Cascade-based Eulerian-to-Lagrangian subgrid-scale modeling of bubble breakup in breaking waves

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1. Motivation and objectives

Breaking waves in oceans produce bubbles of a broad range of sizes (Blanchard & Woodcock 1957; Medwin 1970; Melville 1996; Mortazavi et al. 2016). Knowledge of the production mechanisms behind this broad range of sizes informs the prediction of various maritime and oceanic transport phenomena. However, the broad range of sizes also makes these bubbles immensely costly to directly simulate. In particular, the smallest bubbles are known to be at least four orders of magnitude smaller than the characteristic length scale defining a wave, i.e., its wavelength, such as in the laboratory measurements of Deane & Stokes (2002), who observed $O(100-\mu m)$ bubbles in their breaking wavepacket of center wavelength $O(2 \text{ m})$. A direct simulation resolving all relevant bubble fragmentation and coalescence mechanisms would then require at least $10^{12}$ grid points to simulate a single wave with a computational domain spanning a wavelength in each direction. Physics-based reduced-order models are thus necessary to decrease the computational cost of numerical simulations of breaking waves while maintaining their predictivity. In the present work, a cascade-based subgrid-scale (SGS) model is presented to account for the formation of subgrid bubbles by a turbulent breakup cascade.

Many of the bubbles in breaking waves are produced by turbulent fragmentation in the early wave-breaking stages (Kolmogorov 1949; Hinze 1955; Loewen et al. 1996; Garrett et al. 2000; Deane & Stokes 2002; Rojas & Loewen 2007; Blenkinsopp & Chaplin 2010; Wang et al. 2016; Deike et al. 2016; Mortazavi 2016; Na et al. 2016; Chan et al. 2018, 2021b). In particular, turbulence breaks large bubbles up in a fragmentation cascade, generating small- and intermediate-sized bubbles that are traditionally associated with a $R^{-10/3}$ power-law size distribution, where $R$ denotes the bubble radius. The fragmentation cascade ceases at the Hinze scale, i.e., the scale at which the restoring action of surface tension overcomes breakup by turbulence (Kolmogorov 1949; Hinze 1955). It is emphasized here that the Hinze scale is only an order-of-magnitude length-scale estimate. Recent work (Chan et al. 2021a,b) has provided direct evidence of the breakup cascade by appealing to the size locality of the bubble-mass transfer process from large to small sizes, which may persist even when the $R^{-10/3}$ size-distribution scaling is absent. In particular, the corresponding flux of bubble mass from large to small sizes is quasi-steady and quasi-size-invariant in an intermediate range of sizes, and the corresponding differential breakup rate, or breakup rate per unit size, scales as $R^{-4}$. In addition, contributions to the flux decay as power laws at large and small bubble sizes throughout the active wave-breaking phase. More generally, Chan et al. (2021a,b) draw connections between the models used in earlier simulations to be described in the subsequent paragraphs and the classical ideas of Richardson (1922), Kolmogorov (1941), and Onsager (1945) establishing the energy cascade that underpins single-phase turbulence theories, in order to
relate the breakup dynamics of individual bubbles to the bubble breakup mass flux characterizing the entire bubbly flow. The size locality of this flux, or cascade rate, implies the universality of small-bubble breakup and simplifies the development of SGS models for successive bubble fragmentation in turbulent bubbly flows.

Population balance equations (Smoluchowski 1916, 1918; Landau & Rumer 1938; Melzak 1953; Williams 1958; Friedlander 1960a,b; Filippov 1961; Valentas et al. 1966; Valentas & Amundson 1966) may be used with appropriate model kernels to provide a reduced-order description of a polydisperse bubble population. This approach was incorporated into the two-phase bubbly-flow context by Carrica et al. (1999), who coupled the bubble population balance equation with the Reynolds-averaged Navier-Stokes equations for the two phases to enable a bubbly-flow simulation that accounts for polydispersity. The model for bubble entrainment was refined by Moraga et al. (2008), Shi et al. (2010), and Ma et al. (2011) to incorporate the experimental size distributions of Deane & Stokes (2002). These works either assumed a flat wave surface, or used the level-set or volume-of-fluid (VoF) method to resolve the free surface but not individual subsurface bubbles. Derakhti & Kirby (2014) extended this formulation to large-eddy simulations (LES) that considered the filtered two-phase equations coupled with a polydisperse bubble population, building on the earlier works of Lakehal et al. (2002) and Lakehal & Liovic (2011), and including the entrainment model described earlier. However, as in the abovementioned works, they do not resolve most of the individual bubbles with their VoF method. Liang et al. (2012) attempted a similar LES-based approach, using instead a wave-phase-averaged method that assumes a flat wave surface. By not directly resolving the largest bubbles, many of these works do not harness the full potential of the interface-resolving schemes they employ, and miss the opportunity to emulate the philosophy of single-phase LES (Rogallo & Moin 1984), where the largest structures are resolved, while the smallest structures are modeled since they typically exhibit universality.

Other studies have adopted an Eulerian-and-Lagrangian approach to treat the dispersed phase, where large interfacial structures are resolved by an Eulerian formulation, while small subgrid structures are treated with a Lagrangian description. The representation of small structures as independent Lagrangian particles makes them amenable to further modeling, as existing population balance models assume Markovian—or memoryless—dynamics such that breakup events are independent of one another (Filippov 1961). The Eulerian-and-Lagrangian approach has most commonly been applied to jet atomization. The application of a nascent version of this approach to complex geometries began with the work of Apte et al. (2003b), where the filtered Navier-Stokes equations were coupled with the Lagrangian equations for the dispersed phase for a coaxial combustor. Subsequent works (Herrmann 2010; Tomar et al. 2010) introduced an Eulerian formulation to describe large structures of the dispersed phase, and allowed for the transfer of small and underresolved Eulerian structures to become Lagrangian particles. These works may be distinguished from other Eulerian–Lagrangian schemes in that the dispersed phase is present in both Eulerian and Lagrangian forms and the transfer of dispersed-phase structures is allowed between the Eulerian and Lagrangian formulations. Herrmann (2010), Ling et al. (2015), and Zhou et al. (2016) further allowed two-way transfer between the Eulerian and Lagrangian descriptions, while Zuzio et al. (2018) distinguished between small- and intermediate-sized Lagrangian particles to bridge between the Eulerian and Lagrangian formulations more smoothly, and Evrard et al. (2019) refined the treatment of large Lagrangian particles using a filtering approach. However, the works cited earlier do not model further breakup of the Lagrangian parti-
icles. Apte et al. (2003a, 2009) independently modeled the stochastic secondary breakup of Lagrangian particles using the long-time limit of population balance models, but without transfer between the Eulerian and Lagrangian descriptions. Note that the lognormal limit they employ for the child drop size distribution at large times due to a single parent drop implicitly assumes a size-invariant breakup frequency, even though their discrete breakup model subsequently assumes a size-dependent frequency for each parent drop. Hoppe & Breuer (2020) also only considered a Lagrangian description for the dispersed phase, and used phenomenological breakup models resembling the model breakup kernel of the population balance equation discussed in the preceding paragraph. Kim & Moin (2011, 2020) developed a capillary breakup model for the direct formation of Lagrangian satellite droplets from Eulerian filaments. Eulerian-to-Lagrangian transfer and Lagrangian breakup were eventually implemented simultaneously in the flow solver documented by Kim et al. (2014), Ham et al. (2014), and Bravo et al. (2018), which is employed in this work to enable the subgrid breakup targeted by the proposed model.

This work presents a cascade-based SGS model to account for the formation of subgrid super-Hinze-scale bubbles. The Eulerian-to-Lagrangian transfer process in previous solvers is augmented by a Lagrangian stochastic breakup model that is faithful to the large-scale breakup dynamics and respects the presence of a turbulent breakup cascade. In particular, the prescribed breakup frequency should be consistent with quasi-self-similar and quasi-stationary bubble-mass and turbulent kinetic energy cascade rates in an intermediate range of bubble sizes and scales, and the modeled (small-scale) and resolved (large-scale) bubble-mass cascade rates should be matched. The modeling of small-bubble breakup and direct resolution of large bubbles and structures mirror the approach taken by LES of single-phase turbulent flows (Rogallo & Moin 1984). The universality of small-bubble breakup implied by locality of the flux in bubble-size space suggests that this cascade-based SGS model may also be extended to other turbulent bubbly flows.

Sub-Hinze-scale bubbles are expected to be formed by distinct air entrainment mechanisms (Deane & Stokes 2002; Kiger & Duncan 2012; Chan et al. 2018; Mirjalili et al. 2018; Chan & Mirjalili et al. 2019; Mirjalili & Mani 2020) that are size nonlocal and will need to be addressed by a separate cascade-bypassing SGS model that may be combined with the proposed cascade-based SGS model in an additive fashion. Treatment of a cascade-bypassing SGS model that generates these bubbles via thin film rupture, including the development of a collision detection algorithm to identify locations where the production of microbubbles is feasible and likely, was addressed in earlier works (Chan et al. 2016, 2017, 2018; Mirjalili et al. 2018; Chan & Mirjalili et al. 2019; Mirjalili & Mani 2020). The potential impact of a size-nonlocal bubble breakup mechanism on the size distribution is further elucidated in Section 4.

The remainder of this brief is structured as follows. Section 2 describes the formulation of the cascade-based SGS model, including model inputs and considerations. Section 3 discusses a priori testing of the model through Monte Carlo stochastic breakup of an artificial bubble population. Section 4 highlights the results of the a posteriori implementation of the model in an actual two-phase flow solver through the numerical simulation of a breaking-wave ensemble. Potential contributions of cascade-based and cascade-bypassing SGS models to the size distribution are distinguished. In response to the limitations observed in Sections 3 and 4, the implications of a randomized Hinze scale are briefly discussed in Section 5, while preliminary a priori measurements of the breakup time are introduced in Section 6. Conclusions are provided in Section 7.
2. Model formulation

The proposed cascade-based SGS model comprises two main steps: Eulerian-to-Lagrangian transfer of small and underresolved Eulerian bubbles, and successive stochastic breakup of the resulting Lagrangian bubbles down to the Hinze scale, where the cascade is terminated (Kolmogorov 1949; Hinze 1955). This modeling paradigm relies on the assumption of size locality of the bubble-mass flux in the turbulent breakup cascade and small-scale breakup universality (Chan et al. 2021a). More specifically, small-scale breakup occurs independently and is screened from the details of the large-scale flow geometry, preventing the latter from overtly influencing the former. Because of this mutual independence, an SGS model developed for small-scale breakup is expected to be generally applicable to various turbulent bubbly flows, unless other multiphysics phenomena enter the picture and complicate the dynamics. A schematic of the model is provided in Figure 1. The model comprises the following steps:

(i) Large structures are directly resolved in an Eulerian fashion by a macroscopic two-phase flow solver. In the context of turbulent breaking waves, the wave surface and large subsurface bubbles are directly resolved by a VoF solver. This includes the resolution of large-bubble and large-cavity breakup into bubbles of various resolvable sizes.

(ii) At every simulation time step or some predefined multiple of it, an identification algorithm (e.g., Herrmann 2010; Tomar et al. 2010; Chan et al. 2021b) is used to identify all the bubbles in the computational domain and compute their volume and centroid.

(iii) Small and underresolved Eulerian bubbles are transferred to become Lagrangian particles when their volume is smaller than a predefined threshold dictating the transfer, via the transfer algorithm also detailed by Herrmann (2010) and Tomar et al. (2010). The resulting Lagrangian bubbles are then advected by the flow solver in tandem with the Eulerian phases using particle models (e.g., Apte et al. 2003a; Hoppe & Breuer 2020), which should account for drag, buoyancy, other body forces, and two-/four-way coupling.

(iv) Every time a Lagrangian bubble is created, either by direct transfer from the Eulerian formulation or by fragmentation of a larger Lagrangian parent bubble, a breakup time is assigned to the bubble such that it will be directed to break after this time has elapsed. The breakup time may be prescribed deterministically by ensuring that it scales as $R^{2/3}$, or sampled stochastically such that the mean time satisfies this scaling. The basis
Cascade-based bubble breakup SGS model

for this scaling comes from the conjecture that the characteristic breakup time of a bubble due to turbulent fragmentation should be of the same order as the turnover time of an eddy of comparable size (Hinze 1955; Chan et al. 2018, 2021a). This scaling is also consistent with a bubble breakup flux that is size invariant and local at intermediate bubble sizes (Chan et al. 2021a). The $R^{2/3}$ scaling has been verified experimentally (Martínez-Bazán et al. 1999a; Rodríguez-Rodríguez et al. 2006) and numerically (Chan et al. 2021b).

(v) Once the breakup time has elapsed, the Lagrangian bubble will then be replaced by a number of smaller Lagrangian child bubbles, whose sizes are sampled stochastically such that the total mass is conserved.

(vi) The breakup of Lagrangian bubbles is allowed to continue until the size of the resulting Lagrangian child bubble is smaller than a predefined Hinze scale, at which point the breakup time of this child bubble is set to be infinite and no further breakup occurs.

Regarding the breakup times, one may conceive static and dynamic variants of the model in direct analogy to single-phase LES. In the static variant, breakup times at all sizes are taken with reference to the prescribed breakup time at a reference size, in a similar fashion to how the Smagorinsky constant is prescribed in the static single-phase SGS model. In the dynamic variant, the breakup time is estimated at every time step and possibly spatial location such that the modeled and resolved breakup fluxes are matched, in a similar fashion to how the Smagorinsky constant is dynamically computed in the dynamic Smagorinsky model so that an appropriate rate of energy is dissipated in response to the local and instantaneous production rate (Germano et al. 1991; Lilly 1992). In this preliminary work, we focus on the static variant for simplicity.

Regarding the size of the child bubbles during breakup, we might also conceive quasi-equilibrium and nonequilibrium model variants. In the quasi-equilibrium case, it is assumed that the child bubbles obey the quasi-equilibrium $R^{-10/3}$ power-law size distribution expected when the breakup flux is quasi-steady and quasi-size-invariant (Filippov 1961; Qi et al. 2020; Chan et al. 2021a,b). The number of child bubbles per breakup event depends on the number of breakup generations that are expected to occur: if 1 generation is expected, then $2^1$ bubbles are produced; if $n$ generations are expected, then $2^n$ bubbles are produced. In the nonequilibrium case, no assumption is made about the power-law scaling of the child bubble size distribution. Instead, binary breakup is assumed for simplicity, and the volumes of the two child bubbles are assumed to obey a uniform or beta distribution, or any other suitable surrogate model (Martínez-Bazán et al. 1999b, 2010; Lashears et al. 2002; Liao & Lucas 2009; Solsvik et al. 2013; Qi et al. 2020; Chan et al. 2021a). Here, we investigate the quasi-equilibrium approach, as well as the nonequilibrium approach with uniformly distributed child bubble volumes.

As noted in Section 1, previous works that considered Lagrangian breakup did not include an Eulerian-to-Lagrangian transfer procedure because they treated the dispersed phase exclusively in a Lagrangian fashion. While the model described here is not restricted to Lagrangian point particles and may be extended to finite-sized Lagrangian particles as long as appropriate mass and momentum coupling with the Eulerian fluid is performed for both the transfer and advection procedures, this work assumes exclusive formation of Lagrangian point particles for simplicity. Our SGS model may also be extended to allow coalescence, dissolution, and buoyant degassing of Lagrangian bubbles like other population balance models, but these are beyond the scope of this brief as well.

The stochastic breakup time and nonequilibrium model are tested a priori in Section 3, and then used to justify the adoption of a deterministic breakup time and quasi-equilibrium model in the preliminary a posteriori implementation in Section 4. Note that
Figure 2. Initial bubble size distribution $\tilde{f}$ for the two a priori tests of Section 3 and the a priori test of Section 5. This distribution and subsequent ones are normalized such that $\sum_j \tilde{f}_j \Delta(R_j/L) = N_b$, where $j$ refers to the $j$th histogram bin, $\Delta(R_j/L)$ denotes the nondimensional bin size of the $j$th bin, and $N_b$ is the total number of bubbles at a particular time. The overbar denotes volume averaging over the entire simulation domain, and the distribution is also ensemble averaged over five statistically independent but similar realizations. The error bars in this distribution and subsequent ones denote twice the standard error over the ensemble.

the deterministic breakup time and nonequilibrium model were also employed in a static (as opposed to dynamic) setting by Hoppe & Breuer (2020).

3. A priori testing

To determine the feasibility of various SGS model prototypes and to verify the expected long-time limit of the proposed model, a series of Monte Carlo simulations of successive stochastic breakup of an artificial bubble population was set up. More specifically, the simulation setup serves as a sandbox to determine the response of a bubble population to different breakup-time models and child bubble size model distributions. Note that the Navier-Stokes equations are not time advanced in these simulations. Here, a bubble population initially obeying an $R^{-10/3}$ power-law size distribution is subject to a breakup frequency that scales as $R^{-2/3}$. This procedure successively generates smaller bubbles down to a prescribed Hinze scale, where the breakup process is terminated, and mimics the generation of Lagrangian bubbles from an existing population of fragmenting Eulerian bubbles with a size-invariant breakup flux in an actual flow simulation. A thousand bubbles were seeded with radii $R \in [0.002L, 0.04L]$, where $L$ is the box size used in the simulation, and the bubbles are placed in a physical box of volume $L^3$ such that they do not initially overlap and the bubble population is physically realizable. The minimum bubble radius for the initial distribution is 500 times smaller than the box size, leading to a scale separation comparable to the breaking-wave simulations discussed in Section 4. The initial size distribution of these bubbles is plotted in Figure 2. The Hinze scale is prescribed to be $10^{-4}L$, which is also marked in the plot.

In the Monte Carlo simulations described here, each bubble eligible for breakup, i.e., every super-Hinze-scale bubble, is assigned a probability for breakup equivalent to the simulation time step divided by the mean breakup time corresponding to the bubble size, where the latter scales as $R^{2/3}$. This is approximately equivalent to an exponentially distributed actual breakup time for each bubble size in the limit where this breakup probability is small. The exponential distribution is expected when the breakup events
occur independently of one another (Filippov 1961). This procedure corresponds to the stochastic sampling of the breakup time discussed in Section 2. The time step is taken to be $10^{-5}$ times the mean breakup time corresponding to the smallest allowed initial bubble size ($0.002L$) to keep this probability small. This ensures that the probability is representative of a sample from the aforementioned exponential distribution. In the baseline case, the $R^{2/3}$ scaling holds for all bubble sizes to mimic the situation where the breakup flux is perfectly constant across all sizes. A nonequilibrium model is adopted here such that every successful breakup event is assumed to produce two child bubbles. The volumes of the child bubbles are sampled from a uniform distribution with the restriction that they must have at least 1% the volume of their parent bubble. This restriction was added to suppress the formation of excessively small bubbles and thus prevent the size of the population from exploding, but does not otherwise influence the results.

The size distribution for this baseline case after about one integral time has elapsed is plotted in Figure 3, along with distributions at intermediate times. The plot suggests that the newly formed bubbles smaller than the minimum initial size eventually approach the $R^{-10/3}$ scaling after about one integral time, which is estimated as the mean breakup time of the largest possible initial bubble size ($0.04L$). The result justifies the use of the quasi-equilibrium model variant in the \textit{a posteriori} implementation when bubble statistics averaged over an integral time—rather than the time-instantaneous statistics—are of interest. Note that pileup occurs slightly below the Hinze scale. Sub-Hinze-scale bubbles accumulate in this model system, as they are not allowed to break further, thereby generating a kink in the size distribution around the Hinze scale ($10^{-4}L$). This kink may be mitigated with additional phenomenological assumptions, such as a broadband probability distribution for the Hinze scale (Qi \textit{et al.} 2020). Preliminary efforts to mitigate this kink through a randomized Hinze scale are discussed in Section 5.

A second set of Monte Carlo simulations was performed where the mean breakup time of bubbles smaller than the minimum initial size is set to be 0.3 times shorter than in the baseline case. The goal is to mimic the situation where the small-scale breakup flux does not match the large-scale flux in an actual flow simulation. Figure 4 plots the size distribution for this case after about one integral time has elapsed, along with
Figure 4. The same distributions depicted in Figure 3 for the case where bubbles of radii smaller than $0.002L$ have a shorter mean breakup time (0.3 times the baseline value).

Figure 5. A representative snapshot of the instantaneous air–water interface after the wave has broken, obtained from the breaking-wave simulations of Chan et al. (2021b). Specifically, this is the 0.5 isosurface of the volume fraction field. Note that the outline of the water body is only for illustration. The actual computational domain is about four times as deep.

distributions at intermediate times. Since the small-scale flux ($R < 0.002L$) is larger than the large-scale flux ($R > 0.002L$), the small-scale size distribution is smaller than in the baseline case, as small bubbles fragment and get depleted more quickly. Because of this heightened flux, the distribution also approaches the quasi-equilibrium scaling more quickly as the characteristic response time of the system decreases, and the sub-Hinze-scale pileup is more pronounced as sub-Hinze-scale bubbles are generated more rapidly. The larger kinks in the distributions of Figure 4 relative to those of Figure 3 at the Hinze scale ($10^{-4}L$), as well as the new kinks at $R = 0.002L$, underscore the need for the small- and large-scale fluxes to be matched in order to achieve a continuous size distribution as expected physically. A matched flux is also important for an accurate system response time. Preliminary a priori measurements of the mean breakup time and its probability distribution from the breaking-wave simulations of Chan et al. (2021b), which would inform the prescription of this flux in an a posteriori implementation of the static variant of the SGS model, are presented in Section 6.
4. A posteriori implementation

As a preliminary study, the static quasi-equilibrium SGS model variant with a deterministic breakup time was implemented in the unstructured unsplit geometric VoF flow solver documented by Kim et al. (2014), Ham et al. (2014), and Bravo et al. (2018). The model was used to simulate a 27-cm deep-water wave at atmospheric conditions with an effective grid size of $216^3$. Figure 5 illustrates a representative snapshot of the air–water interface after the wave breakdown and further simulation details are provided by Chan et al. (2018, 2021b). Eulerian-to-Lagrangian transfer occurs when the bubble volume is smaller than 64 grid-cell volumes, which is equivalent to the volume of a bubble whose radius is about 2.4 grid-cell widths. The ensuing Lagrangian breakup is eventually halted when the bubble Weber number is smaller than $0.01$. For the computation of this critical Weber number and its corresponding critical bubble size $R_c$, the characteristic bubble velocity scale is taken to be $(\varepsilon R_c)^{1/3}$, where $\varepsilon$ is the characteristic energy dissipation rate of the wave, or the ratio of the cube of the wave phase speed to the wavelength, which is also discussed by Chan et al. (2021b). Note that this critical Weber number is supposed to be of order unity and is set to be artificially small here for illustration purposes.

Before the results of the a posteriori implementation are introduced proper, it is instructive to discuss what one might expect in the size distribution in an idealized scenario based on the a priori results of Section 3 and additional physical arguments, assuming the grid scale is larger than the Hinze scale. In a simulation with no SGS model, all bubbles are Eulerian and supergrid. Their size distribution is expected to follow an $R^{-10/3}$ power-law scaling at intermediate sizes between the Hinze and integral length scales, provided the two are well separated. In a simulation with an ideal SGS model, all Eulerian bubbles smaller than the Eulerian-to-Lagrangian transfer scale are transferred to become Lagrangian bubbles. Lagrangian bubbles of sizes between the Hinze and transfer scales are also expected to follow an $R^{-10/3}$ scaling. A limited number of sub-Hinze-scale bubbles are expected from the cascade-based SGS model since the cascade terminates at the Hinze scale. The main sources of sub-Hinze-scale bubbles should then be either direct Eulerian-to-Lagrangian transfer, or the implementation of a separate cascade-bypassing SGS model as described in Section 1. The latter is not considered in this work, so most observed sub-Hinze-scale Lagrangian bubbles must be a consequence of the former.

The size distribution resulting from the a posteriori implementation, averaged over the second integral time after breaking, is plotted in Figure 6 for ensembles of simulations that were run with and without the model but are otherwise identical. The time-averaging interval corresponds to the first characteristic time interval of interest identified by Chan et al. (2021b). Five key observations may be made. First, the size distributions of the ensembles with and without the model generally overlap above the Eulerian-to-Lagrangian transfer scale, indicating that the model does not distort the breakup dynamics at these sizes. Second, the sub-transfer-scale size distribution of the ensemble with the model recovers the $R^{-10/3}$ scaling between the Hinze and transfer scales as expected by the model design. Third, the same distribution recovers the $R^{-3/2}$ scaling at smaller bubble sizes. This scaling was observed by Deane & Stokes (2002), Wang et al. (2016), and Mortazavi (2016) in their size distributions. As noted in the preceding paragraph, these bubbles are chiefly a result of direct Eulerian-to-Lagrangian transfer. Fourth, pileup is observed at the Hinze scale concomitantly with its occurrence in the a priori tests of Section 3. Fifth, a smaller discontinuity is observed at the Eulerian-to-Lagrangian transfer scale, suggesting that the resolved and modeled breakup fluxes are not exactly matched. Notwithstanding these discontinuities, the results indicate that a posteriori implementation of the pro-
Figure 6. Bubble size distribution $f^T$ for the a posteriori implementation of Section 4, applied to an ensemble of breaking-wave simulations containing five statistically independent but similar realizations. The distribution is ensemble averaged and time averaged ($\bar{\cdot}$) over the nondimensional interval $t \in (2.30, 3.14)$. The time scale used for nondimensionalization is $\sqrt{L/g}$, where $L = 27$ cm is the wavelength and $g$ is the magnitude of standard gravity. The $R^{-10/3}$ and $R^{-3/2}$ power-law scalings were obtained by Deane & Stokes (2002) in their experimental distributions above and below what they identified to be the Hinze scale, respectively. The symbols H, G, and T respectively denote the Hinze scale, the grid scale, and the Eulerian-to-Lagrangian transfer scale. Bubbles of sizes smaller than $R/L = 2.5 \times 10^{-5}$ are excluded here since the Eulerian-to-Lagrangian transfer procedure did not generate bubbles smaller than this size.

Figure 7. The instantaneous size distribution for the simulations of Section 4 at $t = 2.50$. For details on the time nondimensionalization and other symbols, refer to the caption of Figure 6.

posed SGS model in an actual two-phase flow solver is feasible, and turbulent bubbly flows of practical importance have the potential to be simulated with this model.

In addition to the time-averaged size distribution of Figure 6, Figures 7 and 8 plot the instantaneous size distribution at two time instances, also averaged over the wave ensemble. Even though the quasi-equilibrium model variant is used here, the model also performs reasonably well in a time-resolved sense, except that the flux mismatch has a more pronounced influence on the size distribution at later times.
5. Post hoc tests of the effects of a randomized Hinze scale

The results of Sections 3 and 4 revealed that the size distribution exhibits a kink at the Hinze scale when a sharp cutoff is prescribed. In order to extenuate this behavior and mimic spatial variations in the spatially local Hinze scale in an inhomogeneous environment, a randomized Hinze scale is prescribed in the post hoc tests of this Section. The Hinze scale in the \textit{a priori} test and the critical Weber number in the \textit{a posteriori} test are sampled from a uniform distribution, which is the simplest surrogate model that minimizes further ad hoc assumptions on the underlying dynamics. Future work could entail the implementation of a more involved phenomenological distribution, such as the one considered by Qi \textit{et al.} (2020), or the spatially local and time-instantaneous computation of the breakup rate via a dynamic procedure (see also Pierce & Moin 1998; Aiyer \textit{et al.} 2019). Note that the former approach necessitates a more detailed analysis of the influence of bubbles on the energetics near the Hinze scale, while the latter approach should be interpreted solely as a method to estimate the time scale of interest.

Figure 9 plots the \textit{a priori} size distribution where the baseline case in Section 3 is modified such that the Hinze scale for each generated bubble varies between 0.1 and 1.9 times its baseline value. The kink at the Hinze scale is replaced by a continuous size...
distribution as is expected physically. Figure 10 plots the \textit{a posteriori} size distribution where the configuration in Section 4 is modified such that the critical Weber number for each Lagrangian bubble generated from the Eulerian-to-Lagrangian transfer process varies between 0.1 and 1.9 times its baseline value, and this critical Weber number is carried to all its child bubbles. While the kink at the Hinze scale is smoothed in a similar manner to the \textit{a priori} results, the situation is confounded by the initial presence of sub-Hinze-scale bubbles resulting directly from the Eulerian-to-Lagrangian transfer process. These bubbles did not break when the Hinze scale was prescribed deterministically, but some of them undergo fragmentation when the Hinze scale is prescribed stochastically, thus nudging the resulting distribution towards the $R^{-10/3}$ power-law scaling. Future model refinements will need to be cognizant of the presence and thus careful about the treatment of these directly transferred bubbles.

### 6. Direct measurements of breakup frequency from bubble tracking

Another message conveyed by the \textit{a priori} and \textit{a posteriori} analyses respectively conducted in Sections 3 and 4 is the necessity of accurate breakup frequency information, which is faithful to the actual physical breakup of the bubbles. Failure of a model to comply with the latter might result in unphysical discontinuities in the size distribution due to inconsistencies in the bubble-mass flux across bubble sizes in the breakup cascade. To obtain more realistic information about the breakup time at different sizes, we track the breakup history of individual Eulerian bubbles in time using the simulations presented by Chan \textit{et al.} (2021b), which are similar to those in Section 4. This is a preliminary analysis and higher-fidelity simulations might be utilized in the future to obtain the desired breakup frequency over a larger range of sizes and with higher temporal fidelity. All the bubbles in each simulation are individually tracked in time using the algorithm also detailed by Chan \textit{et al.} (2021b). Breakup events are then detected and used to construct a graph of bubble connections, which contains information on the time elapsed between successive breakup events, using the algorithm of Lozano-Durán & Jiménez (2014).

Figure 11(a) shows the joint probability distribution of the parent bubble size during breakup and the corresponding breakup time, including all breakup events during the nondimensional time interval $[1.20, 4.82]$. The bubble radius is nondimensionalized by the wavelength, $L = 27$ cm, and all times are nondimensionalized by the characteristic
Figure 11. (a) The logarithm of the joint probability distribution of the nondimensional parent bubble radius, \( R/L \), and the nondimensional breakup time, \( t \), of all breakup events detected in the 20-realization subset of the baseline breaking-wave simulation ensemble of Chan et al. (2021b) using the tracking algorithm also detailed therein. (b) The probability distribution of the nondimensional breakup time, conditioned on the two parent bubble radii marked by white dashed lines in panel (a). The square symbols correspond to the larger parent bubble size.

Figure 11(b) further shows the probability density function (PDF) of the breakup time conditioned on two parent bubble sizes. The mean of the PDF increases with parent bubble size in an intermediate range of sizes in corroboration with the results of Chan et al. (2021b), which only consider the size scaling of the mean breakup time and not its magnitude or probability distribution. Note that the theoretical scaling for this mean time is \( R^{2/3} \), i.e., the mean time increases with increasing bubble size. However, the increase in the mean time in the simulations appears to be associated with a growing tail in the PDF, and the mode of the PDF remains close to constant. The current results may be subject to artifacts due to the relatively large time interval between snapshots used for the tracking algorithm, as well as spurious connections in the corresponding graph. These will be tackled in upcoming works, and we expect this bubble tracking approach to aid physics-based refinements of our bubble breakup SGS model.
7. Conclusions

SGS models for bubble breakup are required for cost-effective simulation of turbulent bubbly flows that typically involve a large separation of scales. Since turbulent breakup occurs via a bubble-mass cascade, a cascade-based SGS model is used to account for the formation of subgrid bubbles of sizes larger than the Hinze scale, where the cascade is expected to terminate. The proposed model comprises two main steps: the transfer of small and underresolved Eulerian bubbles to become Lagrangian particles, and the successive breakup of these Lagrangian bubbles down to the Hinze scale. Note that transport of these Lagrangian particles continues in tandem with the Eulerian phases once the particles are generated. The model is first tested in an a priori setting where Monte Carlo stochastic breakup of an artificial bubble population is performed. These Monte Carlo simulations show that the quasi-equilibrium $R^{-10/3}$ power-law scaling in the size distribution is recovered after about one integral time, supporting the use of a quasi-equilibrium a posteriori model implementation in a two-phase flow solver when time-averaged statistics are of interest. In addition, the Monte Carlo simulations underscore the need for the small- and large-scale breakup fluxes to be matched via an appropriate choice of the magnitude of the breakup frequency of the Lagrangian particles. The model is then implemented a posteriori in a VoF solver and used to simulate a breaking-wave ensemble. The implementation preserves the size distribution above the Eulerian-to-Lagrangian transfer scale and recovers the $R^{-3/2}$ power-law scaling for sub-Hinze-scale bubbles that was observed in selected experiments and simulations. However, more investigation is needed into appropriate treatment of breakup at the Hinze scale, as well as the impact of the mismatch between the modeled and resolved breakup fluxes. Preliminary efforts to mitigate these are outlined through the adoption of a randomized Hinze scale and the direct measurement of the breakup time in previous breaking-wave simulations.

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