mathrm{b}}(V_\mathrm{b}, t)\mathrm{d}V_\mathrm{b}$ is the number of bubbles within the small volume interval V_b to $V_\mathrm{b} + \mathrm{d}V_\mathrm{b}$. By definition,

$$\int_0^\infty n_{V_\mathrm{b}}(V_\mathrm{b}, t)\,\mathrm{d}V_\mathrm{b} = N\,. \tag{1}$$

With bubble nucleation and growth (and neglecting resorption) the number density $n_{V_\mathrm{b}}(V_\mathrm{b}, t)$ satisfies a Fokker–Planck equation with respect to the volume domain. Namely,

$$\frac{\partial n_{V_\mathrm{b}}(V_\mathrm{b}, t)}{\partial t} = -U\frac{\partial n_{V_\mathrm{b}}(V_\mathrm{b}, t)}{\partial V_\mathrm{b}} + \kappa\frac{\partial^2 n_{V_\mathrm{b}}(V_\mathrm{b}, t)}{\partial V_\mathrm{b}^2} - S\,, \tag{2}$$

where U [L^3 T^{-1}] denotes a drift speed, a change in volume per unit time, κ [L^6 T^{-1}] denotes a diffusivity, and S [L^{-3} T^{-1}] denotes a sink. From a statistical physics perspective, the drift speed U is an ensemble averaged speed, and the diffusive term in (2) takes into account that bubbles at volume state V_b at any instant grow at different rates due to stochastic effects, as described below.

The drift speed U may be expressed as $U = \mathrm{d}V_\mathrm{p}/\mathrm{d}t$ and it has at least two parts. We thus write $U = U_\mathrm{d} + U_\mathrm{c}$. Here, U_d denotes a contribution to the drift speed due to growth by diffusion of gas to the bubbles, and U_c denotes a contribution due to coalescence of bubbles. For now we set U_d aside assuming this growth rate can be specified based on previous work, and we are neglecting volume expansion due to decompression. Here we focus on U_c and the sink S.

We need to distinguish two sets of bubble volumes. First, we let V_b denote the volume of a "target" bubble to which smaller bubbles are added as coalescence. We then let V_b' denote the volume of a bubble that is added to the target bubble such that $V_\mathrm{b}' \leq V_\mathrm{b}$. Now let λ [T^{-1}] denote a Poisson-like rate constant. Because $n_{V_\mathrm{b}}(V_\mathrm{b}', t)\mathrm{d}V_\mathrm{b}'$ is the number of bubbles within the small volume interval V_b' to $V_\mathrm{b}' + \mathrm{d}V_\mathrm{b}'$, the product $\lambda n_{V_\mathrm{b}}(V_\mathrm{b}', t)\mathrm{d}V_\mathrm{b}'$ describes a Markov birth process. That is, this product gives the rate, the number per unit time, at which bubbles with volume V_b' *could* be added to larger bubbles by coalescence. The actual rate is $\lambda n_{V_\mathrm{b}}(V_\mathrm{b}', t)\mathrm{d}V_\mathrm{b}' n_{V_\mathrm{b}}(V_\mathrm{b}, t)\mathrm{d}V_\mathrm{b}$. That is, for coalescence with target bubbles of volume V_b to occur, there must be bubbles of this volume present. We thus may clarify that the rate λ is a number per small bubble per available target bubble per time. This is entirely analogous to the interactive terms in the Lotka–Volterra (predator-prey) formulation.

Now, the product $V_{\rm b}' n_{V_{\rm b}}(V_{\rm b}', t)\mathrm{d}V_{\rm b}' n_{V_{\rm b}}(V_{\rm b}, t)\mathrm{d}V_{\rm b}$ is the total volume of small bubbles that is added to target bubbles of volume $V_{\rm b}$, and the product $\lambda V_{\rm b}' n_{V_{\rm b}}(V_{\rm b}', t)\mathrm{d}V_{\rm b}' n_{V_{\rm b}}(V_{\rm b}, t)\mathrm{d}V_{\rm b}$ is the rate at which this volume is added. But because this volume is added to $n_{V_{\rm b}}(V_{\rm b}, t)\mathrm{d}V_{\rm b}$ bubbles, the average rate at which the volume of bubbles with volume $V_{\rm b}$ increases is $\lambda V_{\rm b}' n_{V_{\rm b}}(V_{\rm b}', t)\mathrm{d}V_{\rm b}' n_{V_{\rm b}}(V_{\rm b}, t)\mathrm{d}V_{\rm b}/n_{V_{\rm b}}(V_{\rm b}, t)\mathrm{d}V_{\rm b}$. That is, the average rate is simply $\lambda V_{\rm b}' n_{V_{\rm b}}(V_{\rm b}', t)\mathrm{d}V_{\rm b}'$. We thus assume that

$$U_{\rm c} = \int_0^{V_{\rm b}} \lambda V_{\rm b}' n_{V_{\rm b}}(V_{\rm b}', t)\, \mathrm{d}V_{\rm b}' \, . \tag{3}$$

This integral says that the average rate at which bubbles of volume $V_{\rm b}$ grow is given by the rate at which they consume the volume of some proportion of all bubbles smaller than $V_{\rm b}$, that is, via coalescence. Moreover, note that because bubbles of volume $V_{\rm b}$ do not consume the same number of small bubbles per unit time, the variance in growth rates contributes to the diffusivity κ in the diffusive term in (2).

This result suggests the form of the sink S. First, we reverse the meaning of the prime, such that now $V_{\rm b} \leq V_{\rm b}'$. We then observe that when bubbles within any interval $V_{\rm b}$ to $V_{\rm b} + \mathrm{d}V_{\rm b}$ are consumed by larger bubbles, the local density $n_{V_{\rm b}}(V_{\rm b})$ must decrease. Using elements of the development above we assume that within any interval $\mathrm{d}V_{\rm b}$ the rate at which the number of bubbles decreases is

$$\left.\frac{\mathrm{d}n_{V_{\rm b}}(V_{\rm b})}{\mathrm{d}t}\right|_S \mathrm{d}V_{\rm b} = -\int_{V_{\rm b}}^{\infty} \lambda n_{V_{\rm b}}(V_{\rm b}, t)\, \mathrm{d}V_{\rm b} n_{V_{\rm b}}(V_{\rm b}', t)\, \mathrm{d}V_{\rm b}' \, . \tag{4}$$

Because quantities involving $V_{\rm b}$ may be removed from the integral, this leads to

$$S = n_{V_{\rm b}}(V_{\rm b}, t) \int_{V_{\rm b}}^{\infty} \lambda n_{V_{\rm b}}(V_{\rm b}', t)\, \mathrm{d}V_{\rm b}' \, , \tag{5}$$

which represent the loss of bubbles of volume $V_{\rm b}$ to all larger sizes. Note that the rate constant λ might depend on the bubble volume.

Collecting the damage, we now have

$$\frac{\partial n_{V_{\rm b}}(V_{\rm b}, t)}{\partial t} = -\left[U_{\rm d} + \int_0^{V_{\rm b}} \lambda V_{\rm b}' n_{V_{\rm b}}(V_{\rm b}', t)\, \mathrm{d}V_{\rm b}'\right] \frac{\partial n_{V_{\rm b}}(V_{\rm b}, t)}{\partial V_{\rm b}} + \kappa \frac{\partial^2 n_{V_{\rm b}}(V_{\rm b}, t)}{\partial V_{\rm b}^2} - n_{V_{\rm b}}(V_{\rm b}, t) \int_{V_{\rm b}}^{\infty} \lambda n_{V_{\rm b}}(V_{\rm b}', t)\, \mathrm{d}V_{\rm b}' \, . \tag{6}$$

This is a rather interesting expression. As a Fokker–Planck equation with a sink term, it describes the time evolution of the density $n_{V_{\rm b}}(V_{\rm b}, t)$, where the coefficients are nonlocal functions of the bubble volume $V_{\rm b}$.

To explore the behavior of (6) we focus on the possibility of steady-state conditions with $\partial n_{V_{\rm b}}(V_{\rm b}, t)/\partial t = 0$. We assume that the rate λ is fixed across bubble volumes and that the process of coalescence proceeds much faster than growth by gas diffusion. Dividing by N^2 we then have

$$0 = -\lambda \int_0^{V_{\rm b}} V_{\rm b}' f_{V_{\rm b}}(V_{\rm b}')\, \mathrm{d}V_{\rm b}' \frac{\mathrm{d}f_{V_{\rm b}}(V_{\rm b})}{\mathrm{d}V_{\rm b}} + \kappa_N(V_{\rm b}) \frac{\mathrm{d}^2 f_{V_{\rm b}}(V_{\rm b})}{\mathrm{d}V_{\rm b}^2} - f_{V_{\rm b}}(V_{\rm b}) \lambda \int_{V_{\rm b}}^{\infty} f_{V_{\rm b}}(V_{\rm b}')\, \mathrm{d}V_{\rm b}' \, , \tag{7}$$

where $\kappa_N(V_\mathrm{b}) = \kappa/N$ almost certainly varies with volume V_b. To simplify notation we observe that the first integral gives the "partial" mean volume of the density $f_{V_\mathrm{b}}(V_\mathrm{b})$, which we denote as $M(V_\mathrm{b})$, and the second integral is the exceedance probability of the density $f_{V_\mathrm{b}}(V_\mathrm{b})$, which we denote as $R_{V_\mathrm{b}}(V_\mathrm{b})$. Then,

$$\lambda M(V_\mathrm{b}) \frac{\mathrm{d} f_{V_\mathrm{b}}(V_\mathrm{b})}{\mathrm{d}V_\mathrm{b}} - \kappa_N(V_\mathrm{b}) \frac{\mathrm{d}^2 f_{V_\mathrm{b}}(V_\mathrm{b})}{\mathrm{d}V_\mathrm{b}^2} = -\lambda R_{V_\mathrm{b}}(V_\mathrm{b}) f_{V_\mathrm{b}}(V_\mathrm{b}) \,. \tag{8}$$

Note that, in general, the magnitudes of $M(V_\mathrm{b})$ and $\kappa_N(V_\mathrm{b})$ increase with V_b, and the magnitude of $R_{V_\mathrm{b}}(V_\mathrm{b})$ decreases with V_b.

We now assume for argument that the density $f_{V_\mathrm{b}}(V_\mathrm{b})$ is exponential-like and write $f_{V_\mathrm{b}}(V_\mathrm{b}) \sim e^{-V_\mathrm{b}/\mu_{V_\mathrm{b}}}$, where μ_{V_b} denotes the mean bubble volume. We then have

$$-A\lambda M(V_\mathrm{b}) - B\kappa_N(V_\mathrm{b}) = -C\lambda R_{V_\mathrm{b}}(V_\mathrm{b}) \,, \tag{9}$$

where A, B and C are coefficients associated with the probability density $f_{V_\mathrm{b}}(V_\mathrm{b})$ and its derivatives. The first term on the left side converges to $A\lambda\mu_{V_\mathrm{b}}$ with increasing V_b. The magnitude of the term on the right side asymptotically approaches zero with increasing V_b. Because the magnitude of the second term on the left side increase with V_b, an exponential distribution is not admissible. Neglecting the diffusive term does not change this outcome.

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Consider the special case of coalescence, focusing just on the expected (average) behavior under steady-state conditions, neglecting effects of diffusion. Here we assume that the Poisson-like rate λ is volume specific. Namely, we assume to first order that $\lambda = \lambda_0(1 - V_\mathrm{b}'/V_\mathrm{b})$ when $V_\mathrm{b}' \leq V_\mathrm{b}$ and $\lambda = \lambda_0(1 - V_\mathrm{b}/V_\mathrm{b}')$ when $V_\mathrm{b} \leq V_\mathrm{b}'$, where λ_0 is the basic rate. We then have

$$\begin{aligned} &\lambda_0 \int_0^{V_\mathrm{b}} \left(1 - \frac{V_\mathrm{b}'}{V_\mathrm{b}}\right) V_\mathrm{b}' f_{V_\mathrm{b}}(V_\mathrm{b}') \, \mathrm{d}V_\mathrm{b}' \frac{\mathrm{d} f_{V_\mathrm{b}}(V_\mathrm{b})}{\mathrm{d}V_\mathrm{b}} \\ &= -f_{V_\mathrm{b}}(V_\mathrm{b}) \lambda_0 \int_{V_\mathrm{b}}^{\infty} \left(1 - \frac{V_\mathrm{b}}{V_\mathrm{b}'}\right) f_{V_\mathrm{b}}(V_\mathrm{b}') \, \mathrm{d}V_\mathrm{b}' \,. \end{aligned} \tag{10}$$

Canceling λ_0 and expanding the parenthetical terms,

$$\begin{aligned} &\left[\int_0^{V_\mathrm{b}} V_\mathrm{b}' f_{V_\mathrm{b}}(V_\mathrm{b}') \, \mathrm{d}V_\mathrm{b}' - \frac{1}{V_\mathrm{b}} \int_0^{V_\mathrm{b}} V_\mathrm{b}'^2 f_{V_\mathrm{b}}(V_\mathrm{b}') \, \mathrm{d}V_\mathrm{b}'\right] \frac{\mathrm{d} f_{V_\mathrm{b}}(V_\mathrm{b})}{\mathrm{d}V_\mathrm{b}} \\ &= -\left[\int_{V_\mathrm{b}}^{\infty} f_{V_\mathrm{b}}(V_\mathrm{b}') \, \mathrm{d}V_\mathrm{b}' - V_\mathrm{b} \int_{V_\mathrm{b}}^{\infty} \frac{1}{V_\mathrm{b}'} f_{V_\mathrm{b}}(V_\mathrm{b}') \, \mathrm{d}V_\mathrm{b}'\right] f_{V_\mathrm{b}}(V_\mathrm{b}) \,. \end{aligned} \tag{11}$$

As before the first integral gives the partial mean volume and the third integral gives the exceedance probability function. The second integral gives the partial raw variance and the fourth integral gives a partial (exceedance) mean of the reciprocal $1/V_\mathrm{b}$. The magnitudes of the first two integrals increase with V_b and the magnitudes of the third and fourth integrals decrease.

Consider an exponential distribution $f_{V_\mathrm{b}}(V_\mathrm{b}) = ae^{-aV_\mathrm{b}}$ with $a = 1/\mu_{V_\mathrm{b}}$. To be sure, this distribution does *not* satisfy (11). Nonetheless, we can learn key information by allowing the integral coefficients in (11) to vary over V_b according to what is expected for an exponential distribution, as the decay of this distribution defines a separation between light-tail and heavy-tail behavior. We then have

$$\left(\frac{1}{a} - \frac{1}{a}(aV_\mathrm{b}+1)e^{-aV_\mathrm{b}} + \frac{2}{a^2} + \frac{1}{a^2}[-aV_\mathrm{b}(aV_\mathrm{b}+2)-2]e^{-aV_\mathrm{b}}\right)\frac{\mathrm{d}f_{V_\mathrm{b}}(V_\mathrm{b})}{\mathrm{d}V_\mathrm{b}}$$
$$= -\left[e^{-aV_\mathrm{b}} - aV_\mathrm{b}\mathrm{Ei}(-aV_\mathrm{b})\right] f_{V_\mathrm{b}}(V_\mathrm{b})\,, \tag{12}$$

where Ei( ) denotes the exponential integral function. To simplify notation we denote the first parenthetical expression in (12) as $A(V_\mathrm{b})$ and the second parenthetical expression as $B(V_\mathrm{b})$ then rewrite it as

$$\frac{\mathrm{d}f_{V_\mathrm{b}}(V_\mathrm{b})}{\mathrm{d}V_\mathrm{b}} = -\frac{B(V_\mathrm{b})}{A(V_\mathrm{b})} f_{V_\mathrm{b}}(V_\mathrm{b})\,. \tag{13}$$

The coefficient $A(V_\mathrm{b})$ is zero at $V_\mathrm{b} = 0$ then monotonically increases with V_b. The coefficient $B(V_\mathrm{b})$ is unity at $V_\mathrm{b} = 0$ then steadily decreases with V_b. At face value the slope $\mathrm{d}f_{V_\mathrm{b}}(V_\mathrm{b})/\mathrm{d}V_\mathrm{b}$ is unbounded at $V_\mathrm{b} = 0$, which is akin to, say, a Weibull or gamma distribution. The essential reason for this is that the formulation maximizes the transfer of small bubbles to larger bubbles, so there is a rapid loss of small bubbles near $V_\mathrm{b} = 0$. This points to the need to clarify what tiny bubbles do when they are near larger bubbles, and the appropriateness of the approximation that vanishingly small bubbles coalesce with larger bubbles at the maximum rate. If instead we numerically "force" $f_\mathrm{b}(V_\mathrm{b})$ to have a finite value at V_b, then this (non-normalized) distribution decays approximately exponentially over small V_b with $B(V_\mathrm{b})/A(V_\mathrm{b}) \sim$ const. However, because this ratio approaches zero with increasing V_b, the derivative $\mathrm{d}f_{V_\mathrm{b}}(V_\mathrm{b})/\mathrm{d}V_\mathrm{b}$ approaches zero and thus the (non-normalized) distribution $f_\mathrm{b}(V_\mathrm{b})$ flattens, giving it an "extra" heavy tail. The essential reason for this is that with increasing volume V_b and decreasing bubble density $f_\mathrm{b}(V_\mathrm{b})$, there are increasingly fewer larger bubbles available to consume smaller bubbles. That is, the available sink S is decreasing, as reflected by the decreasing value of $A(V_\mathrm{b})$. But simultaneously, smaller bubbles are increasingly adding to the volume (but not numbers) of larger bubbles, as reflected by the increasing value of $B(V_\mathrm{b})$. The effect is to produce ever increasing bubble sizes with no mechanism to remove them.

Now, despite setting up this argument assuming a steady-state condition, it is not likely a steady problem, at least not using the formulation above. Moreover, to the extent that the nonlocal formulation of coalescence and the sink are physically defensible, then aside from the details suggested by an exponential description of the integral coefficients, this nonlocal behavior suggests that a heavy-tail distribution is likely.