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Fragmentation Mechanisms of a Droplet in a Turbulent Flow: a Direct Numerical Simulation Approach

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*A chi cade senza fare rumore,
ma fa tremare la terra quando si rialza.*

Sommario

La rottura di gocce e bolle in flussi turbolenti multifase è un problema classico e tuttora irrisolto della meccanica dei fluidi, con implicazioni che spaziano dall'atomizzazione del combustibile nei motori a combustione interna alla generazione di aerosol all'interfaccia aria-mare.

Questo lavoro studia l'accoppiamento multiscala tra la turbolenza della fase continua (o carrier) e la deformazione dell'interfaccia, isolando sistematicamente il contributo delle diverse scale. Attraverso Simulazioni Numeriche Dirette ad alta risoluzione di una singola goccia in turbolenza omogenea isotropa, vengono condotti esperimenti numerici basati sul troncamento spettrale del campo di velocità al fine di valutare i diversi effetti. In particolare, vengono applicati filtri passa-basso e passa-alto con scale di taglio proporzionali al diametro iniziale della goccia D ($0.5D$, $0.74D$, D e $1.2D$).

I risultati rivelano una profonda differenza nella dinamica di rottura (breakup) in funzione della scala. Le fluttuazioni turbolente a piccole scale (garantite dai filtri high-pass) si dimostrano incapaci di indurre la frammentazione della goccia, registrando un tasso di rottura nullo per quei filtri di taglio inferiore o uguale al diametro D , e appena del 20% per il caso $1.2D$.

Al contrario, le strutture di grande scala (fornite dai filtri low-pass) provocano sistematicamente la rottura nel 100% dei casi, a fronte del 60% riscontrato nella turbolenza non filtrata. Questa discrepanza dimostra che i vortici di dimensioni superiori a quella della goccia sono i principali responsabili dello sforzo necessario a vincere la tensione superficiale.

Tale tensione viene generata dalle fluttuazioni del campo di velocità alle piccole scale e tende a stabilizzare l'interfaccia, garantendo l'integrità della goccia.

Inoltre, l'analisi statistica della distribuzione dimensionale delle gocce generate conferma l'insorgere dei regimi di scala sub-Hinze ($d^{-10/3}$) e super-Hinze ($d^{-3/2}$).

Lo studio del bilancio energetico spettrale scale-by-scale (letteralmente "scala-per-scala") evidenzia come l'interfaccia agisca da volano energetico dinamico, accumulando l'energia cinetica sottratta ai vortici a grande scala sotto forma di energia potenziale superficiale, per poi ridistribuirli alle scale inferiori durante il fenomeno di rottura. Questi risultati forniscono delle basi fisiche per lo sviluppo di modelli sub-grid consistenti nell'ambito delle simulazioni multifase.

Abstract

Droplet and bubble fragmentation in turbulent multiphase flows is a long-standing challenge in fluid mechanics, with profound implications for processes ranging from fuel atomization in industrial combustors to aerosol generation at the air-sea interface.

This work studies the multiscale nature of these processes by systematically isolating the roles of different turbulent scales through spectral filtering of the carrier velocity field. Using high-fidelity Direct Numerical Simulations of a single deformable droplet immersed in homogeneous isotropic turbulence, numerical experiments are performed where the carrier flow field is spectrally truncated. Specifically, low-pass and high-pass filters are applied to the velocity field at multiple cutoff scales proportional to the initial droplet diameter D .

The results reveal a fundamental asymmetry in the scale-dependent breakup dynamics. Isolated small-scale turbulent fluctuations (high-pass cases) are shown to be incapable of triggering droplet breakup on their own, yielding a maximum breakup rate of 20% for cutoff scales slightly larger than the droplet diameter. In contrast, large-scale structures (low-pass cases) consistently drive the droplet to fragmentation in 100% of the runs, compared to a baseline rate of 60% in the unfiltered reference turbulence. This demonstrates that the inertial-range eddies larger than the droplet scale are the primary source of the hydrodynamic strain required to overcome the stabilizing capillary pressure, which is generated by small-scale velocity fluctuations.

Furthermore, statistical analysis of the post-breakup droplet size distribution confirms the emergence of sub-Hinze ($d^{-10/3}$) and super-Hinze ($d^{-3/2}$) scaling laws. Additionally, a scale-by-scale energy budget analysis reveals that the interface acts as a dynamic energy buffer, absorbing kinetic energy from the large-scale forcing eddies and subsequently releasing it at smaller scales during fragmentation. These findings provide a physical foundation for developing scale-aware subgrid-scale models.

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List of Symbols

This list summarizes the primary mathematical symbols, Greek letters, subscripts, and operators used throughout this thesis, along with their physical descriptions and SI units (where applicable).

Latin Characters

Symbol	Description	Units
A, B, C	Arnold-Beltrami-Childress (ABC) forcing coefficients	[-]
Ca	Capillary number	[-]
C_K	Kolmogorov scaling constant	[-]
C_{visc}	Hinze viscosity correction coefficient	[-]
D	Dispersed particle/droplet diameter	m
d_H	Hinze scale (crossover scale)	m
$D(k), \mathcal{D}$	Time-averaged viscous dissipation in the spectral domain	m^3/s^3
$E(k)$	Time-averaged kinetic energy in the spectral domain	m^3/s^2
$F(k), \mathcal{F}$	Time-averaged energy input due to large-scale forcing	m^3/s^3
f_i^σ	Volumetric surface tension (capillary) force component	N/m^3
f_i^T	Volumetric external body (forcing) force component	N/m^3
g_i	Gravitational acceleration vector component	m/s^2
$\hat{G}(k), G(x)$	Filter transfer function (spectral) and kernel (physical)	[-]
k	Wavenumber (spectral domain)	$1/\text{m}$
k_c	Filter cut-off wavenumber	$1/\text{m}$
k_f	Forcing wavenumber	$1/\text{m}$
k_H	Hinze crossover wavenumber	$1/\text{m}$
K	Turbulent kinetic energy	m^2/s^2

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Symbol	Description	Units
ℓ, l	Separation scale (velocity increment length)	m
L	Integral length scale of turbulence	m
n	Order of the velocity structure function	[-]
n_i	Unit interface normal vector component	[-]
n_{bk}	Number of droplet breakup events	[-]
N	Total number of simulation cases/restarts	[-]
Oh	Ohnesorge number	[-]
p, P	Fluid pressure / mean (filtered) fluid pressure	Pa
Q	Forcing coefficient	1/s
r	Separation distance (in two-point correlations)	m
Re	Reynolds number	[-]
S_{ij}	Strain-rate tensor component	1/s
S_n	n -th order velocity structure function	m^n/s^n
$S_\sigma(k), \mathcal{S}_\sigma$	Time-averaged capillary work done by surface tension force	m^3/s^3
St	Stokes number of the dispersed phase	[-]
T_L	Large-eddy turnover time	s
$T(k)$	Time-averaged non-linear kinetic energy transfer in spectral domain	m^3/s^3
$\mathbf{u}, u_i$	Fluid velocity vector and tensor components	m/s
u_i^*	Intermediate (predicted) velocity component	m/s
u_{rms}	Root-mean-square velocity of the carrier phase	m/s
$\tilde{u}_i$	Velocity component in the Fourier (spectral) domain	m^4/s
V	Fluid phase volume	m^3
We	Weber number	[-]
x_i	Cartesian coordinate components	m

Greek Characters

Symbol	Description	Units
α	Dispersed phase volume fraction	[-]
β	Volume ratio of the largest droplet ($V_{\max}/V_0$)	[-]
β_{th}	MTHINC interface thickness parameter	[-]
γ	Breakup rate (ratio of breakups to total restarts)	[-]
Δ	Filter scale / filter width	m
δ	Dirac delta function (interfacial surface density)	1/m
ε	Viscous dissipation rate	m ² /s ³
η	Kolmogorov length scale (turbulent microscale)	m
κ	Interface curvature	1/m
λ	Taylor microscale	m
μ	Dynamic viscosity	Pa · s
ν	Kinematic viscosity	m ² /s
ϕ	Local phase indicator (volume fraction) field	[-]
$\Pi_\sigma(k)$	Cumulative capillary energy flux spectrum in Fourier space	m ³ /s ³
$\Pi(k)$	Cumulative non-linear kinetic energy flux spectrum in Fourier space	m ³ /s ³
ρ	Fluid density	kg/m ³
ρ^*	Density ratio (ρ_d/ρ_c)	[-]
σ	Interfacial (surface) tension	N/m
τ_f	Characteristic carrier flow timescale	s
τ_p	Characteristic dispersed particle response time	s
τ_η	Kolmogorov timescale	s

Subscripts, Accents, and Mathematical Operators

Symbol	Description
$(\cdot)_c$	Continuous carrier phase quantity
$(\cdot)_{crit}$	Critical value of a quantity
$(\cdot)_d$	Dispersed phase quantity
$(\cdot)_f$	Forcing quantity
$(\cdot)_L$	Longitudinal component of a vector / tensor quantity
$(\cdot)^\sigma$	Surface tension / capillary term index
$(\cdot)^T$	Turbulent forcing quantity
$(\tilde{\cdot})$	Fourier-transformed (spectral) variable
$\langle \cdot \rangle$	Ensemble, spatial, or volume average
$\langle \cdot \rangle_t$	Time-averaged quantity

1. Introduction

Predicting the fragmentation of droplets and bubbles has long stood as a challenge in the study of turbulent multiphase flows. Spanning applications from combustion chambers and bioreactors to environmental air-sea interactions and biomedical treatments, the dispersed phase is central to numerous industrial and natural systems, where its dynamics govern transport phenomena and overall performance. This study aims to advance the understanding of these fragmentation mechanisms by analyzing the role of large- and small-scale turbulent structures to improve the predictive modeling of breakup dynamics.

1.1 Multiphase flows

Multiphase flows represent a ubiquitous class of flows defined by the simultaneous co-existence and interaction of two or more distinct phases (solid, liquid, or gas) separated by identifiable boundaries called interfaces.

The dynamics of multiphase systems are governed not only by pressure gradients, shear stresses, and convective acceleration, like the single-phase flows, but they are also dominated by:

- the topological distribution of the phases;
- phase changes and interfacial transport of momentum, mass, and energy;
- surface tension (or capillary) forces;
- complex boundary coupling.

From a theoretical point of view, the main difficulty when analyzing these flows lies in their multiscale nature. The large separation of scales, which can reach up to several orders of magnitude ($\sim 10^5 - 10^6$) between the interface length-scale and the mean-free path, is further magnified when dealing with turbulent flows, broadening the spectrum of scales. At the microscopic level, the interface between two immiscible fluids is a transition zone of finite thickness where density and intermolecular energies undergo rapid variations.

In macroscopic fluid mechanics, this transition zone is typically modeled using two distinct physical and numerical approximations (Scardovelli et al. 1999; Tryggvason et al. 2006):

- **Sharp-Interface Approximation:** the interface is treated as a zero-thickness mathematical boundary layer. Across this surface, physical properties experience discontinuous jumps and the momentum balance is maintained via surface tension acting as a singular boundary force.
- **Diffuse-Interface Approximation:** the interface is represented as a region of finite thickness across which physical properties vary continuously. The phase state is tracked via an order parameter (or phase field) and capillary forces are modeled as a volumetric body force derived from thermodynamic potentials.

A preliminary categorization of multiphase systems can be performed based on three primary topological regimes, which describe the spatial arrangement of the immiscible phases (Clift et al. 1978; Brennen 1995):

- ***Transitional (or Mixed) Flows:*** Characterized by complex, time-varying topologies which undergo transitions between separated and dispersed states, such as the primary atomization of liquid jets.
- ***Separated Flows:*** Consist of continuous streams of immiscible fluids separated by a large, coherent interface. The dynamics are dominated by gravity, wave propagation and shear instabilities. A clear example is given by the free-surface air-sea boundary layers.
- ***Dispersed Flows:*** Consist of a dispersed phase distributed as discrete elements—such as solid particles, liquid droplets, or gas bubbles—within a carrier phase. A typical configuration includes liquid sprays inside a combustion chamber.

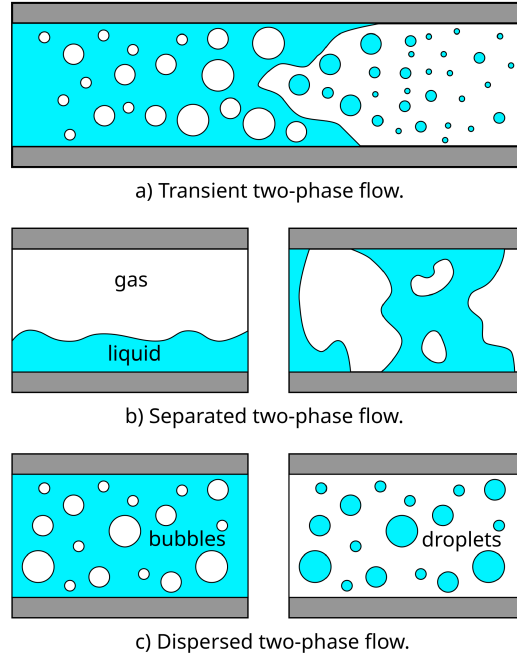


Figure 1: Topological regimes of two-phase flows (Hellmuth 2015).

1.1.1 Coupling Mechanisms in Droplets and Bubbles

Unlike rigid solid particles, the coupling between a dispersed phase of droplets or bubbles and the continuous carrier flow cannot be fully characterized by volume fractions and momentum slip alone. Because the interfaces of fluid particles are highly deformable, they actively exchange energy with the turbulent cascade through topology changes, fragmentation and coalescence. The primary dimensionless parameter governing these deformation and fragmentation dynamics is the Weber number (We), which defines the ratio of the disruptive inertial forces (or hydrodynamic dynamic pressure) to the stabilizing surface tension (capillary) forces:

$$We = \frac{\rho_c U^2 d}{\sigma} \quad (1.1)$$

where ρ_c is the density of the continuous carrier phase, U is a characteristic relative velocity (or velocity fluctuation at the scale of the droplet), d is the droplet diameter, and σ is the surface tension coefficient.

For different Weber number regimes, the behavior and morphology of the dispersed phase vary significantly:

when $We \ll 1$, surface tension forces dominate, and the droplets behave as stable, nearly spherical particles with negligible deformation;

for $We \sim 1$, droplets undergo ellipsoidal deformation and experience capillary-driven oscillations without breaking up;

finally, when $We \gg 1$, external deforming stresses overcome the restoring surface tension, leading to severe interface distortion and eventual fragmentation (Ni 2024).

While spatial transport and slip behavior are classically parameterized by the Stokes number (St), for deformable droplets the coupling is intrinsically scale-dependent and involves a **scale-by-scale energy transfer** across the turbulent spectrum (Crales-Esposito, Chibbaro, et al. 2023). The interface acts as a dynamic energy buffer:

1. **Energy Absorption (Sink at Large Scales):** Large, deforming droplets absorb kinetic energy from carrier-phase eddies and store it as surface potential energy through interface stretching. This process damps the large-scale turbulent kinetic energy (TKE) of the continuous phase.
2. **Energy Release (Source at Small Scales):** Droplets smaller than the stable threshold relax back to spherical shapes through capillary oscillations, and the stored kinetic energy is fed back into the carrier flow at small scales.

This exchange modifies the continuous-phase turbulence by altering the traditional Richardson energy cascade, transferring energy directly from large scales to small scales.

1.1.2 Application fields

Industrial and environmental applications of these complex flows drive the need for a thorough understanding of their dynamics. They are central to several key areas:

- **Power generation and thermal systems:** Two-phase boiling heat transfer must be managed, and cavitation—where local pressure drops trigger vapor bubble formation and violent collapse—must be mitigated to avoid structural damage.
- **Petroleum and process industries:** Control of the viscosity of water-in-oil (W/O) emulsions is essential to ensure flow safety in pipeline transport.
- **Pharmaceutical and food processing:** The stability, shelf-life, and bioavailability of

nanoemulsions, cosmetics, and agricultural sprays depend on the control of the droplet size distribution (McClements 2015).

- **Chemical and bioreactors:** Mass transfer and reaction rates are regulated by bubble breakup and coalescence, which maximize the interphase surface area.

Additionally, multiphase flows govern major natural and geophysical phenomena, including cloud aggregation and precipitation in atmospheric physics, aerosol generation in marine systems, and greenhouse gas transfer at the air-sea boundary.

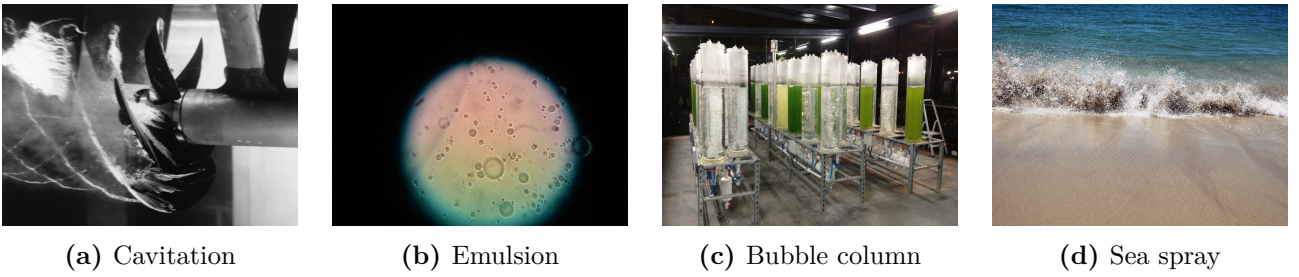


Figure 2: Industrial and environmental applications of turbulent multiphase flows featuring droplets and bubbles.

1.2 The breakup phenomenon

The breakup of droplets and bubbles in a turbulent carrier phase is ultimately the result of two opposing physical mechanisms that govern droplet deformation: the restoring surface tension, which acts to minimize the interfacial area and maintain a spherical shape, and the disruptive hydrodynamic stresses exerted by the surrounding fluid. At the scale of the droplet interface, the stabilizing force is characterized by the Laplace pressure (Clift et al. 1978):

$$\Delta p_L = \frac{2\sigma}{R}$$

where σ is the surface tension of the fluid interface and R is the local radius of curvature of the droplet surface.

The deformation is a dynamic process where external forces stretch the droplets, causing the interface to form elongated structures. Breakup occurs after the external stresses become dominant: these elongated structures, subject to capillary or Rayleigh-Plateau instabilities, lead

to the formation of necks that rapidly pinch off into smaller droplets (Plateau 1873; Rayleigh 1878), causing the final fragmentation.

In a turbulent flow, the balance of these forces is strictly related to the energy cascade. The energy cascade generates multiscale eddies; to understand how they interact with the interface, it is necessary to introduce three key characteristic scales (Pope 2000):

1. **The Integral Scale (L):** The largest scale of the flow. Eddies of this size, much larger than the droplet, do not cause breakup but simply carry or advect the droplet along with the mean flow. (Hinze 1955)
2. **The Kolmogorov Scale (η):** The smallest scale of turbulence, where kinetic energy is dissipated by viscous forces (Kolmogorov 1941).
3. **The Taylor Microscale (λ):** An intermediate scale representing the typical size of the velocity gradients in the flow, often used to characterize the transition region of the turbulent cascade.

1.2.1 The Kolmogorov-Hinze Framework

Despite the wide range of scales involved, the key concepts crucial to understanding deformation and breakup come from the seminal work of Kolmogorov and Hinze, which established the Kolmogorov–Hinze (KH) framework. Within this framework, the Weber number is interpreted as a localized parameter characterizing the balance between turbulent fluctuations and capillary pressure at the droplet scale d :

$$We = \frac{\rho_c u_d^2 d}{\sigma} \quad (1.2)$$

where u_d represents the characteristic eddy velocity fluctuation of scale d .

Assuming homogeneous isotropic turbulence (HIT) and the validity of the Kolmogorov scaling laws, where the velocity increments scale with the average dissipation rate $\langle \varepsilon \rangle$ as:

$$u^2(d) = C_K (\langle \varepsilon \rangle d)^{2/3} \quad (1.3)$$

where C_K is the universal Kolmogorov constant, the Weber number can be rewritten in its

classical formulation:

$$We = \frac{(\rho_c \langle \varepsilon \rangle)^{2/3} d^{5/3}}{\sigma} \quad (1.4)$$

In 1955 Hinze hypothesized that a droplet will break if it is exposed to turbulent fluctuations such that the Weber number exceeds a certain threshold, defined as the critical Weber number We_{crit} , which appeared to be approximately $We_{crit} \approx 1.17$ for HIT cases.

By setting $We = We_{crit}$ the maximum stable droplet diameter can be defined as the one that can survive without breaking and it is known as the **Hinze scale** (d_H):

$$d_H = 0.725 \left(\frac{\sigma}{\rho_c} \right)^{3/5} \langle \varepsilon \rangle^{-2/5} \quad (1.5)$$

The Hinze scale represents the physical boundary dividing the droplet population between the unstable, larger than d_H , that will undergo fragmentation and the stable, smaller than d_H , stabilized by the surface tension.

When the dispersed phase has a significant viscosity, the internal forces resist deformation alongside surface tension: this slows down the droplet's response to fluctuations, meaning higher external stresses are required to cause breakup. This was accounted for by Hinze by introducing the *Ohnesorge Number* (Oh):

$$Oh = \frac{\mu_d}{\sqrt{\rho_d \sigma d}} \quad (1.6)$$

where μ_d and ρ_d are the dynamic viscosity and density of the dispersed phase, respectively. Hence, the We_{crit} can be corrected using the empirical relation proposed by Hinze:

$$We_{crit} = We_{crit,0}(1 + C_{visc}Oh) \quad (1.7)$$

with $We_{crit,0}$ being the critical Weber number for an inviscid droplet, C_{visc} an empirical constant

approximately equal to 3.6. When Oh is large (typically $Oh > 0.1$) the viscous resistance becomes dominant and the droplet requires significantly more energy to break.

1.3 Breakup Regimes

Based on the physical nature of deforming forces and on the ratio between the droplet diameter (d) and the fundamental scales, the breakup subdivision (Ni 2024) is the following:

- **Inertial-Subrange Breakup** ($\eta \ll d \ll L$): The droplet is much larger than the Kolmogorov scale η and this translates into a large bubble/droplet Reynolds number. The disruptive stresses are normal stresses, caused by dynamic pressure fluctuations across the droplet diameter. The viscous contribution can be neglected.
- **Viscous-Subrange Breakup** ($d \ll \eta$): This breakup happens when the droplet is smaller than the Kolmogorov scale η and the size-based Reynolds number is smaller than one. The carrier flow appears locally laminar at the droplet scale and the breakup is driven by the viscous shear and elongation stresses. In this class it is crucial to consider the Capillary number $Ca = \sqrt{\mu_c \rho_c \langle \varepsilon \rangle} d / \sigma$ and the Ohnesorge number Oh .

1.3.1 Inertial-Dominated Regime

In this regime the carrier phase inertia is the primary driving force for interface deformation. Depending on the relative strength of turbulent fluctuations, buoyancy and mean shear, this regime can be subdivided into:

1. **Intense Homogeneous and Isotropic Turbulence:** Breakup is driven purely by local, isotropic pressure fluctuations in the turbulent cascade. The deforming force is associated with local velocity increments at the droplet scale. Capillary forces act as the only restoring pressure, leading to the classical Kolmogorov-Hinze limit.
2. **Buoyancy-Dominated Regimes:** For large bubbles or low-density droplets rising or falling under gravity, buoyancy forces dominate over small-scale turbulent fluctuations. The deformation is driven by hydrostatic pressure differences across bubble height. The bubble transitions from spherical to ellipsoidal, eventually forming a spherical-cap shape where a liquid jet penetrates the bottom interface, leading to toroidal bubble division (Clift et al. 1978).

3. **Shear-Dominated Regimes:** Occur when mean flow shear gradients dominate over local small-scale turbulent fluctuations. This is common in near-wall boundary layers, shear layers or static mixers. The deformation is driven by the spatial gradient of the mean velocity field, stretching the droplets into filaments (Levich 1962).
4. **Mixed Regimes:** Common in most practical turbulent flows, where droplets experience a combination of coherent mean shear and random turbulent pressure fluctuations (like in pipe flows and channel boundary layers). The deformation pathway is complex, combining stretching along the mean shear axis with local wrinkling by turbulent eddies (Rosti et al. 2019).
5. **Viscous Effects in the Inertia-Dominated Regime:** Occur when the dispersed phase viscosity is high. Although the external deforming forces are inertial, the internal viscous stresses damp deformation and delay breakup, requiring the Ohnesorge correction to the critical Weber number.

1.3.2 Viscous-Dominated Regime

This class describes the breakup of droplets smaller than the Kolmogorov scale η or of those systems where the continuous phase is highly viscous. The flow surrounding the droplet is locally linear and laminar, and the viscous shear stresses are the primary deforming force. The process is characterized by:

1. **Negligible Internal Viscosity** ($\lambda = \mu_d/\mu_c \ll 1$): The deforming force is the continuous phase viscous shear stress. The interface deforms into an ellipsoid aligned near 45 degrees relative to the velocity gradient. Since internal viscous resistance is negligible, the breakup occurs easily at low critical Capillary numbers Ca_{crit} through simple pinch-off (Stone 1994).
2. **Large Internal Viscosity** ($\lambda = \mu_d/\mu_c \gg 1$): Droplets with highly viscous cores show a strong suppression of internal circulation and damp deformation by the internal viscous forces. If λ is greater than 4, rotation dominates over stretching and the droplet cannot be broken by shear alone: it is only possible in extensional flows where rotational effects are absent (Grace 1982).

1.4 Research objectives

The primary objective of this thesis is to systematically isolate and quantify the roles of different turbulent scales in the deformation and fragmentation of fluid droplets. While classical frameworks assume that breakup is driven by resonant eddies of size equal to the droplet, and modern models divide breakup into distinct scale regimes, the precise boundaries separating deforming eddies from passive fluctuations remain unresolved. To address this, a numerical strategy is implemented using interface-resolved Direct Numerical Simulations (DNS) combined with spatial filtering of the turbulent velocity field. By decomposing the flow into low-pass and high-pass components at scales both smaller and larger than the droplet size, the critical scale thresholds required to trigger interface instability are determined. The analysis of the resulting breakup statistics, daughter size distributions, and capillary-kinetic energy transfer allows the evaluation of how deformable interfaces modulate the turbulent energy cascade.

2. Methodology

To better comprehend the breakup process and establish a rigorous physical interpretation of the numerical results, it is crucial to outline the governing equations of the multiphase system, the turbulence forcing and the methods used to characterize the energy cascade. This chapter details the mathematical framework implemented in the solver, the filtering selection and the simulations performed.

2.1 Solver and governing equations

The dynamics of a two-phase system composed of two immiscible, incompressible, and Newtonian fluids are governed by the Navier-Stokes equations. In this approach, the two phases are bounded by an infinitesimally small interface and they are treated as a single mixture with physical properties (density and viscosity) that vary discontinuously across the interface.

This study was performed using FluTAS (Fluid Transport Accelerated Solver): a solver for massive Direct Numerical Simulations (DNS) on multi-CPU and multi-GPU specific for incompressible multiphase flows, with heat transfer study possible. This code written in modern Fortran and parallelized using hybrid MPI/OpenMP and accelerated with OpenACC directives has been tested and validated with different multiphase benchmark cases showing a deviation of less than 1% from reference values.

The code uses the finite-difference method in a staggered variable arrangement and it involves also the solution of a Poisson equation to constrain the velocity divergence.

At the base of this code, there are the mass conservation and the momentum equations, which are formulated as:

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (2.1)$$

$$\rho \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + f_i^\sigma + f_i^T \quad (2.2)$$

where u_i is the velocity vector component (with indices $i, j = 1, 2, 3$ representing the spatial

directions), p is the pressure field, ρ is the fluid density, μ is the dynamic viscosity, f_i^σ is the volumetric surface tension force component acting at the interface, and f_i^T is the external body force component (such as large-scale forcing or gravity).

To study thermal transport or buoyancy effects, the temperature field is governed by the energy equation:

$$\rho C_p \left(\frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} \right) = \frac{\partial}{\partial x_i} \left(k_{th} \frac{\partial T}{\partial x_i} \right) \quad (2.3)$$

where T is the temperature, C_p is the specific heat capacity at constant pressure, and k_{th} is the thermal conductivity of the mixture.

The physical properties (ρ , μ , C_p , k_{th}) vary across the interface. Using the one-fluid approximation to model this transition, the local mixture properties are updated dynamically at each spatial point based on a phase indicator field (volume fraction) $\phi(\mathbf{x}, t) \in [0, 1]$:

$$\rho(\phi) = \rho_c(1 - \phi) + \rho_d\phi \quad (2.4)$$

$$\mu(\phi) = \mu_c(1 - \phi) + \mu_d\phi \quad (2.5)$$

$$C_p(\phi) = C_{p,c}(1 - \phi) + C_{p,d}\phi \quad (2.6)$$

$$k_{th}(\phi) = k_{th,c}(1 - \phi) + k_{th,d}\phi \quad (2.7)$$

where the subscripts c and d denote the properties of the continuous carrier phase ($\phi = 0$) and the dispersed droplet phase ($\phi = 1$), respectively.

The capillary force term f_i^σ represents the surface tension acting locally at the interface. It is modeled using the Continuum Surface Force (CSF) approach (Brackbill et al. 1992):

$$f_i^\sigma = \sigma \kappa \frac{\partial \phi}{\partial x_i} \quad (2.8)$$

where σ is the surface tension coefficient and κ is the local interface curvature.

The curvature is defined as the negative divergence of the unit normal vector n_i pointing from

the continuous phase to the dispersed phase:

$$n_i = \frac{\frac{\partial \phi}{\partial x_i}}{\sqrt{\frac{\partial \phi}{\partial x_k} \frac{\partial \phi}{\partial x_k}}} \quad (2.9)$$

$$\kappa = -\frac{\partial n_i}{\partial x_i} = -\frac{\partial}{\partial x_i} \left(\frac{\frac{\partial \phi}{\partial x_i}}{\sqrt{\frac{\partial \phi}{\partial x_k} \frac{\partial \phi}{\partial x_k}}} \right) \quad (2.10)$$

When analyzing buoyancy-driven systems or small temperature-induced density variations, the gravitational force $f_{g,i}$ (represented as part of the external force f_i^T) is modeled using the Boussinesq approximation:

$$f_{g,i} = \rho_0 g_i [1 - \beta_T (T - T_0)] \quad (2.11)$$

where ρ_0 is the reference density, g_i is the gravity vector component, β_T is the thermal expansion coefficient of the fluid, and T_0 is the reference temperature. For buoyancy-neutral emulsions with matched densities ($\rho_c = \rho_d = \rho_0$), the gravity term is neglected.

2.1.1 Phase Advection and VOF-MTHINC Formulation

The spatial distribution of the dispersed phase is tracked implicitly on the Eulerian grid. The transport of the volume fraction $\phi(\mathbf{x}, t)$ is governed by the pure advection equation:

$$\frac{\partial \phi}{\partial t} + u_i \frac{\partial \phi}{\partial x_i} = 0 \quad (2.12)$$

To prevent numerical diffusion from smearing the interface while ensuring strict mass conservation, FluTAS solves this transport equation using the Multi-dimensional Tangent Hyperbola for Interface Capturing (MTHINC) scheme (Xiao et al. 2005; Cialesi-Esposito, Scapin, et al. 2023). MTHINC regularizes the discontinuous indicator function within each cell using a hyperbolic tangent profile. In one dimension, the profile along coordinate x is written as:

$$\tilde{\phi}(x) = \frac{1}{2} \left[1 + \tanh \left(\beta_{th} \left(\frac{x - x_{int}}{\Delta x} \right) \right) \right] \quad (2.13)$$

where β_{th} controls the interface thickness (typically set between 1.5 and 2.5), and x_{int} represents the coordinate of the interface center within the grid cell of size Δx .

2.2 Numerical Discretization and Pressure-Velocity Coupling

2.2.1 Spatial Discretization

The governing equations are discretized on a structured, three-dimensional cubic computational domain of size 2π by 2π by 2π , employing triply periodic boundary conditions in all spatial directions. The spatial discretization is performed on a staggered MAC grid (Harlow et al. 1965) to prevent checkerboard pressure oscillations:

- Scalar quantities (p , T , ϕ , ρ , μ) are located at the cell centers (i, j, k) .
- Velocity components (u_1 , u_2 , and u_3 , representing u , v , and w) are defined at the centers of the cell faces perpendicular to their respective coordinate directions, i.e., u_1 is defined at $(i \pm 1/2, j, k)$, u_2 at $(i, j \pm 1/2, k)$, and u_3 at $(i, j, k \pm 1/2)$.
- Viscous terms and pressure gradients are discretized using a second-order central difference scheme. Convective terms in the momentum equations are discretized using a second-order conservative central scheme.

2.2.2 Time Integration (Fractional-Step Method)

A fractional-step projection method is used to integrate the velocity and pressure fields in time, ensuring that the velocity field remains solenoidal at the end of each time step. The time step is advanced from n to $n + 1$ via the following sequence:

1. **Intermediate Velocity Prediction:** An intermediate velocity field u_i^* is computed without the pressure gradient term:

$$\frac{\rho^* u_i^* - \rho^n u_i^n}{\Delta t} = R_i^n \quad (2.14)$$

where R_i^n represents the discretized convective terms, viscous terms, gravitational forces,

and surface tension forces at time step n (advanced using a second-order Adams-Bashforth scheme), and ρ^* is the predicted density field computed from the updated volume fraction ϕ^{n+1} .

2. **Pressure Poisson Equation:** The final velocity field at $n + 1$ must satisfy continuity ($\frac{\partial u_i^{n+1}}{\partial x_i} = 0$). By taking the divergence of the projection step:

$$u_i^{n+1} = u_i^* - \frac{\Delta t}{\rho^{n+1}} \frac{\partial p^{n+1}}{\partial x_i} \quad (2.15)$$

yielding the variable-coefficient Poisson equation for pressure:

$$\frac{\partial}{\partial x_i} \left(\frac{1}{\rho^{n+1}} \frac{\partial p^{n+1}}{\partial x_i} \right) = \frac{1}{\Delta t} \frac{\partial u_i^*}{\partial x_i} \quad (2.16)$$

3. **Velocity Correction:** Once the pressure p^{n+1} is solved, the divergence-free velocity field is updated:

$$u_i^{n+1} = u_i^* - \frac{\Delta t}{\rho^{n+1}} \frac{\partial p^{n+1}}{\partial x_i} \quad (2.17)$$

2.3 Large-Scale Forcing

To study the interaction between droplet deformation and turbulent eddies in a statistically steady state, the turbulence must be sustained against viscous dissipation. In a triply periodic domain, this is achieved by adding a large-scale volume forcing term f_i^T to the predicted velocity step in the momentum equation:

$$\frac{\rho^* u_i^* - \rho^n u_i^n}{\Delta t} = R_i^n + f_i^T \quad (2.18)$$

In this study, the turbulence is sustained using the Arnold-Beltrami-Childress (ABC) forcing field, which represents the standard forcing scheme implemented in the FluTAS solver (Crales-

Esposito, Scapin, et al. 2023). The forcing acceleration components are defined as:

$$f_x^T = Q [A \sin(k_f z) + C \cos(k_f y)] \quad (2.19)$$

$$f_y^T = Q [B \sin(k_f x) + A \cos(k_f z)] \quad (2.20)$$

$$f_z^T = Q [C \sin(k_f y) + B \cos(k_f x)] \quad (2.21)$$

where $A = B = C = 1$ are the classical coefficients, $k_f = 2$ is the forcing wavenumber, and Q is a positive forcing coefficient, maintained at unity throughout the entire run. By injecting kinetic energy only at the largest scales (wavenumbers $k_f = 2$), the forcing ensures that the turbulent energy cascade develops naturally and remains unforced in the inertial and dissipative subranges, where the droplet-turbulence interactions take place.

2.4 Turbulence Statistics

To characterize the turbulent carrier flow and evaluate the characteristic scales of the system, statistical quantities are computed as volume averages over the entire computational domain. While dense emulsions require phase-conditioned averaging to account for differences in local phase properties (Crales-Esposito, Rosti, et al. 2022), the present study involves a highly dilute system consisting of a single droplet in a triply periodic domain (corresponding to a very small dispersed phase volume fraction $\alpha \approx 0.004$) with matched density ($\rho_d = \rho_c$) and viscosity ($\mu_d = \mu_c$). Under these conditions, the flow properties are uniform across both phases, and global volume averages represent the turbulent state of the entire system.

2.4.1 Volume Averaging

Let $\psi(\mathbf{x}, t)$ be any local flow variable. The volume-averaged value of ψ over the entire domain is denoted by $\langle \psi \rangle$:

$$\langle \psi \rangle = \frac{1}{V} \int_V \psi(\mathbf{x}, t) dV \quad (2.22)$$

where $V = 8\pi^3$ is the volume of the computational domain.

2.4.2 Turbulent Kinetic Energy and Viscous Dissipation

The turbulent carrier phase intensity is characterized by the global turbulent kinetic energy and the global viscous dissipation rate:

- **Turbulent Kinetic Energy (TKE):**

$$K = \frac{1}{2} \langle u'_i u'_i \rangle \quad (2.23)$$

where $u'_i = u_i - \langle u_i \rangle$ represents the local velocity fluctuation relative to the mean flow. Since the mean velocity is zero ($\langle u_i \rangle = 0$) due to periodic boundary conditions and large-scale ABC forcing, the velocity fluctuation matches the instantaneous local velocity: $u'_i = u_i$.

- **Viscous Dissipation Rate:** The local viscous dissipation rate ε is defined as:

$$\varepsilon = 2\nu S_{ij} S_{ij} \quad (2.24)$$

where $S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ is the strain-rate tensor, and $\nu = \mu/\rho$ is the constant kinematic viscosity of the matched phases. The global average viscous dissipation rate is denoted by $\langle \varepsilon \rangle$.

2.4.3 Turbulence Scales

Using the global average dissipation $\langle \varepsilon \rangle$ and kinematic viscosity ν , the characteristic turbulence scales are defined as:

- **Kolmogorov Length Scale (η):**

$$\eta = \left(\frac{\nu^3}{\langle \varepsilon \rangle} \right)^{1/4} \quad (2.25)$$

- **Kolmogorov Time Scale (τ_η):**

$$\tau_\eta = \left(\frac{\nu}{\langle \varepsilon \rangle} \right)^{1/2} \quad (2.26)$$

- **Taylor Microscale (λ):**

$$\lambda = \sqrt{\frac{15\nu u_{rms}^2}{\langle \varepsilon \rangle}} \quad (2.27)$$

where $u_{rms} = \sqrt{\frac{2}{3}K}$ is the root-mean-square velocity.

- **Taylor-Scale Reynolds Number (Re_λ):**

$$Re_\lambda = \frac{u_{rms}\lambda}{\nu} \quad (2.28)$$

These global scales describe the turbulent state of the carrier flow into which the droplet is introduced.

2.4.4 Scale-by-Scale Spectral Energy Budget

To analyze the scale-dependent energy exchange between the fluid interfaces and the carrier-phase eddies, the cumulative scale-by-scale kinetic energy budget in the Fourier domain (wavenumber space) is considered, which integrates the spectral contributions over a sphere of radius k (i.e., for all wavevectors $\boldsymbol{\kappa}$ such that $|\boldsymbol{\kappa}| < k$):

$$\frac{\partial}{\partial t} \sum_{|\boldsymbol{\kappa}| < k} E(\boldsymbol{\kappa}) = \Pi(k) + \sum_{|\boldsymbol{\kappa}| < k} D(\boldsymbol{\kappa}) + \Pi_\sigma(k) + \sum_{|\boldsymbol{\kappa}| < k} F(\boldsymbol{\kappa}) \quad (2.29)$$

where the cumulative fluxes are defined as the sum of the spectral contributions over the wavevectors within the sphere:

- $\Pi(k) = \sum_{|\boldsymbol{\kappa}| < k} T(\boldsymbol{\kappa})$ is the cumulative non-linear kinetic energy flux.

- $\Pi_\sigma(k) = \sum_{|\boldsymbol{\kappa}| < k} S_\sigma(\boldsymbol{\kappa})$ is the cumulative capillary energy flux, representing the work done by the surface tension force.

The individual terms represent the three-dimensional fields in spectral space:

- $E(\boldsymbol{\kappa}) = \langle \tilde{u}_i \tilde{u}_i^* \rangle_t$ is the time-averaged kinetic energy in the spectral domain.
- $T(\boldsymbol{\kappa}) = -\langle \tilde{G}_i \tilde{u}_i^* + \tilde{G}_i^* \tilde{u}_i \rangle_t$ is the time-averaged energy transfer due to the non-linear convective terms.
- $D(\boldsymbol{\kappa}) = -\langle \tilde{V}_i \tilde{u}_i^* + \tilde{V}_i^* \tilde{u}_i \rangle_t$ is the time-averaged viscous dissipation.
- $S_\sigma(\boldsymbol{\kappa}) = -\langle \tilde{f}_i^\sigma \tilde{u}_i^* + \tilde{f}_i^{\sigma*} \tilde{u}_i \rangle_t$ is the time-averaged work done by the surface tension force.
- $F(\boldsymbol{\kappa}) = \langle \tilde{f}_i^T \tilde{u}_i^* + \tilde{f}_i^{T*} \tilde{u}_i \rangle_t$ is the time-averaged energy input due to the large-scale forcing.

This energy budget (Crales-Esposito, Rosti, et al. 2022) provides a thermodynamic definition of the Hinze scale $d_H = 2\pi/k_H$ as the zero-crossing wavenumber where the net capillary energy exchange vanishes:

$$\Pi_\sigma(k_H) = 0 \quad (2.30)$$

For scales larger than the Hinze scale ($k < k_H$, or $d > d_H$), $\Pi_\sigma(k) < 0$, indicating that droplets act as energy sinks, absorbing energy to deform. For scales smaller than the Hinze scale ($k > k_H$, or $d < d_H$), $\Pi_\sigma(k) > 0$, showing that interfaces act as energy sources, releasing stored capillary energy back into the flow through oscillations and pinch-off.

2.5 Simulation process

This section presents a detailed description of the numerical campaign, outlining the physical setup, the spatial filtering configuration, and the simulation parameters that establish the foundation of this research. In total, 136 Direct Numerical Simulations (DNS) were performed on the Leonardo (CINECA) High Performance Computing (HPC) system. The computational campaign started with a single-phase reference, followed by 15 distinct realizations for each selected multiphase configuration to ensure statistical significance.

2.5.1 Filtering

The fundamental distinction between **Reynolds-Averaged Navier-Stokes (RANS)** modeling, **Large-Eddy Simulation (LES)** and **Direct Numerical Simulation (DNS)** lies in the range of turbulent scales that are resolved or modeled.

In this study, this range is controlled systematically through spatial filtering of the velocity field. This approach of using filtered velocity fields to isolate the physical effects of different turbulent scales is inspired by the numerical experiments on scalar transport, entrainment, and mixing conducted by Cimarelli et al. (2021) and Boga et al. (2024). A *Low-Pass Filter (LP)* restricts the velocity field to scales larger than a cut-off length Δ , whereas a *High-Pass filter (HP)* retains only the fluctuations below this threshold. While other filter configurations exist (such as Band-Pass or Band-Reject filters), they are not considered here as the analysis focuses on separating large-scale from small-scale structures.

The filter dimension Δ is related to the *cut-off wavenumber* k_c in spectral space by the relation:

$$k_c = \frac{\pi}{\Delta} \quad (2.31)$$

which determines the size of the turbulent eddies allowed to interact with the droplet interface.

The filters initially selected for this work are: the Gaussian Filter, the Sharp Cut-Off, the Butterworth and the Top-Hat Filter.

Table 1 summarizes the mathematical formulation of these filters in both the physical and Fourier spaces. In turbulence research, spectral space representations are often preferred as they allow for a direct analysis of energy distribution across wavenumbers. The spectral transfer functions (specifically of the LP configurations) are illustrated in Figure 3.

Filter Type	Physical Domain $G(\mathbf{x})$	Fourier Domain $\hat{G}(\mathbf{k})$
Gaussian	$\left(\frac{6}{\pi\Delta^2}\right)^{3/2} \exp\left(-\frac{6 \mathbf{x} ^2}{\Delta^2}\right)$	$\exp\left(-\frac{ \mathbf{k} ^2\Delta^2}{24}\right)$
Top-Hat	$\begin{cases} \frac{1}{\Delta^3} & \text{if } x_i \leq \frac{\Delta}{2} \\ 0 & \text{otherwise} \end{cases}$	$\prod_{i=1}^3 \frac{\sin\left(\frac{k_i\Delta}{2}\right)}{\frac{k_i\Delta}{2}}$
Sharp Cut-off	$\prod_{i=1}^3 \frac{\sin(k_c x_i)}{\pi x_i}$	$\begin{cases} 1 & \text{if } k_i \leq k_c \\ 0 & \text{otherwise} \end{cases}$
Butterworth	-	$\frac{1}{1 + \left(\frac{ \mathbf{k} }{k_c}\right)^{2N}}$

Table 1: Mathematical formulations of the spatial filters in physical and Fourier domains.

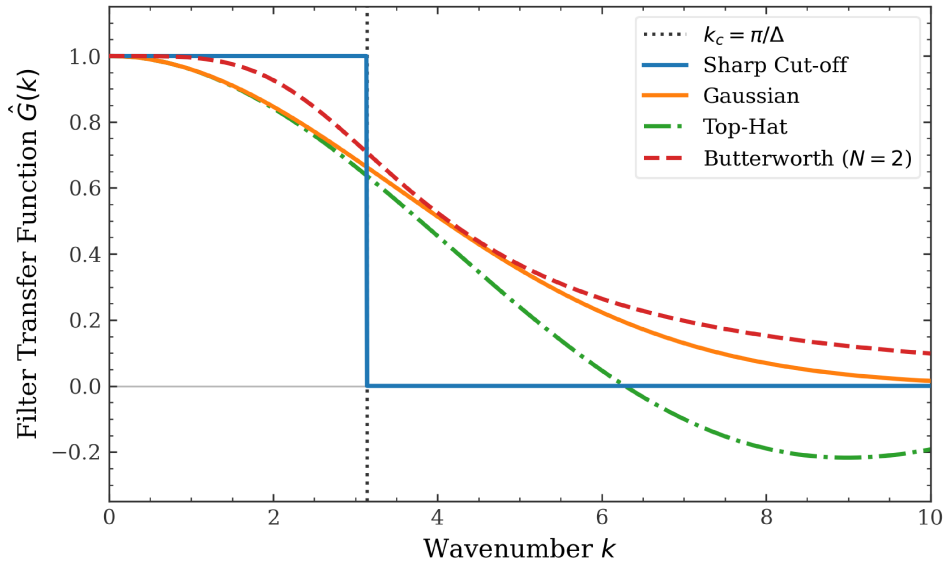


Figure 3: Spectral behavior of the filters tested.

These filters were tested in a single-phase flow, with a domain length $L = 2\pi$, a total number of points per direction of $N = 64$ in the first place and then $N = 96$, and both ρ and μ set to 1.

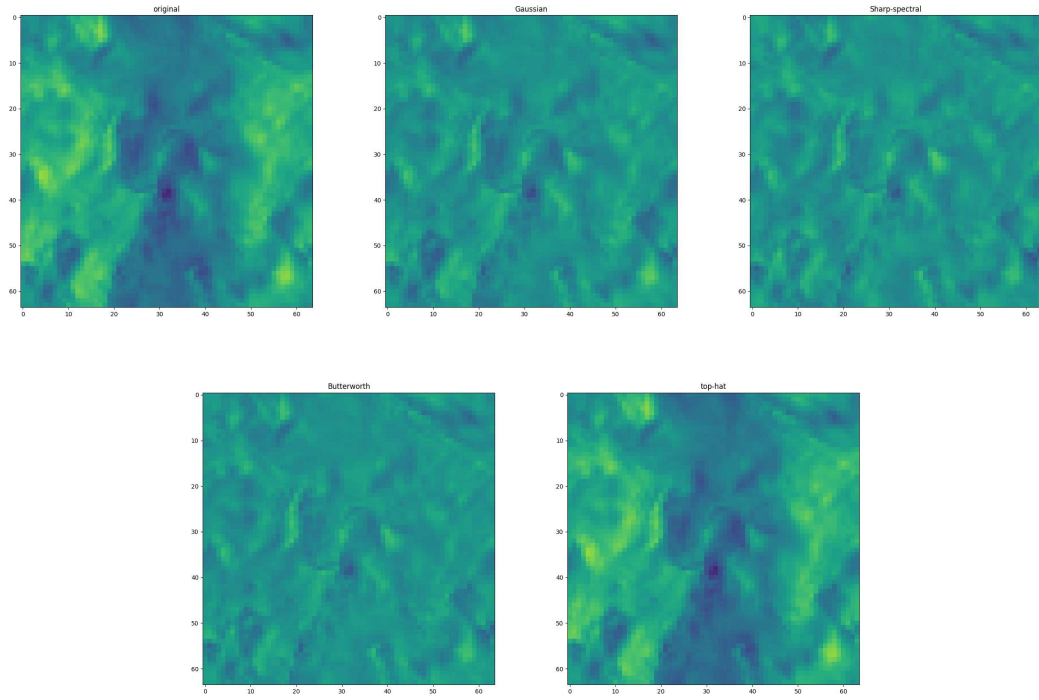


Figure 4: Filters resolution with $N = 64$

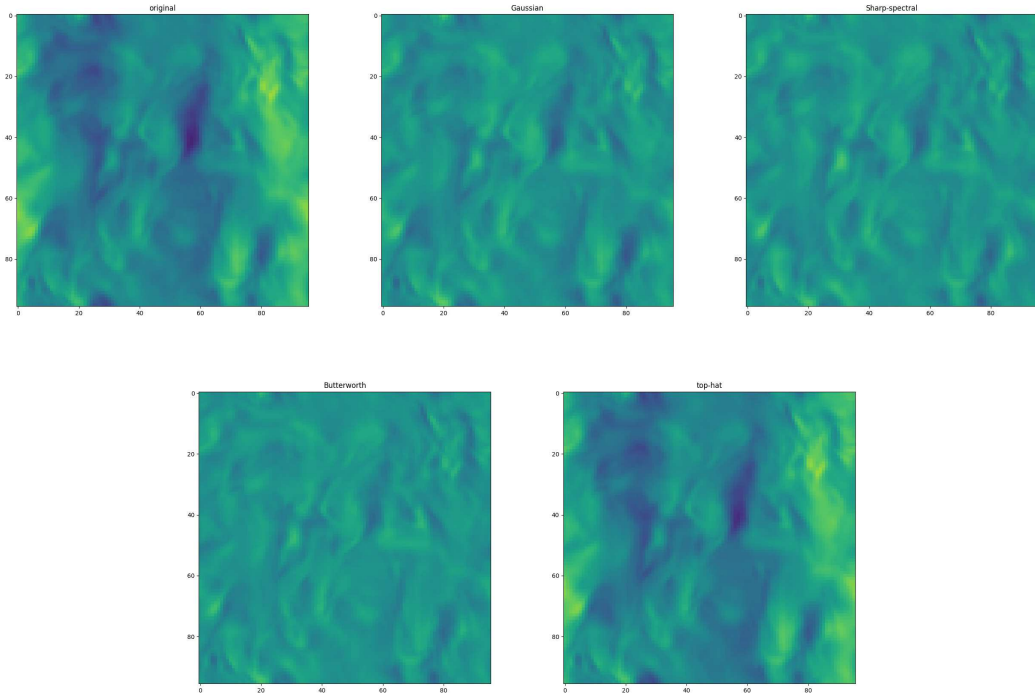


Figure 5: Filters resolution with $N = 96$

Figure 4 and Figure 5 visualize the different response of all filters and a smoothness variation

moving to $N = 96$, as a consequence of the increased number of points.

Given its widespread implementation and superior performance in both the physical and spectral domain, the final choice converged on the Gaussian filter: it reproduces the original velocity field without a high gain, unlike the Top-Hat filter.

To illustrate how the spatial filtering mathematically affects the energy spectrum $E(k)$ of the single-phase flow, the filtering operation is considered in Fourier space. A filtered velocity component $\hat{u}_i(\mathbf{k})$ is obtained by multiplying the unfiltered Fourier coefficient $\hat{u}_i(\mathbf{k})$ by the transfer function of the filter $\hat{G}(\mathbf{k})$:

$$\hat{u}_i(\mathbf{k}) = \hat{G}(\mathbf{k})\hat{u}_i(\mathbf{k}) \quad (2.32)$$

Since the energy spectrum $E(k)$ represents the kinetic energy integrated over a spherical shell of radius k in Fourier space, the filtered energy spectrum $E_{LP}(k)$ for the Low-Pass configuration is given by:

$$E_{LP}(k) = |\hat{G}(k)|^2 E(k) \quad (2.33)$$

Substituting the transfer function of the Gaussian filter $\hat{G}(k) = \exp\left(-\frac{k^2\Delta^2}{24}\right)$ yields:

$$E_{LP}(k) = E(k) \exp\left(-\frac{k^2\Delta^2}{12}\right) \quad (2.34)$$

Conversely, the High-Pass filtered velocity field in physical space is defined by subtracting the filtered field from the original field, $\mathbf{u}_{HP}(\mathbf{x}) = \mathbf{u}(\mathbf{x}) - \bar{\mathbf{u}}(\mathbf{x})$. In Fourier space, this operation yields $\hat{u}_{HP,i}(\mathbf{k}) = (1 - \hat{G}(\mathbf{k}))\hat{u}_i(\mathbf{k})$. Consequently, the High-Pass filtered energy spectrum $E_{HP}(k)$ is formulated as:

$$E_{HP}(k) = |1 - \hat{G}(k)|^2 E(k) = E(k) \left[1 - \exp\left(-\frac{k^2\Delta^2}{24}\right)\right]^2 \quad (2.35)$$

These relations illustrate the mathematical attenuation introduced by the Gaussian filter across the wavenumber range, providing a baseline to interpret the spectral energy content of the filtered simulations.

2.5.2 Setup Identification

Due to its higher resolution, the simulation with $N = 96$ was chosen as the starting single-phase configuration. The subsequent step involved the introduction of the droplet, which was gradually placed over 1000 timesteps to allow pressure and velocity fields to adapt to the droplet interface.

The density and viscosity ratio were kept at unity, but the dynamic viscosity of both phases were modified. This adjustment was made to achieve sufficient spatial resolution, ensuring that the grid spacing $dx = \frac{L}{N}$ remains close to the Kolmogorov scale η to avoid the under-resolution of the smallest scales.

μ	0.01	μ	0.03	μ	0.045
dx	0.06544	dx	0.06544	dx	0.06544
η	0.02122	η	0.04818	η	0.06559
λ	0.49315	λ	0.85402	λ	1.04792
Re_λ	139	Re_λ	81	Re_λ	66
(a)		(b)		(c)	

Table 2: μ variation at $N = 96$.

Varying μ resulted in a reduction of Re_λ while increasing η , thereby achieving a resolution of ratio $\frac{dx}{\eta} \sim 1$. For this specific reason, $\mu = 0.045$ was selected for both carrier and dispersed phases.

Once the single-phase reached convergence, the droplet was placed at the center of the computational domain. The initial diameter was set at $D \approx L/3$ (corresponding to $d = 30dx = 1.96349$), with a surface tension of $\sigma = 14.0261$ and a filter cut-off scale of $\Delta = d/2$.

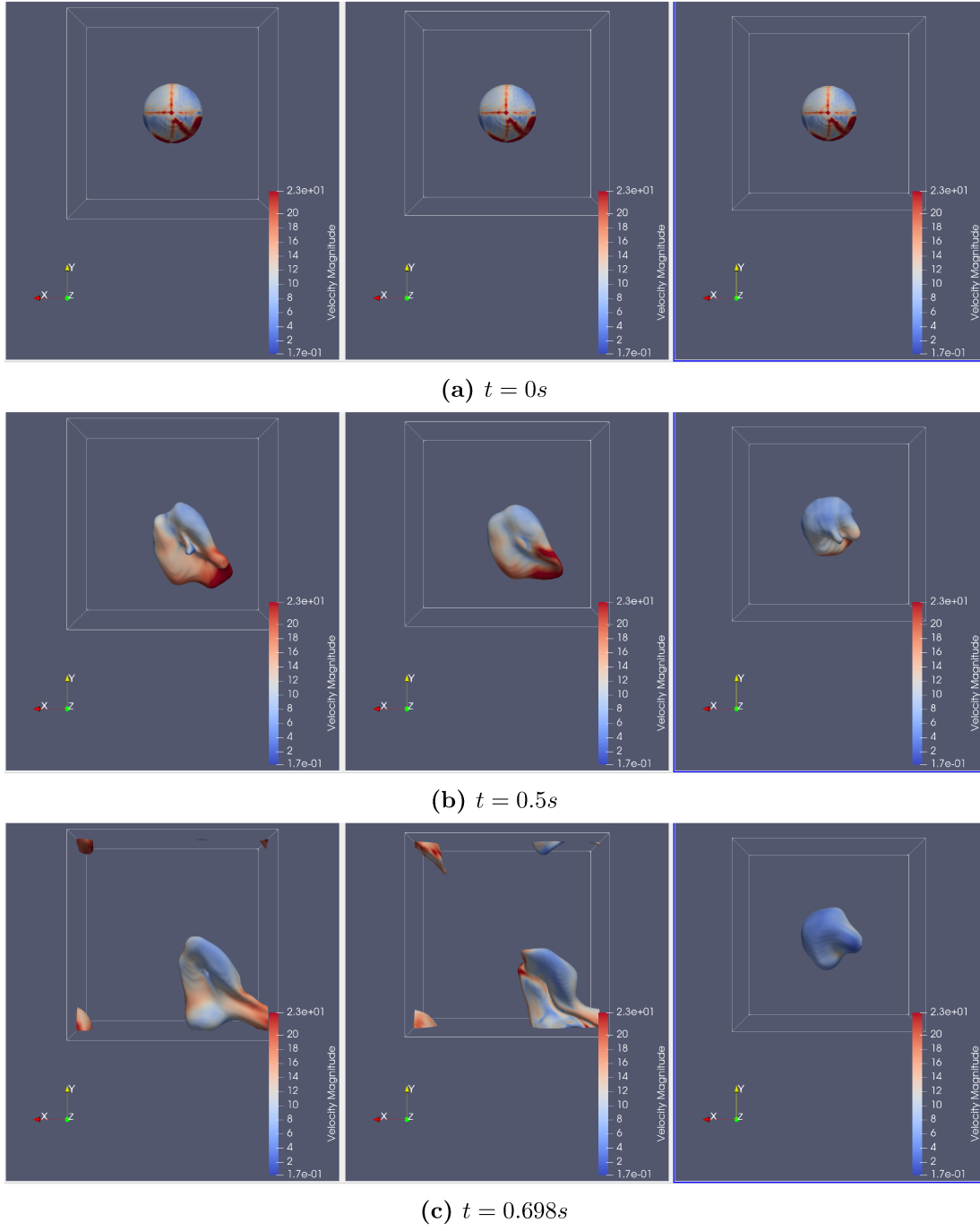


Figure 6: Comparison of the droplet deformation between No Filter (NF), Low-Pass (LP), and High-Pass (HP) configurations (left to right) from $t = 0s$ to $t = 0.698s$.

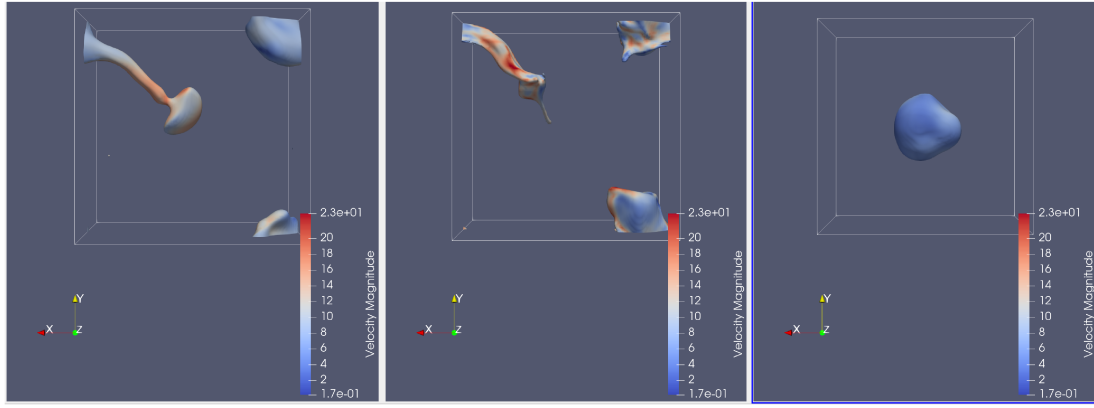
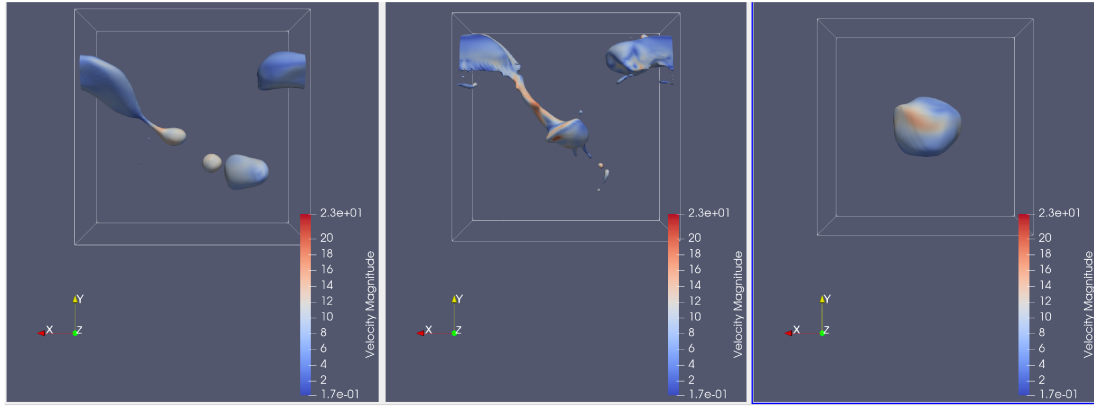
(d) $t = 0.903s$ (e) $t = 1.1s$

Figure 6: Comparison of the droplet deformation between No Filter (NF), Low-Pass (LP), and High-Pass (HP) configurations from $t = 0.903s$ to $t = 1.1s$.

This preliminary setup revealed the potential outcome of the study, giving a first representation of the distinct response of filters with the Low-Pass case (centre of Figure 6) depicting a phenomenology similar to the unfiltered/real reference case (left of Figure 6) leading to the fragmentation. The High-Pass filter exhibited a minor deformation but did not undergo breakup.

2.5.3 Critical Weber number

The Weber number We was addressed as the critical parameter governing the balance between deforming stresses and stabilizing capillary forces. The first formulation (Eq. 1.2) is velocity-dependent but does not account for small-scale phenomena. The formulation used to address this is given by Eq. 2.36, shown below, which introduces the dissipation ε .

$$We = \frac{(\rho_c \langle \varepsilon \rangle)^{2/3} d^{5/3}}{\sigma} \quad (2.36)$$

To calibrate the simulation setup, the surface tension coefficient σ was systematically varied to identify the threshold where the droplet is close to its critical state of stability, ensuring that minor turbulent fluctuations could trigger breakup.

A starting value of $\sigma = 30$ was tested, yielding a Weber number $We = 0.2$, and then progressively reduced down to $\sigma = 3.74387$, which was the exact surface tension needed to obtain $We = We_c = 1$

To ensure a clear separation of spectral scales and preserve the physical integrity of the spatial filtering operation, the droplet diameter was reduced from $D = 2\pi/3$ (1/3 of the domain size) to $D = \pi/3 \approx 1.047$ (1/6 of the periodic domain size $L = 2\pi$).

This choice shifts the characteristic wavenumber of the droplet to $k_D = 2\pi/D = 6$, spectrally decoupling the interface-induced physics (such as capillary work and deformation) from the large-scale turbulent forcing range, which typically acts at wavenumbers $k \leq 3$. Consequently, direct interference between the global energy injection and local capillary mechanisms is avoided.

Furthermore, reducing D shifts the corresponding filtering scales Δ (and thus the cut-off wavenumbers $k_c = \pi/\Delta$) toward higher-frequency, better-resolved spectral regions (for instance, $k_c \approx 6$ for $\Delta = 0.5D$). This extends the resolved inertial subrange prior to the onset of interfacial effects, while ensuring that these scales remain well-resolved within the grid resolution.

The final parameters are summarized below:

N	192
d	1.0472
dx	0.032725
η	0.064645
$\langle \varepsilon \rangle$	5.21798
σ	3.74387
$We_c(\varepsilon)$	1
λ	0.97284
u_{rms}	2.70484
Re_λ	58

(a)

Table 3: Final setup parameters.

2.5.4 Computational Campaign

The simulations were carried out on the Leonardo (CINECA) supercomputer to manage the heavy data load, using a refined grid of 192^3 points. To ensure statistical significance and convergence of the turbulent statistics, an ensemble-based approach was adopted.

The initial campaign, consisting of 5 realizations per category, was extended to 15 independent realizations per configuration. This resulted in a total of 135 multiphase simulations, providing 30 independent runs for each selected filter dimension, detailed in Figure 7.

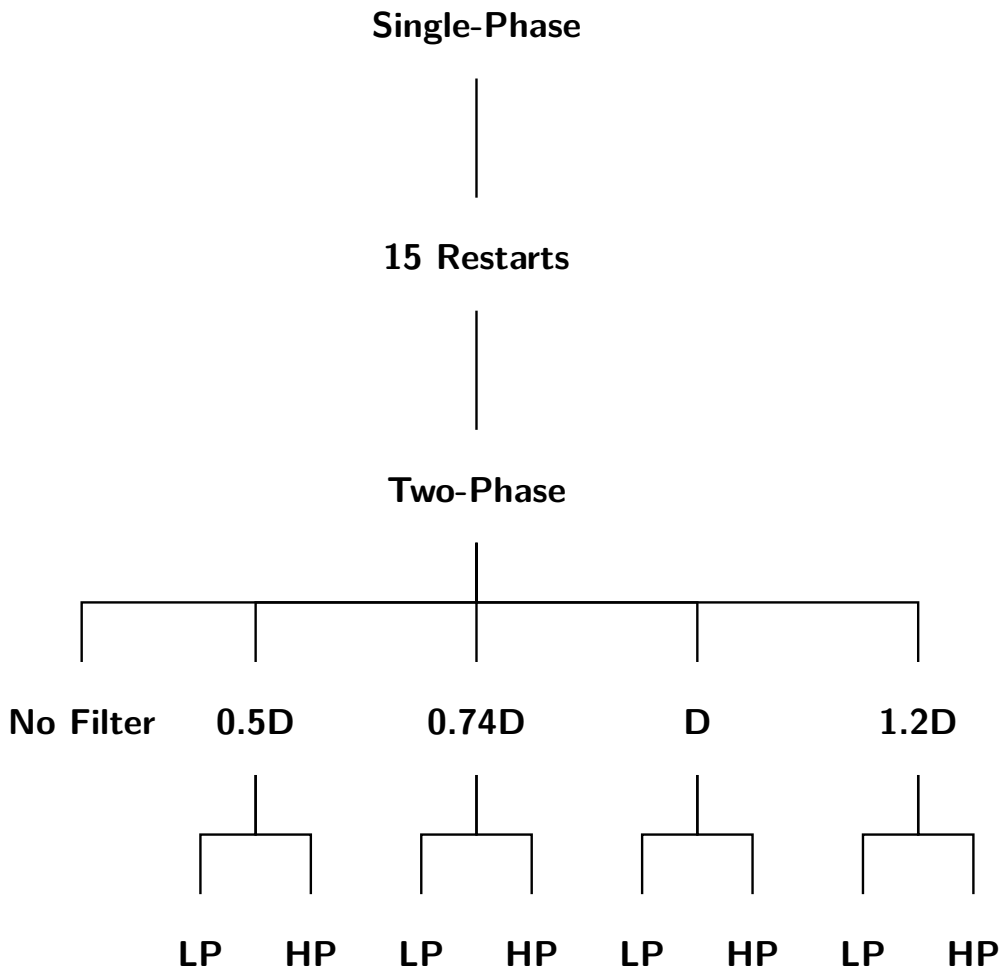


Figure 7: Simulations campaign workflow tree outlining the different execution branches, starting conditions, and filtering configurations.

In order to have the exact same amount of energy exchanged and make the whole study statistically consistent, the duration of each restart has been adequately adjusted to ensure the same dwell time of the droplet.

This statistical approach is schematically illustrated in Figure 8. To establish a consistent statistical ensemble, the single-phase carrier flow is first run until it reaches a statistically stationary turbulent state at t_1 . From this developed single-phase field, multiple independent snapshots (denoted as $SP_1, SP_2, \dots, SP_{15}$) are extracted at regular time intervals during the stationarity window. Because the single-phase statistics (such as the average energy dissipation rate $\langle \varepsilon \rangle$ and turbulent kinetic energy) are constant in time, starting the multiphase runs from these different snapshots guarantees that each droplet is introduced into a carrier flow with the same statistical energy content, ensuring full statistical consistency.

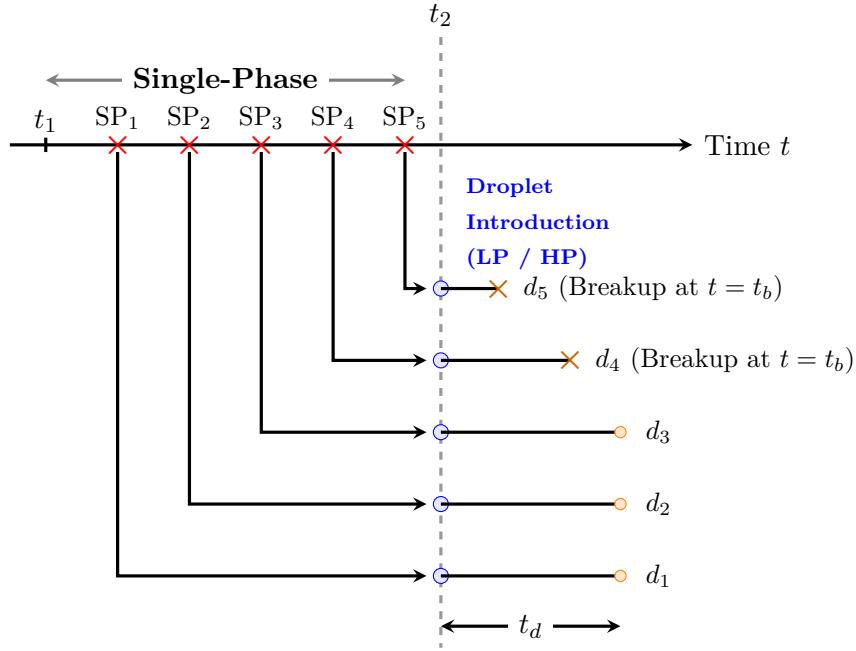


Figure 8: Schematic of the simulation campaign workflow. The single-phase flow is run until a statistically steady state is reached (t_1). During the development period (SP), independent flow field snapshots (SP_1 to SP_5) are extracted. At t_2 , multiphase restart simulations are initialized from these snapshots by placing a droplet in the domain. The restarts are run for a normalized presence time t_d . If breakup occurs, the run ends at $t_b < t_d$ (marked with an $\times$); otherwise, the simulation completes the full duration t_d without fragmentation (marked with a circle).

At the restart time t_2 , a droplet is placed at the center of the domain. In the filtered configurations, the carrier velocity field from the corresponding snapshot is spatially filtered (Low-Pass or High-Pass) prior to the droplet's introduction. The physical time of the multiphase simulations is normalized by the large-eddy turnover time T_L , defined as:

$$T_L = \frac{L}{u_{rms}} \quad (2.37)$$

where $L = 2\pi$ is the size of the computational domain and u_{rms} is the root-mean-square velocity of the turbulent carrier phase. Each multiphase simulation is run for a maximum normalized droplet presence time of $t_d = 4T_L$. If the droplet undergoes fragmentation, the simulation is evaluated at the breakup time $t_b < t_d$ (as shown for cases d_4 and d_5 in Figure 8). Otherwise, the simulation runs for the complete duration t_d without breaking (cases d_1 , d_2 , and d_3). This normalized timeframe ensures that all non-breaking droplets experience the exact same duration of turbulent shear stress and capillary energy exchange, allowing for a rigorous and unbiased comparison across the entire parameter space.

Figure 9 gives an overview of two 0.5D runs, highlighting the different behaviors of the two topologies.

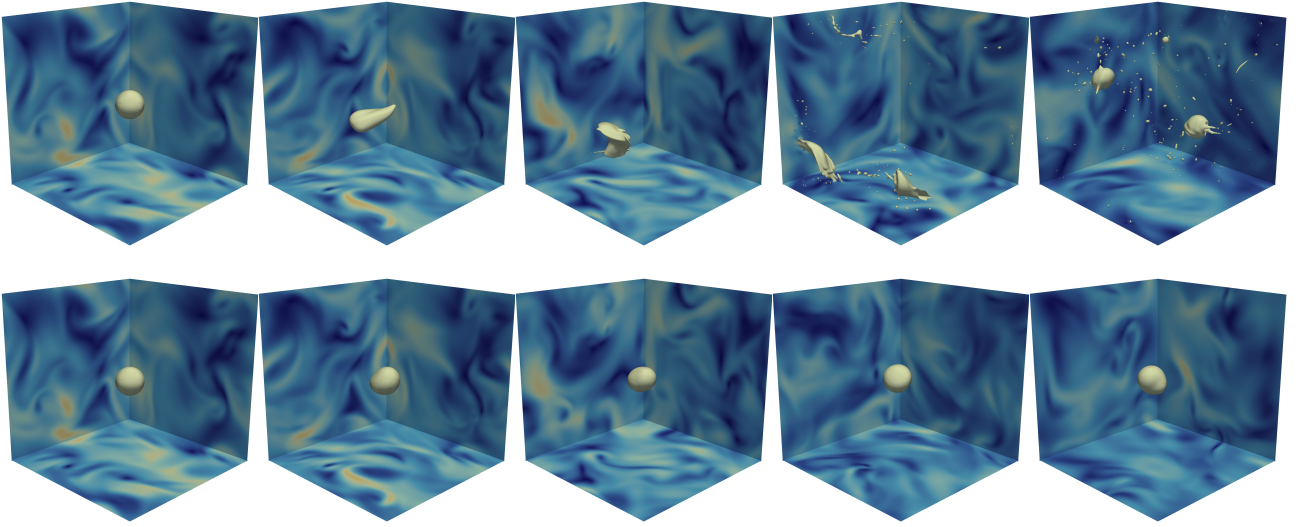


Figure 9: Evolution of the droplet fragmentation from $t_0 = 0s$ to $t_4 = 7.6s$ for the case with filter size $0.5D$: top row represents the Low-Pass topology, while the bottom row represents the High-Pass topology.

3. Results

When a droplet is immersed in a turbulent flow, it undergoes progressive deformation and may eventually fragment. This chapter presents the physical mechanisms underlying breakup, revealing a strongly asymmetric response of the droplet depending primarily on the filter topology and, secondarily, on the cut-off scale.

3.1 Scale Implications on Droplet Breakup

The simulations display a strong dependence of the fragmentation process on the scales seen by the droplet, confirming the hypothesis that eddies of at least the size of the droplet are necessary to trigger fragmentation.

Comparing the low-pass (large-scale) and high-pass (small-scale) filtered cases with the unfiltered reference runs, almost all simulations show the separation of small fluid volumes. However, not all of these events represent physical breakup: some correspond to the shedding of tiny droplets due to local interface fluctuations or numerical discretization effects at the grid level.

In order to properly address real breakups, the criterion adopted is based on the ratio of the biggest droplet volume V_{max} to the initial droplet volume V_0 , defined as β :

$$\beta = \frac{V_{max}}{V_0}$$

A threshold of $\beta = 0.95$ is defined: simulations with higher values are not classified as physical breakup events, even when small droplets are generated.

Figures 10 and 11 show the differences between the unfiltered, Low-Pass, and High-Pass cases in terms of breakup occurrence:

the LP cases display a higher rate of breakups compared to the real unfiltered simulations, generating in almost every case smaller droplets.

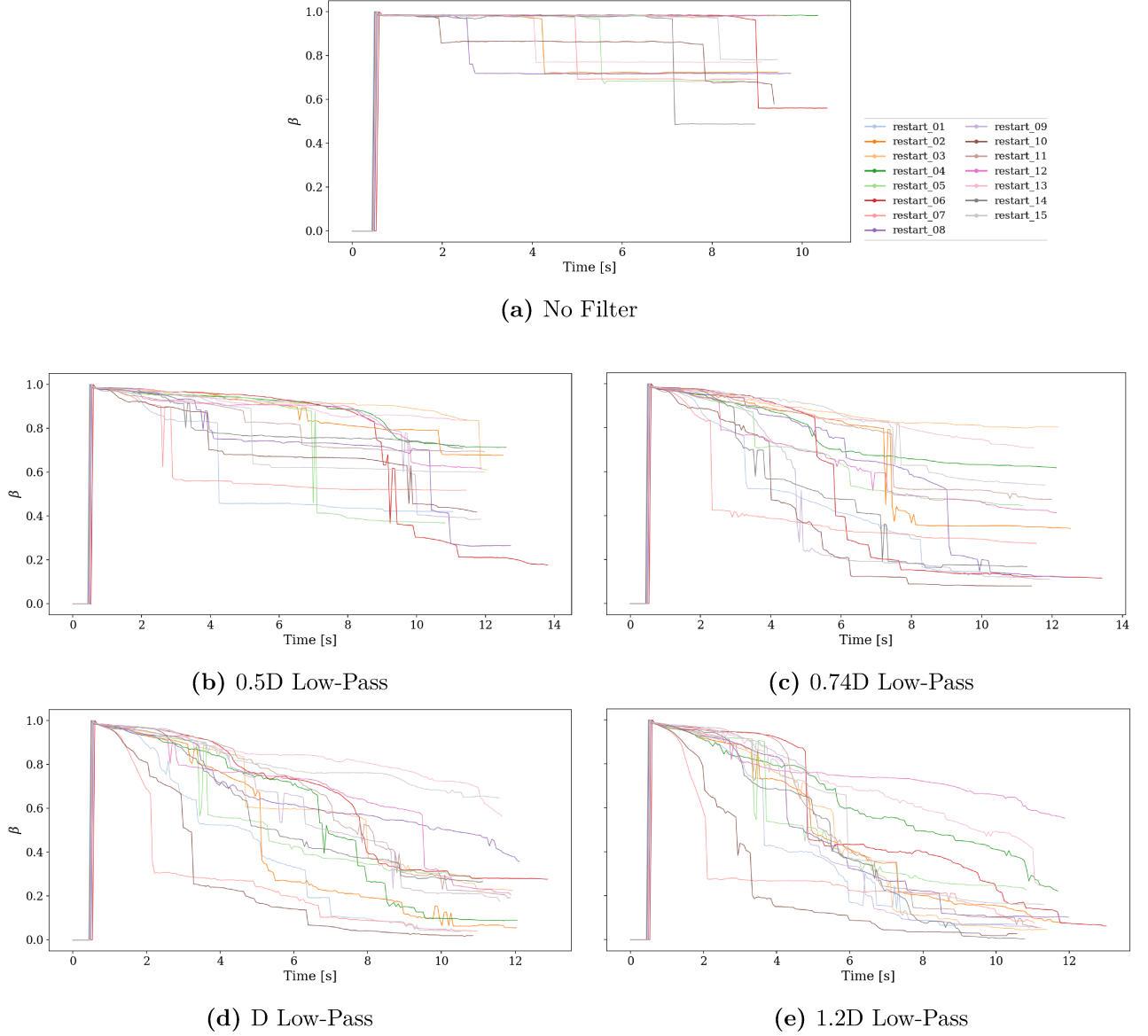
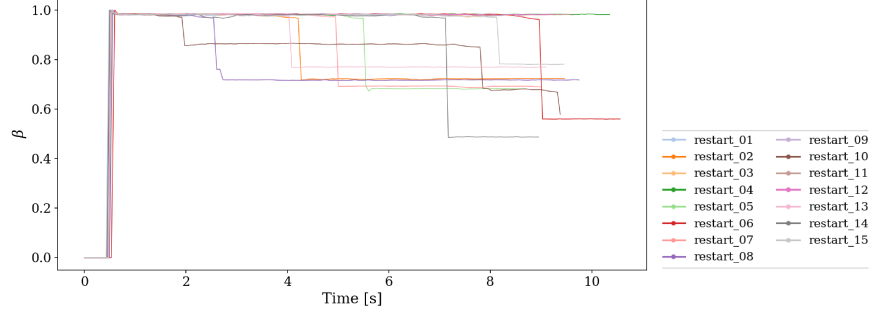
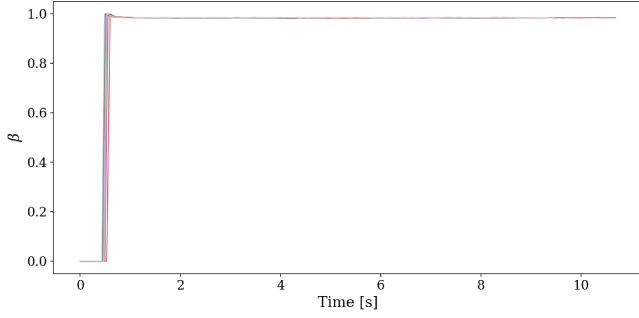
**Figure 10:** Volume ratio Low-Pass

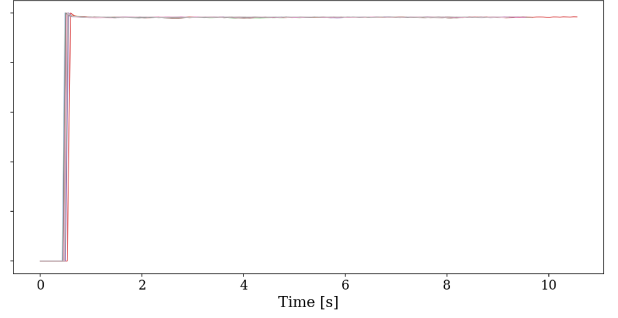
Figure 10 also underlines that varying the filter dimension actively alters the final volume of all the droplets generated: a reduction in droplet diameter is observed as the filter cut-off scale increases from $0.5D$, where less than 50% of runs show $\beta < 0.50$, to $1.2D$, where only 3 simulations have $\beta > 0.20$.



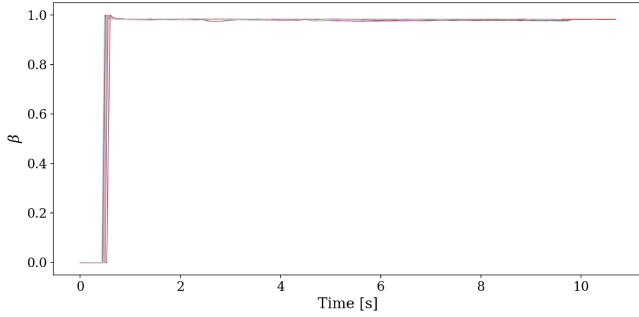
(a) No Filter



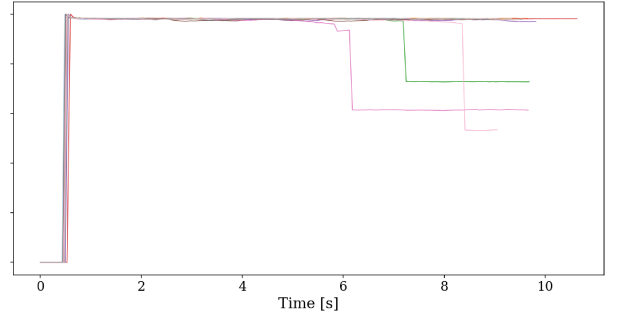
(b) 0.5D High-Pass



(c) 0.74D High-Pass



(d) D High-Pass



(e) 1.2D High-Pass

Figure 11: Volume ratio High-Pass

These data confirm the thesis that turbulent structures must be larger than the droplet diameter d in order to obtain fragmentation. The breakup probability rises to 20% only when the filter lets through scales bigger than the diameter d , as shown in Figure 11e, which allows large-scale deformation. This deformation inevitably increases the likelihood of fragmentation.

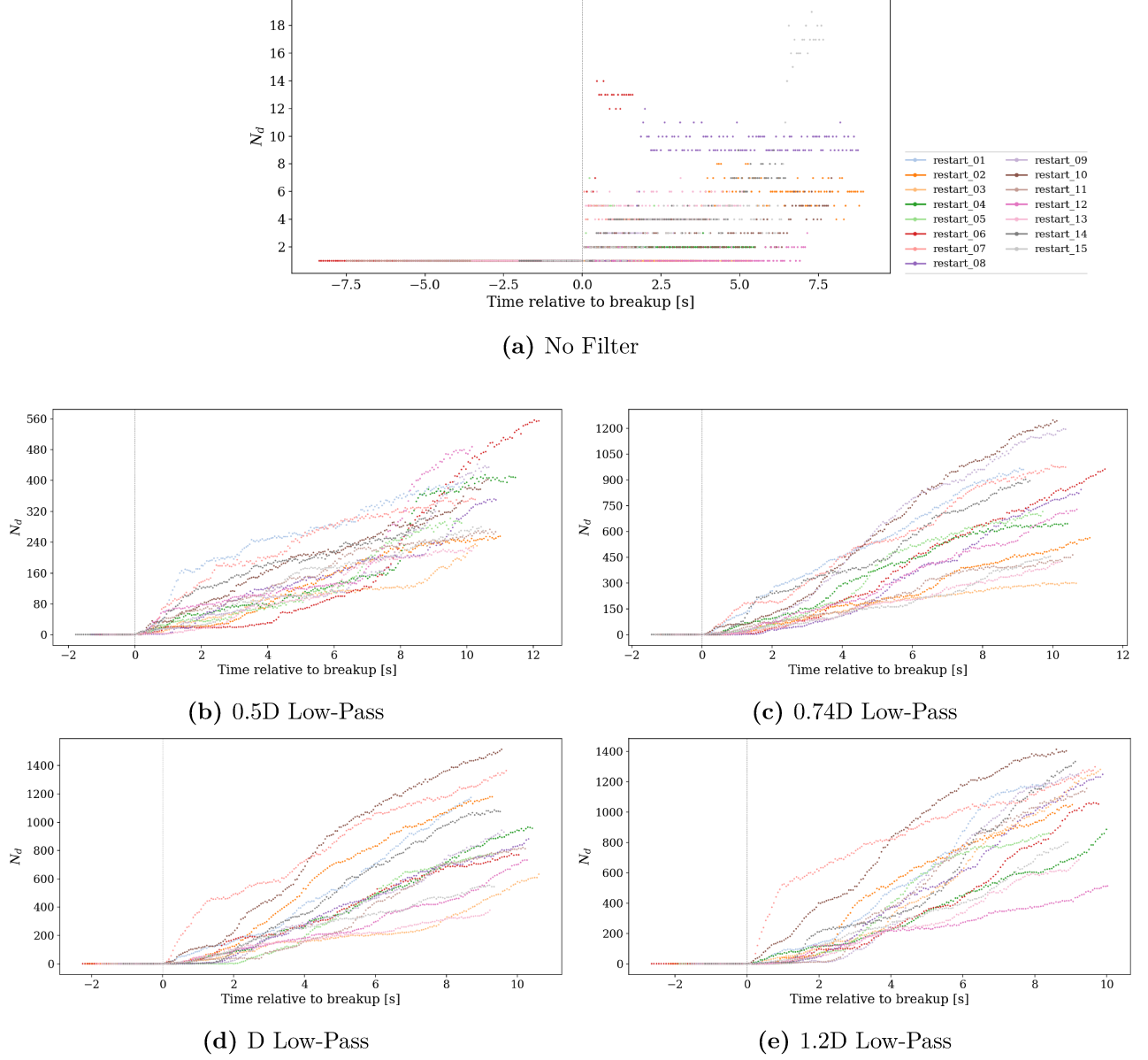


Figure 12: Number of droplets generated by Low-Pass (LP) and Unfiltered Cases

Figure 12 shows the total number of droplets generated, highlighting how the filter size affects their count as a direct consequence of mass conservation. Additionally, Figure 13 underscores how only the High-Pass filter of scale $1.2D$ causes fragmentation, generating fewer droplets than the unfiltered reference cases.

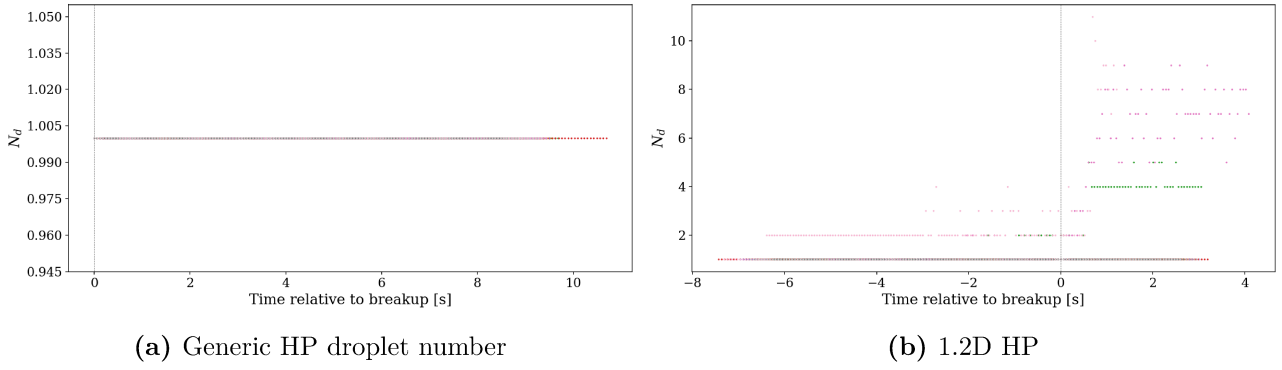


Figure 13: Direct comparison of droplets in: (a) a generic High-Pass (HP) filter case and (b) the only High-Pass (HP) filter case that showed breakup.

3.1.1 Low-Pass (LP) filtering effects

The droplet's deformation generates regions of high curvature κ . Looking at the surface tension term described in Eq. 2.8, high curvature regions generate strong velocity gradients which are extremely localized due to the Dirac's delta δ .

Due to this local nature, when the filtering operation is performed the VOF equation Eq. 2.12 is not able to see the contribution of surface tension forces because the feedback mechanism has been removed. Consequently, the stabilizing effect of surface tension is severely diminished, and the droplet inevitably undergoes fragmentation.

This mechanism explains why larger low-pass filter cut-off scales lead to smaller daughter droplets. Removing the small-scale velocity fluctuations prevents the carrier phase from responding to capillary feedback, allowing the large-scale hydrodynamic strain to deform and fragment the interface unimpeded. On the other hand, shifting the filter towards small scales increases the scales required to mitigate the deforming force effects.

Defining the breakup rate γ as the ratio of successful breakup events n_{bk} to the total number of simulations N , the strongly asymmetric behavior between the Low-Pass and the High-Pass filter is outlined in Table 4, where every Low-Pass case reaches breakup while the highest probability of breakup for High-Pass runs increases up to 20% only for the 1.2D scale.

$$\gamma = \frac{n_{bk}}{N}$$

Simulations	No Filter	0.5D		0.74D		D		1.2D	
		HP	LP	HP	LP	HP	LP	HP	LP
Breakups	9	0	15	0	15	0	15	3	15
Restarts	15	15	15	15	15	15	15	15	15
γ (%)	60	0	100	0	100	0	100	20	100

Table 4: Breakups per simulation type.

3.2 Energy spectra

The energy spectrum directly supports the breakup statistics shown by the volume ratio β , revealing how Low-Pass simulations have a higher energy content at small scales compared to unfiltered and High-Pass simulations and the reason of this outcome lies in the filter itself and the subsequent fragmentation process.

Large-scales allowed by the Low-Pass filter cause the droplet to see strong turbulent structures that will not be counterbalanced by the surface tension force, thus inducing fragmentation into thousands of small droplets. This feedback is missing only inside the *VOF* equation, as previously seen, but it is still present inside the scale-by-scale energy budget: therefore, the fragmentation into smaller droplets increases the total interfacial area, then resulting into an increase of the f_i^σ term at small scales, explaining the higher energy content at high wavenumbers.

This spectral difference is illustrated in Figure 14.

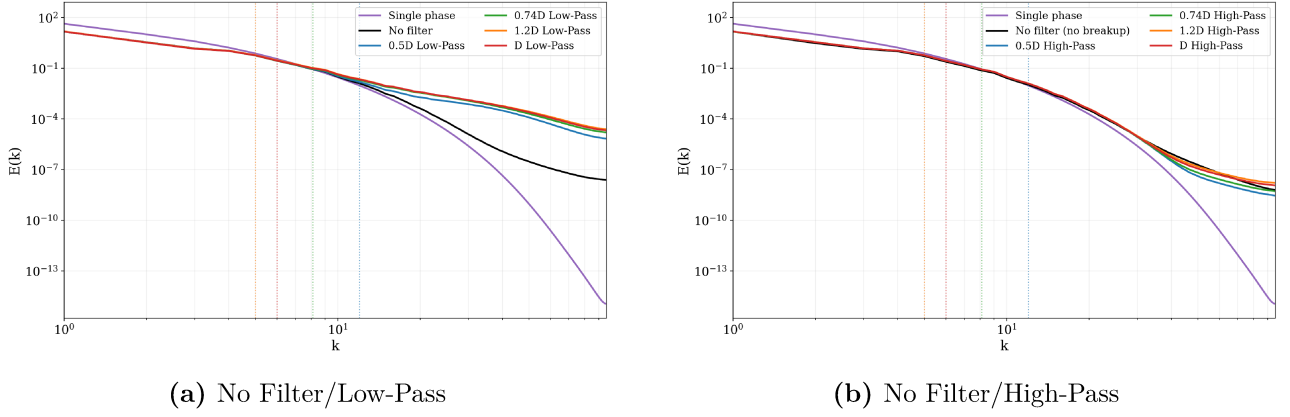


Figure 14: High-Pass and Low-Pass energy spectra compared to Single-Phase and Unfiltered spectra.

Figure 15 shows how the energy content at small scales diminishes with decreasing filter scale, for both topologies. For the Low-Pass topology, this is related to the progressively smaller total number of daughter droplets from $1.2D$ to $0.5D$; for High-Pass filters, this is due to the contraction of the large-scale energy injection range as Δ decreases.

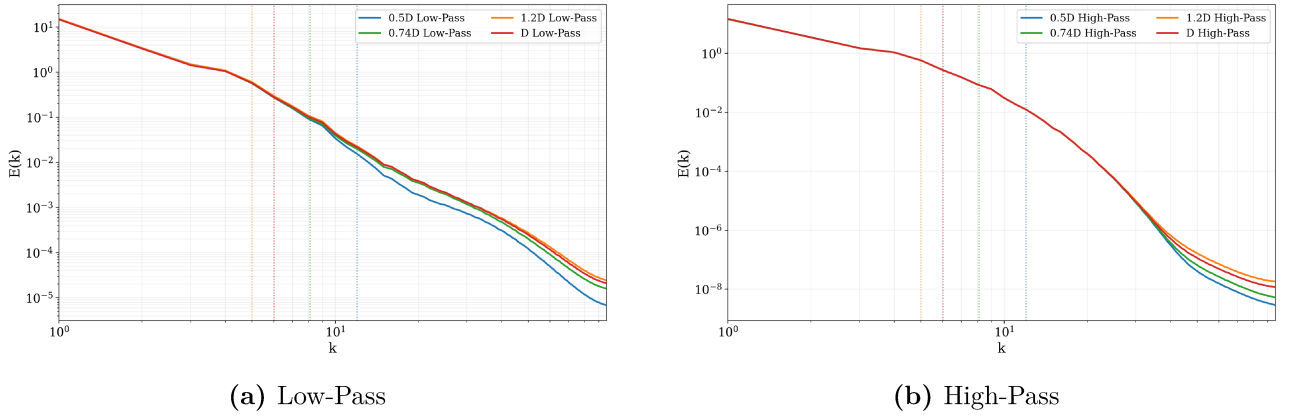


Figure 15: Low-Pass and High-Pass direct energy spectra comparison.

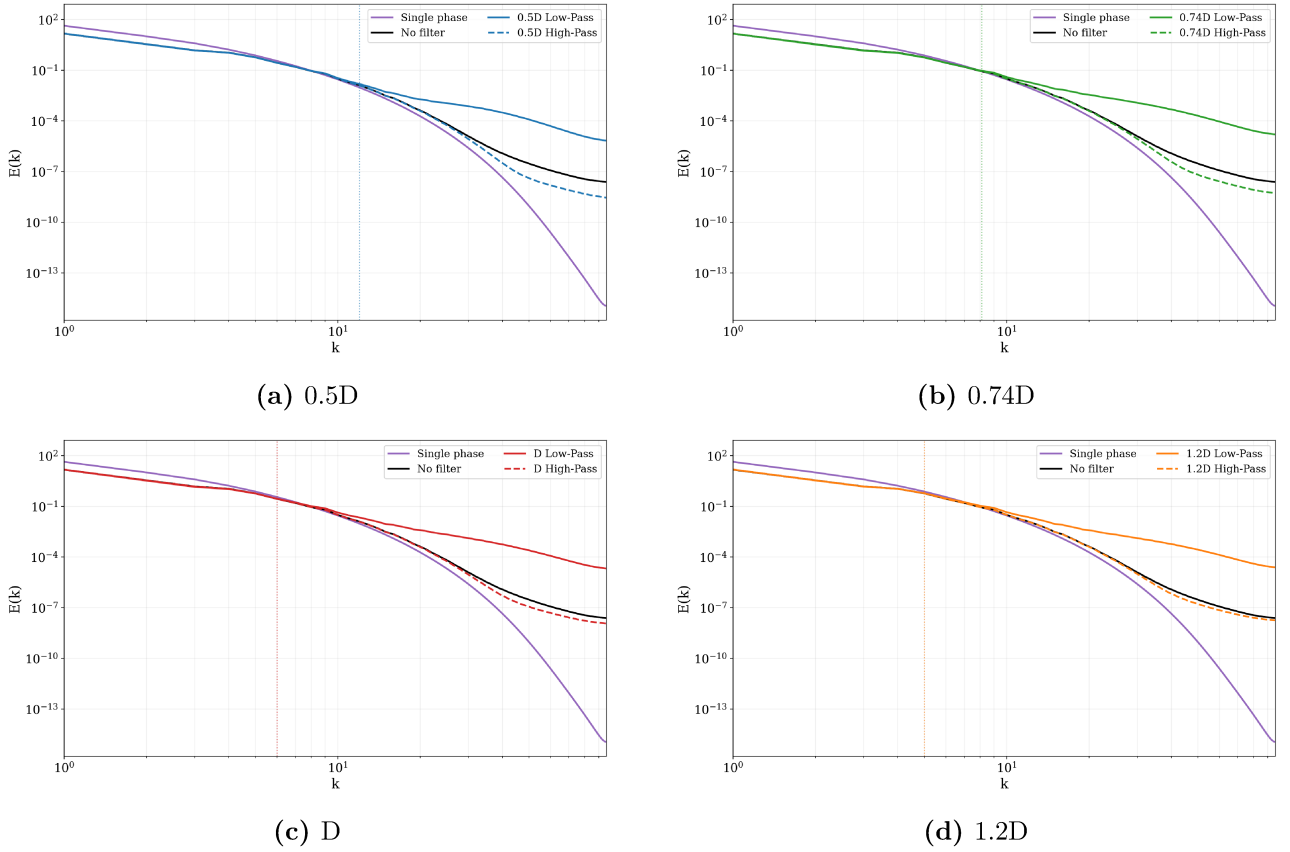


Figure 16: Energy Spectra comparison per filter size. Vertical dashed lines represent the filter scales.

As the HP filter cut-off scale increases, the energy content progressively approaches the unfiltered case. This occurs because a larger cut-off admits more large-scale structures, resulting in stronger turbulent deformations and, ultimately, fragmentation. This explains why some of the 1.2D High-Pass runs reach breakup.

3.3 Structure Functions

The trend illustrated by energy spectra is confirmed by the structure functions S_n . Described as:

$$S_n = \langle [u(x+l, t) - u(x, t)]^n \rangle \quad (3.1)$$

they measure the differences in velocity between two points separated by a distance and they are a statistical observable employed to analyze how velocity fluctuations scale in space.

By modifying the value of the exponent n , different aspects of the turbulent statistics can be analyzed.

For $n = 2$, the second-order structure function $S_2(r)$ represents the scale-by-scale kinetic energy of velocity fluctuations in physical space, which is directly related to the energy spectrum $E(k)$ in Fourier space.

For $n = 3$, the third-order structure function $S_3(r)$ characterizes the spatial kinetic energy flux and is related to the rate and direction of the turbulent energy cascade.

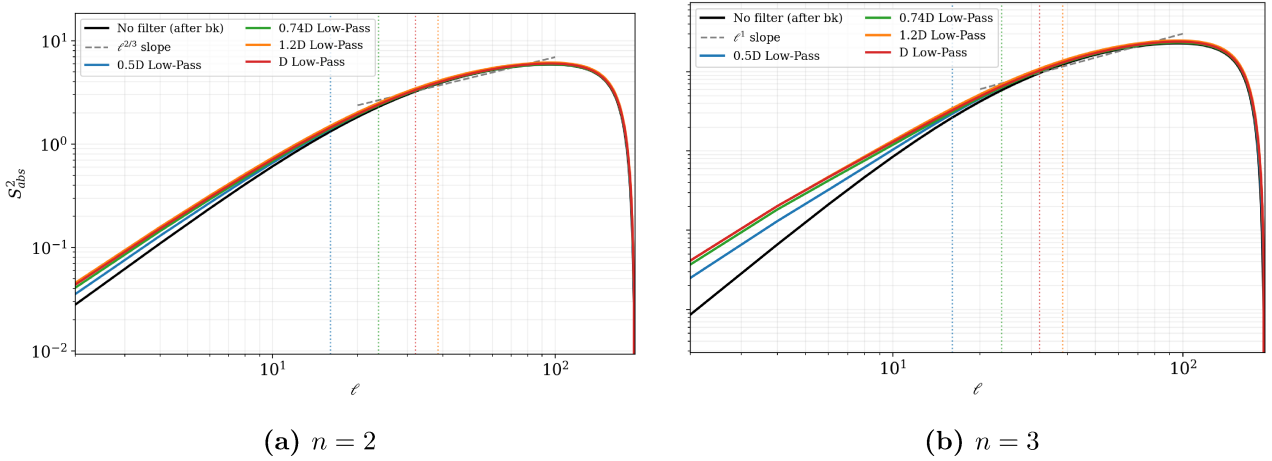


Figure 17: Second-order ($n = 2$) and third-order ($n = 3$) structure functions comparison.

The comparisons of the structure functions for $n = 2$ and $n = 3$ shown in Figure 17 confirm the trends observed in the energy spectra. For the second-order structure function $S_2(r)$ (Figure 17a), the Low-Pass filtered simulations exhibit higher values at small separation distances r compared to the High-Pass and single-phase cases. This upward shift at small scales corresponds to the elevated energy content observed in the high-wavenumber region of the spectral plots, which is driven by the feedback-free, unconstrained breakup of droplets into numerous micro-droplets.

Similarly, the third-order structure function shown in Figure 17b reflects the scale-by-scale energy transfer. Here, the plotted quantity is the absolute structure function $S_a^3(r) = \langle |\delta u|^3 \rangle$, which is positive-definite, rather than the raw signed value. This representation is chosen to permit a clearer comparison of scaling slopes and power-law behaviors in log-log representation. In the present simulations, the Low-Pass curves of $S_a^3(r)$ show a steeper slope at small separations, indicating an enhanced downscale energy transfer flux and a higher rate of local viscous dissipation at those scales. This behavior is consistent with the spectral transfer fluxes and highlights the physical mapping between physical-space velocity differences and the spectral

energy budget.

Additionally, to directly examine the direction of the scale-by-scale energy transfer and align with the JFM methodology of Ciraiesi-Esposito, Boffetta, et al. (2023), the signed third-order structure function $S_3(\ell/L_f) = \langle(\delta u_L)^3\rangle$ is plotted in Figure 18 against the normalized separation scale ℓ/L_f (where $L_f = \pi$ is the characteristic forcing scale).

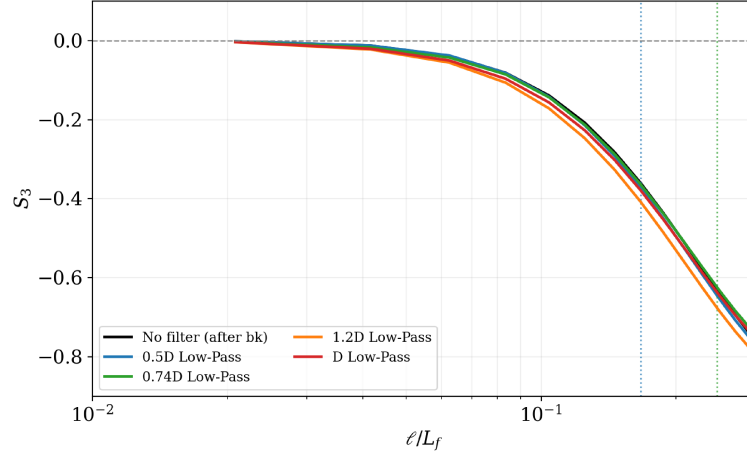


Figure 18: Signed third-order structure function S_3 comparison for low-pass filtered simulations plotted against the normalized scale ℓ/L_f up to 0.3.

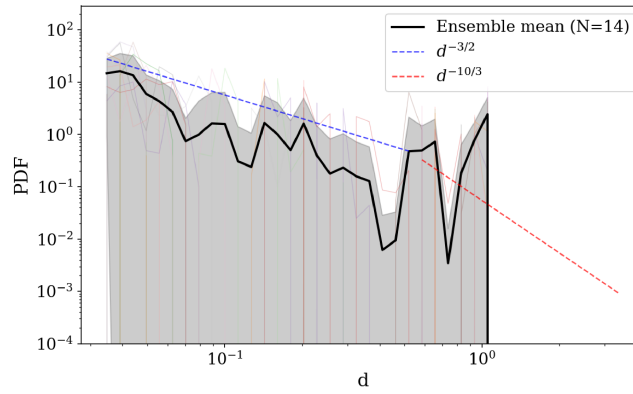
The representation in Figure 18 highlights the physical sign of the third-order structure function, which remains strictly negative across the investigated scale range. According to Kolmogorov’s exact 4/5 law, as discussed by Frisch in his text (Frisch 1995), the signed third-order structure function in the inertial range is negative and proportional to the separation scale ($S_3(r) = -4/5\epsilon r$). This negative sign provides direct physical evidence of a forward (down-scale) energy cascade, directly linking physical-space increments to the constant downscale energy cascade rate. In these low-pass filtered simulations, which retain only the large-scale velocity fluctuations, the magnitude of the negative flux at small separations ($\ell/L_f \lesssim 0.05$) is slightly reduced compared to the unfiltered benchmark, demonstrating that suppressing small-scale structures dampens the local small-scale energy cascade rate.

3.4 Probability Density Function

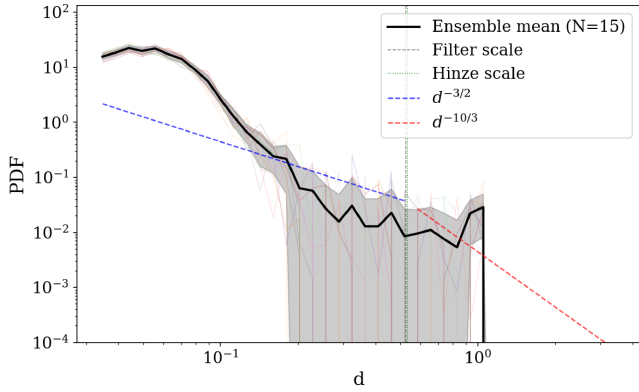
The Probability Density Function (PDF) of the Droplet Size Distribution (DSD) serves as a key statistical observer to characterize the sizes of the daughter droplets generated by the fragmentation process, which subdivide into two distinct regimes separated by the Hinze scale.

For daughter droplets larger than the Hinze scale, the PDF follows a $d^{-3/2}$ power law, which is consistent with the turbulent fragmentation cascade described by Deane and Stokes. In this range, droplet breakup is dominated by large-scale turbulent pressure fluctuations.

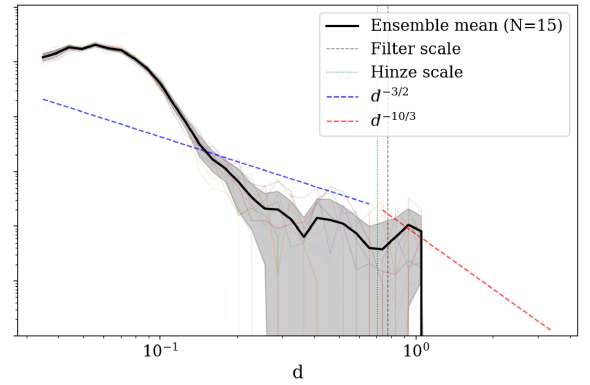
Conversely, for droplets smaller than the Hinze scale, the PDF aligns with a $d^{-10/3}$ power law. In this sub-Hinze regime, droplets are highly stable against turbulent shearing, and their creation is primarily governed by capillary-driven pinch-off and the collapse of thin fluid filaments during major breakup events. To identify the scaling regimes, the two reference power laws are plotted alongside the numerical data.



(a) No Filter



(b) 0.5D Low-Pass



(c) 0.74D Low-Pass

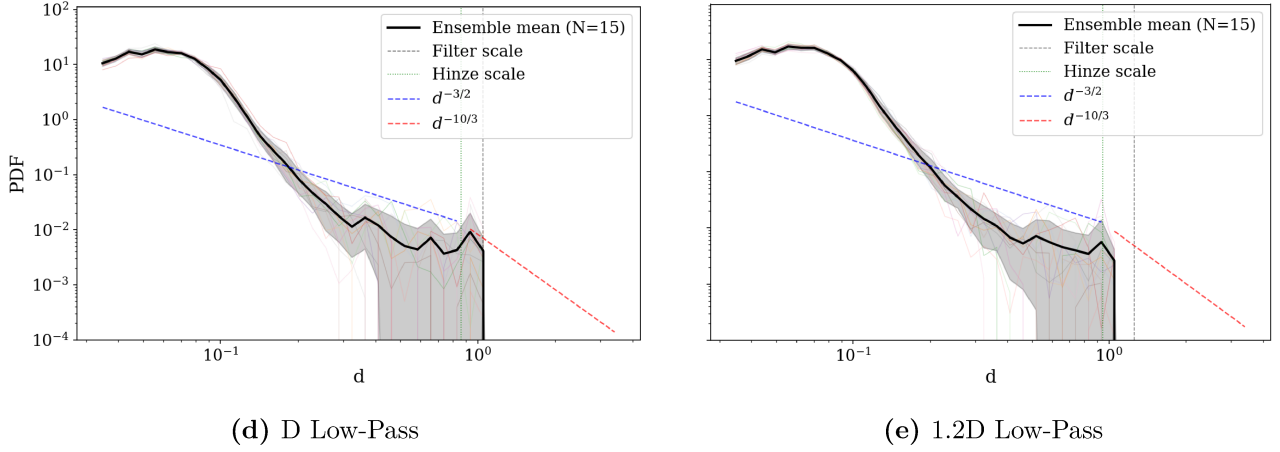


Figure 19: Droplet Size Distribution PDF

Notably, the Low-Pass (LP) simulations display a near-uniform probability across all droplet diameters, indicating a decorrelation of the daughter droplet size from the filter scale.

3.5 Scale-by-scale budget

The scale-by-scale (SBS) kinetic energy budget provides a detailed, wavenumber-resolved characterization of the energy transfer mechanisms, viscous dissipation, and capillary coupling in the two-phase flow. While global energy spectra and physical-space structure functions describe the distribution and scaling of velocity increments, the SBS budget allows one to track how different physical processes compete and balance at each specific spatial scale.

The analysis is formulated by considering the Navier-Stokes momentum equation for a two-phase incompressible flow with dynamic viscosity μ and surface tension σ . Using the Continuum Surface Force (CSF) model (Brackbill et al. 1992), the governing equation is:

$$\rho \left[\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right] = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + f_i^\sigma + f_i^T \quad (3.2)$$

where $f_i^\sigma = \kappa n_i \sigma \delta_s$ is the capillary force acting at the interface, and f_i^T represents the large-scale forcing term used to maintain a statistically steady turbulent state. By performing a spatial Fourier transform and taking the inner product with the complex conjugate velocity $\tilde{u}_i^*$,

the time-averaged kinetic energy budget at wavenumber k is formulated as:

$$\frac{\partial E(k)}{\partial t} = T(k) + D(k) + S_\sigma(k) + F(k) \quad (3.3)$$

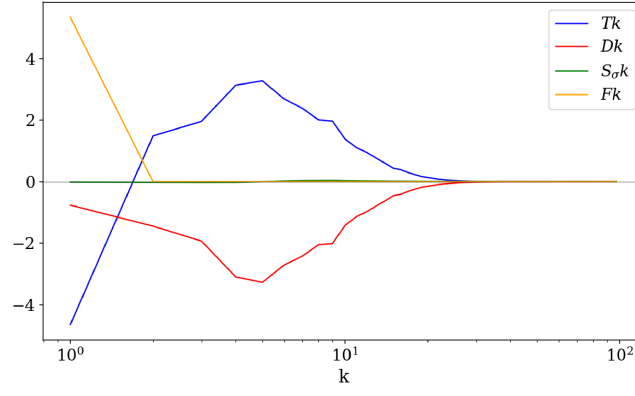
The net rate of energy change vanishes on average, resulting in a balance between all the spectral terms.

The scale-by-scale fluxes for the LP and HP filtered simulations (Figure 20 and Figure 21) show how the different energy budget terms balance across wavenumbers.

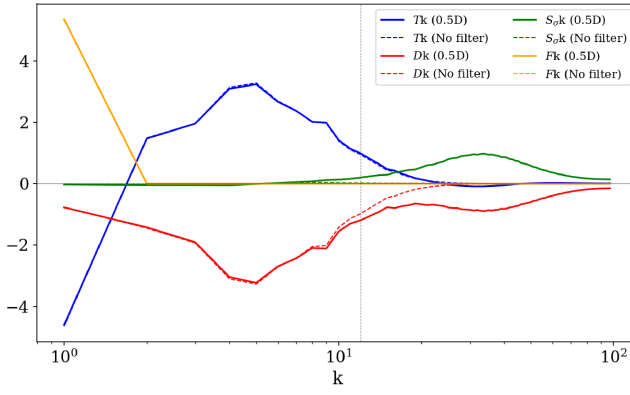
In the unfiltered reference case (Figure 20a), the budget shows that the energy injected by the forcing term $F(k)$ at low wavenumbers is balanced by a combination of convective transfer $T(k)$, which carries energy downscale, and viscous dissipation $D(k)$. Viscous dissipation dominates at higher wavenumbers. The work of surface tension $S_\sigma(k)$ is negative at low wavenumbers, representing kinetic energy absorption (interface-induced dissipation of flow energy) as the interface deforms, and turns positive at high wavenumbers, representing capillary yielding/transfer where stored interface potential energy is released back into the flow as kinetic energy.

For the Low-Pass filtered cases (Figure 20), the convective transfer $T(k)$ exhibits a distinct localized peak just before the filter cut-off wavenumber k_c . This peak represents the accumulation of energy at the smallest resolved scales. Concurrently, both the viscous dissipation $D(k)$ and the surface tension work $S_\sigma(k)$ drop to zero beyond the cut-off k_c , indicating the absence of active subgrid-scale physical mechanisms.

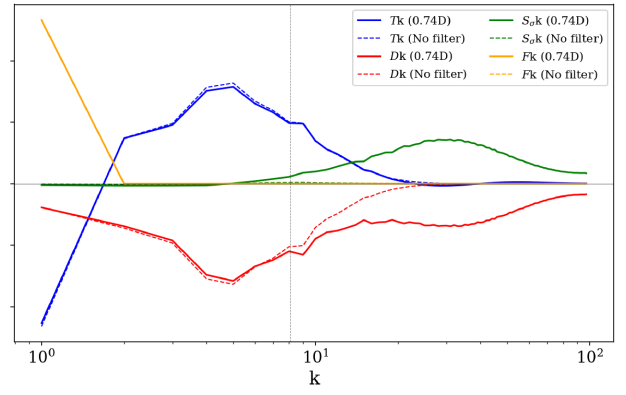
For the High-Pass filtered cases (Figure 21), the energy budget behaves differently depending on the filter size. For the smaller filter sizes ($0.5D$, $0.74D$, and D), the convective transfer $T(k)$ and surface tension work $S_\sigma(k)$ are negligible across all resolved scales. The balance is dominated by a direct equilibrium between the forcing $F(k)$ and the viscous dissipation $D(k)$.



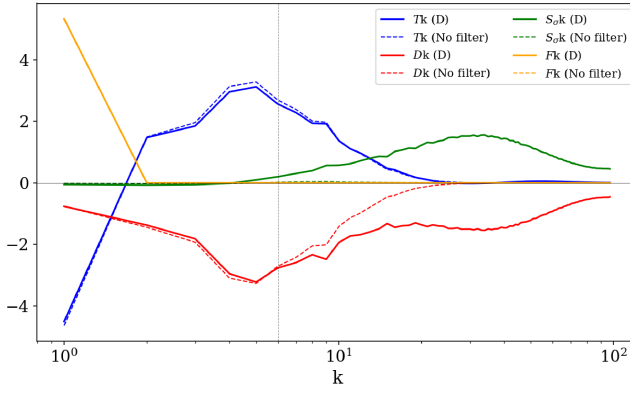
(a) No Filter



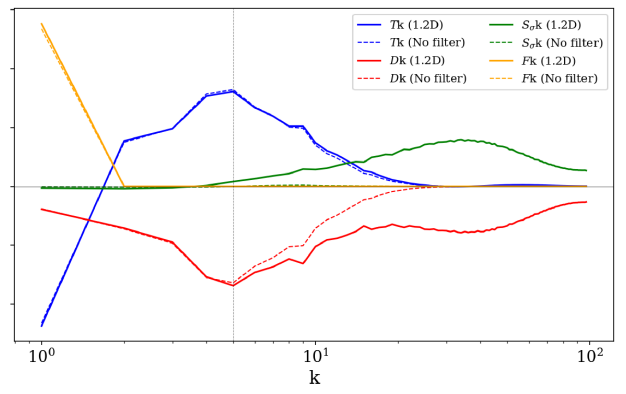
(b) 0.5D



(c) 0.74D

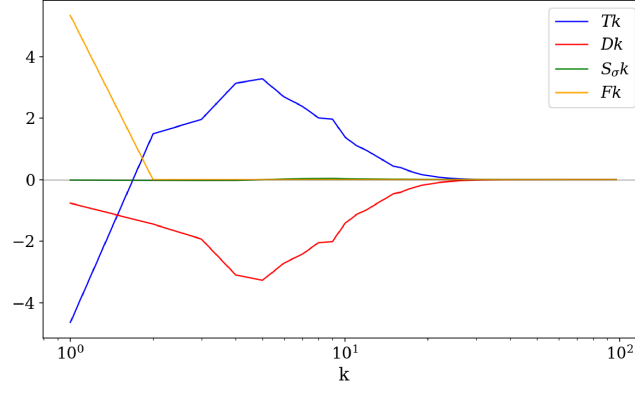


(d) D

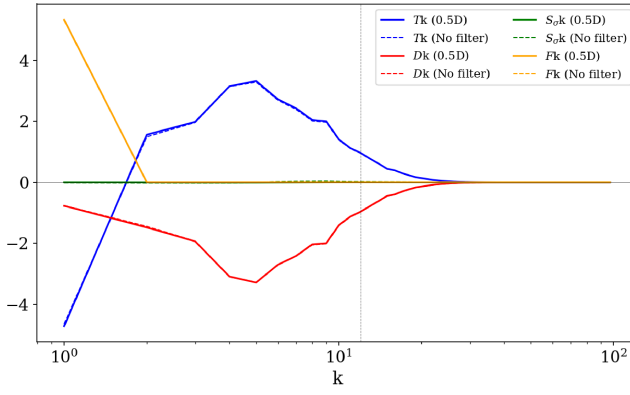


(e) 1.2D

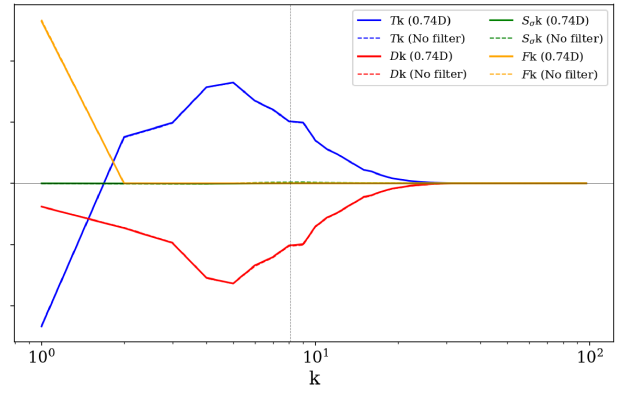
Figure 20: Low-Pass Fluxes.



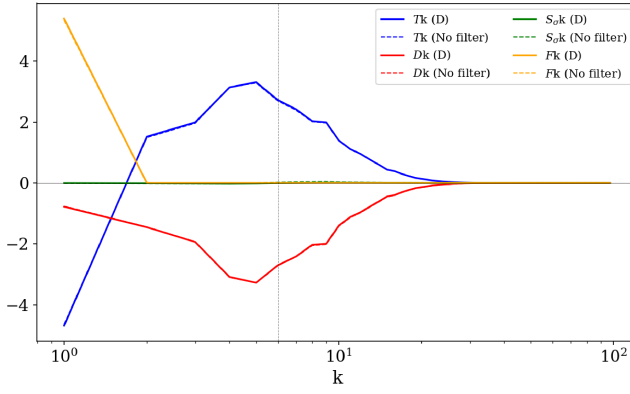
(a) No Filter



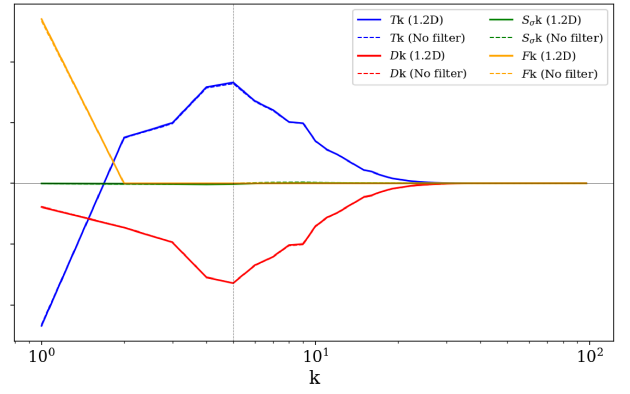
(b) 0.5D High-Pass



(c) 0.74D High-Pass



(d) D High-Pass



(e) 1.2D High-Pass

Figure 21: High-Pass Fluxes.

3.5.1 Surface Tension Term

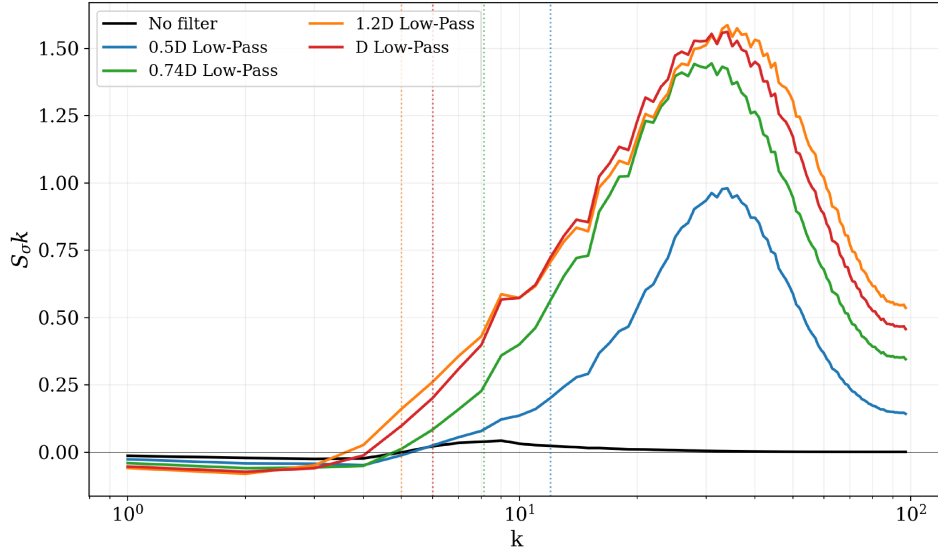


Figure 22: Comparison of Superficial tension term S_σ : No Filter vs Low-Pass Filters.

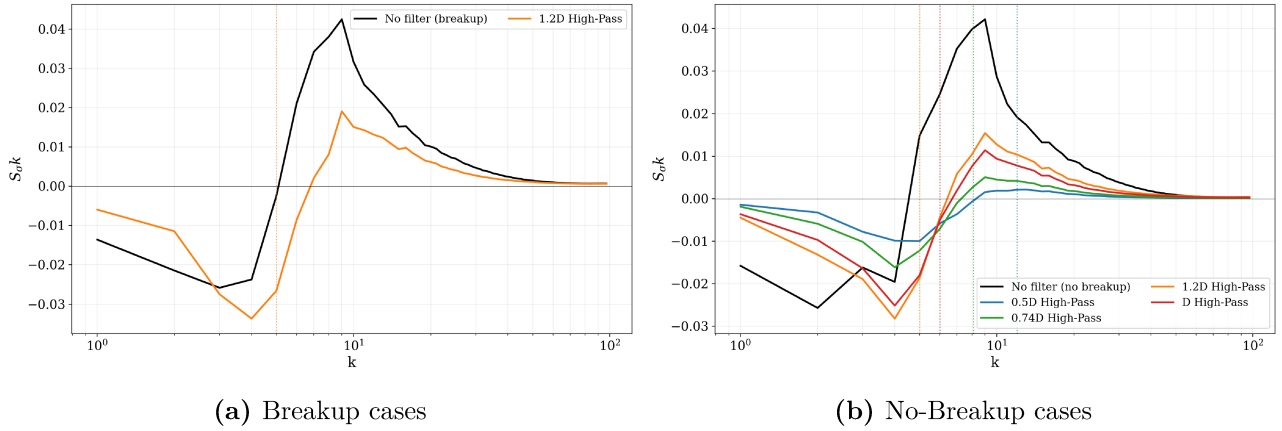


Figure 23: Comparison of Superficial tension term S_σ for High-Pass Filters.

The capillary transfer spectrum $S_\sigma(k)$ exhibits a negative contribution at low wavenumbers (large scales) and a positive contribution at high wavenumbers (small scales). This confirms the dual physical role of the interface as a spectral energy buffer: at large scales, the negative sign corresponds to energy absorption (dissipation of flow kinetic energy into interface potential energy), whereas at small scales, the positive sign denotes capillary yielding (the transfer and release of interface potential energy back into flow kinetic energy through capillary waves and droplet pinch-off).

3.5.2 Dissipative Term

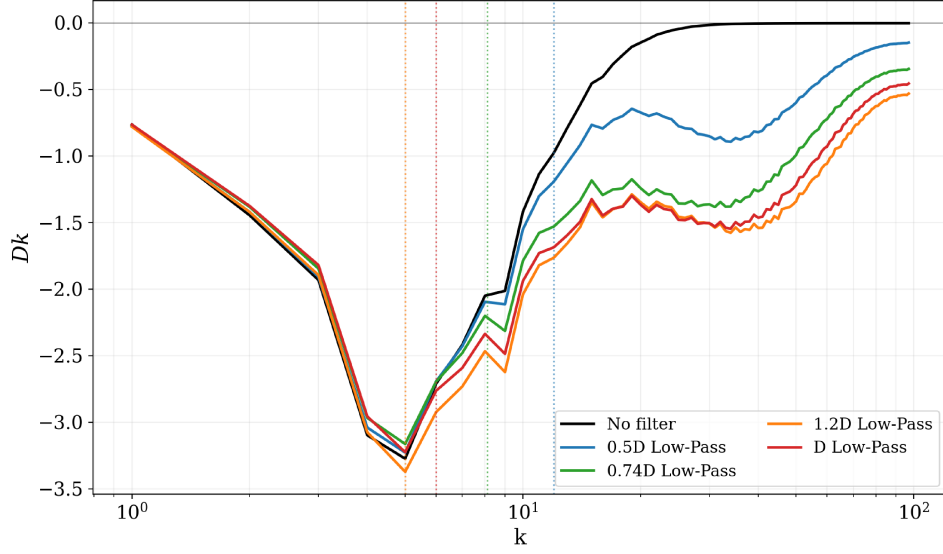


Figure 24: Comparison of Viscous Dissipation term D : No Filter vs Low-Pass Filters.

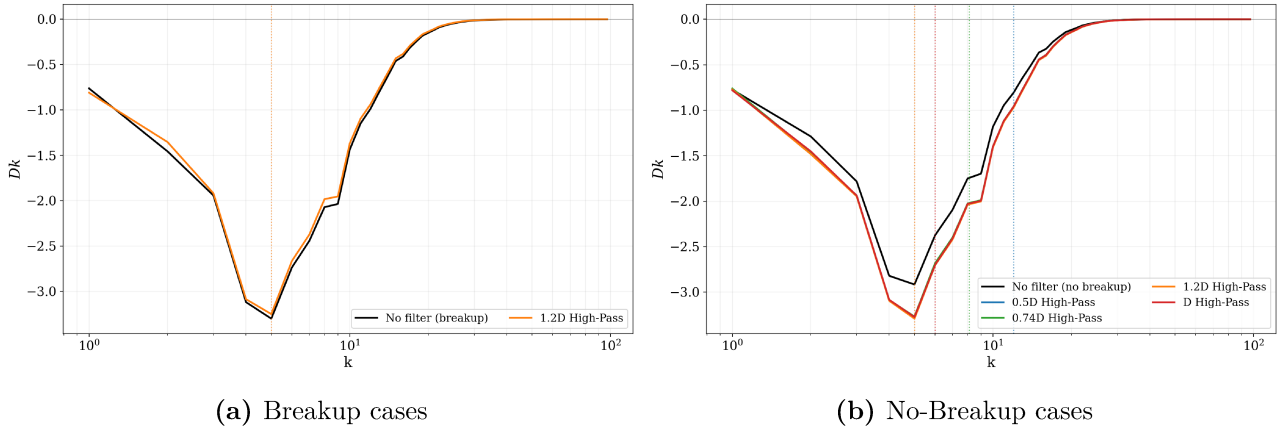


Figure 25: Comparison of Viscous Dissipation term D for High-Pass Filters.

The viscous dissipation spectrum $D(k)$ remains negative across all scales. In the low-pass filtered configurations, the suppression of small-scale structures leads to a significant increase in the magnitude of viscous dissipation compared to the unfiltered baseline, as the high-wavenumber velocity gradients are resolved but unenergized.

4. Conclusions

This thesis presented a systematic investigation into the scale-dependent mechanisms of droplet deformation and fragmentation in homogeneous isotropic turbulent (HIT) carrier flows. While classical theories, such as the Kolmogorov-Hinze framework, attribute droplet breakup to resonant turbulent eddies of scale equal to or larger than the droplet size, the specific contribution of different sections of the turbulent kinetic energy cascade has remained a long-standing open question. To address this, a numerical strategy was implemented coupling interface-resolved Direct Numerical Simulations (DNS) with a spatial filtering method. By separating the turbulent velocity field into low-pass (large-scale) and high-pass (small-scale) components across a range of cut-off widths ($0.5D$, $0.74D$, D , and $1.2D$), the droplet response under isolated spectral bands was examined. The simulations were conducted using the multiphase solver FluTAS, tracking the interface via the MTHINC Volume-of-Fluid (VOF) method. A comprehensive campaign consisting of 136 simulations was carried out on the Leonardo (CINECA) supercomputing cluster, establishing a robust statistical database across multiple independent restarts.

4.1 Summary of the Investigation

The numerical campaign focused on a single droplet of diameter $d \approx L/6 \approx 1.04$ immersed in a triply periodic domain of size $L = 2\pi$ containing statistically steady turbulence. The carrier phase was sustained via the ABC forcing scheme acting at the largest scales ($k_f = 2$). By varying the dynamic viscosity to ensure a grid spacing close to the Kolmogorov scale ($\Delta x/\eta \approx 1$), small-scale motions were fully resolved. The spatial filtering was applied to the advecting velocity field in the phase transport equation, utilizing a Gaussian filter to define the active scale ranges.

The simulations were classified into:

1. **Unfiltered (No Filter) Cases:** Serving as the baseline reference, exhibiting a statistical breakup rate of 60% over the ensemble restarts.
2. **Low-Pass (LP) Cases:** Where the droplet is advected only by large-scale turbulent

structures, and small-scale velocity components are filtered out.

3. **High-Pass (HP) Cases:** Where large-scale advection is removed, exposing the droplet only to small-scale shear and velocity fluctuations.

For each configuration, the filter cut-off width Δ was varied relative to the droplet diameter D , exploring values of $0.5D$, $0.74D$, D , and $1.2D$. To distinguish physical breakup events from minor interface wrinkling or numerical grid-level fragmentation, a volume-ratio threshold criterion of $\beta = V_{\text{max}}/V_0 \geq 0.95$ was successfully implemented.

4.2 Physical Insights and Core Findings

The results of this study reveal a strong asymmetry in the droplet response under low-pass and high-pass velocity filtering, clarifying the physical mechanisms governing turbulent fragmentation and interface-flow coupling.

4.2.1 Validation of the Kolmogorov-Hinze Scale Limit

The High-Pass filtered cases provide direct, statistical validation of the classical Kolmogorov-Hinze hypothesis. As shown by the volume ratio statistics (Figure 11) and the breakup rate summary (Table 4), the simulations yield a 0% breakup rate for all filter cut-offs smaller than or equal to the droplet size ($0.5D$, $0.74D$, and D). Under these configurations, the droplet remains stable, experiencing only mild shape fluctuations without undergoing fragmentation.

Only when the filter cut-off is extended to $1.2D$ does the breakup rate rise to 20% (with 3 out of 15 cases leading to fragmentation). This result indicates that small-scale turbulent fluctuations, which carry lower energy and have spatial coherence scales smaller than the droplet diameter, are insufficient to overcome the restoring surface tension forces. Droplet breakup is primarily driven by large-scale, coherent velocity gradients and pressure fluctuations of scale equal to or larger than the droplet size ($d_{\text{eddy}} \geq D$). These large structures deform the droplet globally, stretching it into unstable ellipsoids or filaments that eventually pinch off.

4.2.2 The Role of Small-Scale Capillary Feedback

Conversely, the Low-Pass filtered simulations exhibit a 100% breakup rate across all filter sizes ($0.5D$ to $1.2D$), generating an extremely large number of daughter droplets (Figure 12). This behavior points to a crucial numerical and physical mechanism: the localized nature of

the surface tension force. The capillary force $f_i^\sigma = \sigma \kappa \frac{\partial \phi}{\partial x_i}$ is concentrated at the interface, generating high-curvature, localized velocity gradients. When the advecting velocity field is low-pass filtered, these small-scale, interface-driven velocity fluctuations are suppressed.

As a result, the stabilizing feedback of the capillary force is removed from the Volume-of-Fluid transport equation. Lacking this local cohesive mechanism, the droplet is unable to resist the large-scale deforming stresses. The interface undergoes unconstrained deformation, leading to runaway stretching and fragmentation into a massive population of sub-grid-scale droplets. This effect becomes more pronounced as the filter width increases (from $0.5D$ to $1.2D$), which progressively removes more of the stabilizing capillary feedback, resulting in increasingly smaller fragments.

4.2.3 Scale-by-Scale Energy Transfer and Budget

The spectral energy analysis clarifies the thermodynamic role of the interface in modulating turbulence. The scale-by-scale kinetic energy budget formulated in the Fourier domain:

$$\frac{\partial E(k)}{\partial t} = T(k) + D(k) + S_\sigma(k) + F(k) \quad (4.1)$$

shows that the surface tension work term $S_\sigma(k)$ acts as an energy buffer. At large scales (low wavenumbers $k < k_H$), $S_\sigma(k) < 0$, indicating that deforming droplets absorb kinetic energy from the large-scale turbulent eddies and store it as surface potential energy. At small scales (high wavenumbers $k > k_H$), $S_\sigma(k) > 0$, showing that the interface releases this stored potential energy back to the carrier phase as kinetic energy during capillary relaxation and pinch-off.

This dual behavior creates an energy "bypass" mechanism, routing kinetic energy directly from large scales to small scales, thereby circumventing the traditional Richardson cascade. In the Low-Pass simulations, the unconstrained fragmentation into a massive number of micro-droplets increases the total interfacial surface area. This results in a significant increase in the surface tension term at high wavenumbers, leading to an elevated energy content at small scales (Figure 14) and a corresponding increase in local viscous dissipation.

4.3 Future Perspectives and Outlook

The findings from this thesis open several research directions in the study of turbulent multiphase flows, both at the level of fundamental physics and numerical modeling:

- **Subgrid-Scale (SGS) Modeling for Multiphase LES:** The dramatic increase in breakup rates under Low-Pass filtering highlights a critical challenge for Large Eddy Simulations (LES) of multiphase flows. In LES, the grid resolution is insufficient to resolve small-scale interface dynamics, which is equivalent to applying a low-pass filter. The lack of unresolved capillary feedback leads to artificial, runaway fragmentation. To address this, new subgrid-scale models must be developed to represent the unresolved surface tension force feedback, ensuring that under-resolved interfaces maintain physical cohesion.
- **Exploration of the Parameter Space:** The current study utilized matched density and viscosity ratios ($\rho_d/\rho_c = 1$, $\mu_d/\mu_c = 1$) to isolate the scale effects of the velocity field. Future investigations should extend this framework to non-unity density and viscosity ratios. High viscosity ratios ($Oh > 0.1$) will introduce internal viscous damping, which is expected to delay the breakup process and alter the critical scale thresholds.
- **Coalescence and Dense Emulsions:** While this work isolated a single droplet to study breakup mechanisms, realistic industrial and environmental flows involve dense emulsions where coalescence competes with fragmentation. Extending the spatial filtering methodology to multi-droplet systems will reveal how scale-resolved turbulence modulates the collision frequency, film drainage, and coalescence rates, ultimately determining the steady-state Droplet Size Distribution (DSD).
- **Thermal and buoyancy effects:** The incorporation of buoyancy forces (non-matched densities) and temperature gradients will allow the study of mixed regimes, such as rising bubble columns or boiling flows. Investigating how temperature-induced surface tension gradients (Marangoni stresses) couple with filtered turbulent fields represents an important direction for industrial heat-transfer applications.

In conclusion, this research provides a statistical and spectral characterization of the scale-dependent interactions between deformable interfaces and turbulent flows. The quantitative validation of the Kolmogorov-Hinze scale limit and the identification of the runaway fragmentation mechanism—driven by the suppression of small-scale capillary feedback—constitute

concrete steps toward more physically consistent predictive models for turbulent multiphase flows.

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