Is biofuel HVO an alternative in aviation? An Infodynamic Comparative Analysis

M.R.O. Panão[1],*, I.A.S. Ferrão[2,3,4], A.S.O.H. Moita[3]

1: ADAI, LAETA, Dept. of Mechanical Engineering, University of Coimbra, Portugal
2: AEROG, LAETA, University of Beira Interior, Portugal
3: IN$^+$, Instituto Superior Técnico, University of Lisbon, Portugal
4: IDMEC-LAETA, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal
*Corresponding author: miguel.panao@dem.uc.pt

Keywords: Biofuels, Sprays, Infodynamics, Phase-Doppler Interferometry.

ABSTRACT

The transition from fossil fuels to sustainable alternatives is imperative. This research evaluates Hydroprocessed Vegetable Oil (HVO) as a substitute for Jet A-1 in aviation. Focusing on droplet sizes in fuel sprays, which are critical for optimizing combustion, we explore an informational perspective for comparative analysis. Integrating information theory principles, we introduce the terms informature, infotropy, and infosensor that quantify and capture the non-deterministic nature of physical systems. Our analysis reveals similar drop size distributions for HVO and Jet A-1, with the Gamma function effectively characterizing the distributions. Both fuels exhibit spray complexity evolving toward higher states, emphasizing the role of aerodynamic forces and minimum development distance in atomization. We propose a novel lexicon, infodynamics, viewing sprays as networks of information flows, with infotropy providing context-rich insights. HVO is endorsed as a viable alternative, with broader implications for sustainable aviation solutions and understanding complex engineering processes.

1. Introduction

Climate change is a real issue affecting the entire world. It is essential to address it urgently to protect living beings and ecosystems. The longer we wait, the more difficult it will be to solve the problem. The leading causes of climate change are the heavy reliance on industrialization and non-renewable energy sources. Additionally, political actions have been taken to ensure the global energy economy, supply, and security. In 2015, the Paris Agreement focused on restricting the global temperature increase to below $2^{\circ}\mathrm{C}$ above pre-industrial levels and efforts to restrict it to $1.5^{\circ}\mathrm{C}$ (Cabrera & de Sousa, 2022). The purpose is to achieve net carbon neutrality by 2050. However, energy systems in developing nations persist in relying heavily on fossil fuels, a non-renewable energy source (Yang et al., 2023). In particular, the transportation sector relies on petroleum fuels, which account for around 19% of worldwide energy usage and contribute to approximately 23% of greenhouse gas emissions (Ershov et al., 2023). The primary fuel source for the transportation sector is liquid fuels provided by petroleum due to their high energy density, ease of transport and storage, and the extensive global infrastructure established over the past century to maintain this system (Khan et al., 2023).

Consequently, exploring sustainable and alternative energy sources is imperative to mitigate environmental issues. In this context, air transportation has focused on the energetic transition allied with reducing greenhouse gas and pollutant emissions. Aviation is mainly sourced from a finite fossil fuel, denoted as jet fuel, which is responsible for air pollution. To change this perspective, sustainable aviation fuel (SAF) has been investigated and introduced in this industry. Several alternatives have been discussed, mainly focused on drop-in biofuels, batteries, hydrogen, and fuel cells (Afonso et al., 2023).

The International Air Transport Association (IATA) has recognized that drop-in biofuel is the most favorable strategy, particularly in the short term, to mitigate the environmental impact of the aviation sector (Cabrera & de Sousa, 2022). Drop-in biofuels generally refer to fuels derived from biomass sources and renewable feedstock acquired from biological, thermal, and chemical conversion methods (Afonso et al., 2023). Drop-in fuels are related to a direct replacement or blend for conventional jet fuel (typically Jet A or Jet A-1) without demanding any aircraft engine or fuel infrastructure modification (Okolie et al., 2023). Biofuels are crucial to achieve carbon neutrality since plants absorb the CO_2 during their biomass growth, which is practically identical to the amount of carbon dioxide released to the atmosphere by the combustion of aero engines. The mixture of jet fuel and biofuel has already been tested, and favorable findings were reported. Current legislation permits certified SAF to be blended to a maximum ratio of 50% with fossil-based jet fuel, depending on the feedstock-production pathway considered.

Regarding the SAF pathway, the HEFA conversion process is a fully commercialized and mature technology already operating in aviation gas turbines (Abrantes et al., 2021). Besides these advantages, biofuels can possess unique properties that affect the atomization process, depending on the feedstock-production pathway, influencing the combustion emissions. It is essential to ensure that fuel is atomized efficiently to achieve optimal combustion. Poor atomization can lead to larger droplets, resulting in localized fuel-rich combustion. This process can produce soot and nitric oxides in combustion systems, as noted by Chong & Hochgreb (2015). Therefore, thoroughly understanding spray dynamics is necessary for developing combustion chambers and injection systems.

Following the earlier discussion, exploring alternative and sustainable solutions for the aviation sector to address environmental concerns is fundamental. In this perspective, within complexity science, the present work introduces an infodynamic comparative analysis to investigate the differences between alternative and conventional fuel sprays. In conventional data analysis on the spray characteristics, the focus is on droplets' average sizes and velocities, from which one determines dimensionless numbers relating several forces and energy components involved in liquid atomization. However, due to its reductionist nature, once the analysis proceeds with average quantities, all the information contained in the distributions is no longer part of the analysis. Fig. 1 illustrates the distinction between drop statistics expressed through the known Sauter Mean Diameter (SMD) and an infodynamic parameter defined in section 3 that quantifies the amount of information in $nats$ of a frequency probability distribution (f) of drop sizes. On the left, the SMD is blind to the distribution of drop sizes, and different distributions can result in the same SMD. However, on the right, if one mirrors the frequency probabilities relative to size classes, the amount of information is blind to the position of frequency probabilities, but not the SMD. Therefore, a counterposition between conventional drop statistics and infodynamic analysis is misleading because these methods address different levels of interpreting spray data.

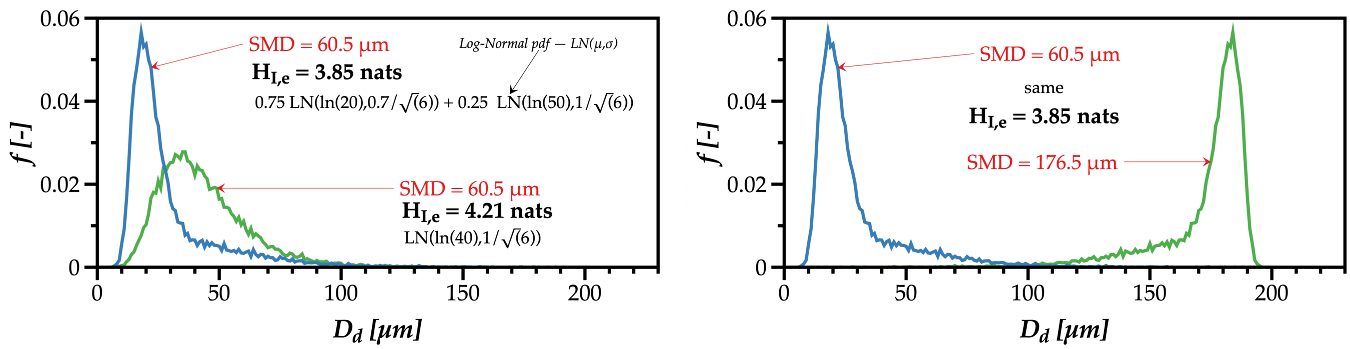


Figure 1. Example of distinction between drop statistics and infodynamic analysis.

One frequently reads how sprays are complex flows, but little has been done to quantify this complexity rooted in the amount of information on the spray. An infodynamic analysis represents a step forward in the quantification and understanding of the complexity of liquid atomization and spray dynamics from the perspective of its information content.

After this introduction and the presentation of the experimental setup and laser diagnostic technique, this paper introduces the background concepts of an infodynamic analysis adapted to engineering. Afterward, the results focus on the mathematical nature of drop size distributions of conventional and alternative aviation fuel using infodynamics and present an attempt to measure the spray complexity and infodynamic properties.

2. Experimental Setup and Diagnostic Technique

In this study, a comparison between conventional and alternative jet fuel is performed. Jet A-1 is a liquid fuel derived from kerosene designed for applications in the aeronautical industry. For aviation purposes, Jet A-1 is enriched with several additives that aim to inhibit the hazard of static charges, reducing the oxidizing and corrosive potentials while increasing the lubricity and improving the cold flow properties (Chuck & Donnelly, 2014). Moreover, aero-engines must be powered by fuels with high energy content, good flow characteristics, thermal stability, and restrictions to ensure reliability, safety, and security (Blakey et al., 2011). The alternative jet fuel used in this work is a NEXBTL (HVO) acquired from NESTE. This liquid biofuel is obtained by converting vegetable oils and animal fat into paraffinic hydrocarbons. HVO presents acceptable cold flow properties, a high cetane number, a reasonable distillation range, and high thermal stability. It is free of aromatic and sulfur content. Additionally, it presents a stable storage resistance to microbial growth, avoiding the formation of engine deposits. According to the literature, using HVO has shown advantages in reducing greenhouse gases and pollutant emissions (Pinto et al., 2023; Mikkonen et al., 2013; Aatola et al., 2008). Table 1 shows the properties of Jet A-1 and HVO fuels.

Table 1. Jet A-1 and HVO properties (Ferrao et al., 2021)

Parameter	**Jet A-1**	**HVO**
Density (Kg/m^3) (at 20°C)	789	780.6
Surface Tension (N/m) (at 20°C)	0.0247	0.0265
Kinematic Viscosity (mm^2/s (at 25°C)	1.40	4.33
Sulfur (wt. %)	0.3	0.09
Aromatics (wt. %)	13.8	0
Flash Point (°C)	38	99
Final Boiling Point (°C)	237	308
Cloud Point (°C)	-26	-30
Lower Heating Value (MJ/kg)	43	43.9
Higher Heating Value (MJ/kg)	47	47.1
Destillation 10 vol. % (°C)	170	262
Hydrogen Content	14.5	15.4
Carbon Content	84.6	85.5
H/C Ratio	1.91	2.18

Figure 3 schematically represents the experimental setup used to characterize the spray. As for spray visualization tests, an air-assisted SCHLICK Two-Substance Nozzle Model 0/2 atomizer with external mixing and swirl grooves was used. The atomizer was placed vertically downwards, avoiding overlapping droplets in recirculation. The liquid fuel and air atomization flow rate was controlled by two different rotameters ABB PurgeMaster. A maximum volumetric capacity of 1.15 L/h was employed for the fuel rotameter. A rotameter with a capacity of 54 L/min was used for the air atomizing. For Jet A-1 and HVO, the same rotameter was used to control the flow rate.

Consequently, a calibration was required to assess the effective flow rate dispensed by the atomizer, as shown in Figure 2. The theoretical flowrate is related to the volumetric flowrate that should be released by the rotameter. However, when a specific theoretical flowrate is imposed, fuel flowrate release departs from the expected value. Consequently, the effective flowrate was evaluated, which corresponds to the fuel volumetric flowrate released by the flowmeter. This analysis was carried out for each fuel and flowrate condition three times, with each examination lasting two to three minutes.

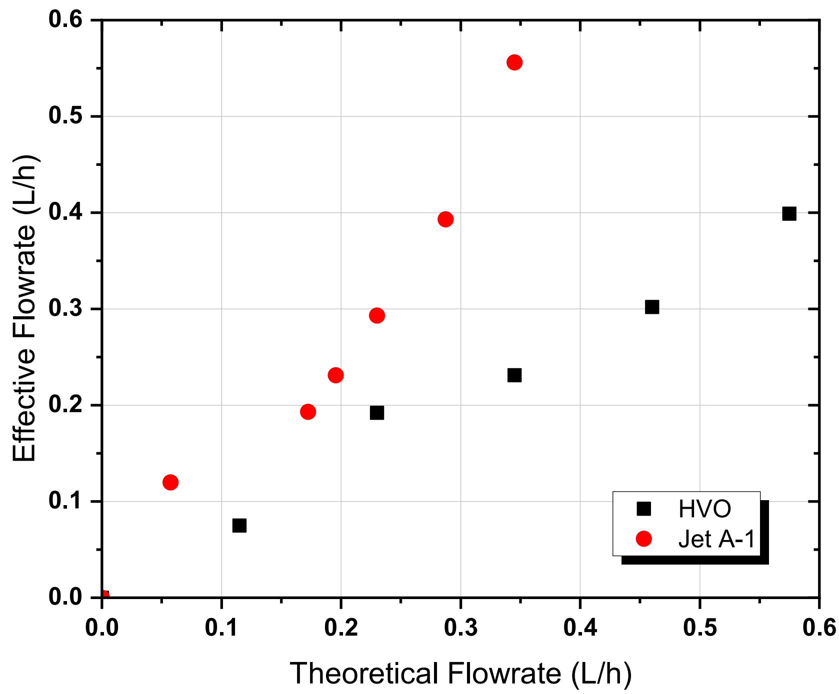


Figure 2. Rotameter calibration for alternative and conventional jet fuel

The delivery of liquid fuel is performed with the aid of a pressure tank at 1 bar. Additionally, a nitrogen bottle was used to pressurize the fuel tank at 1 bar; then, a manually regulated valve was used to regulate the fuel that goes through the rotameter to feed the atomizer. The air flowing to the atomizer was pressurized by a compressor to the value of 2 bar and regulated by a manual valve. Concerning the operating conditions, the liquid and air interaction occurred under ambient and atmospheric conditions. The atomizer has free movement in rx, ry, and z, allowing it to change its position. Phase Doppler measurements were performed at the axial locations of $z = 5, 10, 15,$ and $20\ mm$ from the atomizer exit $z = 0\ mm$. The selection of these distances was correlated to the breakup structure of the spray. For each z, a set of measurements was performed along the radial-x and radial-y axes in 2 mm steps for the two perpendicular axes.

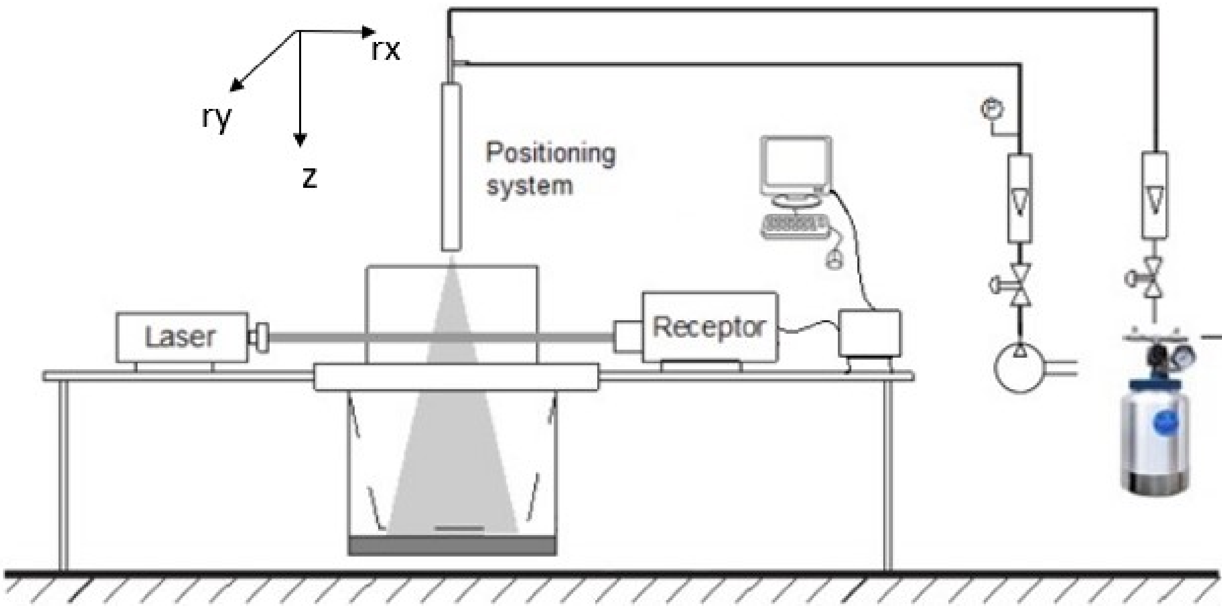


Figure 3. Experimental Setup: Phase Doppler Interpherometry

The droplet size and velocity distributions were measured using a phase Doppler interferometry system (a FlowExplorer 1D transmitting and receiving optics connected to a BSA F100 processor from Dantec Dynamics). The system is used for transmitting optics laser power of 90 mW for the axial (U) velocity component measurements, with a wavelength of 660 nm. The focal length is 500mm, the beam spacing is 37mm. The receiving optics was a fiber PDA, with a receiver focal length of 400mm. The scattering angle used was 31°. Table 2 summarizes the PDI measurement configuration.

3. Infodynamic Analysis Background

When Claude Shannon (1948) deduced his formulation for the amount of information produced by a process affected by randomness due to its nature or the influence of noise, he expressed it as a *"measure of information, choice and uncertainty"* (see Shannon & Weaver (1949), p. 50).

$$H = -K \sum_i f_i \log_2(f_i) \tag{1}$$

with K as an arbitrary constant and f_i the probability (frequency) of occurrence of x_i, $\sum_i f_i = 1$. This parameter has all the characteristics of an uncertainty (Shannon & Weaver, 1949), and according to Tribus & McIrvine (1971), K determines the unit of information and usually takes the form of $\ln(2)$ to change the logarithm base to e. Still, the most common expression for H is *Shannon entropy*, due to its similarity with Boltzmann H-theorem function. Also, Tribus & McIrvine (1971) revealed that Shannon's designation of his formulation as an "entropy" was the suggestion of John von

Table 2. PDI Measurement Configuration

Transmitting Optics	
Beam System	U1
Laser power	90 mW
Wavelength	660 nm
Focal length	500 mm
Beam spacing	37 mm
Receiving Optics	
Receiver Type	Fiber PDI
Scattering angle	31°
Receiver focal length	400 mm
Software Parameters	
Photomultiplier Sensitivity	900 V
Signal Gain	16 dB
Center Velocity	-16.34 m/s
Velocity Span	43.03 m/s

Neumann. However, Denbigh (1981) argued this suggestion as a disservice to the work of Shannon because functions with the same formal structure do not necessarily represent the same. To overcome this misleading designation, we introduce two neologisms: *informature* and *infotropy*.

3.1. Informature, Infotropy and Complexity

Informature is the block in Shannon's formulation that measures the amount of information from the knowledge of the probability distribution

$$H_{I,b} = -K_b \sum_i f_i \log_2(f_i) \tag{2}$$

with K_b as the first part of $K = K_b \cdot K_c$ that established the logarithm base. Therefore, if $K_b = \log_2(2) = 1$, the logarithm is the original base-2 of Shannon's formulation, and *informature* is in "binary units" or $bits$. If $K_b = \ln(2)$, the base changes to the natural logarithm and *informature* is in "natural units" or $nats$. One should consider *informature* measurements of the amount of information in a stochastic system in $bits$ or $nats$, as one considers temperature measurements in Kelvin or mass measurements in grams. In this sense, while Shannon's formula is an extensive property of the non-deterministic system it characterizes because K is size-dependent, *informature* is an intensive property because it does not depend on the size of the system, only on the probabilities describing it.

In Shannon's formula, the second part of K, K_c, is what contextualizes the informature, leading to the second neologism of *infotropy*, synthesizing "information" (*info-*) and transformation (from the Greek *trope*, as in Clausius invention of the word "entropy"). For example, when $K_c = k_B$ (Boltzmann's constant), $K_b = \ln(2)$ and $f_i = 1/W$ is constant, and W corresponds to the number of molecules in a gas, $H_e = S = k_B \ln(W)$, which is Boltzmann's formula for the thermodynamic entropy, a gaseous *infotropy* where Boltzmann's constant contextualizes the maximum *informature* obtained for a fully chaotic physical system, such as a gas at a microscopic level in Boltzmann's perspective. These neologisms overcome the shortcomings of Neumann's ill suggestion and avoid mistaking Shannon's measure of information for a concept similar to thermodynamic entropy. Thus, one rewrites Shannon's *infotropy* as

$$H_b = K_c \times H_{I,b} \tag{3}$$

In this new terminology, the H in Eq. (1) is H_2 because Shannon applied a base-2 logarithm. When applying the *infotropy* to a continuous function, $H_b \to \infty$. Therefore, Stone (2015) explains how one can ignore this infinity if considering the differential part of the measure of information, $H_{\Delta,e}$. In discrete probability distributions, the differential *informature* is given by

$$H_{\Delta,e}[nats] = -\sum_{i=1}^{N_k} f_i \ln(p_i) \tag{4}$$

with N_k as the number of classes and $p_i = f_i/\Delta x_i$ as the probability density dividing the frequency of a class (f_i) by its size (Δx_i). In this case, unlike the *informature* defined in Eq. (2), this measurement becomes an extensive property of the system because it depends on the size of classes defined for the system. For a continuous function, the differential *informature* adapted to drop size distributions corresponds to

$$H_{\delta,e} = \int_0^\infty p(x) \ln\left(\frac{1}{p(x)}\right) dx \tag{5}$$

According to Stone (2015), as the number of classes increases, $H_{\Delta,e} \to H_{\delta,e}$ and this approximation is the ground for the approach followed in this work.

If one considers the relative information, also known as the Kullback-Leibler information distance or information gain, it measures the distance between the maximum informature, $H_{max,b} = K_b \cdot \log_2(N_k)$, where all possible configurations (N_k) are equally probable, and the actual informature given by Eq. (2), becoming

$$D = H_{max,b} - H_{I,b} \tag{6}$$

According to Feldman & Crutchfield (1998), one can quantify the complexity of a finite-size system as the product between its informature and the relative information as

$$C = H_{I,b} \times D \tag{7}$$

Systems without information ($H_{I,b} = 0$) have no complexity ($C = 0$) as well as fully indeterminate systems ($D = 0$). However, if one divides the complexity by the square of the maximum informature, this quantity becomes dimensionless

$$C_n = H_n \cdot R_n \tag{8}$$

with $R_n = (1 - H_n)$ as the redundancy, which measures the amount of structure present in the spray information. Suppose there is only one mechanism leading to droplets of a single size. In that case, the heterogeneity degree (how many different sizes are relevant in the spray) is low, implying regularity in the atomization mechanisms, leading to a well-defined spray structure with droplets of regular sizes. On the contrary, if more than one physical process is atomizing the liquid, for example, a combination of aerodynamic forces of an air-assisted jet, stretching of ligaments, and bag breakup, the multitude of physical mechanisms leads to a less structured spray is a lower redundancy.

What exactly is the statistical complexity measuring? Statistical complexity measures the degree of organization on the spray. It is the combined effect of:

- the non-deterministic part associated with the polydispersion degree of drop size diversity (see M. O. Panão et al. (2020)) expressed by the normalized informature
- and the deterministic part associated with the degree of structure expressed by redundancy, given by the hydrodynamic morphology of instabilities or a certain dispersion pattern resulting from the interaction between droplets and the environment, implying a diversity of physical mechanisms spatiotemporally organizing the spray propagation.

A highly complex spray is not an unexplainable spray unless empirically but a spray formed and developed with a high balance between the diversity of drops' characteristics and the physical mechanisms structuring the spray development. In the context of a spray's drop size distribution, a high C_n value indicates a distribution that is both diverse and structured, suggesting a well-organized system with moderate indeterminacy. Conversely, a low C_n value suggests either a fully controlled atomization with low indeterminacy and well-defined atomization mechanisms or a fully uncontrolled atomization with high indeterminacy and a multitude of physical mechanisms structuring the spray. Both indicate lower organization levels of drops' dispersion. Thus, C_n serves as a useful metric for evaluating the organization of droplet distributions in various engineering physical systems containing deterministic and non-deterministic elements.

How is the measure to be used? What questions might it help answer? Statistical complexity in the infodynamic analysis of sprays can be seen as part of the broader evolutionary trend of natural systems toward higher degrees of organization. By measuring and monitoring the statistical complexity of droplet size distributions, we can gain insights into how spray systems evolve and adapt over space and time. Specifically, it can help answer questions such as: *How does the droplet size distribution in a spray evolve towards higher complexity under different operating conditions and nozzle designs?* This understanding aligns with the natural tendency of systems to move towards more organized complexity. Additionally, it can address: *What are the optimal conditions under which the spray achieves a balanced state of diversity and structure, ensuring both efficient atomization and desired droplet characteristics?* By framing these questions within the context of infodynamics, one clarifies the role of statistical complexity in driving the development of more sophisticated and effective spray systems, similar to the progression seen in natural systems.

Fig. 4 structures the *complexity domain* map and what characterizes each region. The limits of the complexity domain with no complexity are made of *fully regular* physical systems (*e.g.*, all droplets in the spray have the same size or the same velocity), and *fully chaotic* (*e.g.*, all classes of drop sizes have the same sample size resulting in a uniform distribution). A spray is often considered a complex flow, but its complexity has not yet been quantified. One of the goals of this work is to introduce an infodynamic perspective of measuring the spray complexity.

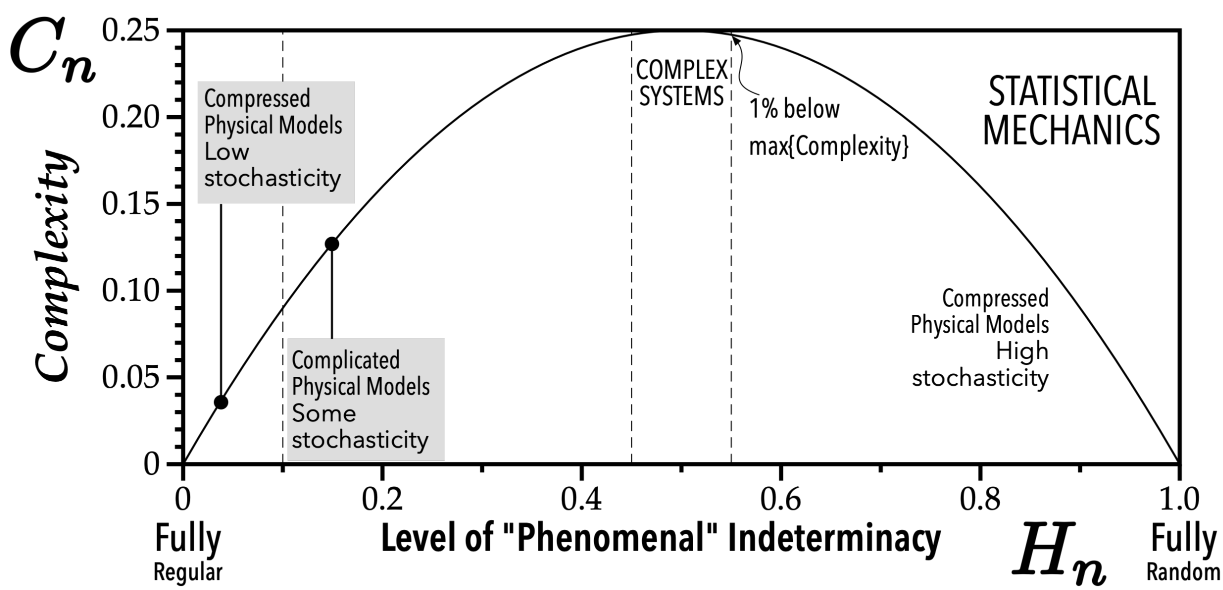


Figure 4. Map of the dimensionless complexity domain inspired by David Krakauer's lecture on "What is complexity?".

In the following section, the Phase-Doppler Interferometer is considered an *infosensor*, which requires an explanation of what this concept and its application to the measurement of more than one characteristic of the physical system. In the case of a spray, how can one know that the *infosensor* measured enough information of drop size and velocity?

3.2. Considerations on *infosensors*

The thermocouple is a sensor used to measure temperature through the electromotive force generated by the temperature difference between two junctions formed by two materials of different compositions. Since *informature* is also an intensive property of a physical system, its measurement requires an *infosensor*, where the measurement principle is its ability to capture the statistical nature of a physical system. While the Seebeck effect explains how a thermocouple operates, statistical analysis is what explains the operation of an *infosensor*. The two most relevant procedures in *infosensors*, as occurs with any sensor, are their calibration and response time.

Calibrating an *infosensor* means designing the best way to express the statistical nature of the physical system. For example, M. Panão (2022) showed how the decimal part of drop size measurements is redundant. Considering the microscale (μm) as the one that best describes drop sizes, it implies that building frequency probabilities of classes with less than $1\ \mu m$ is pointless. Therefore, calibrating an *infosensor* means identifying the scales of the elements in the phase space of the physical system and choosing an appropriate method to define the number of classes.

In the case of one measured characteristic of the physical system under infodynamic analysis, the *informature* should be enough to assess the *infosensor* response time, as explored in M. R. O. Panão (2012). However, suppose more than one characteristic is needed to ensure that one acquires enough information (not data). In that case, we should use the mutual informature ($mH_{I,e}(d,u)$), which means the amount of information contained in drop size and velocity simultaneous measurements does not exceed the amount of information associated with each of these characteristics – $mH_{I,e}(d,u) \leq H_{I,e}(d) + H_{I,e}(u)$. This quantity depends on the joint probability between the measured quantities, $p(d_i,u_j)$, which corresponds to the frequency probability associated with the class d_i, and class u_j, such that $\sum_i \sum_j p(d_i,u_j) = 1$. The mutual informature corresponds to (Stone, 2015)

$$mH_{I,b}(d,u) = \sum_{i=1}^{k_d} \sum_{j=1}^{k_u} p(d_i,u_j) \cdot \log_b \left(\frac{p(d_i,u_j)}{p(d_i) \cdot p(u_j)} \right) \tag{9}$$

with k_d, k_u as the number of size and velocity classes, respectively, b is the logarithm base (e.g., e leads to $mH_{I,e}$ measured in *nats*), $p(d_i) = \sum_{j=1}^{k_u} p(d_i,u_j)$ and $p(u_j) = \sum_{i=1}^{k_d} p(d_i,u_j)$. Fig. 5 shows an example of calibrating the response time.

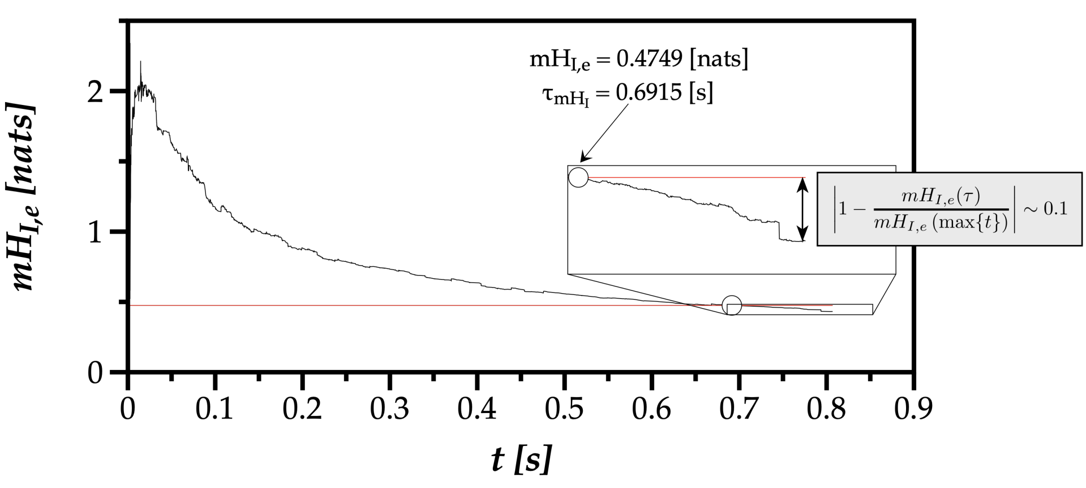


Figure 5. Example of obtaining the response time for one measurement point.

All measured points resulted in response times lower than the maximum measurement time to acquire $N = 5000$ samples with droplets' characteristics. Fig. 6 exemplifies maps of the response time measurement and corresponding mutual informature.

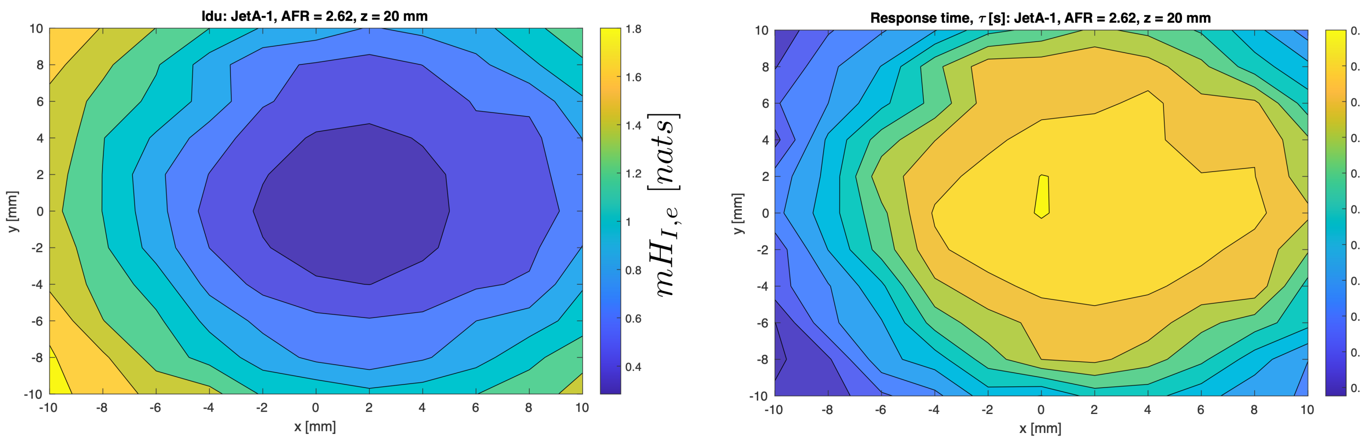


Figure 6. Example of the mutual informature ($mH_{I,e}$ $[nats]$) map and corresponding the response time for HVO with an AFR=2.62 at the $z = 20$ $[mm]$ measurement plane.

The larger response time in the center and its lower mutual informature value indicate a region of high variability and independence between the sizes and velocity of corresponding droplets. From the center of the spray to its outskirts, the amount of information of the size reduces the amount of information needed for the velocity, which is the meaning of a higher mutual informature. Relative to the acquisition time (Δt), PDI mutual informature response times (τ) have two clusters. Fig. 7 evidences a first cluster from locations at the outskirts of the spray that needed less than 25% of the total acquisition time to stabilize the mutual informature. In contrast, locations inside the spray require almost all samples acquired to ensure data contains enough information. These results for the PDI's informational response time are coherent with the lower data rates where the spray density is higher, requiring more time to stabilize the amount of the local size-velocity mutual informature in the spray.

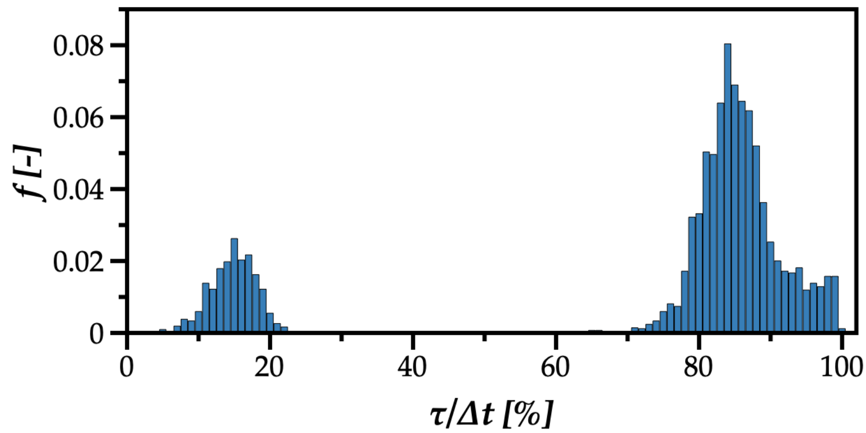


Figure 7. Histogram of percentual response times in all measurement locations relative to the total measurement time taken to acquire 5000 samples.

4. Results and Discussion

In the first part of this section, the informational results of the spray explore the infodynamic nature of liquid atomization and whether discrete representations of drop sizes correspond to any of the common mathematical probability distribution functions associated with sprays. In the second part, one performs a first attempt to investigate informational properties based on infotropies as "contextualized" informatures to address the challenge of quantifying the spray complexity.

4.1. Infodynamic Nature of Liquid Atomization

The purpose of fitting probability mathematical functions to discrete drop size distributions should be to understand the nature of liquid atomization processes. In the present Jet A-1 and HVO comparison, most properties are similar, except for the dynamic viscosity, as shown in table 1. If this property affects the nature of liquid atomization using the same atomizer and liquid breakup strategy, it could mean that different mathematical functions would fit the experimental data.

The three essential probability mathematical functions typically used to fit drop size distribution data are Log-normal, Gamma, and Weibull. The best and most known goodness-to-fit test is the Kolmogorov-Smirnov (K-S), which compares two continuous distributions and is sensitive to the test sample size. Other methods consider comparing two discrete distributions. However, in these tests, if the null hypothesis should not be rejected for two of the continuous functions, how does one know which function best describes the measured results? In the K-S method, the function with the minimum value of the maximum deviation observed between the discrete and the continuous is decided as the one that best describes data. However, Fig. 8 shows a case where the Log-Normal surpassed the Gamma PDF by a marginal value (see magnification in the plot), implying that the KS test indicates the Log-Normal as the best PDF that describes drop sizes, failing to capture how it fails to capture the distribution behavior for sizes smaller than $5\ \mu m$. For this reason, KS-test methods are unable to capture the nature of the mathematical probability distribution function underlying the sizes resulting from liquid atomization. Therefore, in this work, we introduce and explore a method based on information theory using the differential informature defined in section 3.

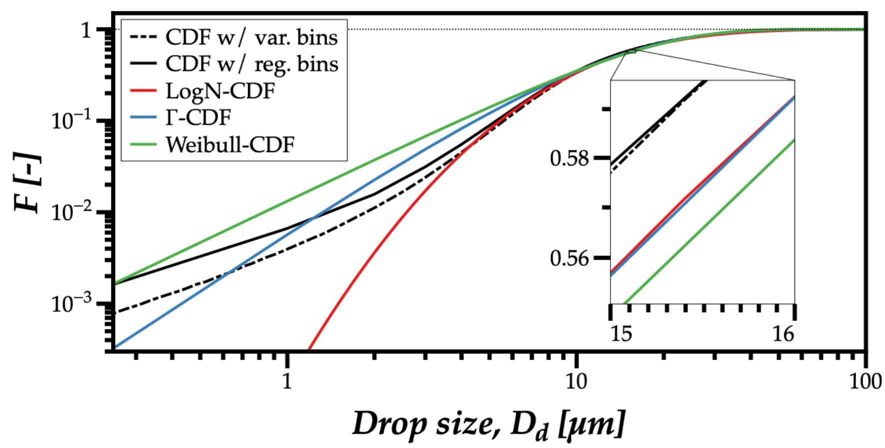


Figure 8. Example of the Cumulative Distribution Function (CDF) with regular and variable bin sizes compared to the Log-Normal, Gamma and Weibull that best fitted the entire spray of HVO with AFR = 6.56 at $z = 10\ mm$.

Table 3. Drop size mathematical distribution used to fit discrete histograms in spray science.

Type	Function, $p(d)$	$H_{\delta,e}$
Log-Normal	$\frac{1}{\sqrt{2\pi} s D_{50}} \exp\left(-\frac{\ln(d/D_{50})^2}{2s^2}\right)$	$\frac{1}{2}\ln\left(2\pi e s^2 D_{50}^2\right)$
Gamma	$\frac{d^{a-1}}{b^a \Gamma(a)} \exp\left(-\frac{d}{b}\right)$	$\ln(b\Gamma(a)) + (1-a)\psi(a) + a$
Weibull	$\frac{b}{a}\left(\frac{d}{a}\right)^{b-1} \exp\left(-\left(\frac{d}{a}\right)^b\right)$	$\ln(a/b) + ((a-1)/a)\gamma + 1$

If one analyzes each measurement point to compare the differential informature retrieved from data ($H_{\Delta,e}$) with the analytical differential informature ($H_{\delta,e}$) of the best adjustment of each mathematical function in Table 3, both Log-Normal and Gamma distribution functions appear in the grid as the ones that best describe the measured drop size distributions. The Weibull does not produce any best adjustment. Although a local exhaustive analysis is beyond the scope of the present work, one notes that increasing AFR and the spray propagation plane z, the dominant distribution describing all points in the measurement plane tends to be the Gamma. Therefore, instead, all data of drop sizes measured in a plane is accumulated into a single sample to express the spray crossing a plane as an event.

Table 3 also includes the analytical solution for the *differential informature* (Michalowicz et al., 2013) where $\psi(x)$ is the digamma function, and γ represents the Euler-Mascheroni constant. The reasoning behind the *differential informature* explored is spray characterization is to compare the value obtained from the discrete drop size distribution with the analytical value obtained for the three continuous mathematical functions considered. The best mathematical distribution function describing the discrete probability distribution is the one with the minimum difference between these values.

Fig. 9 depicts the ratio between the discrete *differential informature* ($H_{\Delta,e}$) and the analytical value ($H_{\delta,e}$) for the three distribution mathematical functions considered. Each data point contains the data for the entire measurement plane. In general, and with both fuels, the Gamma distribution function is the one that best describes the drop sizes formed in this air-assisted swirl atomizer. Above a differential *informature* of $4\ nats$, both Log-Normal and Gamma distribution functions produce similar fittings.

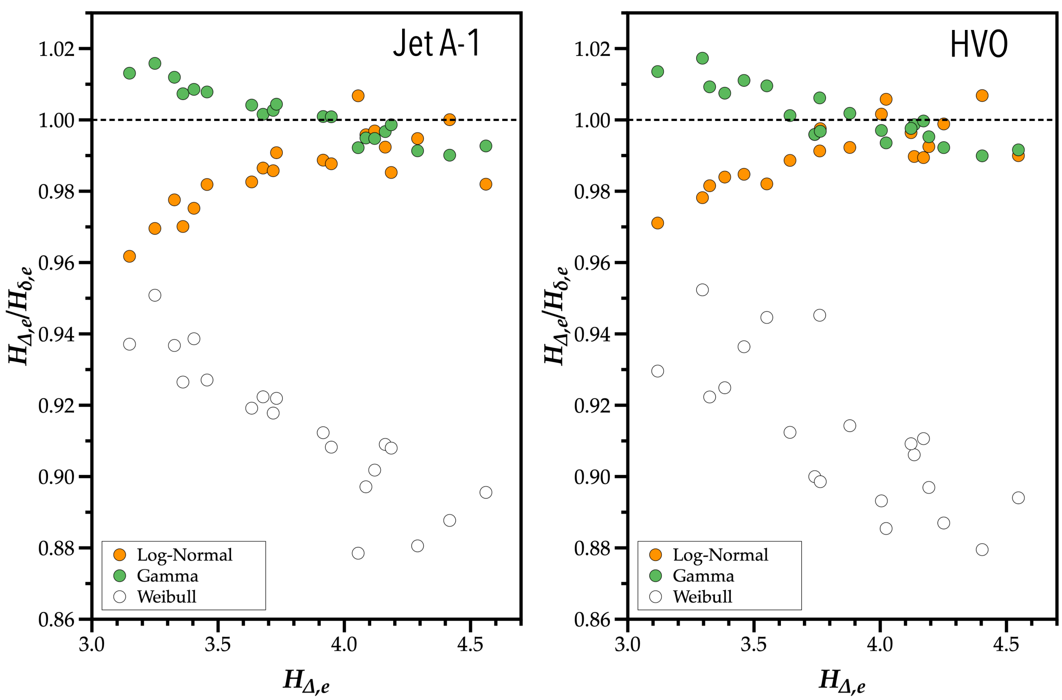


Figure 9. Comparison between the discrete and analytical differential informature based on drop size. The Log-Normal is best in 80% of the cases, but only in one case is this difference significant.

Recently, Cejpek et al. (2023) argued in favor of the Log-Normal distribution using the visual similarity between the discrete and continuous drop size distributions. Earlier, Tratnig & Brenn (2010) argued in favor of the Gamma distribution, modifying it by empirically adding a second exponential term to cover the larger drop sizes present in the spray. However, the authors evaluate the similarity using moments of the distribution, which is not an accurate strategy (M. Panão & Moreira, 2008). The background reason for using the Gamma distribution is rooted in the work of Villermaux et al. (2004) that associated the gamma distribution function with the outcome of ligament temporal fragmentation, modeling each ligament as an aggregation of sub-droplets arranged in several sub-layers. Later, Dumouchel (2006) used the Maximum Entropy Formalism (a designation we disagree with for the reasons exposed in section 3) and also arrived at a Gamma distribution. Although the conclusions of Cejpek et al. (2023) and Tratnig & Brenn (2010) seem contradictory, the fact that the later authors added an exponential term to their Gamma distribution function points to the hypothesis that the actual distribution function could be a weighted average of two physical effects: 1) the exponential growth process of drop size diversity leading to a Log-normal, as explained in M. Panão (2023); 2) and the liquid temporal fragmentation leading to a Gamma distribution function. However, this research hypothesis suggested by the infodynamic analysis is the subject of future work. Henceforth, since the Gamma PDF is the dominant one from the differential informature point of view, we consider it in the comparative infodynamic analysis of the two fuels.

Fig. 10 compares the ratios between the discrete and the analytical differential informatures of both fuels as a function of the discrete value. The plot shows the informational similarity of the sprays produced with different fuels and evidence a $\pm 2\%$ marginal difference when adjusting a Gamma distribution function to the experimental values, validating the dominant nature of liquid atomization associated with the temporal event of ligament fragmentation.

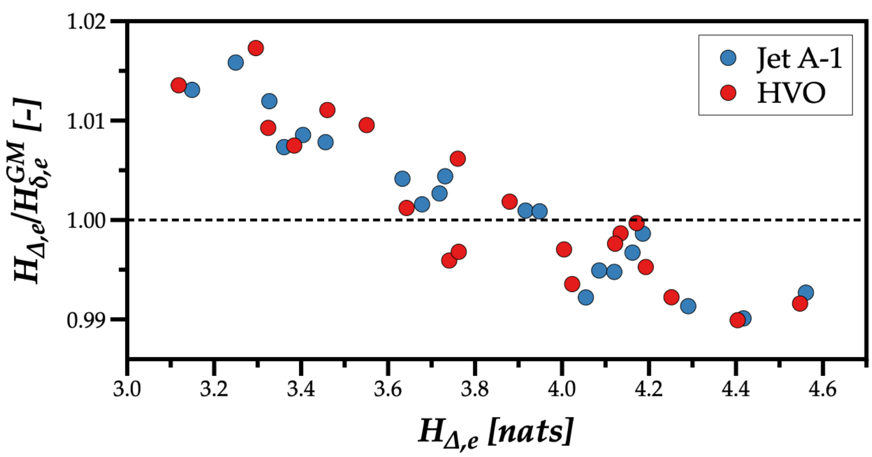
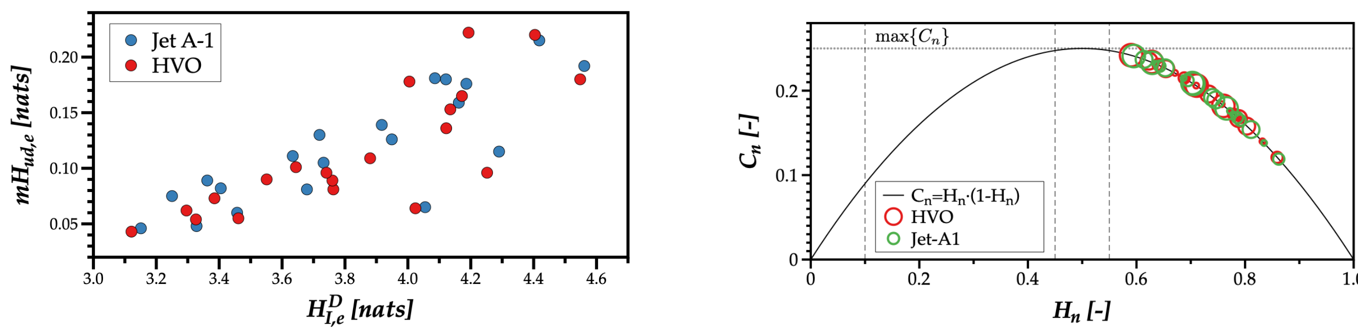


Figure 10. Comparison of the ratios between the discrete and analytical differential informatures and the discrete differential informatures of Jet A-1 and HVO.

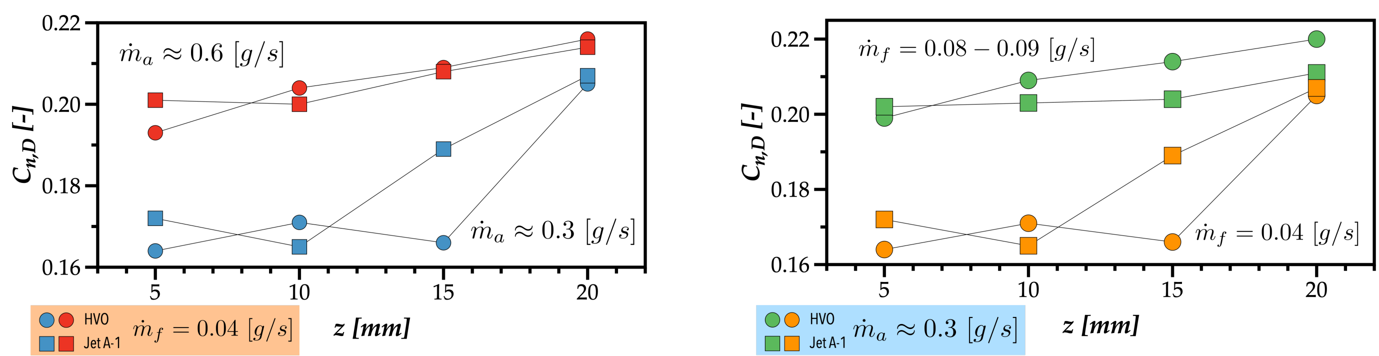
In terms of the mutual informature, Eq. (9), Fig. 11a evidences a proportional relation with drop size informature and similar for both fuels. A large drop size informature indicates higher variability of drop sizes, and a high mutual informature means that a high amount of information on drop size is shared with the information on drop velocity. As shown previously in Fig. 6, the lower levels of informature are in the center of the spray planar pattern, and globally, the uniformization of informature occurs as the spray develops in its propagation path (z-direction). This uniformization of the spray spatial information, while it develops, appears correlated with the trend for increasing its complexity, as Fig. 11b depicts, where the larger the symbol is, the farther the measurement plane is from the nozzle. In fact, although not included in this paper, the spray complexity maps tend toward a uniform distribution with z and AFR.



(a) (b)

Figure 11. Relation between (a) the mutual informature ($mH_{ud,e}$) for both fuels and the several operating conditions and measurement planes, and (b) the corresponding results of the spray statistical complexity with symbols' size proportional to the z distance.

To understand how the fuel or the air flowrates produce change in spray information, Fig. 12 considers both fuels and shows consistent results for the evolution of the spray complexity toward a higher balance between variability and order. The organization levels as the spray develops and propagates in the z-direction depend on droplet formation and dispersion in the environment. A larger air mass flowrate means aerodynamic forces begin to dominate liquid atomization, lowering the amount of information in the spray. For the lower fuel mass flowrate, Fig. 12a evidences a significant increase in spray complexity when duplicating the air mass flowrate, and the same change occurs when maintaining the air mass flowrate and duplicating the fuel mass flowrate, as shown in Fig. 12b.



(a) (b)

Figure 12. Evolution of the spray complexity (a) for a constant mass flow rate and varying air flow rate and (b) similar air flow rates and different mass flow rates.

The purpose of this work is to use an infodynamic analysis to compare a conventional fuel (Jet A-1) with an alternative one (HVO). So far, the results presented point to the production of similar sprays. Therefore, for the higher fuel mass flowrate ($\dot{m}_f = 0.08 - 0.09\ [g/s]$) and varying the air mass flowrate, one would expect similar complexity maps for the aerodynamic effect on the spray complexity while it propagates. However, Fig. 13 shows some differences between fuels. Namely, with HVO, aerodynamic forces produce a different initial complexity condition, but the $z = 10\ mm$

plane represents a common transition of a similar amount of complexity, above which the spray seems to evolve in the sense of returning to the initial condition until $z = 15\ mm$. After this plane, the evolution of the spray complexity follows a similar informational pattern until $z = 20\ mm$. These results suggest, that only after $15\ mm$ below the injector nozzle are the sprays of both fuels actually similar. Also, if one assumes the principle of evolution of physical systems toward higher levels of complexity, as observed in the natural world, this direction in sprays requires higher dominance of aerodynamic forces and a minimum development distance.

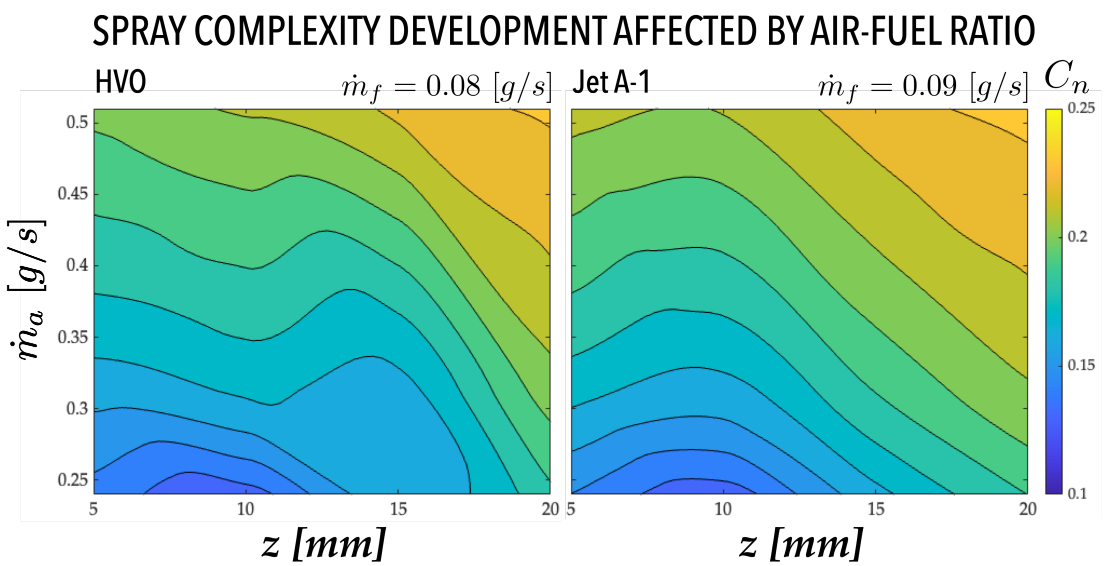


Figure 13. Comparison between HVO and Jet A-1 in terms of the spray complexity.

The following section presents a new approach to spray characterization focused on droplets as information carriers. With the advent of Artificial Intelligence, a synthesis between thermofluid engineering and information theory is needed if one aspires to produce intelligent systems capable of adapting their operating conditions toward the best performance. Also, although providing data on average sizes, velocity distributions, and spray angles is helpful for the combustion chamber design, these parameters might not capture the complexity and diversity of the spray dynamic characteristics. An example of information theory's insights in spray characterization lies in quantifying the Drop Size Diversity of the spray. M. O. Panão et al. (2020) showed how the normalized *informature* (although designated in the paper as Shannon entropy), H_n, combined with the standard deviation of a volume-weighted drop size distribution, SD_v, allows distinguishing the polydispersion and heterogeneity degrees of drop size diversity, respectively. However, while the *informature* is proportional to the amount of information needed due to the diversity of drop sizes, its formulation lacks context. The following section considers the implications of this approach for the meaning of concepts such as entropy and explores a conceptual framework to add context to spray indeterminacy. The expectation is to develop new characterization methods when using laser diagnostic techniques as *infosensors* and improve our understanding of spray dynamics from the point of view of changes captured by information flows.

4.2. Spray Infodynamics

According to Grunwald (2005), *infodynamics* captures the dynamics of information in its transformation into knowledge by intelligent agents. A system is *intelligent* if it follows the cycle of perception, reasoning, feedback, and knowledge update. In spray infodynamics, droplets are objects that contain the spray knowledge (their size and velocity characteristics). Information flows throughout the spray propagation path through these droplets as objects, and interaction events with the surrounding environment change the conveyed information. The Phase-Doppler Interferometer is the communication channel that interfaces with the processing unit and software as agents that provide access to the object's knowledge (perception) to understand it (reasoning). With that understanding, one can adjust operating conditions if needed (feedback), leading to a knowledge update expressed by droplets (objects) with altered characteristics.

The *informature*, $H_{I,b}$, quantifies the amount of information one needs to describe a parameter without context because it depends solely on the probability distribution. The higher this parameter is, the more droplets of different sizes are relevant to describe the spray. The opposite would mean that droplets have a dominant single size in the spray, as produced by a monosize injector.

Shannon (1948) described the term introduced here in Eq. (3), H_b, as a measure of uncertainty but later decided to designate it as *entropy*. The Gibbs and Boltzmann entropies are particular cases of H_b, with Boltzmann introducing the constant with his name (k_B) to maintain the units of the original concept by Clausius. Later, Gibbs obtained a general form for the thermodynamic entropy, considering that microstates could have different probabilities of occurrence. Based on Clausius' intuition that entropy is related to the transformation occurring in a system, we introduced in section 3.1 the concept of as *infotropy* as a *contextualized measure of information*. For example, when the context is Thermodynamics, the corresponding parameter K_c in Eq. (3) is the Boltzmann constant k_B. We will apply the as *infotropy* concept within the spray science context, comparing the two fuels under research, to understand how information flows in the liquid atomization process.

Consider K_c a spray contextual scale parameter affected by the non-deterministic nature of the liquid atomization process. The *infotropy* defined as the contextual transformation of a spray characteristic is a combination of context (K_c) and indeterminacy ($H_{I,b}$), as defined in Eq. (3), $H_b = K_c \cdot H_{I,b}$. If the variation of H_b generates an *infodynamic flow*, it implies that

$$dH_b = dK_c H_{I,b} + K_c dH_{I,b} \tag{10}$$

where dK_c represents a change in context and $dH_{I,b}$ a change in the degree of indeterminacy.

Assuming as a diffusive approximation that the sensibility of the infotropy to its context is

$$\frac{dH_b}{dK_c} = \kappa \tag{11}$$

with κ constant. Applying Eq. (11) in (10) and integrating the outcome between a reference and a subsequent event (in space or time), one could determine the constant κ as

$$\kappa = \frac{(K_c/K_{c,0})\, H_{I,b} - H_{I,b,0}}{K_c/K_{c,0} - 1} \tag{12}$$

with $K_{c,0}$ and $H_{I,b,0}$ as the scale context and *informature* of the reference event. Using the plane at $z = 5\ mm$ as the reference event and planes $z = 10, 15, 20\ mm$ as subsequent events through which information flows, one can determine, in principle, the value of κ.

We considered several contexts: 1) the aforementioned heterogeneity degree of drop size diversity, SD_v; 2) the Sauter Mean Diameter, SMD, because it is the physical measure related to the atomization efficiency (M. Panão, 2022); 2) and the Weber number because of its essential role in drop formation and association with the classification of atomization regimes. The contextual ground for the scale parameter K_c that fulfilled the assumption in Eq. (11) was the Weber number.

The median Weber number ($K_c = \mathrm{We}_{d50}$) is obtained from the discrete distribution of Weber for each measurement plane considering variable size classes due to the changes in the order of magnitude of droplets Weber number ($\mathrm{We}_d = \rho u_d^2 d/\sigma$). For the Jet A-1, $\kappa = 3.94 \pm 5.1\%$ and for HVO, $\kappa = 4.06 \pm 6.6\%$ using Eq. (12). However, for both fuels (Jet A-1 and HVO), Fig. 14 depicts the linear relation of the infotropy and the contextual parameter (Weber in this case). From the linear fitting, it is noteworthy that the sensitivity of the infodynamic entropy contextualized by the Weber results in $dH_e/d\mathrm{We}_{d50} = 3.6$ with a $R^2 = 0.997$, which is similar to the previous values obtained by analyzing the information flow for each fuel between events/planes.

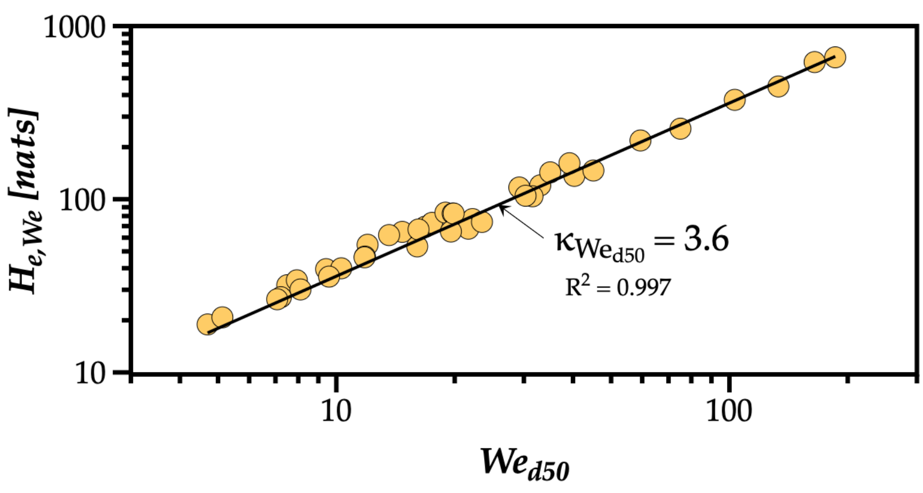


Figure 14. Relation between the infotropy of the Weber number for both fuels (Jet A-1 and HVO), showing the linear variation assumed in Eq. (12).

The similar sensitivity of the infotropy to its context in both fuels indicates that the liquid atomization process affects more the spray's ability to transport information than differences in the fluid's properties. The similarity between drop size distributions explored in the previous section and the similarity of information flows allows for hypothesizing that the differences in the dynamic viscosity (see Table 1) are irrelevant in this liquid atomization strategy. A possible reason could be the dominant effect of aerodynamic mechanisms in the swirl fluidic structure on the spray formation, already observed from the complexity point of view in the previous section. Therefore, the infodynamic comparative analysis suggests that considering HVO as an alternative fuel in aviation might depend on choosing the appropriate atomization strategy that makes the effects of the parameters with the more prominent differences meaningless.

5. Conclusions

After the 28th Conference of Parties (COP28), the urgency of transitioning from fossil fuels to more sustainable alternatives is underscored. This research pivots on evaluating biofuels, explicitly focusing on Hydroprocessed Vegetable Oil (HVO) as a potential substitute for conventional aviation fuels such as Jet A-1. Central to our analysis is comparing droplet sizes in fuel sprays, a parameter critical to optimizing the combustion process. If the atomization process becomes more efficient, it reduces fuel emissions related to droplet sizes in a spray. In light of this, decarbonization is a relevant topic since introducing sustainable aviation fuel is imperative to mitigate environmental concerns. Will the sprays produced by alternative aviation fuels work on injectors optimized for conventional fuels?

Our approach to answering this question integrates principles from information theory in spray science, introducing the appropriate terminology of *informature* (and differential informature) that quantifies the amount of information in a physical system with a non-deterministic nature, *infotropy* as a contextualized informature and *infosensor* as the Phase-Doppler Interferometer that captures the non-deterministic nature of the physical system. We apply these concepts innovatively to analyze and compare discrete and continuous probability distributions of droplet sizes, employing the differential informature as a cornerstone of this analysis. Our findings reveal a striking similarity in the drop size distributions of HVO and traditional Jet A-1 fuel. Notably, although the Gamma mathematical function adeptly characterizes the drop size distribution in swirling sprays, the Log-Normal presented close results to the Gamma, indicating that liquid atomization could hybrid a temporal fragmentation of ligaments and an exponential growth pattern in drop size diversity. We also evaluated the spray complexity and showed that both fuels produce spray evolving toward higher complexity states, balancing variability of drop sizes and order imbued in the interactive atomization mechanism between the fuel and the air flows. However, from the spray complexity point of view, the similarity between the sprays requires dominance of aerodynamic forces in liquid atomization and a minimum development distance.

Finally, we propose a novel lexicon for spray characterization – *infodynamics* – which conceptualizes a spray as a network of information flows among droplets and their interactive events. Further, the *infotropy* concept introduced provides context-rich insights into spray dynamics. In this work, we searched for the contextual scale that expressed a constant sensibility of infotropy to its context. From the several relevant parameters characterizing a spray, the contextual scale based on the Weber number aligned with the constant sensibility assumption. It means spatial variations of the context generated by the interaction events in the atomization process produce linear variations in the infodynamic transformation of the physical system expressed by its infotropy.

Our exploration endorses HVO as a viable alternative to traditional aviation fuels, especially from the perspective of spray infodynamics. The broader implications of this study extend beyond fuel selection that offers sustainable solutions in aviation and related fields. It offers a transformative perspective on understanding engineering complex processes containing elements of deterministic and non-deterministic nature.

Acknowledgements

The authors would like to acknowledge the Fundação para a Ciência e Tecnologia (FCT) for partially financing the research through project PTDC/EMETED/7801/2020 and UIPD/50022/2020 (DOI: 10.54499/UIDP/50022/2020) and UIDB/50022/2020 (DOI: 10.54499/UIDB/50022/2020).

Nomenclature

a, b	Scale and shape parameters in probability distributions
C, C_n	Complexity [$nats^2$] and normalized by the maximum informature
D	drop size [μm]
D_{50}	Median drop diameter [μm]
f	Frequency probability of a distribution
F	Cumulative frequency of a distribution
H_b	Infotropy of a non-deterministic physical system [a.u.]
H_δ	analytical differential informature [a.u.]
H_Δ	discrete differential informature [a.u.]
H_I	Informature [a.u.]
$H_{max,b}$	Maximum informature [a.u.]
H_n	Normalized informature
K_b	Logarithm-base conversion constant
K_c	Arbitrary contextual scale of an infotropy
$\dot{m}$	Mass flowrate [g/s]
$nH_{ud,b}$	Mutual informature between velocity u and size d [$nats$]
p	probability density [μm^{-1}]
R_n	Normalized redundancy
s	log-normal standard deviation [μm]
u_d	Drop velocity [m/s]
We_d	Weber number

Subscripts

0	Initial event
a	Air
b	Logarithm base
d	droplet
$d50$	Median representative quantity
e	Exponential base
f	Fuel

Greek symbols

Δt	Total measurement time [s]
κ	Contextual infodynamic parameter [a.u.]
ρ	Density [kg/m^3]
σ	Surface tension [N/m]
τ	Infosensor response time [s]

Acronyms

AFR	Air-Fuel Ratio [-]
HVO	Hydrotreated Vegetable Oil
KS	Kolmogorov-Smirnof
LN	Log-Normal
PDF	Probability Density Function
SMD	Sauter Mean Diameter

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