

Inferred Binary Mixture Fraction via Physics-Informed Filtered Rayleigh Scattering

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ABSTRACT

Understanding mean passive scalar transport in non-reacting flows is a complex task, in part due to measurement difficulties outside of controlled, lab-scale environments. This work seeks to use a combination of filtered Rayleigh scattering to yield non-intrusive, high spatial resolution measurements of the mean field of a Mach 0.8 air-helium mixture and physics-informed machine learning to denoise the experimental data and provide mass fraction of helium. This yields a simultaneous result for axial and radial velocity, static temperature and density, and mass fraction of helium without measurements of a reference Rayleigh scattering signal of each gas in the mixture. Specifically, it was found that the derived mass flow from probe measurements, CFD, and the physics-informed FRS method agree within ± 0.01 kg/s.

1. Introduction

The capability to measure mixture concentration has implications across science and engineering because it imparts a greater understanding of the turbulent phenomena that govern active transport in a fluid. From creamer mixing with coffee to aircraft engine exhaust particle matter mixing with the surrounding atmosphere, understanding the mixing begins with the capability to measure concentration, or more generally, a passive scalar in a fluid Sreenivasan (2019). Because the term passive scalar refers to a quantity that is convected by the fluid, but has no effect on the fluid itself, passive scalar can generally refer to temperature or gas species concentration Warhaft (2000). This work specifically focuses on average mass fraction of helium in a binary gas mixture and will be referred to as mixture fraction. Because the analysis is confined to the region near the jet exit, it is assumed that motion is dominated by initial momentum and buoyancy effects are minimal Michaux & Vauquelin (2009).

Concentration can be observed in a qualitative manner through smoke/dye injection Raissi et al. (2020). Concentration is measured quantitatively using a non-intrusive optical technique or sampled at a point using a probe C. Ground et al. (2018). Probe measurements for gas concentration are

straightforward to implement and do not require many assumptions about the flow itself; however, they are limited in that they only provide this measurement at a point and typically cannot be deployed in harsh environments due to limited survivability.

Optical-based techniques offer an advantage because their interaction with the flow is limited, and usually have a higher spatial resolution. However, most optical techniques are inverse techniques that require solving an inverse problem, necessitating additional information or assumptions about the flow field to determine molecular concentration. Particle image velocimetry (PIV) and planar laser-induced fluorescence (PLIF) have been previously implemented for concentration measurements in reacting and non-reacting flows but typically require volumetric correlation, defining a calibrated relationship, or using a combination of the techniques Nguyen et al. (2012); Sarathi et al. (2012). Notably, Clemmens & Mungal Clemmens & Mungal (1995) utilized PLIF to characterize the structure and concentration field in axisymmetric mixing layer flows. Raman spectroscopy is an additional optical technique that has had success in characterizing gas species concentration, particularly for combustion applications Danehy et al. (2003). However, these optical techniques are difficult to implement outside of a lab environment because they either require seeding particles or increasingly complex instrumentation Raffel et al. (2018); K.P.Geigle et al. (2022). Background-oriented Schlieren (BOS) has also been applied to measuring concentration, but is limited to qualitative observations without supplementary information Kotchourko et al. (2014).

Rayleigh scattering is a technique that can overcome these limitations because the signal is generated based on laser light scattering off of molecules present in the gas and is proportional to the size and number of scatterers Sorensen (2022). Rayleigh scattering techniques mitigate the issue of limited spatial resolution, but most techniques can only be applied assuming either constant temperature Shirinzadeh et al. (1992), pressure C. Ground et al. (2018), or both Seasholtz et al. (1997). Despite the required assumptions about the thermodynamic state of the measurement, filtered Rayleigh scattering (FRS) and laser Rayleigh scattering (LRS) are predominant optical techniques for measuring mixture fractions because of the relatively straightforward measurement setup and the versatility of the technique as a whole C. R. Ground et al. (2023). Their widespread deployment for mixture fraction measurement applications is supported by the fact that they are a molecular scattering technique, eliminating the need for seeded flow Miles et al. (2001). This makes it an ideal tool to measure the concentration of a gas species in a mixture. FRS can also be used to determine static temperature, density, and three-component velocity of the mean flow field Boguszko & Elliott (2005).

FRS and LRS are not excluded from the primary limitation of optical techniques: they are inverse problems. This often results in an ill-conditioned problem Grauer et al. (2022). Solving for three-component velocity, static temperature, and static density requires three different observations of the FRS signal from different viewing angles to deterministically solve for all five quantities

C. Ground et al. (2018). Adding an additional variable (mass fraction) increases the ill-posedness of the problem. Traditionally, Rayleigh scattering-based approaches to determine the concentration of a flow field employ a simpler ratiometric method. This method takes advantage of the fact that both the differential scattering cross-section and the number of scatterers are intensity-based scaling factors on the signal. This approach, while easier in practice, necessitates separate measurements of the scattering signal of both gases in the binary mixture at the same pressure and temperature Gopal & Maddalena (2021); George et al. (2014). There are some approaches to the FRS measurement model (to be discussed in Section 2) that would yield concentration for non-isobaric, non-isothermal cases but their implementation, in general, is limited to lab environments because they do not circumvent the requirement of reference measurements for the components of the mixture.

This work seeks to introduce an additional measurement capability to FRS such that the measurands include velocity, static density, static temperature, and mass concentration in a binary mixture. An additional requirement is to eliminate the need for gas-specific reference measurements and to require minimal assumptions about the mean flow field. This is done via incorporating physics-informed machine learning with FRS. Physics-informed machine learning acts as an FRS data assimilation technique that utilizes a fully-connected deep neural network that accepts spatial coordinates as inputs and outputs three-component velocity, static density, static temperature, and mass fraction for both helium and air.

A statistical approximation of a function is created using penalties defined by the measured FRS data and the governing fluid dynamics. More directly, the deep neural network learns the appropriate combination of weights and biases by minimizing two loss components: a data loss term and a physics loss term. The data loss corresponds to an observation or measurement of the flow field and the physics loss term consists of a residual of the differential equations that govern the physics of the flow. Physics-informed neural networks (PINNs) are rapidly gaining notoriety in fluid diagnostics because of their capabilities to reduce spatial noise and recover missing information Raissi et al. (2019). To complete this task, PINN's require knowledge of the velocity field from a diagnostic technique (most commonly PIV) or boundary conditions in the form of mean field properties along a defined region of the measurement domain to reconstruct the mean field with reduced noise and recovered missing information Steinfurth & Weiss (2024); Molnar et al. (2023); Raissi et al. (2020). Previous implementations of FRS with PINNs have been focused on the noise-reduction capabilities and have not sought to expand FRS measurands beyond static density, static temperature, and velocity Bundy et al. (2026). Because this work is the first such implementation, a major objective is to determine the influence of added information through boundary conditions or additional assumptions.

Section 2.1 will provide a description of the FRS measurement model with supporting context on how FRS yields mean field properties and binary mixture concentration. This is followed with a

description on how the FRS measurement model is integrated into the PINN model, with brief discussion on the governing fluid dynamics and underlying assumptions incorporated into the FRS-PINN model (Section 2.2). An overview of the setup procedure for the CFD simulation used for initial validation is then provided (Section 3.2), followed by a similar description of the experimental FRS measurement setup (Section 3.1). Results from the FRS-PINN model and CFD simulation are provided and discussed (Section 4), followed by conclusions and outlooks.

2. Methods

2.1. Rayleigh Scattering

LRS refers to the elastic scattering of coherent light from sources that are much smaller than the wavelength of light Sorensen (2022). The scattering source is the molecules of the gas mixture. The Rayleigh scattering signal is related to the molecules in the gas through the following Pitts & Kashiwagi (1984):

$$S_{LRS} = AI_0N \left(\sum_{j=1}^J \frac{\partial \sigma}{\partial \Omega_j} X_j \right) + C \quad (1)$$

where A is a constant related to optical parameters, C is a constant related to image background intensity, N is number density of the mixture, I_0 is the incident laser intensity, X is the mole fraction of each species in the mixture, $\frac{\partial \sigma}{\partial \Omega}$ is differential scattering cross section, or a representative size of the scatterer that is a function of the index of refraction, number density, the wavelength of light, and the measurement setup Pitts & Kashiwagi (1984). It should be noted that several significant assumptions are involved in Eq. 1. The first is that all components of the gas are at the same number density. This is a standard limiting assumption of using LRS to determine mixture fraction C . Ground et al. (2018). If this cannot be assumed (which is the case for the measured data to be presented), the measurement becomes significantly more complex. For a more detailed overview on the appropriate measurement model for variable number density between components of the mixture, readers are referred to Gopal *et al.* Gopal & Maddalena (2021). A final assumption is that the flow measured in this work is a binary gas mixture, which treats air as a single species gas. This is widely considered to be an appropriate assumption for Rayleigh scattering measurements of air Pitts & Kashiwagi (1984).

The key takeaway from Eq. 1 is that the LRS signal is a function of gas mixture composition. To yield quantitative gas mixture fraction measurements, Eq. 1 can be manipulated since several properties are known. Given a measurement of each component of the mixture at the same pressure, temperature, and laser conditions, mixture fraction can be determined by rearranging Eq.

1. The first step is formalizing the assumption that gas mixture is binary and composed only of helium and air, which is the measured LRS signal of the mixture:

$$S_{mix} = AI_0N \left(\frac{\partial \sigma}{\partial \Omega_{He}} X_{He} + \frac{\partial \sigma}{\partial \Omega_{air}} X_{air} \right) + C \quad (2)$$

This can be further simplified with the knowledge that, because the mixture is binary:

$$X_{He} + X_{air} = 1 \quad (3)$$

Substituting Eq. 3 into Eq. 2, gives the following:

$$S_{mix} = AI_0N \left[\frac{\partial \sigma}{\partial \Omega_{He}} X_{He} + \frac{\partial \sigma}{\partial \Omega_{air}} (1 - X_{He}) \right] + C \quad (4)$$

It follows from Eq. 1 that LRS signal for helium and air only can be written as:

$$S_{air} = AI_0N \frac{\partial \sigma}{\partial \Omega_{air}} + C \quad (5a)$$

$$S_{He} = AI_0N \frac{\partial \sigma}{\partial \Omega_{He}} + C \quad (5b)$$

Using Eqs. 2-5, and reiterating that a constant number density between all S_{mix} , S_{air} , and S_{He} is assumed, it follows that:

$$\begin{aligned} S_{mix} - S_{air} &= \left(AI_0N \left[\frac{\partial \sigma}{\partial \Omega_{He}} X_{He} + \frac{\partial \sigma}{\partial \Omega_{air}} (1 - X_{He}) \right] + C \right) \\ &\quad - \left(AI_0N \frac{\partial \sigma}{\partial \Omega_{air}} + C \right) \\ &= AI_0N X_{He} \left(\frac{\partial \sigma}{\partial \Omega_{He}} - \frac{\partial \sigma}{\partial \Omega_{air}} \right) \end{aligned} \quad (6a)$$

$$\begin{aligned} S_{He} - S_{air} &= \left(AI_0N \left[\frac{\partial \sigma}{\partial \Omega_{He}} \right] + C \right) \\ &\quad - \left(AI_0N \frac{\partial \sigma}{\partial \Omega_{air}} + C \right) \\ &= AI_0N \left(\frac{\partial \sigma}{\partial \Omega_{He}} - \frac{\partial \sigma}{\partial \Omega_{air}} \right) \end{aligned} \quad (6b)$$

Thus mixture fraction can be defined using three distinct LRS measurements at the same number density: one with air only, one with helium only, and one of the whole mixture:

$$X_{He} = \frac{S_{mix} - S_{air}}{S_{He} - S_{air}} \quad (7)$$

Several problems arise when implementing this approach. The first is that, outside of a highly controlled environment, it is exceedingly difficult to obtain measurements of the mixture and each of its components at the same pressure and temperature Gopal & Maddalena (2021). A second key problem that arises is that the LRS signal can be easily overwhelmed by scattering contributions from larger particles or reflections in the image. To mitigate this, a molecular absorption filter is employed, which attenuates signal contributions from unwanted sources and retains sensitivity to the Rayleigh scattering signal. This is called filtered Rayleigh scattering.

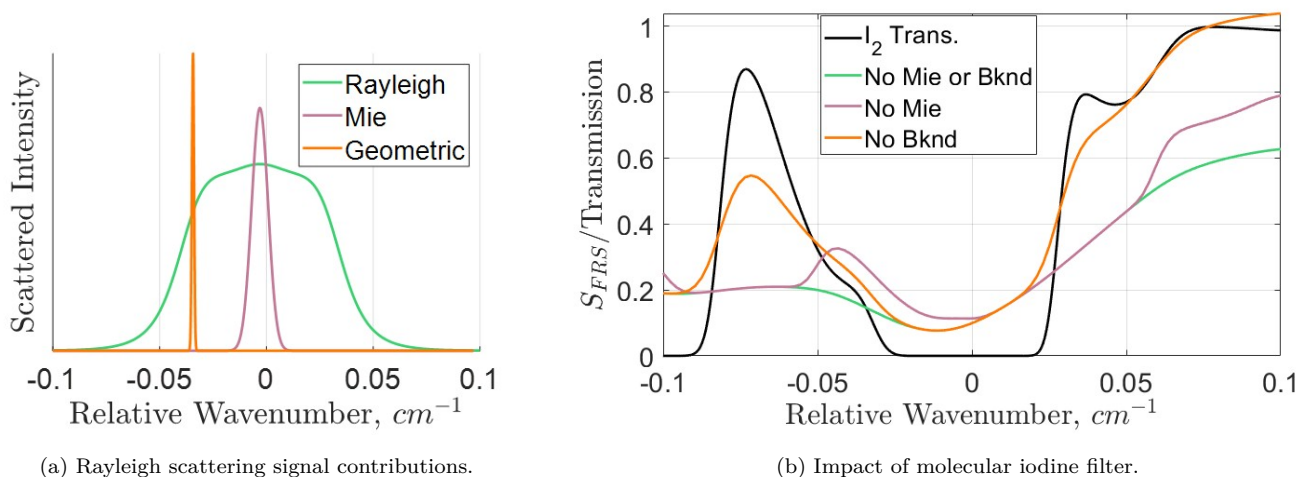


Figure 1. Theoretical description of FRS.

This is described through Figs. 1a and 1b. Figure 1a shows the spectra of the three major types of scattering signal contributions. Geometric scattering (or scattering from the background in the image) is the highest intensity signal in Fig. 1a and does not experience a Doppler shift proportional to the bulk motion of the gas (indicated by the orange line), unlike Rayleigh and Mie scattering. Mie scattering is the higher intensity scattering from larger particles and is indicated by the narrower, Gaussian signal in Figure 1a. To generate the FRS spectra, the light source is frequency tuned through a high to low transmission feature in the molecular filter, illustrated in Figure 1b. The black line shows the frequency-dependent transmission profile of the molecular iodine filter (I_2). The green line corresponds to a case with all Rayleigh scattering, i.e., no Mie or background contribute to the convolved signal. The pink line represents a convolved signal with Rayleigh and background scattering and no Mie scattering. The orange line represents a convolved signal Rayleigh and Mie scattering but no background. As can be seen in Figure 1b the Mie and background signals make no contribution to the convolved signal (the two lines collapse with the green,

or all Rayleigh scattering, line) in a low transmission region of the iodine feature. The result is a FRS signal that retains sensitivity to the properties of the gas and mitigates influence from particle and background scattering.

The ideas conveyed in Figure 1b can also be written mathematically in the form of an FRS measurement model:

$$S_{FRS} = AI_0N \left(\sum_{j=1}^J \frac{\partial \sigma}{\partial \Omega_j} X_j \int_{-\infty}^{+\infty} r(X_j, Y_j) \tau(\nu + \nu_l + \Delta\nu_D) d\nu \right) + C \quad (8)$$

where A is a signal calibration constant that encompasses parameters related to the optical collection system, τ is the iodine transmission, ν is the relative optical frequency, ν_l is the central frequency of the incident laser light, $\Delta\nu_D$ is the Doppler shift. This is similar to the LRS measurement model defined in Eq. 1, but in this case, the scattering is not directly proportional to Rayleigh scattering intensity but instead is proportional to the convolution of the Rayleigh spectra and the iodine transmission. The Rayleigh lineshape is represented by $r(X, Y)$. This is dependent on two non-dimensional parameters that are related to the mean properties of the gas:

$$X = \frac{2\pi\nu}{\sqrt{2}Ku_0} \quad (9a)$$

$$Y = \frac{Nk_B T}{\sqrt{2}Ku_0\eta} \quad (9b)$$

where u_0 is thermal velocity, η is the dynamic viscosity of the gas, and K is the interference wave vector, defined as:

$$\vec{K} = (2\pi/\lambda)(\hat{o} - \hat{i}) \quad (10)$$

where $\hat{o}$ is the observation vector and $\hat{i}$ is the laser propagation vector. The results in this work treat mass fraction as the passive scalar, not mole fraction. To achieve this, Eq. 8 must be modified to reflect this. Mass fraction is defined as:

$$X_j = \frac{\chi_j M_{mix}}{M_j} \quad (11)$$

where M is molar mass. Substituting Eq. 11 into the FRS measurement model yields:

$$S_{FRS} = AI_0N \left(\sum_{j=1}^J \frac{\partial \sigma}{\partial \Omega_j} \frac{\chi_j M_{mix}}{M_j} \int_{-\infty}^{+\infty} r(X_j, Y_j) \tau(\nu + \nu_l + \Delta\nu_D) d\nu \right) + C \quad (12)$$

This is simplified by removing molar mass of mixture, M_{mix} , from summation:

$$S_{FRS} = AI_0 N M_{mix} \left(\sum_{j=1}^J \frac{\partial \sigma}{\partial \Omega_j} \frac{\chi_j}{M_j} \int_{-\infty}^{+\infty} r(X_j, Y_j) \tau(\nu + \nu_l + \Delta \nu_D) d\nu \right) + C \quad (13)$$

Using the relationship between number and mass density ($N = \frac{\rho N_A}{M}$, where N_A is Avogadro's number), the FRS measurement model can be written in terms of mass density (ρ):

$$S_{FRS} = AI_0 \rho N_A \left(\sum_{j=1}^J \frac{\partial \sigma}{\partial \Omega_j} \frac{\chi_j}{M_j} \int_{-\infty}^{+\infty} r(X_j, Y_j) \tau(\nu + \nu_l + \Delta \nu_D) d\nu \right) + C \quad (14)$$

Simplifying this for the case of a binary air-helium mixture:

$$S_{FRS} = AI_0 \rho N_A \left[\frac{\partial \sigma}{\partial \Omega_{He}} \frac{\chi_{He}}{M_{He}} \int_{-\infty}^{+\infty} r(X_{He}, Y_{He}) \tau(\nu + \nu_l + \Delta \nu_D) d\nu + \frac{\partial \sigma}{\partial \Omega_{air}} \frac{(1 - \chi_{He})}{M_{air}} \int_{-\infty}^{+\infty} r(X_{air}, Y_{air}) \tau(\nu + \nu_l + \Delta \nu_D) d\nu \right] + C \quad (15)$$

With the knowledge that the differential scattering cross section for helium is approximately 73 times smaller than air, it is assumed that its contribution is small, if not negligible C . Ground et al. (2018). This allows (15) to be simplified to:

$$S_{FRS} = AI_0 \rho N_A \frac{\partial \sigma}{\partial \Omega_{air}} \frac{(1 - \chi_{He})}{M_{air}} \int_{-\infty}^{+\infty} r(X_{air}, Y_{air}) \tau(\nu + \nu_l + \Delta \nu_D) d\nu + C \quad (16)$$

Laser intensity, Avogadro's number, differential scattering cross section for air, and molar mass of air can be lumped into A to yield the final form of the FRS measurement model considered in this work:

$$S_{FRS} = A \rho (1 - \chi_{He}) \int_{-\infty}^{+\infty} r(X_{air}, Y_{air}) \tau(\nu + \nu_l + \Delta \nu_D) d\nu + C \quad (17)$$

where χ_j is now mass fraction. The result is a mixture dependent FRS signal model for a binary mixture of helium and air that is dependent on the thermodynamic properties of air and a signal scalar that represents the amount of the mixture that is not air (mass fraction of helium). This is again a product of assuming that the contribution to the Rayleigh signal from the helium portion of the mixture is insignificant because differential scattering cross section is much smaller than air. It is noted that this form of the measurement model only requires one measurement, that of the mixture; however, the problem of limited information still remains. Instead of using multiple measurements of the mixture to resolve concentration, this approach uses the governing flow physics

to add more information to the problem. The integration of the measurement model defined in this Section (Eq. 17) with a physics-informed neural network is described in Section 2.2. This is a substantial departure from the LRS approach (Eq. 7), which requires three different measurements of the mixture at constant number density and retains sensitivity to background/particle scattering. This also differs from previous FRS-based mole fraction measurements in that these require at least a measurement of air and the mixture C. Ground et al. (2018); C. R. Ground et al. (2023).

2.2. Physics-Informed Neural Network

Physics-informed neural networks (PINNs) are a machine learning technique that use a combination of governing physics and experimentally measured data. They have gained notoriety in fluid diagnostics due to their ability to reduce measurement noise and increase measurement output Raissi et al. (2020). PINNs in general, have a wide application space in scientific computing and can be applied in any scenario that incorporates partial differential equations with measured data Raissi et al. (2019). The basis of this work is a PINN that combines the FRS measurement model (Eq. 17) with the Reynolds-averaged Navier-Stokes (RANS) equations. The FRS-PINN takes inputs of spatial coordinates and outputs mean field properties, namely static temperature, density, and three-component velocity. The technique is pictorially summarized in Figure 2.

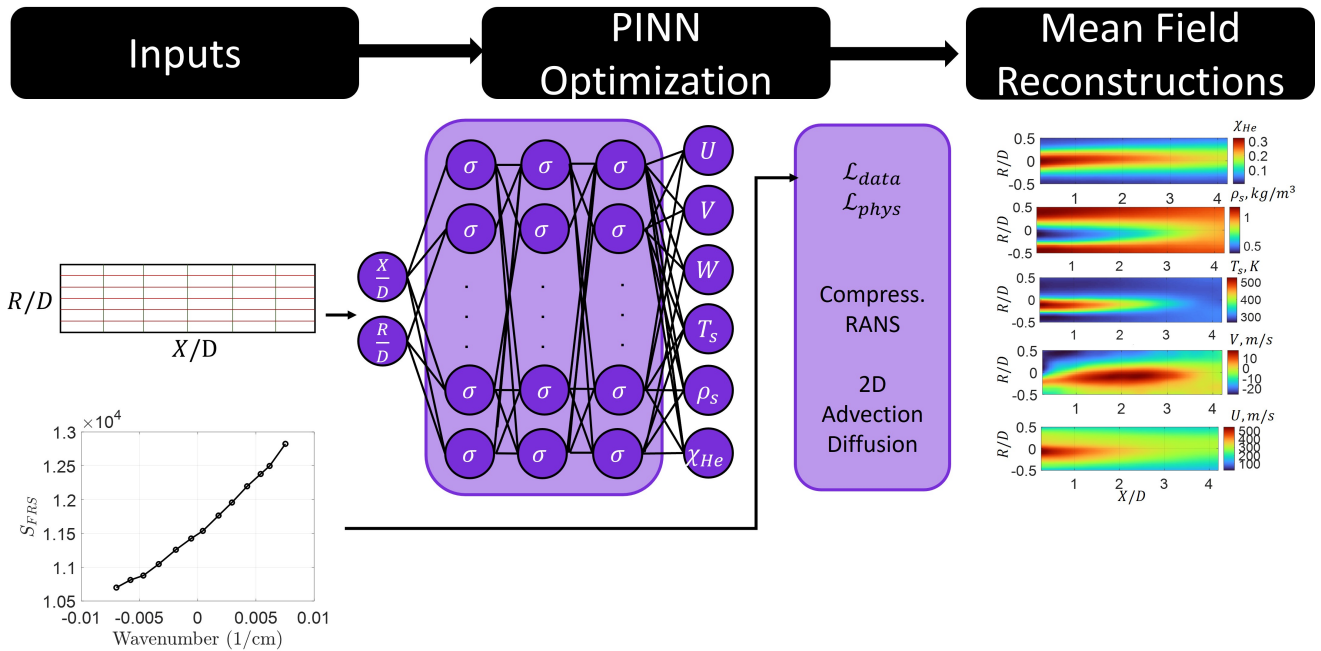


Figure 2. FRS-PINN summary.

The FRS-PINN differs from other PINN techniques in that it also requires inputs that describe the measurement setup such that an FRS signal can be modeled from the PINN outputs at each training iteration. The modeled signal from the PINN outputs is then used to compute a loss term,

$\mathcal{L}_{data}$, relative to the measured FRS signal. $\mathcal{L}_{data}$ is defined as:

$$\mathcal{L}_{data} = \frac{1}{N_{FRS}} \frac{1}{N_\nu} \left[\sum_i^{N_{FRS}} \sum_j^{N_\nu} (S_{FRS_{mod_{i,j}}} - S_{FRS_{meas_{i,j}}})^2 \right] \quad (18)$$

The second loss term, $\mathcal{L}_{phys}$ is formed from the RANS equations for an axisymmetric, compressible jet and the advection-diffusion equation. The RANS equations are not provided for brevity. The advection-diffusion equation is how the passive scalar, in this case mass fraction (χ_{He}), is accounted for in the physics loss. For a passive scalar in an axisymmetric turbulent jet flow, this is defined as Pope (2000):

$$\frac{\partial(r\rho V \chi_{He})}{\partial r} + \frac{\partial(r\rho U \chi_{He})}{\partial x} - \frac{1}{Re} \left[\frac{\partial}{\partial x} \left(r\rho \frac{\partial \chi_{He}}{\partial x} \right) + \frac{\partial}{\partial r} \left(r\rho \frac{\partial \chi_{He}}{\partial r} \right) \right] = 0 \quad (19)$$

where Re is Reynolds number, and all quantities are in non-dimensional form. The two losses are then combined with a weight parameter to yield the total loss:

$$\mathcal{L}_{total} = \omega_{phys} \mathcal{L}_{phys} + \omega_{data} \mathcal{L}_{data} \quad (20)$$

For this work, a constant $\omega_{phys} = 1 \times 10^{-3}$ and $\omega_{data} = 1$ are applied. These were selected based on previous FRS-PINN implementations. A hyperparameter tuning process was performed to ensure that a primary emphasis is placed on the measured FRS data, which is a direct product of the flow of interest, and the physics loss regulates the solution. The network continues to train on random batches of spatial locations and measured FRS data until both losses are minimized. The trained model is then used to produce mean field reconstructions.

The performance of this model will be evaluated on two different data types: simulated FRS data from the CFD solution for this field and measured FRS data on a Mach 0.8 jet with helium injection. FRS-PINN results will be compared to the CFD solution. This mean field result and the specific measurement configuration defined in Section 3.1 are then used as inputs to the FRS measurement model (Eq. 17). These FRS data are then used as inputs to the PINN model to benchmark the capability of the approach to yield simultaneous, full-field estimates of static density and temperature, axial and radial velocity, and mass concentration of helium in a binary gas mixture. In short, there are two different approaches to arriving at $S_{FRS_{meas}}$ used to compute the data loss term that guides the training process (Eq. 18):

1. $S_{FRS_{meas}}$ is measured experimentally on the jet flow described in Section 3.1, with results presented in Section 4.2.
2. A noise free representation of the flow field is used to define $S_{FRS_{meas}}$, which is computed via the following steps:

- (a) The field is simulated with CFD, based on gauge total pressures during rig operation. This procedure is described in Section 3.2.
- (b) The mean field from the CFD result is used as inputs to the FRS measurement model, specifically to define the X and Y parameters (Eq. 9) that define the FRS signal that results from the mean field properties (Eq. 17). Setup specific parameters such as scattering angle and laser propagation direction are kept constant between the measurement and simulation, i.e., the scattering angle from the measurement is used to simulate the data.
- (c) These FRS data that result from the CFD mean field solution are taken to be $S_{FRS_{meas}}$ in the data loss parameter. This allows for a model performance benchmark without measurement noise.

It was conventionally selected to produce all reconstructions with ten hidden layers, 50 neurons per output, and 256 Fourier features with a standard deviation of one. The size of the network is selected by training the network on an exact field loss for 1000 iterations, i.e., the ground truth or CFD solution is used to construct a mean square error. It was found that this configuration (ten hidden layers, 50 neurons per output) is capable of reconstructing the mean field with root mean square error of 4.81×10^{-2} in mass fraction, 13.1 m/s in axial velocity, 6.1 m/s in radial velocity, 3.0×10^{-2} kg/m³ in static density, and 3.0 K static temperature. These are slightly high, but this is 1/10 of the training period used to produce the mean field reconstructions. Training on an exact field loss is done purely to gauge that the network size is sufficient enough to reconstruct the mean field to an admissible level of detail. Finally, the model performance on experimentally measured data without reference measurements or boundary conditions will be discussed.

3. Test Setup Description

The following section describes the experimental setups and associated uncertainties. This is inclusive of the jet and its instrumentation, as well as the FRS measurement configuration. The description of the jet and measurement configuration is then followed by an overview of how rig instrumentation informed the boundary conditions for a CFD simulation, which will serve as a guideline for the expected mean field behavior from the nozzle exit, extending to the near-jet region, but remaining within the potential core.

3.1. FRS

FRS measurements were taken on a Mach 0.8 jet flow with helium injection at Virginia Tech's Advanced Propulsion and Power Lab *Advanced Propulsion and Power Lab* (2025). This was achieved using the nozzle assembly seen in Figure 3. Air at ambient temperature (298 K) was delivered

through the primary nozzle ($D = 38.1 \text{ mm}$) at a mass flow rate of 0.3440 kg/s . Helium was delivered through a secondary nozzle ($D = 8.38 \text{ mm}$) at a mass flow rate of approximately $1.1 \times 10^{-2} \text{ kg/s}$. Helium was regulated from 2000 psi to 300 psi using a Prostar high pressure/high flow regulator, this was followed by a low pressure Harris Model 425-50 regulator that regulates the pressure from 300 psi to approximately 12 psi, thus controlling the mass flow rate of helium to the nozzle exit. In between the regulator and the nozzle exit, helium passes through a Lambda Square Inc. orifice meter, to provide an estimated mass flow rate of the secondary stream before it mixes with air. The secondary nozzle exhausts approximately two jet diameters before the exit of the nozzle assembly Daniel et al. (2019). This allows for the two streams to mix before the beginning of the measurement. The effect of this is that the mass fraction is not exactly one at the jet exit and is seen in both the CFD and FRS results in Section 4. The entire helium delivery procedure is summarized in Figure 3.

Figure 3 additionally depicts the FRS measurement configuration. The measurement plane originates at the exit of the nozzle assembly and extends axially to an $X/D \approx 4$ and radially to $R/D \approx \pm 0.5$. The polarization state of the laser, defined by $\hat{p}$ in Figure 3 is parallel to the measurement plane. The cameras were placed at roughly 45, 90, and 135 degrees relative to the measurement plane (θ in Figure 3). The cameras had an exposure time of 20 seconds with 35 frequency points in each scan which resulted in a data acquisition period of approximately 15 minutes. To create the measurement plane, a 532 nm wavelength, continuous wave, Coherent Verdi-V18 frequency-doubled Nd:YVO₄ diode-pumped, solid-state laser was operated at a power level of approximately 10 watts Coherent (n.d.).

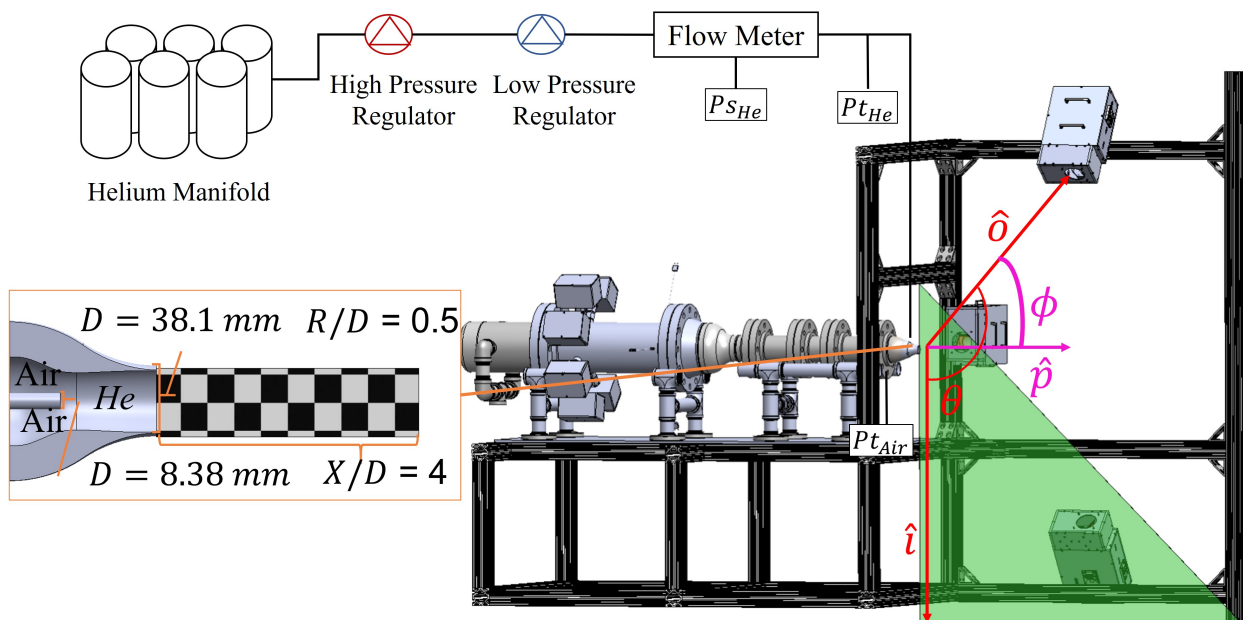


Figure 3. Relevant setup information for the measurement on Virginia Tech’s heated free jet rig.

For rig instrumentation, a National Instruments (NI) 9213 thermocouple module in a NIcDAQ-

9184 chassis was used to record the temperature data and pressures were recorded a Scanivalve Corporation ZOC17IP/8Px-APC. Readers are referred to Daniel *et al.* Daniel et al. (2019) for a more detailed overview of jet instrumentation. Because of recent calibration before data acquisition, bias error associated with these values are considered to be negligible. Based on manufacturer specifications, the error associated with pressure readings is $\pm 0.08\%$ of the full scale reading of the sensor. This corresponds to ± 0.3 psi or approximately ± 2000 Pa. Similarly, the error associated with the temperature data is ± 2.2 K, which is the standard error for type K thermocouples DwyerOmega (2026). The spatial uncertainty of the FRS measurement is taken to be ± 0.14 mm. This is based on the reprojection error resulting from the camera calibration procedure and the known resolution of the measurement to be 7.8 ± 1 pixels/mm. This value accounts for uncertainty in the location of the measurement plane relative to the cameras, but it is noted that there may be additional uncertainty in the position of the nozzle exit relative to the Cartesian grid of the FRS measurement, which is assumed to be minimal for this experiment.

A source of bias error that is non-negligible is the error incurred by the open-loop control system used to deliver the mass flow rate of helium. This was continuously adjusted throughout the experiment to maintain a consistent flow rate; however, the resolution of the regulator is 2 psi. To appropriately account for this uncertainty in the pressure of helium at the nozzle exit, it is assumed that there is a bias error of ± 2 psi or approximately $\pm 14,000$ Pa. The impact of this bias error on the accuracy of results is discussed thoroughly in Section 4.2. To reduce bias error in future measurements, a mass flow rate controller with higher precision could be implemented.

3.2. CFD

A computational fluid dynamics (CFD) simulation was performed to provide high spatial resolution data for comparison to both the stand alone FRS results and the FRS-PINN results. Ansys Fluent *ANSYS Fluent - Fluid Simulation Software* (2025) was used along with the computational domain seen in Figure 4a which extends $50 X/D$ downstream and $10 X/D$ in the radial direction. A pressure-based solver was employed for the 2D-axisymmetric simulation which also used a two-equation SST $k - \Omega$ turbulence model with both the turbulence intensity and turbulent viscosity ratio set at Fluent's standard values of 5% and 10, respectively. The species transport model was turned on to model the mixing of helium (coming from the core nozzle) and air (coming from the bypass nozzle). The energy equation was turned on, and, as such, both the individual gas species and the mix were modeled using the ideal gas assumption, and the viscosities were determined using the built-in three-coefficient Sutherland model. It should be noted that the helium viscosity table was manually entered into Fluent using the information from Ref. *Helium Gas Dynamic Viscosity* (2025). The shape of the nozzle is the same as that depicted by Mayo *et al.* Mayo Jr et al. (2019) and can be seen in Figure 3. The exception being that the core flow (C) is centered around the revolving axis (center of jet). The jet exhausts into freespace where the pressure outlet boundary

conditions allow for the passage of flow in/out of the domain.

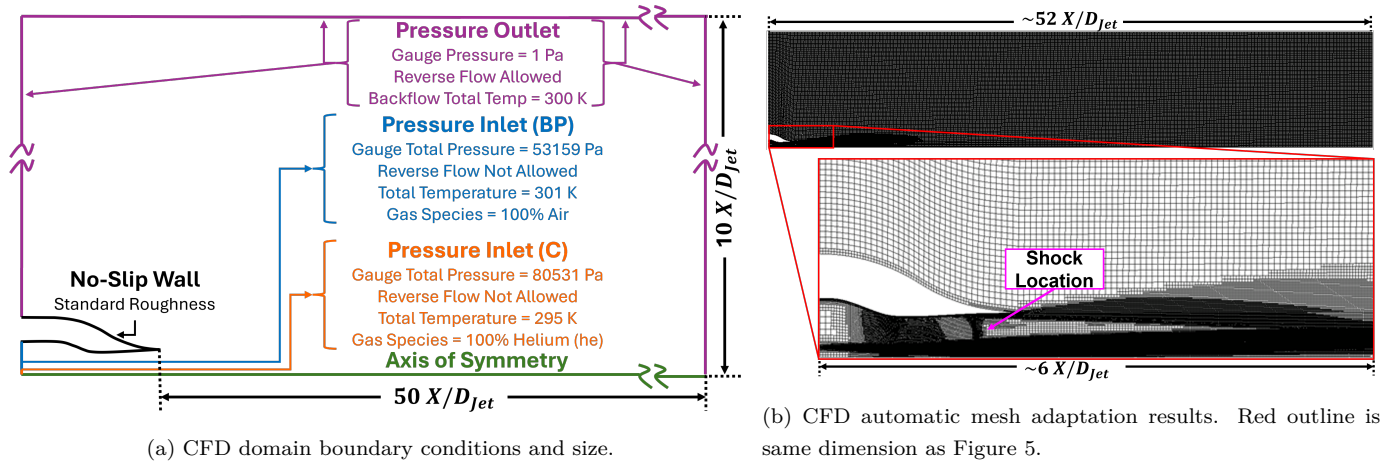


Figure 4. Relevant boundary conditions and mesh information for CFD simulation of Virginia Tech's heated free jet rig with air and helium. Gauge pressures are to Blacksburg, VA STP.

The mesh was initially very coarse with an average cell size of 0.0025 m by 0.0025 m for a total cell count of approximately 120,000. This was allowed to run for 1000 initial iterations by which the time the residuals had leveled out below $1e^{-4}$ for all variables of interest. Then Fluent's built-in Y-plus mesh adaptation tool was implemented. The limits for the allowable values of Y-plus were 1-10. The mesh was allowed to adapt every 250 iterations for a total of 2000 iterations. After all adaptations were completed, all Y-plus values fell in between the specified range. The solution was run for another 1000 iterations to converge using the newly adapted wall mesh using approximately 170,000 cells. The mesh was then adapted for the velocity gradient, where a maximum gradient of 5 m/s cells to cells was specified. Again, the mesh was allowed to adapt every 250 iterations for a total of 1000 iterations. Once completed, the mesh was approximately 650,000 cells and the solution was again allowed to converge for another 1000 iterations using the newly refined mesh. Then the mesh was refined for the gas species mass fraction gradient where a maximum allowable change from cell to cell was 0.001. The mesh was again adapted every 250 iterations for a total of 1000 iterations and then allowed to converge for another 1000 iterations. The result was a mesh size of approximately 1.6 million cells. Finally, the mesh was adapted using the density gradient to refine the shock in the nozzle (since the nozzle was run at off design conditions) where a maximum change of 0.01 kg/m^3 from cell to cell was specified. This time the mesh was allowed to adapt every 500 iterations for a total of 1000 iterations and then was allowed to converge for 2000 iterations before the residuals no longer dropped. This resulted in a mesh with approximately 2.5 million cells which can be seen in Figure 4b.

Figure 5 depicts six key results from the CFD simulation. The plots have been cropped to approximately match the same axial distance that will be shown with the FRS results in Section 4. The top left image shows axial velocity, the top right depicts radial velocity, the middle left is static density, the middle right is static temperature, the bottom left is static pressure and the bottom right is

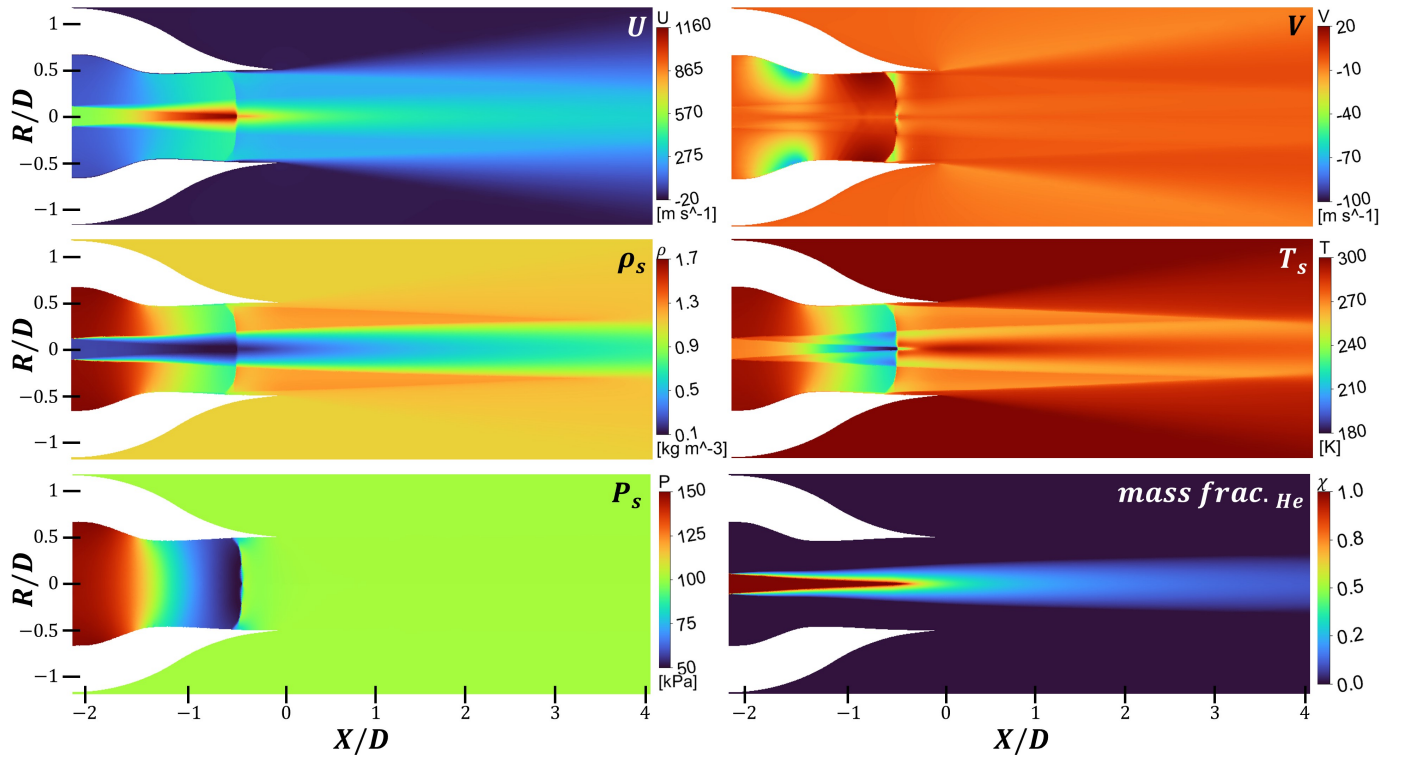


Figure 5. Six key CFD results at Blacksburg, VA ambient conditions for comparison from $X/D = -2$ to 4 including nozzle internals for reference.

helium mass fraction. The Mach disk and oblique shock can be seen about three quarters of the way between the throat and nozzle exit with a clear separation point. This results in the exit Mach number of approximately 0.8 in the bypass region. The mixing of the core (helium) and bypass (air) flows also compounds the complexity of the shock interaction within the nozzle and resulting flow downstream. The mass fraction of helium and Mole fraction of Helium show similar results with a large majority of the mixing having occurred before the nozzle exit. Finally, the ambient conditions are approximately quiescent, as expected. As mentioned earlier, greater comparison and discussion will be presented in Section 4.

4. Results

The results from the FRS-PINN approach are presented and discussed in the following section. Two variations of flow field results are compared. The first is a case with random error only (no bias) which uses simulated FRS data from the CFD solution. The process for simulating the data is described in Section 2.2. The second is a case with random and bias error, which focuses on the experimentally measured data with measurement uncertainties discussed in Section 3.1. The result from the experimentally measured data is then presented and compared to mass flow estimates based on what was recorded during rig operation. More discussion on areas of incurred bias for

each scenario can be found in their respective sections, Sections 4.1 and 4.2.

4.1. Simulated Field

In order to create a noise-free, baseline solution with an exactly known exit condition, FRS data were generated using the measurement model defined in Eq. 17 and the CFD solution presented in Section 3.2. In order to match the experimental data as closely as possible, the data were simulated using the same measurement setup as the experiment. This is described with more detail in the methods section. Additionally, the CFD data are downsampled to match the spatial resolution of the experimental configuration. This can be seen in Figure 6a.

The results from the FRS-PINN can be seen in Figure 6b. This is compared to the mean-field CFD result (Figure 6a). Uncertainty estimates were derived by training the network with five different random initializations. In general, uncertainty quantification for PINNs is a complex procedure Zou et al. (2025). The ensemble averaging of five different initializations is done to gain an initial estimate of random error in the FRS-PINN outputs, but it is noted that a more thorough uncertainty quantification approach is needed for future work. The 95% confidence estimates are seen in Figure 7 and represent the random error associated with the FRS-PINN approach. The highest uncertainty in all results occurs near the jet exit. It is expected that the highest amount of error would occur where the influence from helium is the highest. This relates to how the measurement model is defined. As derived in Section 2.1, the measurement model assumes the contribution from helium is negligible and that all of the Rayleigh scattering is due to air only. This adds some uncertainty in the region where there is a larger helium concentration, as evident in Figure 7. Additionally, the lowest amount of signal in the measured data occurs where there is primarily helium because the differential scattering cross section is much lower than air, which can impact the amount of information available from the spectra.

The axial velocity, static density, and mixture fraction results agree well with the CFD solution in regions further downstream from the jet exit and in regions with minimal gradients for all mean field quantities. This finding is consistent with previous PINN implementations with PIV and FRS and was generally expected for the result here Eivazi et al. (2022). FRS-PINN performance can likely be improved in future iterations by increasing the spatial resolution in these regions either when acquiring FRS data or via spatially upsampling with the PINN Gao et al. (2021).

The impact of an exit condition on the entire mean field can be summarized by the root mean square error (RMSE) of the FRS-PINN result with and without an exit condition, listed in Table 1.

Table 1. Comparison of RMSE of FRS-PINN outputs relative to CFD solution with and without exit conditions

ε_U	ε_V	ε_T	ε_ρ	$\varepsilon_{\chi_{He}}$
3.81	3.73	2.85	3.80×10^{-2}	3.64×10^{-2}

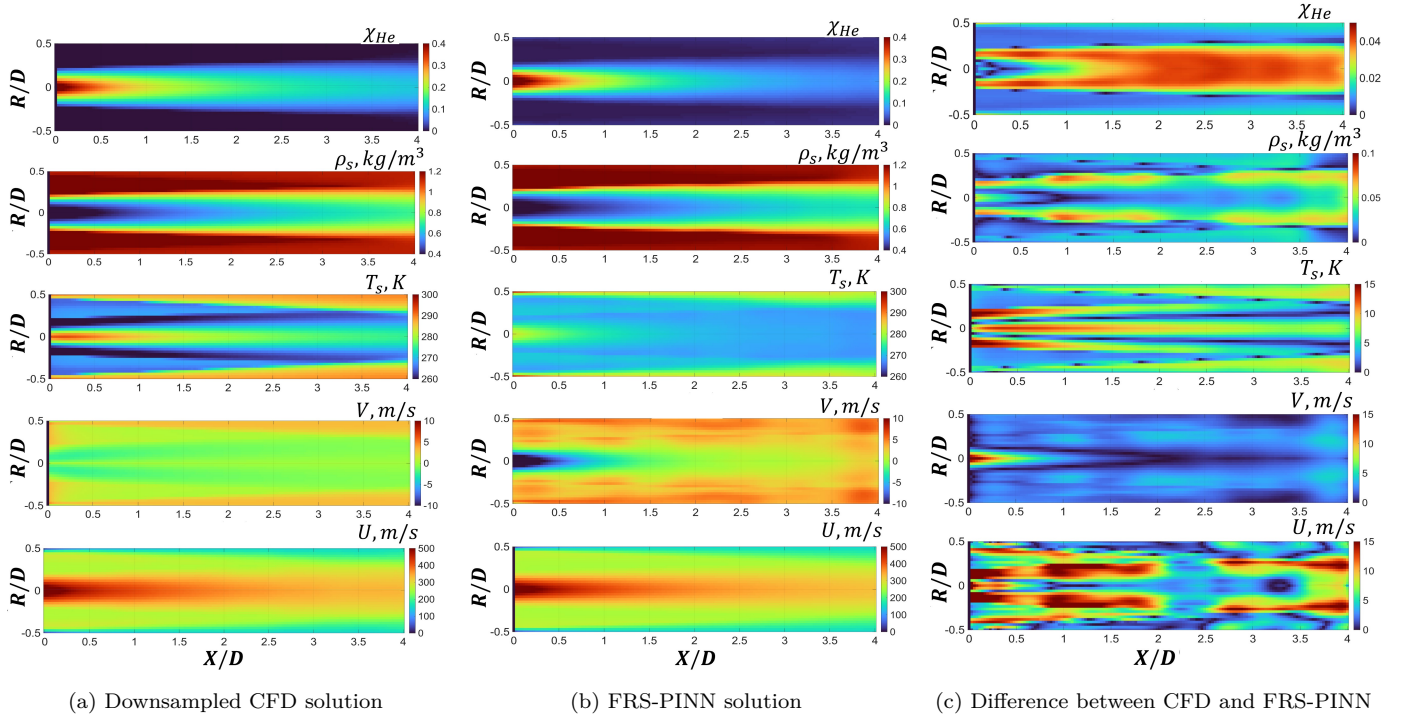


Figure 6. Mean field CFD solution and resulting FRS-PINN reconstructions

The relatively low errors in Table 1 indicate that the inverse problem of solving for static temperature and density, axial and radial velocity, and mixture fraction using solely FRS data from the mixture is achievable. By leveraging flow physics as prior information, the FRS-PINN approach mitigates the need to take independent reference measurements at the same number density of the different contributions to the mixture, which is an advancement over previous implementations of FRS to measure mixture composition C. Ground et al. (2018); Seasholtz et al. (1997). Bypassing the requirement of reference measurements and a controlled number density by using the FRS-PINN approach allows for the technique to be applied outside of highly-controlled, lab-scale environments.

4.2. Experimental Field

The same approach as seen in Section 4.1 is applied to experimentally measured data, from the configuration defined in Section 3.1. This case differs from the previous section in that there is bias error due to the open-loop control and the 2 psi resolution of the regulator. The results presented here discuss the performance of the FRS-PINN with random and systematic measurement error and how this impacts the mean field result.

To demonstrate the effect of measurement bias on the field, particularly in regions with and without high helium concentrations, mean-normalized experimentally measured and simulated signals

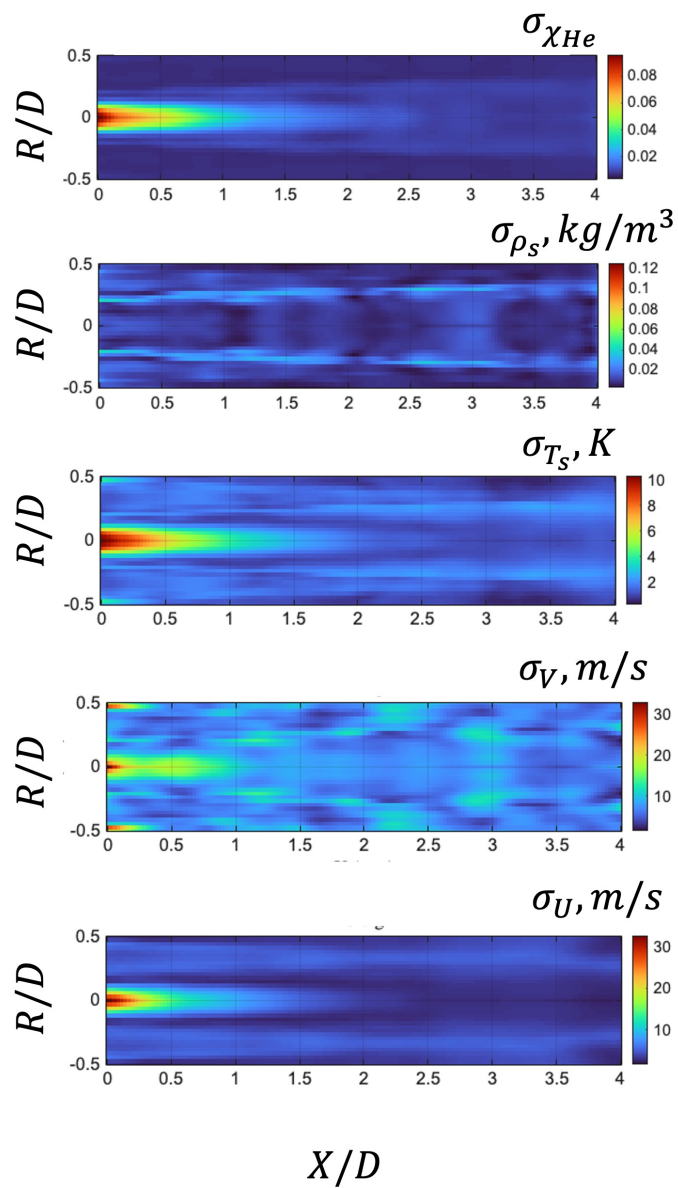


Figure 7. Estimated uncertainty in FRS-PINN outputs

in the primary regions of the jet are compared. Fig. 8a illustrates the relative difference between the expected FRS signal behavior from the CFD simulation and the measured signal in areas with high helium concentration (near the jet exit), low concentration (outside the jet) a region downstream of the jet exit still within the potential core.

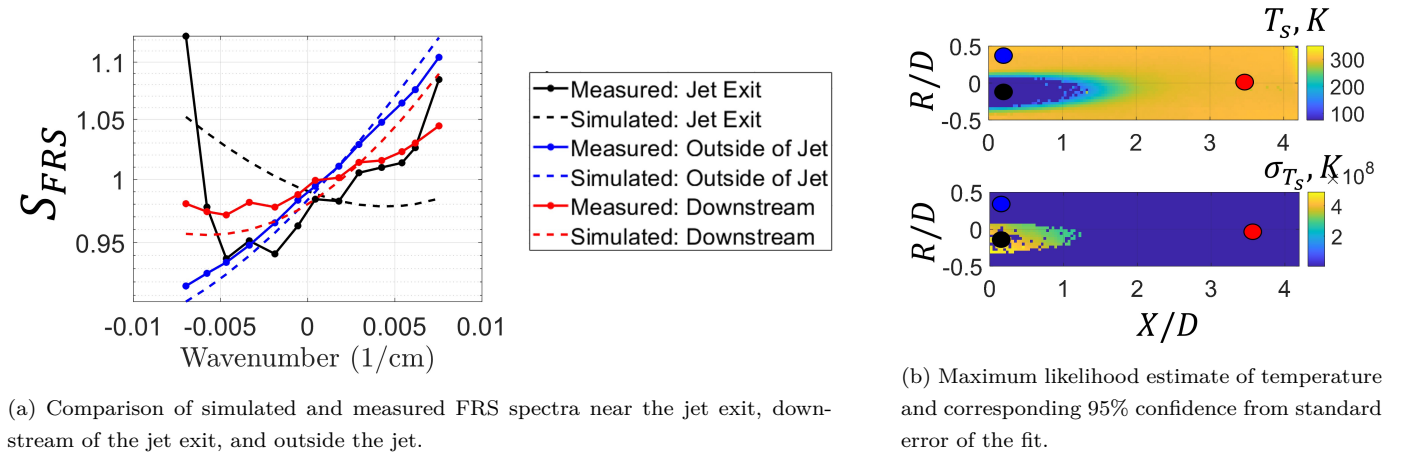


Figure 8. Effect of measurement noise on FRS data

Figure 8a trends as expected, with the bias in total pressure causing the highest amount of bias in the measured data closest to the jet exit, with limited influence outside the jet. The persistent effect of bias error on the FRS signals, particularly in primarily helium regions, is further confirmed by examining the result from a conventional nonlinear least squares solver. Temperature and the resulting 95% confidence from the standard error of the fit can be seen in Figure 8b. Temperature is shown because it is the mean field quantity most directly related to the shape of the spectra Miles et al. (2001). All mean field quantities that result from the conventional nonlinear least squares solver have substantial uncertainty near the jet core.

It is known that PINNs are effective at mitigating measurement noise, but this is primarily limited to random errors. It is clear that the assimilated result also contains bias in regions of higher helium concentration and it is expected that this bias propagates to the FRS-PINN results. The axial velocity result at the jet exit matches within 0.21 m/s of the CFD exit velocity, radial velocity matches within 9 m/s, static density matches within 0.07 kg/m³, static temperature matches within 228K, and mixture fraction matches with 0.12. The full-field results from the FRS-PINN approach can be seen in Figure 9. The results in Figure 9 compare well to the expected values based on the CFD result for axial velocity, static density, and mixture fraction. There is, however, a bias in the temperature result which is expected based on the effect of bias in the MLE result in Figure 8b. The preliminary conclusion can be drawn that the FRS-PINN approach is effective at mitigating random error due to measurement noise, however, this cannot be extended to bias error.

To further compare the estimated field quantities, the mass flow rate of helium can be derived using the magnitude of velocity, static density, and the exit diameter of the pipe. This value for the

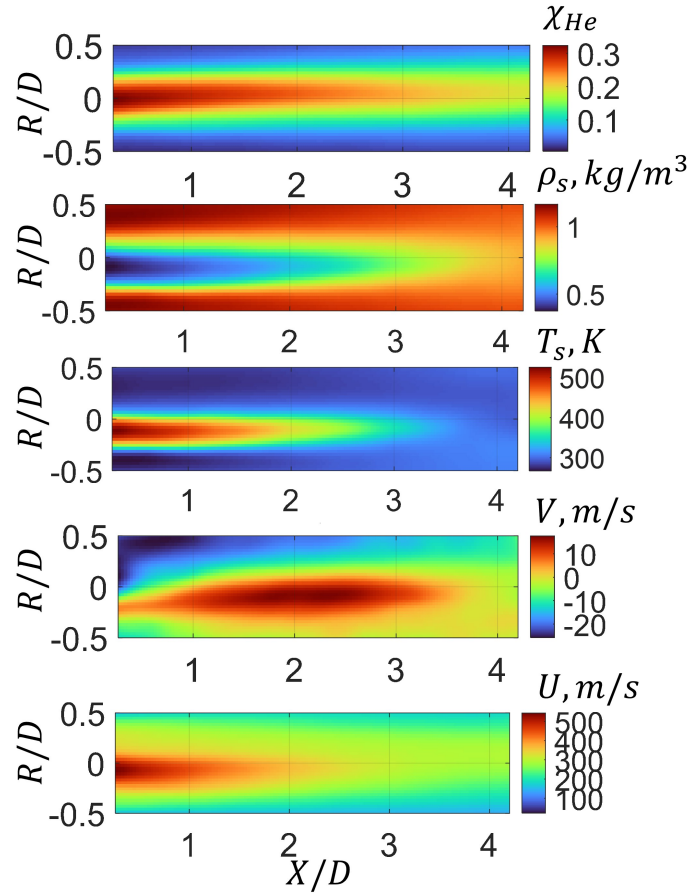


Figure 9. Mean field results from FRS-PINN using experimentally measured data

CFD result, FRS-PINN result, and rig instrumentation can be found in Table 2.

Table 2. Comparison of estimated mass flow rate in kg/s

Probe	CFD	FRS-PINN
0.011	0.009	0.019

The mass flow rate estimates for all cases match within ± 0.01 and ± 0.002 without a constant static pressure loss, but further examination of the bias in temperature requires investigation before a claim on accuracy to four significant figures can be made. Additionally, the mass flow result from CFD is calculated with the downsampled data. When calculated using all available points, the result for mass flow from CFD is 0.012 m/s.

The most direct comparison to rig instrumentation that can be made, for this data, is partial pressures of the mixture. The total and static pressures of the mixture and its components can be derived using the axial velocity, static density, static temperature, and mass fraction (converted to mole fraction) from the FRS-PINN, using isentropic flow relations and the ideal gas law for a mixture. This result can be seen in Figure 10.

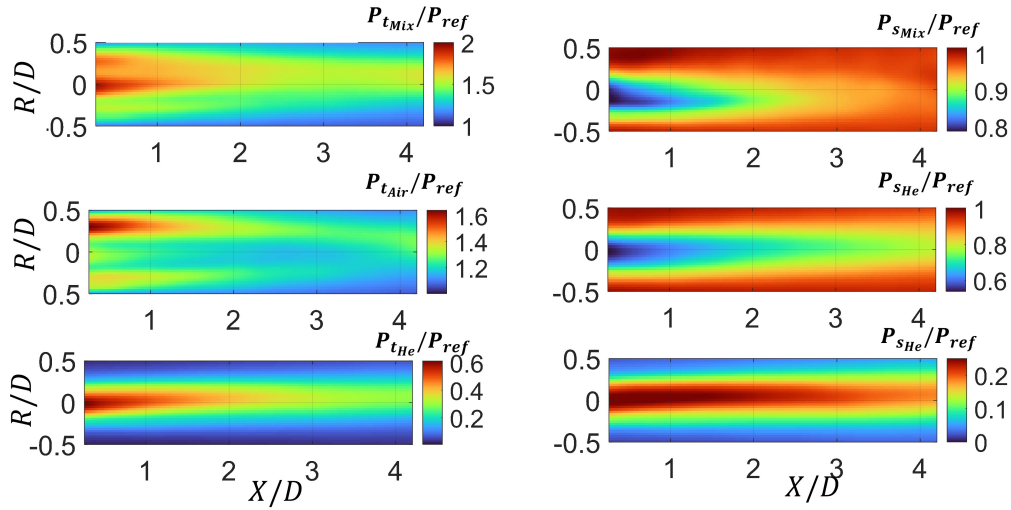


Figure 10. Mixture and partial pressures

The total pressure of air in the jet plenum was constant at 1.5×10^5 Pa. This matches the result for the total pressure of air in Figure 10. Additionally, the ambient static pressure during data acquisition was 9.5×10^4 Pa. This matches the result for static pressure, with the major exception of a lower static pressure inside the jet core. The static pressure inside the jet core, which is a product of the biased temperature result, is non-physical but it corresponds to a deviation of approximately 2.5 psi. This is well within the bias error defined in Section 3.1. This uncertainty arises due to the precision of the mass flow regulator for helium. The total pressure of helium during data acquisition ranged between 2×10^4 Pa. The FRS-PINN result for the total pressure of helium is significantly lower than this. It is noted that this does not account for losses that might have occurred from the location where total pressure was measured and the nozzle exit. Regardless of losses, this partial pressure value provided is too low to accurately match the measured total pressure of helium in the jet plenum.

The static pressure of air is slightly lower than the ambient condition, but this difference is less than the total bias error of the measurement. The agreement between the probe data and the FRS-PINN result for air indicate that this technique is effective at resolving the mean field because pressure is not a direct output, but derived from the mean field result. The disagreement between probe and FRS-PINN result for helium total pressure indicate the effects of noise induced by total pressure fluctuations. This conclusion, in tandem with high accuracy results on simulated data, provide future evidence that the FRS-PINN approach is capable of resolving mass fraction, axial velocity, radial velocity, static temperature, and static density without boundary or reference conditions with high SNR FRS data. This conclusion is limited for this work because of the high bias error, particularly at the jet exit. However, static and total pressure results in areas not affected by helium total pressure fluctuations were resolved within 1.8% of ambient and 1.6% of total pressure.

Ultimately, this result demonstrates a capability to solve for vector velocity, static density, static

Table 3. Comparison of static and total partial pressures in Pa, where all pressure results have a bias error of $\pm 1.4 \times 10^4$ Pa

Pressure	Probe	FRS-PINN
$P_{t_{Air}}$	1.5×10^5	1.5×10^5
$P_{t_{He}}$	1.8×10^5	4×10^4
$P_{s_{Air}}$	9.4×10^4	9×10^4
$P_{s_{He}}$	9.4×10^4	2×10^4

temperature, and mass fraction with solely noise-free FRS data of the mixture. This alleviates some measurement complexity and greatly expands the potential application space for mixture fraction. It also demonstrates the limitations of the approach in the presence of measurement bias error, which increases uncertainty and decreases accuracy. However, the source of bias for this measurement can be mitigated by using a higher precision mass flow controller.

5. Conclusions

This work seeks to enable full-field, non-intrusive measurements of mass fraction of a mixture outside of a lab environment and particularly for mixtures where reference measurements of the components in the mixture are not available. This is done via extending the measurement output of FRS to include mass fraction in a binary mixture in addition to vector velocity, static density, and static temperature. The methodology for this involves a derived measurement model in terms of mass fraction of a binary mixture and its integration into a physics-informed neural network that uses the RANS equations and the advection-diffusion equation to assimilate the FRS data. The performance of this technique was evaluated was simulated data from the CFD solution for this field and measured FRS data. These two sets of results are compared to probe data and a CFD simulation of the field. The following key outcomes resulted from this work:

1. Using FRS data simulated from the CFD solution, the FRS-PINN approach solves the inverse problem for axial velocity with an error of 3.81 m/s, radial velocity with an error of 3.73 m/s, static temperature with an error of 2.85 K, static density with an error of 3.80×10^{-2} kg/m³, and mass fraction with an error of 3.64×10^{-2} .
2. The FRS-PINN approach is capable of mitigating measurement errors due to random error, but cannot mitigate bias error.
3. Derived static and total pressure for air with and without a constraint on static pressure match the ambient and jet plenum total pressure with 1.8% and 1.6% error, respectively. Derived mass flow rate was found to be 0.01 kg/s consistently across all approaches (CFD, probe data, FRS-PINN from experimental and simulated data).

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Data Availability

The data cannot be made publicly available upon publication due to legal restrictions preventing unrestricted public distribution. The data that support the findings of this study are available upon reasonable request from the authors.

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