

**Assessment of the viability of VISR: a mid-wavelength  
infrared (MWIR) multispectral imaging-based approach for  
remote flare CE quantification**

by

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## **Author's Declaration**

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

## Abstract

In the upstream and downstream petrochemical industry, flaring is a common practice to dispose of the redundant by-products of crude oil extractions, including associated gas and highly reactive volatile organic compounds (HRVOCs), for a variety of regulatory, safety and economic purposes. The current consensus among government regulators and industry experts is that flaring typically occurs at a combustion efficiency (CE) higher than 98%. Recent studies, based on real-world observations and computational simulations, have called this into question. For example, a recent study, based on airborne sampling observations and unlit flare prevalence surveys, reported a mean flare CE of 91%, accounting for both inefficient flaring and unlit flares in the three largest basins in the US. This represents a five-fold increase in fugitive hydrocarbon emissions, primarily comprised of methane, compared to the presumed release rates, highlighting an opportunity for developing robust flare CE monitoring techniques to mitigate the adverse health and environmental impacts of the underappreciated flaring emissions.

This study presents a numerical assessment of video imaging spectro-radiometry (VISR), a mid-wavelength infrared (MWIR) multispectral technique, proposed for remote flare combustion efficiency quantification applications. The present analysis utilizes a series of computational fluid dynamics (CFD) simulations of a crosswind steam-assisted industrial flare, with a focus on three aspects: how approximations in the radiometric model impact the local “pixel-wise” CE, the validity of the approach for computing flare global CE using inferred local CE values, and the ability and limitations of VISR instrument to capture fuel that may be aerodynamically stripped from the combustion zone under crosswind conditions. The current assessment is conducted on a simplified version of the VISR instrument model using simulated broadband images generated over spectral bands adjusted for the key absorption features of three main by-products of flare combustion reaction: CO<sub>2</sub> (4.2–4.4 μm), CO

(4.5–4.9  $\mu\text{m}$ ), and  $\text{CH}_4$  (3.2–3.4  $\mu\text{m}$ ). The results highlight the accuracy of the proposed simplified VISR approach in predicting local CE within the VISR region-of-interest (ROI) yet flawed in terms of converting these values into a flare global CE, potentially leading to large biases from the actual flare CE. Ultimately, the VISR technique, due to reliance on mid-wavelength infrared imaging, is inherently incapable of quantifying unburned (cold) methane, allegedly stripped from the flare stack, without participating in the combustion process, due to the presence of a high crosswind over the flare stack, leading to a considerable overestimation of the true flare performance.

**Keywords:** Flares, Combustion Efficiency, Remote Sensing, Verification and Validation, Radiometric Measurements, Uncertainty Analysis, Bayesian Inference.

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## **Dedication**

*To my beloved family, for helping me through the ups and downs*

*And to you, who find yourself reading this thesis*

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## List of Abbreviations

|                  |                                                   |
|------------------|---------------------------------------------------|
| AFTIR            | Active Fourier Transform Infrared                 |
| AC               | Alternating Current                               |
| AGL              | Above Ground Level                                |
| BC               | Black Carbon                                      |
| CE               | Combustion Efficiency                             |
| CEM              | Continuous Emissions Monitoring                   |
| CFD              | Computational Fluid Dynamics                      |
| CH <sub>4</sub>  | Methane                                           |
| CI               | Confidence Interval                               |
| CO               | Carbon Monoxide                                   |
| CO <sub>2</sub>  | Carbon Dioxide                                    |
| CRDS             | Cavity Ringdown Spectrometers                     |
| DC               | Direct Current                                    |
| DOM              | Discrete Ordinates Method                         |
| DRE              | Destruction Removal Efficiency                    |
| EGC              | Enclosed Ground Combustor                         |
| EPA              | Environmental Protection Agency                   |
| ESF              | Emission Scaling Factor                           |
| FTIR             | Fourier Transform Infrared                        |
| GHG              | Greenhouse Gas                                    |
| GKDME            | Generalized Kernel Density Maximum Entropy        |
| GWP              | Global Warming Potential                          |
| H <sub>2</sub> O | Water                                             |
| HC               | Hydrocarbon                                       |
| HITRAN           | High-Resolution Transmission Molecular Absorption |
| HPD              | Highest Posterior Density                         |
| HRVOC            | Highly Reactive Volatile Organic Compound         |
| HS               | Hyper-Spectral                                    |

|                 |                                                           |
|-----------------|-----------------------------------------------------------|
| HV              | Heating Value                                             |
| HWHM            | Half-Width at Half Maximum                                |
| ICV             | Image Correlation Velocimetry                             |
| ID              | Identification                                            |
| IFTS            | Imaging Fourier Transform Spectrometer                    |
| IID             | Independent and Identically Distributed                   |
| ILS             | Instrument Lineshape function                             |
| IMACC           | Industrial Monitor and Control Corporation                |
| IR              | Infrared                                                  |
| LBL             | Line-by-Line                                              |
| LES             | Large Eddy Simulation                                     |
| LNG             | Liquid Natural Gas                                        |
| LOS             | Line-of-Sight                                             |
| LWIR            | Long-wavelength Infrared                                  |
| MCMC            | Markov Chain Monte Carlo                                  |
| ME              | Maximum Entropy                                           |
| MOPD            | Maximum Optical Path Difference                           |
| MS              | Multi-Spectral                                            |
| MWIR            | Mid-wavelength Infrared                                   |
| NESR            | Net equivalent Spectral Radiance                          |
| NETD            | Net Equivalent Temperature Difference                     |
| NHV             | Net Heating Value                                         |
| NG              | Natural Gas                                               |
| NO <sub>x</sub> | Nitric Oxide (NO) and Nitrogen Dioxide (NO <sub>2</sub> ) |
| OGI             | Optical Gas Imaging                                       |
| PFTIR           | Passive Fourier Transform Infrared                        |
| PM              | Particulate Matter                                        |
| QOGI            | Quantitative Optical Gas Imaging                          |
| QOI             | Quantity-of-Interest                                      |
| RCCE            | Rate-Controlled Constrained Equilibrium                   |

|                 |                                             |
|-----------------|---------------------------------------------|
| RE              | Relative Error                              |
| ROI             | Region-of-Interest                          |
| RTE             | Radiative Transfer Equation                 |
| SCA             | Scene Change Artifacts                      |
| SF <sub>6</sub> | Sulfur Hexafluoride                         |
| CF <sub>4</sub> | Tetrafluoromethane                          |
| SO              | Sulfur Monoxide                             |
| SP              | Soot Photometer                             |
| TCEQ            | Texas Commission on Environmental Quality   |
| TDLAS           | Tunable Diode Laser Absorption Spectrometer |
| THC             | Total unburnt Hydrocarbons                  |
| TM              | Trademark                                   |
| TNG             | Tulas Natural Gas                           |
| TRI             | Turbulent-Radiation Interactions            |
| VIIRS           | Visible Infrared Imaging Radiometer Suite   |
| VISR            | Video Imaging Spectro-Radiometry            |
| VOC             | Volatile Organic Compound                   |
| VR              | Vibrational-Rotational                      |

## List of Symbols

### Combustion

---

|            |                                                  |
|------------|--------------------------------------------------|
| $a-h$      | Chemical reaction balancing coefficients         |
| $M$        | Molar mass                                       |
| $\dot{m}$  | Mass flow rate                                   |
| $n_C$      | Intermediate hydrocarbon, number of carbon atoms |
| $p$        | Pressure                                         |
| $T$        | Temperature                                      |
| $\chi$     | Molar fraction                                   |
| $\sigma$   | Column number density                            |
| $s$        | Location along the line-of-sight (LOS)           |
| $L$        | Length of the prescribed line-of-sight (LOS)     |
| $x$        | Fuel molecule's number of carbon atoms           |
| $y$        | Fuel molecule's number of hydrogen atoms         |
| CE         | Combustion Efficiency                            |
| DRE        | Destruction Removal Efficiency                   |
| $[\Delta]$ | Peak enhancements                                |

### Subscripts

---

|          |                                                     |
|----------|-----------------------------------------------------|
| $\infty$ | Ambient conditions                                  |
| C        | Carbon                                              |
| $m$      | Intermediate hydrocarbons' number of carbon atoms   |
| $n$      | Intermediate hydrocarbons' number of hydrogen atoms |
| fuel     | Refer to the state of the pure flare fuel stream    |
| plume    | Refer to the combustion products inside the plume   |
| local    | Local CE                                            |
| soot     | Soot (Black Carbon)                                 |
| $j$      | $j$ th pixel in the flare plume image               |
| $k$      | $k$ th species                                      |
| $X$      | DRE target species                                  |

### IR Spectroscopy and Radiative Transfer Equation (RTE)

---

|                |                                                            |
|----------------|------------------------------------------------------------|
| $e$            | Level of energy                                            |
| $\eta_{ij}$    | $ij$ th molecule transition's central line wavenumber      |
| $f$            | Lineshape function                                         |
| $\gamma$       | Line half-width at half-maximum (HWHM)                     |
| $\eta$         | Wavenumber                                                 |
| $\kappa_\eta$  | Spectral absorption coefficient                            |
| $I_\eta$       | Spectral intensity measured at the wavenumber $\eta$       |
| $L$            | Optical path (LOS) length                                  |
| $s$            | Distance parameter along the optical path (LOS)            |
| $S_{ij}$       | Spectral line intensity of the $ij$ th molecule transition |
| $x_V$          | Ratio of Lorentz-to-Voigt lineshape HWHM                   |
| $\sigma_0$     | Normalized center-line strength                            |
| $C_{\eta,abs}$ | Molecular spectral absorption cross-section                |

|                                                                |                                                                                |
|----------------------------------------------------------------|--------------------------------------------------------------------------------|
| $N$                                                            | Local number density (concentration)                                           |
| <b>Subscripts</b>                                              |                                                                                |
| $p$                                                            | Refers to Photons                                                              |
| $i,j$                                                          | Energy states $i$ and $j$                                                      |
| $\eta$                                                         | Measured at wavenumber $\eta$                                                  |
| $L$                                                            | Lorentzian profile                                                             |
| $D$                                                            | Doppler profile                                                                |
| $V$                                                            | Voigt profile                                                                  |
| $bg$                                                           | Refers to Background radiation                                                 |
| $B$                                                            | Refers to Blackbody emission                                                   |
| $m$                                                            | $m$ th species in the plume                                                    |
| mix                                                            | Referring to the gas mixture                                                   |
| <b>VISR Camera Model (Radiometric + Instrument sub-models)</b> |                                                                                |
| $S_k$                                                          | Broadband signal (intensity) corresponding to channel $k$                      |
| $C_{cal}$                                                      | Broadband filter's Calibration constant                                        |
| $\tau$                                                         | Optical thickness                                                              |
| $\alpha_\eta$                                                  | Spectral absorption line strength                                              |
| $\Delta\eta$                                                   | Broadband filter's spectral width                                              |
| $N_{ROI}$                                                      | Number of pixels located within the VISR region-of-interest (ROI)              |
| $\mathbf{b}$                                                   | Set of Broadband signal for all the camera spectral channels                   |
| $\delta\mathbf{b}$                                             | Set of Broadband signal noise for all the VISR spectral channels               |
| $\mathbf{\Gamma}$                                              | Covariance matrix                                                              |
| $\mathbf{u}$                                                   | Local mass-weighted projected crosswind velocity                               |
| $\hat{\mathbf{n}}$                                             | Crosswind projected velocity unit vector, normal to the integration line       |
| <b>Subscripts</b>                                              |                                                                                |
| $\eta_k$                                                       | Indicates the averaging over wavenumber within the $k$ th channel spectrum     |
| $j$                                                            | $j$ th pixel in the flare plume image                                          |
| $k$                                                            | $k$ th broadband channel                                                       |
| VISR                                                           | Refers to the VISR camera model                                                |
| NETD                                                           | Refers to Net Equivalent Temperature Difference                                |
| <b>Superscripts</b>                                            |                                                                                |
| exact                                                          | Refers to exact broadband signal with no interference (noise)                  |
| meas                                                           | Refers to the measured broadband signal by the VISR instrument                 |
| noise                                                          | Refers to the broadband signal noise                                           |
| <b>Bayesian Uncertainty Analysis</b>                           |                                                                                |
| $\delta\mathbf{b}$                                             | Set of Broadband signal errors for all the VISR spectral channels              |
| $p()$                                                          | Probability density function                                                   |
| $\langle \rangle_s$                                            | Averaged along the optical path (LOS) over parameter $s$ (location on the LOS) |
| $\mathbf{x}$                                                   | Quantities-of-Interest (QOIs)                                                  |
| <b>Subscripts</b>                                              |                                                                                |
| pr                                                             | Refers to Prior distribution/knowledge                                         |
| $j$                                                            | $j$ th pixel in the flare plume image                                          |
| <b>Superscripts</b>                                            |                                                                                |

---

|          |                                                                                 |
|----------|---------------------------------------------------------------------------------|
| meas     | Refers to Ground Truth (RTE-driven) broadband signal                            |
| model    | Refers to broadband signal post-processed by the VISR instrument                |
| modified | Refers to modified VISR Global CE model based on the updating prior information |

---

**Physical Constants**

---

|       |                    |
|-------|--------------------|
| $A$   | Avogadro's number  |
| $c$   | Speed of light     |
| $h$   | Planck's constant  |
| $k_B$ | Boltzmann constant |

# Chapter 1

## Introduction to Gas Flaring

Flaring Petrochemical industries use flaring to dispose of the surplus hydrocarbon (HC) and other redundant gas-phase products of crude oil extractions, by converting them into less harmful species, with significantly lower global warming potential (GWP), mainly carbon dioxide ( $\text{CO}_2$ ) and water vapor ( $\text{H}_2\text{O}$ ) [1].

Flaring is used in three sectors of the petrochemical industry: (1) upstream, comprised of crude oil and natural gas (NG) drilling and extraction operations; (2) midstream, where the extracted crude oil and natural gas is transported to refineries; and (3) downstream, where the raw natural resources are transformed into commodity chemical compounds. The redundant fuel processed in the flaring operations may originate from chemical compounds from purged gases and effluents from downstream refining facilities, such as highly reactive volatile organic compounds (HRVOCs), and associated gas, comprised primarily by methane ( $\text{CH}_4$ ), as a by-product of the upstream crude oil production. This study focuses on the upstream flaring of associated gas, although it can be applied to other types of flaring.

The practice of flaring in oil and gas industries is generally incentivized by safety, health, environmental, economic, and operational factors. In contrast to onsite gas flaring, alternative approaches, with more favorable and climate-friendly outcomes for utilizing the redundant extracted associated gas and other flammable by-products of crude oil productions exist, including power generation, favorably onsite at the petrochemical facilities, the production of pressurized liquid natural gas (LNG) or methanol ( $\text{CH}_3\text{OH}$ ) from the refinement of unwanted associated gas [2]. However, due to problematic factors, including the intermittency of the gas flow, the lack of appropriate infrastructure

to store and transport the associated gas [3], and the low heating value of some of the flare vent gas components [4–6], these alternative methods are mostly considered to be impractical or lack economic incentive [7]. Therefore, gas flaring is often viewed as the safest and most environmentally benign approach to comply with the EPA regulations for the disposal of the redundant flammable gas in production sites. The preference for utilizing gas flaring, in comparison to direct venting of the unwanted gas into the atmosphere, is mainly due to the considerably higher GWP of the components in the flared gas, in contrast to its combustion products, particularly CO<sub>2</sub> and water vapor [8,9].

Several types of flaring exist. The most common ones are: (1) start-up flaring, a short period combustion of sample hydrocarbon fuel to test the performance and readiness of the flaring equipment, (2) continuous (routine) flaring, typically used in off-shore oil rigs to dispose of redundant associated gas onsite, (3) operational (planned) flaring, during the planned maintenance, shutdowns, and emergency, due to equipment failures and other unexpected operational issues.

The equipment used for flaring depends on the type of flaring process. Flares designed for the upstream oil and gas facilities, including onshore and offshore oil and gas production sites, are typically simple and have fewer components in comparison to their downstream counterparts. Flares at upstream sites consist of an elevated stack with an attached electric pilot (igniter), and a barricade surrounding the stack exhaust, to obstruct the undesirable impact of crosswind on flare performance and occasional blow-outs. Air-assisted flare tips are sometimes used to improve the mixing process between the fuel stream and the ambient air, suppressing the formation of smoke (soot) [10]. Approximately 90% of the global oil and gas flaring processes are designated to dispose of redundant associated gas, primarily composed of methane (CH<sub>4</sub>), extracted during upstream oil and gas drilling and production operations, with the remaining 10% of the flaring facilities utilized in the midstream and downstream sectors [3]. Mitigating the pollutant emissions from the flaring of relatively heavier hydrocarbons in downstream

facilities requires additional equipment, including steam- and air-assistance technologies and auxiliary fuel streamlines to enable more effective control of the fuel mixture flow rate to regulate the combustion process. To facilitate the efficient combustion of associated gas and overcome similar operational issues, these types of equipment can also be found in upstream gas flaring facilities.

Additionally, several emission compliance regulations imposed by the Environmental Protection Agency (EPA) [11,12], require continuous emission monitoring (CEM) systems [13] or instrumentation to ensure that the pilot remains lit (e.g., PilotEye 2000™ by John Zink Co. [14]). Moreover, flaring operations in the downstream sector face several human health implications, both direct and indirect, given the combustion of toxic compounds such as highly reactive volatile organic compounds (HRVOCs), that would otherwise be released directly into the environment.

## 1.1 Flaring Effluents: Health and Environmental Implications

Flare plumes often contain significant traces of unburned or partially-pyrolyzed hydrocarbons in both the gas-phase and particulate matter (PM), due to poor mixing of the fuel and ambient air, and the aerodynamically stripped unburned fuel from the combustion zone, among other factors. These types of emissions, both visible and invisible to the naked eye, detrimentally affect the environment and human health.

Soot (black carbon, BC), a major pollutant with adverse impacts on the human respiratory and cardiovascular systems [15]. Additionally, this pollutant is considered one of the most critical climate-forcing agents, playing a major role on both local and global scales [8,16]. Among all the combustion by-product species, only soot formation can be readily visible to the naked eye. The visible flame is caused by the incandescence of soot particles and the chemiluminescence of gas-phase radicals within the visible flame, while the opacity of the flare plume downwind of the combustion zone is linked to soot formation. Many jurisdictions have regulations and rules regarding flaring operations based on the opacity of this plume, in which flare operators are responsible for complying with certain regulations for maintaining “smokeless” flaring requirements by adjusting flare operating parameters, including the injection flow rates of the auxiliary fuel and assisted steam and air streams to achieve smokeless flames [17,18].

Although the injection of steam and air into the flare combustion zone is intended to promote the suppression of soot formation through turbulent mixing between the hydrocarbon and oxidizer steam flow rate [19], too much assistance can lower the net heating value of the combusted fuel and steam mixture, leading to partial/ complete quenching of the flame [20]. Since gaseous hydrocarbon emissions are invisible to the bare eye, operators may over-assist to suppress the formation of visible smoke (soot) at the cost of excessive gas-phase emissions. Hence, these regulations not only do not address the

implications caused by flare gas-phase emissions, but they are also often linked to excessive gas-phase emissions, which is especially prevalent when flaring the heavier hydrocarbons, typically found in the downstream petrochemical processes. These emissions are reported to directly cause several adverse environmental and human health complications. Due to a lack of reliable instruments to measure these harmful emissions, less strict regulations exist regarding these gas-phase emissions.

In upstream flaring operations, CH<sub>4</sub>, the dominant constituent of associated gas with a simple chemical structure, possessing a characteristically high GWP (86 and 24 times that of CO<sub>2</sub> over a 20 and 100-year lifespan, respectively [8]), is often considered as the primary species-of-interest for flare performance evaluations. In the case of downstream flaring, the comparatively larger volumes of flared gas in the upstream sector usually overshadow the impact of downstream flaring on climate change, leading to the implications of downstream flaring, with around 10% contribution to the total global flare emission estimates, to be often disregarded [3]. However, the adverse health impacts of heavier unburned or partially-pyrolyzed hydrocarbon flare emissions in the downstream sector, particularly highly reactive volatile organic compounds (HRVOCs), which are reported to cause the formation of toxic air pollutants such as formaldehyde and ground-level ozone, could pose far greater concerns [16,21,22]. An air quality survey conducted in the Houston-Galveston-Brazoria area in 2006 estimated that 76% of the VOC and HRVOC emissions could be linked directly to nearby refinery flaring operations [21], assuming that the flare combustion efficiency remains constant within 98-99% [22]. While the health effects of downstream flaring are a concern due to the complex species in the flare plume and the proximity of many refineries to residential areas, there is also growing evidence that VOCs, nitrogen oxides (NO<sub>x</sub>), sulfur dioxide (SO<sub>2</sub>), carbon monoxide (CO), and particulate matter (PM) from upstream and midstream flaring can also cause health complications for the nearby communities [15,23].

## **1.2 Future of Gas Flaring: Global and Regional Perspectives**

According to global GHG emissions, reported by the World Bank, in 2023, over 147 billion cubic meters of gas were flared in the upstream oil and gas facilities around the globe, with a significant 6.5% increase compared to 2022, resulting in emissions with a global warming potential (GWP) equivalent to the release of nearly 470 million tons of carbon dioxide (CO<sub>2</sub>) over a 20-year span [24].

In Canada, flaring constituted only 1% of the overall greenhouse gas (GHG) emissions in 2023, with the majority originating from the upstream sector [25]. Despite the marginal contribution to Canada's total GHG emissions, mitigating all sources of anthropogenic carbon emissions, including the flaring emissions, is crucial for the Canadian government, as a signatory of the Global Methane Pledge [26], to fulfill: (1) net zero emissions by 2050 and (2) decrease annual GHG emissions to 40% to 45% of the 2005 levels, by 2030 [9].

### 1.3 Motivation

For a long time, the compliance regulations for upstream flaring operations imposed an expected flare performance of 96.5% or higher flare combustion efficiency (CE), 98% or higher destruction removal efficiency of methane ( $DRE_{CH_4}$ ), a common metric for characterizing the performance of a flaring process, given the conditions of continuous flaring and pilot flame remaining lit [24,27,28]. This standard was originally established based on a series of studies conducted by the US Environmental Protection Agency in the 1980s [27,29]. Recent studies shed light on the shortcomings of this standard and challenged the 96.5% CE figure, to the extent that Plant et al. reported a mean CE value as low as ~92% for the routine flaring operations in the Permian Basin [28]. According to this study, since GHG emissions from the oil and gas sector are commonly estimated, assuming a flare CE of 96.5%, such discrepancies can potentially lead to a five-fold rise in the US annual methane emissions [28]. This drop in the performance of gas flaring processes has been linked to multiple operational conditions, including strong crosswind over the flare stack [5,30], excessive steam and air assistance in the assisted flares, to prevent soot formation and smoke suppression [4,10,31], and low heating value (HV) of some of the components in the flare gas [4–6,30,32].

Unreliable global flaring emission estimates [9,33] paired with the growing awareness of adverse impacts of flaring effluents on human health in short and long terms and the push for modernizing the environmental regulations regarding the flaring operations in oil and gas upstream and downstream sectors, requires an urgency to develop monitoring instruments, to provide a robust quantification of flare performance. Such instruments can be found in infrared (IR) optical gas imaging (OGI) approaches.

Compared to traditional flare performance quantification approaches, infrared OGI techniques, particularly mid-wavelength (MWIR) and long-wavelength (LWIR) infrared imaging technologies, are

well-equipped for remote flare CE sensing applications, potentially capable of reporting a flare CE estimate without independent knowledge of the injected fuel gaseous constituents and flow rates [34–38].

Passive Fourier transform infrared (PFTIR) spectroscopy, introduced in 1985 [39], is one of the earliest remote sensing techniques. This technique utilizes an open-path FTIR spectrometer to infer the participating gaseous species concentrations along a single line-of-sight (LOS), which is then converted into a local CE estimate [40–43]. By assuming a homogeneous plume composition, the local CE estimate can be interpreted as an overall flare CE. PFTIR instruments operate at a spectral resolution of approximately  $0.5\text{ cm}^{-1}$  [44], sufficient to resolve key absorption lines of the various participating species inside the plume. Additionally, the inferred flare CE depends strongly on the aiming point/LOS through the plume. A common strategy among industry experts and regulators is to aim the FTIR camera at the point one flame length downstream of the visible flame tip [44]. This approach suffers from several critical limitations, including the undermined dynamic nature of the flame geometry, ignorance of the inherently heterogeneous composition of the plume, and the fluctuating crosswind stream over the flare stack, potentially resulting in the formation of an undetected cold fuel-rich region under the visible flame, downstream of the plume, due to aerodynamic fuel stripping [32].

The advent of commercially available MWIR and LWIR hyperspectral (HS) imagers has enabled spectrally resolved intensity measurements of the entire flare transient plume. These measurements can infer the species column density along the LOS associated with each pixel in the generated images of the flare, ideally capturing the gaseous species distribution through the flare plume. The post-processing of this information may provide a quantitative evaluation of flare performance in terms of flare combustion efficiency (CE) or species-specific destruction removal efficiency (DRE), Section 2.3.

Imaging Fourier transform spectrometers (IFTSs) [45–47], which utilize interferometry, as well as line-scan [48] and light-field (plenoptic) cameras [49], which use dispersion spectroscopy, are among

the most prominent infrared OGI technologies. Imaging Fourier transform spectrometers (IFTSs) operate according to the same principle as PFTIR spectrometry, except the captured scene is recorded as the interferogram is generated and converted to irradiance using a Fourier transform mechanism; the outcome is a data cube comprised of thousands of images, each at a distinct wavelength. While IFTSs have a lower spectral resolution (typically  $\sim 1 \text{ cm}^{-1}$ ) compared to the PFTIR instrument, the generated data cubes are usually sufficient for fingerprinting various species inside the plume and obtaining robust estimates of the temperature and species column densities along each pixel's LOS. The first study to deploy IFTS technology for remote quantification of flare CE was Savary et al. [50], utilizing two distinct types of IFTS cameras for simultaneous measurements, with spectral ranges of 1.5–5.5  $\mu\text{m}$  (MWIR) and 8–12  $\mu\text{m}$  (LWIR). This approach was further explored through computational fluid dynamics large eddy simulations (CFD-LES) data of air- and steam-assisted flares [35,51], lab-scale heated vent experiments [35,36], and measurements of diffusion flares and ground combustors [36]. Recently, Lapeyre et al. [52] compared the performance of MWIR and LWIR IFTS instruments for measuring steam-assisted flares and found that the LWIR spectrum provides a better dynamic range.

While IFTS instruments provide a high degree of spatial and spectral resolution, they suffer from several key drawbacks. First, an interferogram consists of thousands of images; even though the images are captured by a high frame rate camera ( $\sim 1 \text{ kHz}$ ), each interferogram requires tens of seconds to minutes to acquire depending on the spectral resolution. Moreover, turbulent fluctuations in the flare plume contaminate the interference patterns in the interferogram data cube, leading to scene change artifacts (SCAs) [47,53]. In the case of a stationary plume, these artifacts may be mitigated by median-filtering multiple interferograms [47], which further lowers the temporal resolution of the hyperspectral images.

Other types of OGI remote sensing technologies include line-scan and light-field cameras, which can provide faster responses compared to IFTSs, due to their significantly lower spectral resolution. In 2016, Zeng et al. [48] proposed using a four-channel light field imager to quantify flare CE; this technique is referred to as the “video imaging spectro-radiometry (VISR)”. The light field imager would use a microlens array to project four copies of the scene through corresponding broadband filters located adjacent to a camera sensor subdivided into quadrants. The filters are positioned behind the cold shield to minimize signal interference due to the filters’ blackbody emissions, which would otherwise dominate the image. The filter windows would be aligned with key vibrational-rotational (VR) bands of CO<sub>2</sub> (4.5–4.9 μm), CH<sub>4</sub> (4.2–4.4 μm), and CO (3.2–3.4 μm), with an additional band aligned with a transparent window corresponding to the atmospheric background radiance. Through several assumptions and simplifications, the broadband intensities are correlated to the corresponding species column density along the LOS of each pixel inside the plume. The column densities are then converted into a local CE for each pixel. Finally, this approach approximates the flare CE as the mean local CE of the detectable pixels located outside the flame envelope, representing the visible flame where the combustion is happening inside the plume.

Zeng et al. [38] implemented this approach using a commercial line-scan camera (SOC 750 [54]) that generates a data cube of 42 uniformly spaced spectral channels between 2 to 5 μm at a rate of 11 data cubes (256 pixels × 240 pixels × 42 bins) per second. They assessed the performance of this approach on steam- and air-assisted flares burning various gaseous mixtures of propane, propylene, and

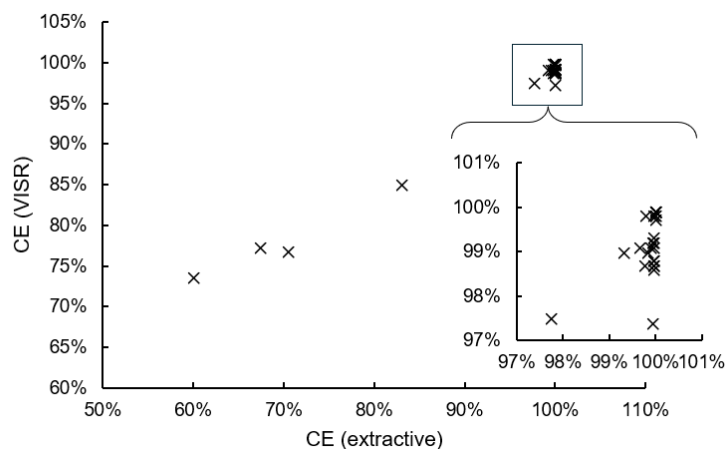


Figure 1.1 Comparison of global CE, estimated using VISR with their respective extractive sampling values, adapted from Zeng et al. [38].

natural gas. A comparison between the VISR-inferred flare CEs and CE estimates obtained from the extractive sampling, using an exhaust hood located downstream and on top of the flare plume, showed excellent quantitative agreement, claiming the VISR as “1% accurate” (Figure 1.1) based on the absolute difference between the measured CE values under efficient flare operating conditions ( $CE > \sim 97\%$ ) [55]. VISR technology has been commercialized as the FlareGuardian™ system [56], which replaced the line-scan imager with a light field instrument, equipped with a similar number of channels and operating within a nominal spectral range of 3–5  $\mu\text{m}$ , with band spacings optimized to capture key absorption features of the species-of-interest inside the plume.

The veracity of the proposed VISR approach for remote flare CE quantification applications, and its physical relevance requires further evaluations. The main concerns regarding the VISR technique can be summarized into three main research objectives: (1) Assess the impact of radiometric simplifications and assumptions applied to the VISR radiometric model, including the plume heterogeneity and optically-thin plume approximation, on the local CE estimates; (2) Analyze the veracity of VISR global CE inference model, based on the estimated local CE; (3) Verify the

capabilities of VISR instrument model in terms of detecting cold (unburned) stripped HC gases, downwind of the flare stack below the plume, and its potential impact on the estimated flare CE.

It is difficult to answer these questions through physical experimentation due to the inherent uncertainty associated with the extractive sampling method mainly due to collected data predicting the flare plume composition only at a certain location, usually downwind of the visible flame [32,57]. Moreover, these measurements cannot be used to isolate the errors originating from the simplifications made to the radiometric model, the flare CE inference method by averaging the local CE, and the limited hardware detection capabilities.

## 1.4 Research Objectives and Thesis Layout

While Zeng et al. [38] used experiments with extractive sampling to assert the veracity of VISR, this study instead uses modeled measurements, computed using temperature and species concentration field datasets generated by CFD-LES simulations of a steam-assisted flare tip in crosswinds, to assess the veracity of the proposed VISR model for remote quantification of flare CE, a flare performance metric which quantifies the effectiveness of flaring process for transforming unwanted hydrocarbons in the fuel stream into more environmentally desirable compound, such as  $\text{CO}_2$  and  $\text{H}_2\text{O}$ . The rationale behind this approach comes down to the two main drawbacks of extractive sampling; innate systematic errors associated with the extractive gas sampling method [32,57], and lack of information to filter-out and analyze the impact of applied simplifications and assumptions in the VISR radiometric model and its potential impact on the local CE and estimated flare CE outcomes. Note that this study attempts to evaluate the preliminary four-channel configuration of the VISR instrument, presented in the original VISR patent [48], not the more advanced and complex methods utilizing the SOC 750 multispectral imager, explained in Zeng et al. [38], or the commercialized FlareGuardian<sup>TM</sup> system [56].

Moreover, an uncertainty analysis, using a hierarchical Bayesian inference model, is conducted on the VISR estimated local CE. The analysis aims to determine the contribution of the innate VISR model error to the overall uncertainty associated with the inferred local CE and provide an observation-based statistical inference of the accuracy associated with the VISR approach for general remote flare CE quantification applications. Finally, an optimized format of the four-channel VISR model, based on the proposed Bayesian analysis, is presented to potentially overcome the flaws in the current VISR model and provide a more accurate flare CE estimate.

Chapter 2 provides a discussion on the various metrics used to quantify flare performance. These metrics include flare combustion efficiency (CE) and destruction removal efficiency (DRE) of methane

or any species-of-interest. This chapter also summarizes the most problematic operational conditions, including heavy crosswind over the flare stack, low heating value of fuel constituents, and excessive air and steam assistance during the flaring process, resulting in a significant drop in the flaring performance.

Chapter 3 provides a literature review on potential techniques for flare CE quantification, which are commonly utilized by industry experts and regulators. These techniques can be categorized into two general groups: (1) invasive, namely the extractive gas sampling methods, and (2) non-invasive techniques, including PFTIR, IFTS, and VISR.

Chapter 4 provides an introduction to infrared spectroscopy, followed by a discussion of the non-scattering radiative transfer equation (RTE) that connects the state of the flare plume to the spectral intensities measured by the remote sensing devices. This discussion is followed by a description of the implemented radiometric assumptions and the governing equations in the VISR radiometric model, used to estimate the local CE value for each pixel within the VISR region-of-interest (ROI). Finally, the VISR model for inferring global CE based on the VISR-estimated local CE within the ROI is discussed.

Chapter 5 describes the computational fluid dynamics (CFD)-large eddy simulations (LES) framework (Uintah-Arches), along with the configurations of the four CFD-LES cases of a John Zink SKEC<sup>®</sup> steam-assisted flare tip under four various crosswind conditions used in this study. This section includes the CFD-LES configurations, boundary and initial conditions, LES mesh and domain size, incorporated solvers and physical models for chemical reactions, radiation heat transfer, etc. This description is followed by the original four-channel VISR instrument model, which, together with the temperature and species concentration fields from the CFD-LES datasets, is utilized to generate synthetic VISR broadband images.

Chapter 6 presents the results for the assessment of the VISR instrument model's veracity in estimating the flare CE using the synthetic VISR broadband images. The results are broken down into the three sub-sections, each describing the evaluation of a unique performance criterion of the VISR four-channel model, the three research objectives provided in Section 1.4, for remote off-situ flare combustion efficiency quantification of a steam-assisted industrial flare under varying crosswind conditions, details provided in Chapter 5.

Chapter 7 conducts an uncertainty analysis on the estimated local CE by the VISR instrument model, provided in section 4.4, based on a proposed hierarchical Bayesian inference model. Additionally, based on the inferred posterior probability density function of the local CE, for pixels located within the VISR ROI, an optimized data-driven format of the VISR global CE inference model is developed, aiming to potentially overcome the inherent simplified VISR model. These inferred posterior distributions are obtained from the Bayesian inference framework presented earlier in this chapter.

Finally, Chapter 8 provides the conclusions and key takeaways of this thesis and presents a series of suggestions for potential future work.

## **Chapter 2**

### **Quantification of Flare Performance**

Quantifying the performance of industrial flares can be a challenging endeavor given several factors, including limited physical access to the flare plume and numerous unknown operational variables, mainly fuel stream composition and flow rate, that must be measured simultaneously. This chapter starts by reviewing the impact of operational conditions, resulting in inefficient flare performance, followed by a brief discussion on the combustion of associated gas in upstream industrial flares. Finally, the chapter presents two key flare performance quantification metrics, flare combustion efficiency (CE) and destruction removal efficiency (DRE) of a specific species. These metrics can report an estimated quantity for the ongoing or time-averaged performance of the flaring process, using the measured species concentrations within the flare plume.

## **2.1 Inefficient Flaring**

The performance of flaring processes in the upstream oil and gas industry depends heavily on several operational and environmental conditions. These include: (1) the presence of a crosswind over the flare stack, generating an unburned fuel-rich region downwind of the flame due to the aerodynamic fuel-stripping phenomenon; (2) over-utilization of complementary air and steam injections in the air- and steam-assisted flares to suppress visible black carbon; and (3) low heating value (HV) fuel components.

### **2.1.1 Aerodynamic Fuel Stripping**

In the presence of a significant crosswind over the flare stack, the primary source of inefficient flaring is linked to a phenomenon known as aerodynamic fuel-stripping. Figure 1 shows the impact of the fuel-stripping phenomenon on the turbulent wake-stabilized flames, by demonstrating the evolution of unburned fuel pockets, which are substantially carried away to the downstream of the flare plume [30]. Initially, given the turbulent perturbations caused by the crosswind flow over the stack, the exhaust fuel gas is entrained within localized flame pockets, which are characteristic of the wake-stabilized turbulent flames. Due to the low fuel concentration between these flame pockets, the local flame is extinguished, resulting in the formation of localized pockets of unburned fuel. The low pressure in the recirculation zone creates turbulent vortices that drive the unburned fuel pockets downwind into a region beneath the flame. Since the horizontal velocity of the flame pockets and unburned fuel are identical, the generation of unburned fuel local pockets occurs along the entire length of the flare plume. However, the buoyancy of the hot combustion products pushes the flame pockets upward, whereas the relatively colder unburned fuel pockets move horizontally with the surrounding ambient air. Therefore, the amount of unburned fuel remains more prominent beneath the flame, in comparison to the region downstream of the flare plume, which only constitutes a minor source of unburned fuel.

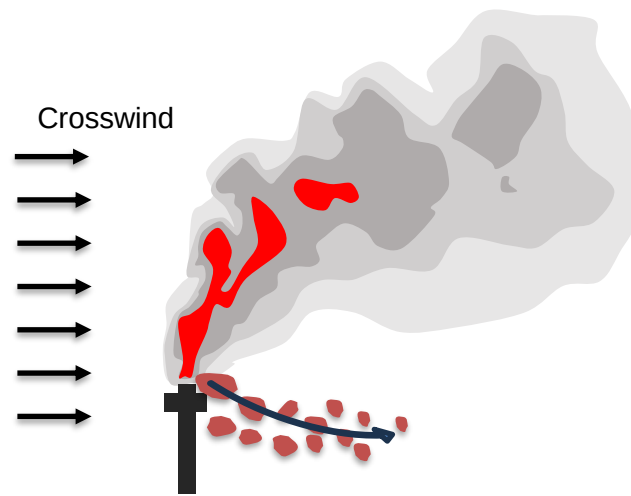


Figure 2.1 Evolution of unburned fuel pockets formation, created due to the fuel-stripping mechanism, in a wake-stabilized turbulent flame. The black line indicates the displacement path for a series of cold unburned fuel-rich pockets moving downward of the flare plume.

### 2.1.2 Steam and Air Over-Assistance

Injecting air or steam at the flare tip can improve the efficiency of the combustion process and suppress the formation of black carbon. Supplementary air or steam flow increases the flare gas exit velocity and enhances mixing with the surrounding air, resulting in improved combustion of the injected fuel stream [58]. Moreover, this mixing process reduces soot formation, luminosity, and thermal irradiation from the plume [59]. Steam assistance is considered to be more effective in smoke suppression compared to air assistance [60]. Several pathways can be associated with the reaction of the injected water vapor during the combustion process, including the primary mechanism, referred to as thermolysis or water splitting [19]. As a result, the Hydrogen and hydroxyl radicals produced by dissociation of water vapor during the combustion process [61] facilitate conversion of carbon into gaseous  $\text{CH}_2$ - and -CHO radicals, subsequently reducing the formation of soot within the flare plume.

While lower injection rates may reduce gas-phase emissions through improved mixing, excessive amounts of air- or steam-assistance lead to partial localized extinction of the flame, resulting in considerable unburned fuel released into the atmosphere [31].

Conveniently, the effects of excessive steam and air assistance on flare performance and gas emissions can be replicated and examined using laboratory-scale flare setups [4]. For instance, Torres and coworkers conducted a series of full-scale flare CE measurements based on extractive sampling and optical measurements [5,10]. The studies focus on low flow and low fuel heating value conditions. The authors used stack diameters of 610 mm and 915mm (24" and 36"), which were air-assisted and steam-assisted, respectively. The fuel was diluted with nitrogen to control the fuel's lower heating values. One of the main objectives of this study was to assess the possibility of flares achieving a CE of 98% or above in real-world operational conditions. Another objective was to evaluate the viability of quantifying gas emissions using competing remote sensing techniques. The reported CE for all flares

ranged between 50% to 99% and typically over 90% and 95% for air- and steam-assisted flares, respectively. However, flare CO<sub>2</sub> equivalent emission rates were several times above those estimated using emission factors under identical experimental conditions.

### **2.1.3 Low Heating Value of Fuel Stream**

The low fuel flow rate and heating value of fuel stream components can play a significant role in the reduction of overall flare performance. Multiple large-scale investigations on assisted flares, with design and operational conditions typical of air- and steam-assisted flares used in refineries and downstream facilities, conducted throughout the 1980s and 2010s, showed that low fuel flow rates and low heating value of the fuel stream constituents have a significant impact on the performance of the air and steam-assisted flares [27,29,62,63].

Fewer studies have been conducted on non-assist flares in upstream and midstream facilities, which are common in locations with limited access to power such as offshore/onshore extraction sites, storage tanks, and some refining facilities, where the fuel stream is typically considered to have very low flow rates, typically less than 50 thousand cubic feet per day (MSCFD), with heating values ranging drastically from 1000 to 2500 Btu/scf. Pohl et al. [63] conducted outdoor pilot experiments on 3", 6", and 12" flare tips injected with propane-nitrogen mixtures, diluted with various quantities of nitrogen, as the fuel stream over a wide range of flare tip exhaust velocities, with low crosswind conditions, less than 8 miles per hour (MPH). Results show that flaring occurred with high combustion efficiency (CE) values, above 95%, for fuel mixtures with a heating value greater than approximately 500 BTU/scf. However, flaring processes utilizing higher heating value fuels, with relatively higher combustion efficiency, generated more smoke, which is in contempt of EPA regulations [12].

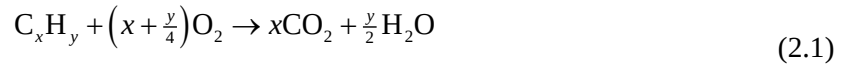
Additionally, other studies focused on the performance of non-assisted flares in wind-tunnel environments. Johnson and Kostiuk [64] studied 0.5" to 2" non-assisted flares in a closed-loop wind tunnel setup, investigating the influence of varying flare gas flow rates, fuel composition, burner diameters, and crosswind velocities on flare performance. This research suggests that smaller flare pipes, higher crosswind velocities, and lower heating value gases all reduce the overall performance,

while increased flare gas exhaust velocity enhances flare performance by negating the effects of crosswind on the turbulent flame. Another study by Howell [65], expanded their work by examining 1" to 4" NG pipe flares, achieving similar results. Gogolek [66] performed pipe flares, ranging from 1" to 6" in diameter, experiments within an open-loop wind tunnel; introducing a new scaling parameter and concluding that flares with diameters less than 3" did not scale similarly to larger diameter ones. More recently, Burt [67] conducted experiments on 1" to 4" diameter pipe flares in a wind tunnel with a turbulent crosswind, comparing various scaling parameters and developing empirical models for 2" to 4" diameter pipe flares with less than 20% volumetric inert gas in the flare gas.

While wind tunnel studies provide useful data on the performance of non-assist flares within controlled environmental conditions, they do not capture the impact of field-specific effects, such as dynamic flare operation and changing environmental conditions, on the overall flare performance. Previous work by Stolzman et al. [68] tested various non-assisted flare tips and analyzed the effects of varying heating values, gas flow rate, crosswind velocities, and tip geometry on flare performance. The experiments were performed in an indoor calorimeter facility, providing a closed controlled environment to measure flare performance, equipped with a fan, capable of generating up to 13 MPH crosswind at the flare tip. Like other studies, they concluded that higher flare-gas flow rates and heating values enhanced the flare combustion efficiency, compared to low gas flow rate conditions with lower heating values, which showed significantly higher impact by crosswind. More recent work by Stolzman et al. [69], who conducted similar experiments in an outdoor environment with higher crosswind velocity, reached similar conclusions in terms of decreased flare performance, at lower fuel flow rates and low heating values.

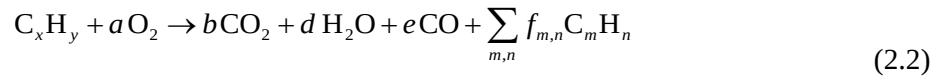
## 2.2 Gas Flaring: Combustion Process

The performance of an industrial flare is directly linked to the efficiency of combustion of the injected fuel into the stack, which is usually natural gas in the case of upstream flaring operations. This section provides a brief introduction to the chemical processes associated with the combustion of natural gas in upstream flaring operations, which ultimately aim to transform unwanted hydrocarbon constituents into more environmentally benign CO<sub>2</sub> emissions. Under ideal stoichiometric conditions, the combustion of hydrocarbon gas may be expressed by

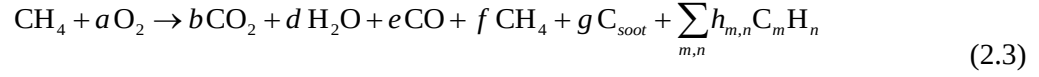


where  $x$  and  $y$  are the numbers of carbon and hydrogen atoms in hydrocarbon molecules, respectively.

During the combustion reaction, formation of nitrogen oxides (NO<sub>x</sub>) occurs through thermal dissociation of N<sub>2</sub> and other Nitrogen-containing fuel components, under higher flame temperature and residence time conditions [ref]. Oxygen insufficiency is one of the main factors that can lead to such conditions within the combustion zone [ref]. Under ideal conditions, enough oxygen is provided to convert all hydrocarbons into CO<sub>2</sub> and H<sub>2</sub>O. However, the oxygen supply can be locally limited by air and fuel mixing implications. Therefore, other combustion products can be formed in the process via



Additionally, new hydrocarbon by-products, not initially present in the reactant fuel, can be formed during inefficient combustion reactions, which are then released into the atmosphere in the gas-phase. Additionally, partially pyrolyzed fuel elements can potentially condense into BC and create soot. Considering methane (CH<sub>4</sub>) as the primary component of the associated gas, the following expression describes the inefficient combustion,



where methane and soot are isolated from the other scarce hydrocarbon by-products to emphasize on their expectedly higher concentrations. These species play a significant role in determining flare performance in terms of flare CE or destruction removal efficiency. For more information on flare CE and DRE, refer to sections 2.4 and 2.3, respectively.

Moreover, crosswinds over the flare stack may disturb this combustion process. The mixing caused by the crosswinds affects the transition from laminar to turbulent flow at the flare tip, thereby altering the mixing of the combustion reactants in Eq. (2.3).

### 2.3 Destruction Removal Efficiency (DRE)

There are several metrics used for quantifying the flare performance. The selection of appropriate metrics relies on the research objectives, whether it is to analyze the efficiency of converting certain compounds in the flaring process or to report the overall performance of the flares for regulatory or evaluation purposes; for instance, flare CE is more suitable for scenarios where the overall performance of the flare is the primary focus of the assessment, while the DRE is primarily used to assess the efficiency of a flaring process in terms of the disposal of a target species. Methane ( $\text{CH}_4$ ) is a primary species-of-interest, targeted by many regulatory and industrial experts, given its status as the main constituent of natural gas, a typical fuel for upstream flaring, and its high GWP, 84 times larger than  $\text{CO}_2$  in a span of 20 years. Other common target species for the DRE metric include the total hydrocarbons (THC), and accumulated soot (BC).

In contrast to flare CE, the DRE metric provides a means for quantifying the effectiveness of the flaring process in terms of specific fuel components disposal by transforming it into less environmentally benign chemical compounds, mainly  $\text{CO}_2$  and  $\text{H}_2\text{O}$  [18,70]. In other words, the DRE of a target species represents how effectively this specific component of the flared gas participates in the flare combustion reaction and is converted into nonhydrocarbon compounds, e.g.  $\text{CO}$ ,  $\text{CO}_2$ , and  $\text{H}_2\text{O}$ .

For instance, in 2010, the Texas Commission on Environmental Quality (TCEQ) conducted a series of experiments to assess various techniques for measuring flaring performance and emissions. This study utilized both flare performance metrics, flare CE and DRE of several VOC compounds, to evaluate the veracity of remote sensing technologies, refer to Section 3.2 for more information, for flare CE quantifications, by comparing with the results obtained from extractive sampling [62]. Other studies and regulatory reports focused on the impact of upstream flaring on climate change, can benefit more

from a flare performance metric that can provide an estimate of the unburned fugitive  $\text{CH}_4$  emissions into the atmosphere, in other words, estimating the efficiency of the flaring processes in terms of methane removal from the fuel stream,  $\text{DRE}_{\text{CH}_4}$ . Note that  $\text{DRE}_{\text{CH}_4}$  is equivalent to flare CE, assuming  $\text{CH}_4$  as the dominant component of the associated gas, processed in most upstream flaring scenarios [29,62].

According to this general definition, the DRE for a target species  $X$  may be expressed by [70,71]

$$\text{DRE}_X = 1 - \frac{\dot{m}_{X,\text{plume}}}{\dot{m}_{X,\text{fuel}}} \quad (2.4)$$

where  $\dot{m}_{X,\text{plume}}$  and  $\dot{m}_{X,\text{fuel}}$  denote the mass flow rates of the target species  $X$  leaving the flare plume into the atmosphere post-combustion and the fuel stream leaving the flare stack, respectively.

Additionally, for the carbon-containing species, a more practical concentration-based alternative form of the DRE is commonly used, which may be denoted by

$$\text{DRE}_X = 1 - \frac{\chi_{X,\text{plume}}}{\chi_{X,\text{fuel}}} \quad (2.5)$$

where  $\chi_{X,\text{plume}}$  and  $\chi_{X,\text{fuel}}$  denote the overall molar fraction of carbon affixed to the target species  $X$ , leaving the flare plume, measured at post-combustion steady state, and the fuel stream gas, exiting the flare stack, respectively [70]. The carbon mole or mass fraction may be inferred through local point concentration measurements, assuming a spatial and temporally averaged uniform plume composition.

## 2.4 Flare Combustion Efficiency (CE)

In contrast to DRE, combustion efficiency (CE) defines the effectiveness of a flaring process by converting the unwanted hydrocarbons inside the vent gas into desirable combustion products, e.g., CO<sub>2</sub> and H<sub>2</sub>O. Considering this definition, a general definition for flare CE may be provided as the fraction of carbon mass flux in the fuel stream supplied to the flare stack, which is ultimately converted into CO<sub>2</sub> and released into the atmosphere. This definition may be denoted by the following expression

$$CE = \frac{\dot{m}_{C,CO_2}}{\dot{m}_{C,fuel}} \quad (2.6)$$

where  $\dot{m}_{C,CO_2}$  and  $\dot{m}_{C,fuel}$  are mass flow rates of the carbon affixed to the carbon dioxide, as the primary flare combustion product, and the fuel stream injected into the flare stack.

In many practical scenarios the fuel composition and mass flow rate is unknown, in which case the mass flow rate of the carbon affixed to the injected fuel stream may be inferred according to a mass balance of all carbon-containing species leaving a control volume surrounding the flare plume. This method is commonly used for flare CE quantifications using remote sensing techniques [36,52]. In this case, flare CE can be expressed by

$$CE \approx \frac{\dot{m}_{C,CO_2}}{\dot{m}_{C,CO_2} + \dot{m}_{C,HC} + \dot{m}_{C,CO} + \dots} \quad (2.7)$$

where “HC” refers to the unburned hydrocarbon components of the flared gas. Carbon mass flow rates are found by multiplying the total mass flow rates by the molecular mass fraction of carbon-containing species. Theoretically, while the denominator in Eq. (2.7) includes all carbon-containing combustion unburned reactants and products in the flare plume, it is primarily dominated by CO<sub>2</sub> and unburned hydrocarbon components of the fuel stream [72,73].

In principle, the mass flow rates in Eq. (2.7) can be obtained by integrating mass fluxes along the control volume (CV) surrounding the plume region, as demonstrated in Figure 2.2.

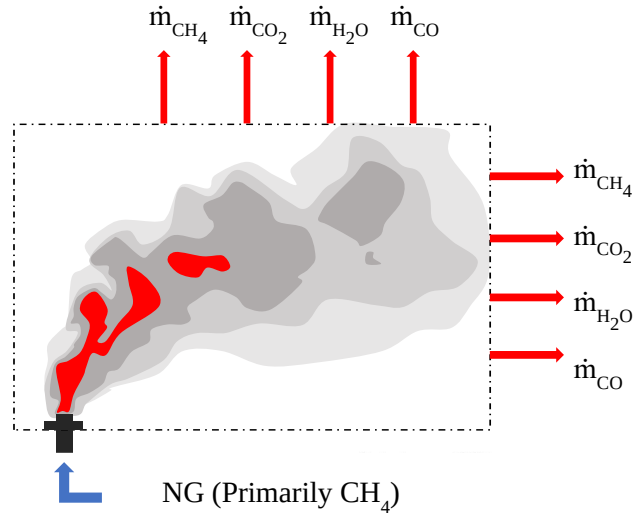


Figure 2.2 Carbon-containing species mass flow rates, leaving an arbitrary control volume (CV) surrounding the flare plume.

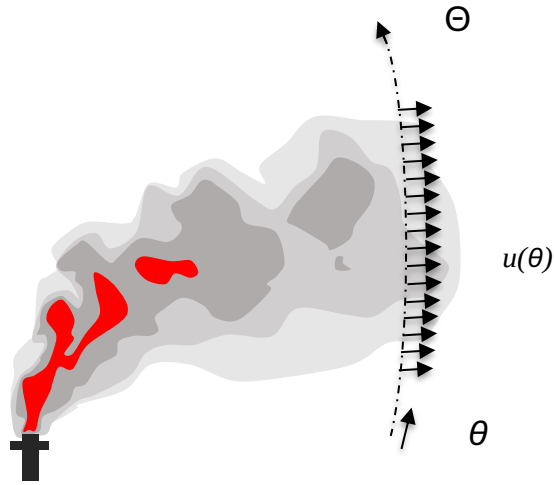


Figure 2.3 Mass flux in Eq. (2.8), calculated by integrating the product of species column densities and projected intensity-weighted crosswind velocities along a control surface.

The local mass fluxes at the boundary of the CV surrounding the plume can be estimated as the product of species column densities and intensity-weighted projected crosswind velocity at the edge of the control surface confining the plume, as demonstrated by Figure 2.3. The local mass flux may be expressed by

$$\dot{m}_{C,k} = \frac{M_C}{M_k} \dot{m}_k = \frac{M_C}{M_k} \int_0^\Theta \rho_k \sin \theta u \sin \theta d\theta \quad (2.8)$$

where  $\rho_k$  and  $u$  are the column density of species  $k$  and intensity-weighted projected velocity along the control surface, respectively.

Furthermore, infrared imaging measurements performed along a line-of-sight (LOS) passing through the flare plume, provide the opportunity to obtain localized (pixel-wise) combustion efficiency at certain locations within the plume; for more information refer to Section 4.2. In comparison to the definition of global flare CE, Eq. (2.6), using mass flow rates of carbon affixed to combustion reactants and products, local flare CE can be defined based on the ratio of carbon-containing species column densities multiplied by the number of carbon atoms per molecule,  $n_{C,k}$ . More precisely, the local CE along the LOS corresponding to the  $j$ th pixel in the flare plume image may be denoted by the following expression

$$CE_{local,j} = \frac{\sigma_{CO_2,j}}{\sum_k n_{C,k} \sigma_{k,j}} \quad (2.9)$$

where  $\sigma_{k,j}$  is the column number density of the  $k$ th species along the  $j$ th pixel LOS (molecules/m<sup>2</sup>),

$$\sigma_{k,j} = \int_0^L \frac{\chi_{k,j}(s) p_{atm}}{k_B T_j(s)} ds \quad (2.10)$$

where  $k_B$  is Boltzmann's constant,  $\chi_{k,j}(s)$  and  $T_j(s)$  are the mole fraction and temperature profiles at a location  $s$  along the  $j$ th LOS, and  $L$  is the plume width (into the image plane). The atmospheric pressure,  $p_{\text{atm}}$ , is taken to be uniform through the plume.

Due to the distinct nature and measurement techniques associated with the “local” CE, Eq. (2.9), and the “global” CE, Eq. (2.6), no direct links can be established between these two metrics, without certain assumptions in regards to plume composition, e.g., isothermal plume, uniform distribution of species within the plume and etc. In this context, Zeng et al. [38,48] suggest that the overall flare CE could be estimated by the mean local CE of pixels located within an envelope surrounding the combustion zone, rationalizing that these pixels contain gaseous by-products of the complete combustion process. They define the inner envelope surface as the region in the vicinity of the flame where the CE increases abruptly, indicating the completion of the combustion reaction, while the outer surface corresponds to areas with almost undetectable broadband intensity [38]. This procedure may be reasonable, provided that: (i) the averaged pixels are representative of the entire post-combustion flare plume; (ii) the turbulent plume is well-mixed so that a “plug flow” velocity model applies; and (iii) radiative emission from all carbon-containing species in the plume are detectable and quantifiable by the MWIR camera.

Finally, compared to flare CE measurements, knowledge of plume composition alone is insufficient for quantifying the DRE of a specific species. In other words, the composition of the fuel stream, injected into the flare stack, is the key to obtaining the DRE, whether this information is based on reported fuel stream composition or estimated through reasonable assumptions [71]. Evidently, for a specific flare, the DRE of a target flared gas component, Eq. (2.4), can be expected to be greater than or equal to the flare CE, Eq. (2.6).

## **Chapter 3**

### **Flare CE Quantification**

This chapter provides a discussion on several common approaches used to quantify flare performance in terms of flare combustion efficiency (CE) or destruction removal efficiency (DRE). A brief background on each technique is provided, along with its advantages and disadvantages, and fundamental, technical, and operational sources of uncertainty associated with these measurement methods.

#### **3.1 Extractive Gas Sampling**

Techniques used for quantifying flare CE or DRE of a combustion product generally work by obtaining the plume composition, in terms of absolute or relative combustion product concentrations within the plume, through either examining gas samples extracted directly from the plume or inferring the concentration ratios via spectrally-resolved or broadband IR emission measurements.

The “gold standard” approach is near-field extractive gas-phase sampling, in which samples from the gas plume are collected and analyzed to estimate combustion product species concentrations via online or offline methods [29,43,71,74,75]. Typically, the plume is sampled using an extractor (hood) suspended above and downwind of the flame, using a crane or a lift. Continuous emission monitors, such as tunable diode laser absorption spectrometers (TDLAS) or cavity ringdown spectrometers (CRDS), enable real-time (online) measurements of species, such as VOCs, CO, CO<sub>2</sub>, O<sub>2</sub>, and NO<sub>x</sub> [5,28,76–79]. While these methods provide temporal resolution (often 1 Hz), the sampling process introduces time lags and temporal blending. Alternatively, samples may be collected and analyzed offsite (offline) using precise gas chromatography/mass spectrometry techniques [75], which is

particularly effective for trace species analysis. To prevent potential contamination of the collected samples via water vapor condensation, equipping the sample lines with heating systems and moisture traps is essential for accurate analysis of the “dry” analyte. In some tests, inert tracers are added to the flare fuel stream to quantify diluent introduced during sampling, which must be corrected to accurately relate analyte composition to plume composition and combustion species concentrations [74,75]. Correlations of plume species can also be leveraged to infer air entrainment, assuming a consistent dilution rate [71,75]. However, the reactivity of intermediate species can be a crucial factor, given that it introduces additional uncertainty, as these species tend to decompose or react post-extraction.

Near-field sampling is not practical for in-service flares, especially in remote upstream or midstream facilities where accessibility and infrastructure are limited. Nonetheless, this approach remains a critical benchmarking tool for validating other flare CE or DRE quantification techniques [38,40,80]. Despite the questionable reliability of flare CE and DRE estimates acquired from the analysis of near-field extractive measurements, given that these calculations rely on measurements of CO, CO<sub>2</sub>, and target species concentrations in the plume, assuming a well-mixed, steady-state turbulent plume, the DRE and flare CE values obtained from this method are typically considered as ground truth to verify the results obtained from other approaches for quantifying the flare performance. These ground truth values are typically used in controlled-environment experiments, where flare vent gas composition and flow rate are well-defined.

Uncertainty in near-field measurements often stems not only from instrument accuracy but also from flare plume dynamics, which are difficult to capture due to the limited spatial and temporal resolution of sampling methods. Plume heterogeneity and intermittency pose significant challenges. For instance, hood extractors placed above the flame may miss fuel-rich regions caused by fuel stripping below the flare or intermittent phenomena, e.g., flare sputtering [40]. These limitations raise

questions regarding the accuracy of flare CE or DRE estimates, particularly in distinguishing between values such as 98% and 99.5%, given the assumptions and approximations required to extrapolate point concentration measurements to overall flare performance.

There are several inherent limitations to near-field gas sampling approach, which can be linked to spatial inhomogeneity of flare plumes [32], “rogue” events, such as the BC/H<sub>2</sub>O concentration ratios, as shown in Figure 3.1, tend to be skewed to lower values which undermines the underlying assumptions of highly correlated and well-mixed combustion products within the plume [57], and finally the low resolution of extraction probes [73]. Such limitations necessitate caution when interpreting the results using a near-field sampling approach. Despite near-field sampling capabilities for differentiating between acceptable (efficient) and unacceptable flare operating conditions (e.g., under over-utilization of steam assistance or high crosswind over the flare stack), its robustness for finer quantification of flare CE and DRE has yet to be demonstrated adequately.

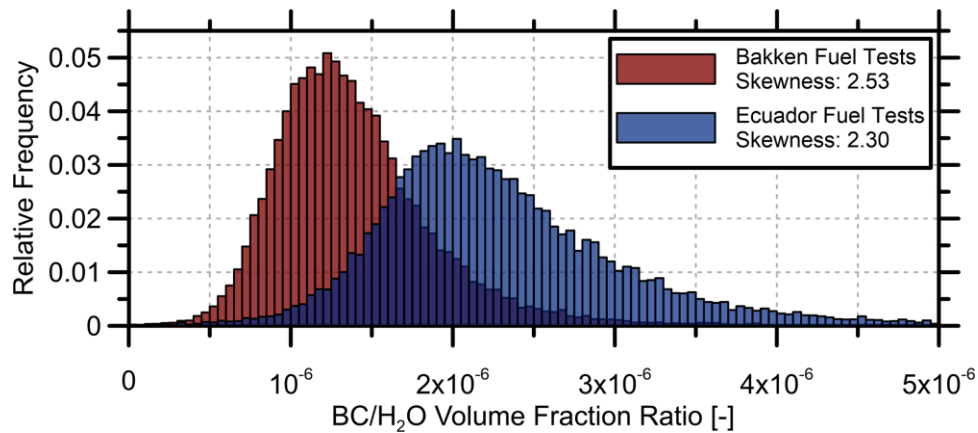


Figure 3.1 Aggregated BC/H<sub>2</sub>O ratio distributions for the two types of fuel, adapted from Seymour et al. [57].

Far-field sampling, another variation of extractive gas measurement techniques, involves collecting gas samples at a greater distance downstream from the flare plume. These far-field measurements are commonly conducted as part of environmental monitoring campaigns and might often occur without the collaboration of the flare operator [5,62]. Unlike the near-field sampling approach, far-field sampling methods benefit from additional mixing as the plume travels downstream, allowing a more reasonable assumption of a homogeneous plume in most scenarios [62]. Despite all the merits, this approach suffers from several limitations, including the reduced concentrations of target species due to mixing and dilution with ambient air, limited temporal resolution, in addition to difficulties associated with accurately locating the gas plume and distinguishing emissions from a specific flare from those of other nearby sources. For DRE estimates, the flare fuel stream composition is typically unknown and must be estimated. Hence, these measurements may rely on annual emission inventories provided by flare operators for downstream refining flares [70] or assume representative associated gas compositions, typical of the basin for upstream flaring [23,28].

Far-field measurements can be conducted either from the surface or from aircraft. Wood et al. [70] performed ground-based mobile measurements of flare plumes in the Houston area using an Aerodyne Mobile Laboratory, which was stationary during sampling. Assuming plume release heights of 65-70 m, they modeled atmospheric mixing to transport the plume to the ground. Measurements were taken 400-800 m downstream from the flare, a distance chosen to balance plume homogenization with minimizing interference from other sources. Flare CE values were estimated based on Eq. (2.7) by scaling and regressing concentrations relative to CO concentrations to separate flare-generated carbon species from industrial background emission levels. Moreover, DRE values were estimated on a concentration basis, Eq. (2.5).

Aircraft measurements are increasingly employed to quantify plume emissions and flare CE/DRE [28,76,78,81]. Typically, aircraft equipped with onboard sensor packages perform multiple transects

across a single plume. These packages typically contain cavity ring-down spectroscopy (CRDS) for high-sensitivity measurements of  $\text{CH}_4$ ,  $\text{C}_2\text{H}_6$ , and  $\text{CO}_2$ , as well as sensors for  $\text{NO}_x$  and particulate matter (PM). Peak enhancements of  $\text{CO}_2$  ( $[\Delta\text{CO}_2]$ ),  $\text{CH}_4$  ( $[\Delta\text{CH}_4]$ ), and other species in the plume are quantified as the difference between the observed plume concentrations relative to background (ambient) concentrations measured outside the plume. Flare CE and DRE estimates are then obtained by regressing  $\Delta\text{CH}_4$  against  $\Delta\text{CO}_2$ . These studies typically focus on deriving  $\text{DRE}_{\text{CH}_4}$  from the observed peaks of  $\text{CH}_4$  and  $\text{CO}_2$ , which may be expressed by [76,78]

$$\text{DRE}_{\text{CH}_4} = 1 - \frac{[\Delta\text{CH}_4]}{\chi_{\text{CH}_4} [\Delta\text{CO}_2] + [\Delta\text{CH}_4]} \quad (3.1)$$

where  $\chi_{\text{CH}_4}$  is the molar fraction of  $\text{CH}_4$  in the flare fuel stream. The threshold sensitivity and uncertainty of this measurement technique are obtained from the threshold sensitivity of the onboard  $\text{CH}_4$  and  $\text{CO}_2$  sensors [78], along with the statistical variability of the concentration enhancements measured from the set of transects.

Airborne sampling studies have reported a wide range of CE and DRE values for upstream flares across various regions. These differences reflect both the uncertainties inherent to the measurement techniques and the regional variability of the flare fuel composition. One of the earliest airborne studies, conducted by Caulton et al. [78] measured  $\text{DRE}_{\text{CH}_4}$  for 10 flares in North Dakota's Bakken Formation and one in Pennsylvania's Marcellus Formation using a CRDS-equipped aircraft. The aircraft flew directly above the flare plumes, measuring  $\text{CH}_4$  and  $\text{CO}_2$  enhancements across multiple transects. Enhancement factors were determined by regressing  $[\Delta\text{CH}_4]$  against  $[\Delta\text{CO}_2]$ , with the slope used to estimate DRE via Eq. (3.1). While all DRE values exceeded 99.8%, significant variability in enhancement factors was reported, and the quantification limit was constrained by the challenge of

measuring CO<sub>2</sub> enhancement. This study also found that enhancement factors decreased nonlinearly with increasing crosswind speed, with negligible impact on the high DRE values.

Gvakharia et al. [76] expanded on this work by surveying 37 flares in the Bakken region, employing a CRDS, TDLAS, and SP2 system aboard the aircraft to measure gas-phase combustion species and particulate matter (PM). Plumes were sampled at altitudes of 400-600 m (and occasionally 1,000 m) above ground level, with measurements taken hundreds of meters to a kilometer downwind to allow plume dispersion. DRE was calculated using a similar approach to Caulton et al. [78], solely utilizing the peak enhancements per transect of the species in the calculations. This study also reported a weak dependence for flare performance efficiency on crosswind velocity, despite a much lower and more broadly distributed DRE<sub>CH<sub>4</sub></sub>, with a median of 96-97% and a strong lognormal distribution. This finding highlights the disproportionate influence of low-efficiency flares on overall emissions, a difference attributed to the smaller sample size of the earlier study.

Plant et al. [28] conducted the most extensive airborne sampling of upstream flares to date, covering over 600 transects of more than 300 flares across the Permian, Eagle Ford, and Bakken formations. Using similar instruments, the aircraft collected samples 200-2000 m downwind of the plumes and calculated DRE from CH<sub>4</sub> and CO<sub>2</sub> peak enhancements using Eq. (3.1). Their results confirmed the lognormal distribution reported by Gvakharia et al. [76], with a median and mean DRE of 98% and 95%, respectively, demonstrating the influence of a long distribution tail. A bootstrap analysis showed mean DRE, with 95% confidence intervals of around  $\pm 1\%$ , less than 98% across all basins, contrasting the underlying assumption of 98% DRE, from earlier large-scale extractive tests [27,29]. Additionally, accounting for emissions from unlit flares reduced the mean effective DRE to 91%. Moreover, in contrast to the earlier studies [27,29,74], Plant et al. [28] observed no significant relationship between wind speed and DRE.

In terms of shipborne far-field sampling techniques, several studies have employed these methods to measure VOC, NO<sub>x</sub>, and other pollutant emissions from offshore oil and gas production platforms in the North Sea and infer the flare CE and DRE associated with these offshore flares [82–84]. Among all these studies, Shaw et al. [81] is the only study to simultaneously quantify CO<sub>2</sub> concentrations, and infer flare CE and DRE, assuming the flared gas composition and flow rate, using several measurement methods including CRDS, TDLAS, and other custom sensors. Sampling 58 offshore platform plumes, this study highlighted the limitations of earlier shipborne CH<sub>4</sub> measurements, which failed to capture emissions from buoyant flare plumes rising into the atmosphere. Flare CE was estimated by comparing peak enhancements of CO<sub>2</sub> [ $\Delta\text{CO}_2$ ], CH<sub>4</sub> [ $\Delta\text{CH}_4$ ], and C<sub>2</sub>H<sub>6</sub> [ $\Delta\text{C}_2\text{H}_6$ ] relative to background intensity, denoted by

$$\text{CE} = \frac{[\Delta\text{CO}_2]}{[\Delta\text{CO}_2] + [\Delta\text{CO}] + 2[\Delta\text{C}_2\text{H}_6]} \quad (3.2)$$

while DRE<sub>CH<sub>4</sub></sub> and DRE<sub>C<sub>2</sub>H<sub>6</sub></sub> were defined in a format similar to Eq. (3.1). Shaw et al. [81] analyzed DRE<sub>CH<sub>4</sub></sub> and DRE<sub>C<sub>2</sub>H<sub>6</sub></sub> using a method distinct from linear regression between co-located measurements. Instead, they utilized time- or path-integrated concentration enhancements, arguing this approach is less affected by temporal misalignments between species concentration measurements. Their findings indicated mean and median combustion efficiencies of 97.9% and 98.4%, respectively, with a skewed distribution. Mean and median DRE<sub>CH<sub>4</sub></sub> values were reported at 97.6% and 98.5%, respectively, aligning with results from Plant et al. [28] and Gvakharia et al. [76] but lower than those reported by Caulton et al. [78]. Like Plant et al. [28], Shaw et al. [81] found no significant correlation between wind speed and CE for wind speeds up to 15 m/s. Additionally, they noted a linear relationship between NO<sub>x</sub> production and CE, attributed to higher flame temperatures driving thermal NO<sub>x</sub> formation.

The reliability of CE and DRE estimates from airborne sampling depends on critical assumptions, including that the flare plume is well-mixed, steady, and originates solely from the flare. Under these conditions, the measured concentration enhancements represent emissions from the plume. However, discerning CO<sub>2</sub> enhancements relative to background concentrations is a major challenge, especially at high CE/DRE levels. Gvakharia et al. [76] highlighted that transects need to be far enough downwind for a clear plume profile but close enough to minimize the impact of noise on CO<sub>2</sub> measurements, which can make distinguishing DRE values above 99% particularly difficult. Plant et al. [28] further examined the effects of inert CO<sub>2</sub> and incomplete combustion products, estimating that these could contribute to errors of approximately 0.1%.

A key takeaway from airborne sampling studies of upstream flares is the wide distribution of CE and DRE values across regions, with poorly performing flares disproportionately affecting overall emissions. The variability in results across several studies [28,76,78] underscores the significant impact of sampling error on the average estimates of the flare performance. This variability suggests that understanding the true environmental impact of upstream flaring requires large-scale measurement campaigns. While airborne sampling may be less sensitive than near-field techniques, it excels at assessing large numbers of flares across wide geographic regions, reinforcing the notion that there is no universal method suitable for measuring flare performance.

### **3.2 Remote Sensing Radiometric Technologies**

Remote (stand-off) infrared optical gas imaging (OGI) techniques offer significant advantages, particularly in overcoming the challenges associated with direct plume gas extractive sampling techniques. Stand-off methods are generally considered to be safer, more cost-effective alternatives, which can support fence-line monitoring, enabling automated and continuous assessment of flare performance. Among all the radiometric techniques discussed in this section, passive approaches are generally preferred due to their simplicity, lower cost, and minimal physical access requirements.

Stand-off radiometric techniques rely on spectrally resolved intensity measurements, which may target either the flame itself or the hot plume gases. Flame-based measurements infer quantities of interest (QOIs) indirectly through correlations with parameters such as flame temperature, area, and shape, often supplemented by reported flaring volumes and calibration via extractive sampling or computational fluid dynamics (CFD). Conversely, radiometric measurements of plume gases provide more reliable information on the species gas-phase emissions by the flare.

### 3.2.1 Open-path FTIR spectroscopy

Open-path FTIR spectroscopy is currently the most prevalent stand-off technique for measuring flare CE or DRE. This method utilizes an FTIR spectrometer equipped with a telescope to measure spectral intensity along a single line-of-sight (LOS) intersecting through the flare plume at a specified point relative to the flame tip. The resulting spectrum is analyzed to estimate species column densities and subsequently, the flare CE or DRE via Eqs. (2.6) and (2.5), respectively.

In 1984, Industrial Monitor and Control Corporation (IMACC) developed the first proprietary PFTIR instrument, designed for flare plume measurements, and underwent refinements during experimental field campaigns in 2003, 2009, and the 2010 TECQ study [40,62]. In 2000, Blackwood [41] utilized the open-path FTIR technique to infer the DRE of CO of two distinct flares simultaneously; meanwhile, Haus et al. [43] independently conducted measurements of CH<sub>4</sub>, CO<sub>2</sub>, CO, NO, and H<sub>2</sub>O concentrations within the NG flares, using the same equipment as Blackwood.

Generally, Fourier Transform Infrared (FTIR) spectrometers operate by splitting a broadband light beam into two separate paths: one reflects off a stationary mirror, while the other reflects off a moving mirror. The two beams are recombined to produce an interferogram, an oscillatory pattern representing wavelength-dependent information derived from optical path differences. This interferogram is Fourier-transformed to generate a spectrum. The measured spectrum reflects the result of a convolution of the true intensity and the instrument lineshape function (ILS). The spectral resolution depends on the maximum optical path difference (MOPD), which is required to be adjusted by balancing between the desired spectral resolution and temporal (acquisition) rate.

Currently, there are two distinct variants of the open-path FTIR technology employed in field campaigns: passive (PFTIR) or active (AFTIR). PFTIR relies on the sky as a background source, with plume characteristics determined by comparing spectral measurements inside and outside the plume.

Atmospheric transmittance is calibrated using a blackbody source, and plume temperature is estimated through the analysis of temperature-sensitive spectral features, including CO absorption features at  $2150\text{ cm}^{-1}$  [44]. Path-integrated species concentrations are then inferred by fitting a modeled plume transmittance to the observed FTIR spectrum. Conversely, AFTIR uses an active light source or a retroreflector to indicate the terminal point of the LOS, as exemplified by Haus et al. [43], who employed an IR light source (globar), and an IMACC AFTIR instrument, which combines a controlled fluctuating light source with an FTIR unit. This instrument isolates emission and background components of the transmitted spectra, hence reducing the calibration requirements for this technique [40]. On the other hand, removing the effect of fluctuating ambient background irradiation greatly reduces the uncertainty associated with the observed transmittance spectra from the plume. Despite considering the AFTIR to be more accurate than PFTIR, the challenges associated with adequately positioning a globar or a retroreflector at the prescribed location behind the flare plume make the AFTIR method impractical for field measurements.

A specialized variant of the AFTIR, referred to as solar occultation flux, utilizes the sun as an active light source. Mellqvist applied this AFTIR approach to measure ethylene ( $\text{C}_2\text{H}_4$ ) emissions from polyethylene plant flares [85]. In this study, the AFTIR system was mounted on a mobile platform, equipped with a sun tracker. The modeled absorption spectra from a select number of species,  $\text{C}_2\text{H}_4$ ,  $\text{H}_2\text{O}$ , and  $\text{NH}_3$ , were fitted onto the transmittance spectra to infer combustion species column densities, including  $\text{C}_2\text{H}_4$ . Emission rates were computed by combining the estimated column densities with crosswind measurements. While unable to directly obtain vent gas flow rates, this method used  $\text{N}_2\text{O}$  as a tracer to estimate flare CE, which ranged from 50% to 97%, depending on operating conditions, whereas low CE values correspond to over-utilization of steam assistance, generating high steam to  $\text{C}_2\text{H}_4$  flow rates ratios.

FTIR spectroscopy offers the distinct advantage of detecting (fingerprinting) and quantifying a diverse range of species within its operational spectrum. For instance, a study conducted by the US Environmental Protection Agency (EPA) between 2014 and 2016 [86], the IMACC PFTIR and Telops MWIR IFTS instruments were utilized to quantify the flare CE of the enclosed ground combustors (EGCs). The PFTIR successfully quantified multiple species, including CO, CO<sub>2</sub>, H<sub>2</sub>O, NO<sub>x</sub>, and various hydrocarbons, e.g. CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>3</sub>H<sub>6</sub>, and C<sub>4</sub>H<sub>10</sub>, despite the challenges posed by the lower temperature and heterogeneity of EGC plumes, compared to NG flares. Additional uncertainties can be associated with the open path FTIR-based techniques due to factors such as atmospheric CO<sub>2</sub> interference, temperature-sensitive detection limitations, and assumptions of isothermal plume and plume homogeneity.

Wormholdt et al. [40] compared CE values derived from PFTIR and extractive sampling techniques during the 2010 TECQ tests [62]. While PFTIR results aligned with extractive sampling at higher CE values, greater discrepancies arose at lower CE levels due to increased plume inhomogeneity. This undermines the underlying assumption of the PFTIR method, that the plume is considered to be homogeneous and at a steady state. A comparison of PFTIR and extractive sampling methods, employed on propylene-fueled flares, showed significant discrepancy in the results, which may be associated with measuring the collected propylene (extremely low quantities) through extractive sampling, errors originating from the radiometric model for processing PFTIR data, missing the cold fuel-rich regions, undetectable by the PFTIR instrument, in addition to extra uncertainty from the plume heterogeneity. Moreover, Wormhoudt et al. [40] reported considerable temporal fluctuations in species column density, yet flare CE estimates suffered from much less uncertainty and were deemed robust. They rationalized this phenomenon based on the strong temporal covariance between species column densities within the plume. Later studies, conducted by Seymour and Johnson [57], reported

contradicting results, where the recorded BC and H<sub>2</sub>O column densities within the plume showed no temporal correlation but rather high skewness toward lower BC/H<sub>2</sub>O concentration ratios.

In conclusion, FTIR measurements may fail to detect fuel-rich regions beneath the visible flame, primarily due to insufficient thermal contrast, compared to the background, and the alignment of the PFTIR, which is typically pointed downstream of the flare plume, not beneath, where due to fuel-stripping phenomenon, refer to Section 2.1.1, an unoxidized, cold, fuel-rich zone is formed under the visible flame. Additionally, the extractive sampling methods face the same technical challenge, as the extractive hood is normally suspended downwind and above the flare plume, missing the fuel-rich region beneath the plume. As a result, both PFTIR and extractive sampling methods might systematically overestimate flare CE, particularly under specific operational conditions, such as the presence of heavy crosswind over the flare stack. Despite all the shortcomings, PFTIR technology has become a staple in the flare performance monitoring methods among industry regulators and experts, given its flexible, safe, and convenient operation, compared to extractive sampling [23].

### 3.2.2 Imaging Fourier Transform Spectrometer (IFTS)

Imaging Fourier Transform Spectrometers (IFTSs) have been widely used to quantify flare gas emissions, particularly methane, and infer flare CE from stand-off (remote) settings. This technology has attracted a great deal of interest due to its robust capability of capturing the transient development of the entire flare plume region through spectrally resolved measurements, potentially providing accurate instantaneous estimates of the flare CE, with no requirement of fuel compositions and flow rate prior knowledge.

Commercially available mid-wavelength (MWIR) and long wavelength (LWIR) infrared IFTSs, developed by Telops Inc. [45], have proven effective for analyzing the composition of post-combustion flare plumes. Unlike a traditional PFTIR spectrometer, which conducts its measurement along a single LOS, IFTSs capture intensity across the whole plume domain, comprised of thousands of nearly parallel LOSs, producing an interferogram cube. Applying the Fourier transform on the interferogram data cube yields a dataset containing hundreds of spectral intensity measurements, each corresponding to a distinct wavenumber. Although the spectral resolution of IFTSs ( $\sim 1 \text{ cm}^{-1}$ ) is lower than that of PFTIR ( $\sim 0.5 \text{ cm}^{-1}$ ), it is significantly higher than other remote sensing radiometric technologies, including light field or light-scan hyperspectral cameras, e.g., SOC750 with  $\sim 70 \text{ cm}^{-1}$  close to the  $3.5 \mu\text{m}$  [54].

Spectral data of selected pixels can be analyzed to infer species column number densities. As with the PFTIR method, this approach enables the identification (fingerprinting) of species post-combustion within the flare plume, with an indeterminate composition. However, while PFTIR spectrometers cover most of the IR spectrum, IFTS instruments typically operate over a narrower range, restricted to either the mid-wavelength infrared (MWIR) or long-wavelength infrared (LWIR) spectrum. This limited coverage may potentially complicate the species fingerprinting process. Typically, the assembly of an IFTS interferogram takes approximately 30 seconds, depending on the designated spectral resolution,

while individual frames are recorded at hundreds of frames per second. Intensity-weighted velocity fields can be computed by applying optical flow [87,88] or image correlation velocimetry (ICV) [89] techniques on the recorded frames. The combination of inferred velocity fields and species column density data facilitates the process of estimating species mass fluxes, which are essential for calculating the flare CE.

However, performing regression calculations for each pixel's LOS is deemed computationally intensive due to complications arising from the temperature dependency of the absorption cross-section calculations. To optimize computational resources, column densities are often computed along specific vertical "integration lines" intersecting the plume rather than creating a full two-dimensional (2D) map of the plume domain. These column densities are then multiplied by their corresponding velocity components, normal to the line and pixel height, where the results are summed across the pixels, located on the integrating line, shown in Figure 2.3, to provide estimated mass flow rates needed for flare CE quantification via Eq. (2.7).

Studies have demonstrated the utility of IFTS in estimating emission rates for various species. For example, Savary et al. [50] used both MWIR (1.5–5.5  $\mu\text{m}$ ) and LWIR (8–12  $\mu\text{m}$ ) IFTS instruments to measure emissions of  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{SO}_2$ , and hydrocarbons found in the refinery flare plumes, subsequently deriving flare CE estimates. Gagnon et al. [90] employed an LWIR IFTS to map  $\text{SO}_2$  and  $\text{CH}_2\text{O}$  column densities in a flare plume but could not measure  $\text{CO}_2$  within this spectral range, precluding CE calculation. Later studies [36,91] primarily focused on MWIR instruments due to their inherent capability for capturing prominent  $\text{CO}_2$  absorption features, essential for quantification of the flare CE, and having minimal spectral overlap with the absorption lines associated with atmospheric water vapor.

As part of the 2010 Texas Commission on Environmental Quality (TCEQ) study [62], an MWIR IFTS was used to conduct CE measurements of steam- and air-assisted flares. In this study, two independent contractors conducted plume measurements using an imaging Fourier transform spectrometer (IFTS) (Telops Inc.), and a passive and active Fourier transform infrared (PFTIR, AFTIR) spectroscopy (Industrial Monitor and Control Corporation). The PFTIR and AFTIR provide the spectral data along a single LOS, in contrast to the IFTS, which provides the spectral data in a two-dimensional array of LOSs, represented by pixels. The PFTIR and IFTS record the radiation emitted from the gas plume, against an ambient background, while the AFTIR records absorption measurements and requires an artificial radiative source, acting as a background. While the requirement of a radiative source significantly complicates the experimental apparatus and would be infeasible under most realistic conditions, the absorption-only measurement is more straightforward, and it facilitates the quantification of colder gases that may not be visible in strictly emissions-based measurements. The test description of PFTIR and AFTIR can be found in Wormhoudt et al. [40]. The average flare CE values inferred using PFTIR and AFTIR were within 2.5% of probe-derived (extractive sampling) measurements, while IFTS-estimated CE values were 15% lower than its counterpart. This may be justified considering that despite the Telops MWIR IFTS generating the same amount of data as the PFTIR for each camera pixel, the much longer integration time required to record a data cube, increases the errors associated with scene change artifacts (SCAs) [47]. This, in addition to the significant computational demand, over six weeks of data processing, required to calculate CE estimates, primarily due to the enormous amount of data collected by the IFTS, making the IFTS generally less reliable.

A similar study conducted by the Environmental Protection Agency (EPA) [86] employed the Telops MWIR IFTS instrument to measure plume-generated VOC emissions, particularly benzene, toluene, xylene, ethylbenzene, and other combustion products, including CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, and N<sub>2</sub>O,

at a spectral resolution of  $0.25\text{ cm}^{-1}$  within a  $128 \times 128$  pixels focal plane array subdomain. While this study revealed significant plume heterogeneity and temporal emission "bursts," the large volume of data again hindered reliable CE estimation.

Several recent studies assessed the reliability of flare CE measurements using MWIR IFTS instruments. Miguel et al. [35] evaluated the feasibility of MWIR IFTS for CE quantification under three scenarios: a simulated industrial flare in crosswind using CFD-LES modeling, a laboratory-scale heated exhaust vent, and industrial-scale controlled-release steam- and air-assisted flares. Their results showed strong agreement between IFTS-estimated and controlled-release  $\text{CH}_4$  flow rates for the heated vent, despite the measured spectra from lab-scale flares being contaminated by soot emissions and other artifacts. On the other hand, MWIR IFTS identified species overlooked by gas chromatography/mass spectrometry (GC/MS), particularly  $\text{CO}$ , which can undermine the CE estimates. Lapeyre et al. [36] utilized the same MWIR IFTS instrument to assess the CE of multiple flare configurations, including natural gas, enclosed ground, and refinery steam-assisted setups. While carbon mass flow rates for the ground flare aligned with the supplied fuel stream flow rates, quantitative analysis of exposed flares was compromised by veiling glare from hot  $\text{CO}_2$  inside the active combustion zones. This issue is less impactful on the operation of LWIR IFTS instruments, e.g., the Telops mini xLW ( $7.4\text{--}12.5\text{ }\mu\text{m}$ ), as these instruments capture fewer  $\text{CO}_2$  absorption features within their nominal spectral range, ultimately mitigating this artifact [52].

On the other hand, uncertainties associated with the IFTS-estimated flare CE and DRE values remain inadequately quantified. These uncertainties arise primarily from errors in column density retrievals through radiometric calculations and the velocity field estimates used to convert the column densities into mass flow rates. Benchmarking by Miguel et al. [91] and Lapeyre et al. [36] illustrated that IFTS-estimated mass flow rates generally fell within 10% of known values, indicating acceptable

accuracy. Note that while utilizing these flow rates to compute CE via Eq. (2.7), these uncertainties may be partially reduced due to the correlated errors in the projected velocity fields. Column density uncertainties depend on spectral resolution, plume composition, atmospheric transmittance, and the parameterization of temperature and species concentrations along each pixel's LOS. Neglecting nonlinear couplings in these parameters introduces additional model errors. Furthermore, scene change artifacts (SCAs), caused by turbulent fluctuations during interferogram construction, manifest as broadband spectral artifacts. These can be addressed through median filtering or bandpass filtering, at the cost of reduced temporal resolution.

### 3.3 Conclusion

IFTS, in its current state, can be considered unfit for real-time flare CE monitoring due to the time-consuming computational processing required for inferring species column densities throughout the plume domain. While this technology excels in experimental campaigns by identifying combustion species and mapping the species column density throughout the flare plume, thereby suitable for research and regulatory assessments, the issues associated with the data storage and processing requirements remain significant limitations for this technology.

To address some the shortcomings of IFTS measurement techniques, Video Imaging Spectro-Radiometry (VISR) was presented by Zeng et al. [38,48] as a quick and accurate alternative for remote quantification of flare performance. This OGI approach utilizes a MWIR multispectral instrument to capture and analyze the flare plume evolution in real time. As promising as this approach may appeal to industry experts and regulators, further assessments are required to determine the veracity of this technology in terms of reported flare CE and identifying its underlying limitations and detection capabilities for combustion products IR emissions.

## Chapter 4

### Video Imaging Spectro-Radiometry (VISR)

Species concentrations and temperature distribution vary spatially and temporally within the plume region. As discussed in the previous chapter, limited physical access to the flare plume creates several challenges for deploying direct measurement techniques in the field. This has led to the popularity of optical gas imaging (OGI) approaches for standoff (remote) flare measurement applications, to surge, as a more feasible alternative to direct sampling methods.

This chapter introduces Video Imaging Spectro-radiometry (VISR) technology, starting by reviewing the principles of infrared spectroscopy, specifically the non-scattering radiative transfer equation (RTE), along with a short discussion on computing gas mixture absorption coefficient based on the HITRAN database. This discussion is followed by a review of the VISR radiometric model, including the governing equations, approximations and assumptions incorporated in the non-scattering RTE to establish the multispectral four-channel VISR radiometric model, the original version of the VISR method. This version of VISR approach is used in this thesis to estimate the flare combustion products, mainly the species column number density along a LOS, for pixels located within the VISR region-of-interest (ROI), using the VISR broadband signals, to ultimately infer local CE values. This section also discusses the means to estimate flare CE as a function of local CE for pixels located within the VISR ROI.

Finally, the section provides the details of CFD-LES simulations of an upstream steam-assisted flare used in this study to generate synthetic VISR broadband images to assess the veracity of the proposed VISR radiometric model.

## 4.1 Infrared spectroscopy

IR Infrared (IR) spectroscopy aims to identify and potentially quantify gas molecules, found within a gas mixture, by analyzing the interactions between light and matter as a function of wavelength or frequency. The molecular absorption coefficient of the gas species strongly depends on their emitted wavelength, given that the gas molecules are only permitted to occupy discrete (quantized) energy levels. On the other hand, within the IR spectrum, temperature, pressure, and concentration of the species within the gas mixture could potentially impact the absorption coefficient beyond its dependence on the quantum spacing of the energy levels. Figure 4.1 provides a schematic of the potential transitions between discrete quantum energy states.

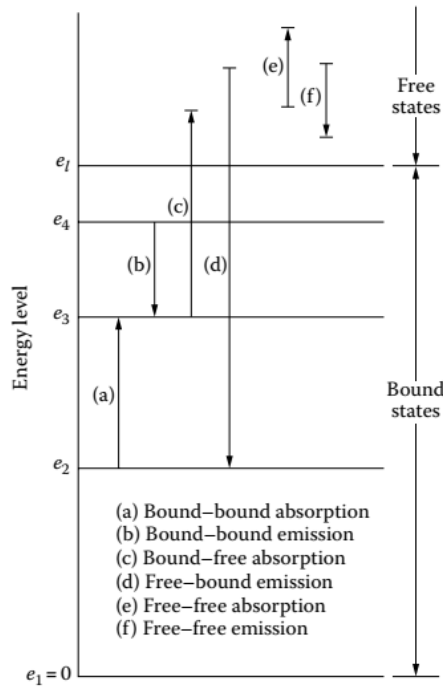


Figure 4.1 Schematic of the potential transitions between discrete quantum energy states. Adapted from Ref. [92].

For wavelengths within the IR spectrum, gas molecules can undergo transitions between bound energy states. However, only photons having the exact amount of energy required for the molecule to

transition from one state to another can be absorbed. For instance, if a photon with quantum energy equal to  $e_3 - e_2$  is absorbed, the molecule will change its energy state from  $e_2$  to  $e_3$ , denoted as the energy jump (a) in Figure 1. Meanwhile, a molecule changing state from  $e_3$  to  $e_2$  will emit a photon having a quantum energy equal to  $e_3 - e_2$ . Therefore, for photons with valid quantum energy,  $e_p$ , the corresponding electromagnetic wavelength,  $\lambda$ , or wavenumber,  $\eta = 1/\lambda$ , can be acquired according to the following expression

$$e_p = e_j - e_i = hc\eta_{ji} \quad (4.1)$$

where  $h$  is Planck's constant,  $c$  is the speed of light, and  $\eta_{ij}$  is the central line wavenumber,  $e_j$  and  $e_i$  are the final and initial particle energy states of this transition [92].

In the case of polyatomic molecules, simultaneous transitions between vibrational and rotational states correspond to the emission of photons having energies corresponding to the infrared spectrum. Typically, low-energy photons participate in transitions between rotational levels of the same vibrational level in the same electronic state, which correspond to spectral lines in the far-IR (LWIR) region. Meanwhile, transitions between rotational levels of different vibrational states involve photons in the near to mid-IR (closer to MWIR) region. Note that these types of IR absorption and emission only occur in diatomic or polyatomic molecules, given their molecular structures, allowing vibrational-rotational states' transitions. Subsequently, molecules with more atoms can generate a higher number of spectral lines compared to simpler molecules. The difference in spectral lines generates a distinct molecular characteristic, referred to as spectroscopic "fingerprint", which allows for the identification, and possibly quantification, of various chemical compounds within a mixture via IR spectroscopy applications.

#### 4.1.1 Radiative Transfer Equation

This section provides the details of the non-scattering radiative transfer equation (RTE). Figure 4.2 shows the schematic of a spectroscopic measurement of the IR irradiation emitted from both background and flare plume sources and their interactions within the plume. The influence of absorption and emission along the atmospheric layer between the flare and the camera aperture is excluded from the present analysis. This effect can be accounted for by examining a “background” pixel at a similar distance from the camera as the flare plume, e.g., the flare stack, in combination with the signal measured by the “transparent” channel. Assuming negligible molecular gas scattering at mid-infrared wavelengths over the measurement pathlengths, the spectral intensity incident on the camera aperture at wavenumber  $\eta$  is expressed by

$$I_{\eta,L} = I_{\eta,bg} \exp\left[-\int_0^L \kappa_{\eta,mix}(s) ds\right] + \int_0^L \kappa_{\eta,mix}(s) I_{\eta,B}[T(s)] \exp\left[-\int_s^L \kappa_{\eta,mix}(s') ds'\right] ds \quad (4.2)$$

where  $I_{\eta,bg}$  is the background irradiation,  $I_{\eta,b}$  is the spectral blackbody emission,  $L$  is the plume thickness,  $\kappa_{\eta,mix}$  is the absorption coefficient of the gas mixture and  $T(s)$  is the plume temperature at a parametric location  $s$  along the pixel LOS.

The absorption coefficient of the gas mixture is the sum of the absorption coefficients of all participating species at location  $s$  along the pixel LOS, driven by the sum of the absorption coefficients of all participating species at the same location

$$\kappa_{\eta,mix}(s) = \sum_m C_{\eta,abs,m}[T(s)] N_m(s) \quad (4.3)$$

where  $N_m$  and  $C_{\eta,abs,m}$  are the local number density, derived along the corresponding pixel LOS at location  $s$ , and the molecular spectral absorption cross-section of the  $m$ th component inside the plume, respectively. The spectral absorption cross-section can be computed as a function of the local temperature using parameters obtained from the HITRAN database [93].

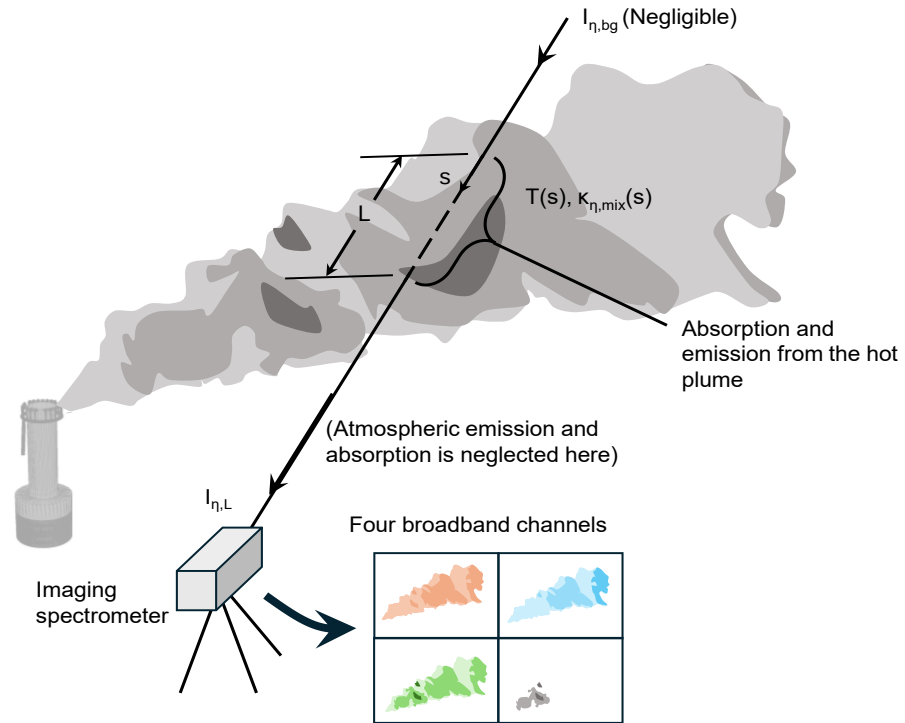


Figure 4.2 Schematic of a four-channel VISR radiometric measurement.

#### 4.1.2 Spectral Absorption Coefficient

The spectral absorption coefficient is proportional to the probability of a photon encountering a molecule along the optical path having a quantum transition that matches the photon's energy. In principle, the spectral absorption coefficient should thus be represented by a series of infinitesimally thin vertical lines at the specific wavenumbers corresponding to possible transitions between quantized energy levels. However, in reality, various phenomena cause the spectral lines to broaden, as shown in Figure 4.3. The broadened line structure is defined by the line intensity,  $S_{ij}$ , the line width, along with the line shape; these parameters relate the spectral absorption coefficient with the temperature and concentration of the gas species.

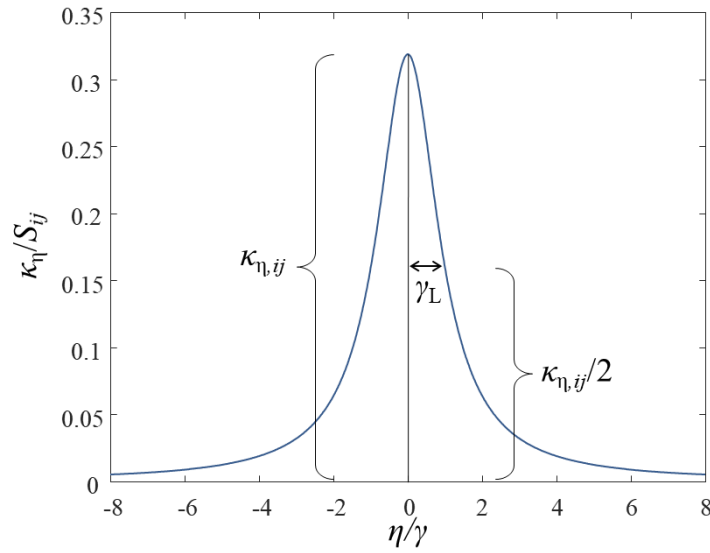


Figure 4.3 Lorentz line profile. Adapted from Ref. [92].

The broadening mechanisms are natural broadening, Doppler broadening, Stark broadening, and collision broadening. In most molecular gases, broadening is dominated by collision and Doppler broadening.

Collision broadening is caused by the varying repulsive or attractive forces between colliding molecules, which change the energies required to transition from one energy state to another. Collisions between neutrally-charged particles result in a Lorentzian line shape, expressed by

$$\frac{\kappa_{\eta,ij}}{S_{ij}} = \frac{\gamma_L/\pi}{\gamma_L^2 + (\eta - \eta_{ij})^2} \cdot \frac{\chi P}{k_B T} \quad (4.4)$$

where  $S_{ij}$  is the line intensity, which is the area under the line profile, and  $\gamma$  is the line half-width at half maximum (HWHM), as shown in Figure 4.3. The half-width is determined by the collision rate, which depends on the pressure and molecule absorption cross-section. To obtain accurate results, for gas mixtures, in addition to common collisions between molecules of the species-of-interest, referred to as self-broadening, interactions of other species' molecules should also be considered.

On the other hand, Doppler broadening is caused due the velocity differences associated with the thermal energy of the gas molecules, which alters the photon wavenumber, known as “red shift”, depending on the velocity of the molecule relative to the observer, which subsequently depends on the gas temperature. Since the velocity of the molecules obeys a Maxwell-Boltzmann distribution, the effect of Doppler broadening can be considered as a Gaussian line shape. Under the typical conditions within the flare plume, the impact of Doppler broadening is negligible compared to collision broadening. Figure 4.4 shows the Gaussian line shape generated by the Doppler broadening in comparison to the Lorentz line shape profile due to collision broadening.

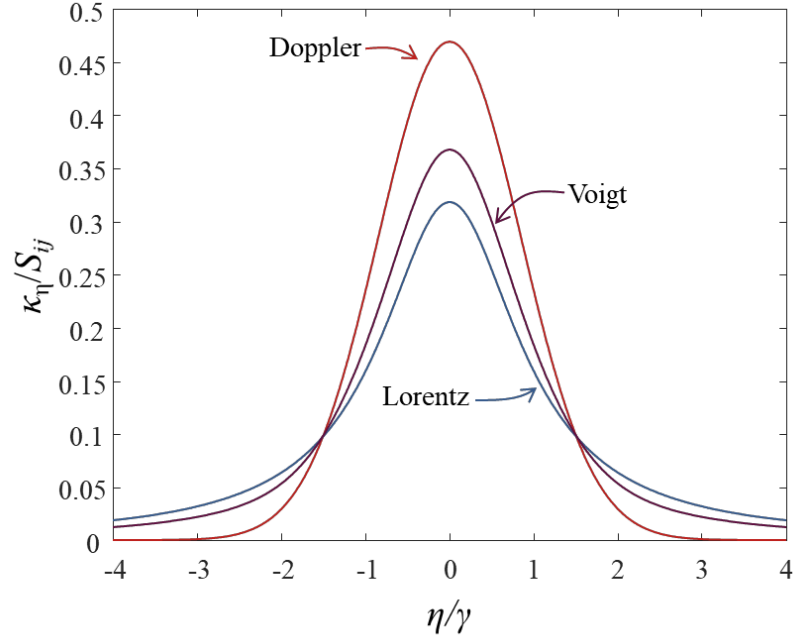


Figure 4.4 Doppler, Lorentz, and Voigt lineshape for the same HWHM and line strength. Adapted from Ref. [92].

Finally, the Voigt lineshape accounts for the effects of both collision (Lorentzian lineshape,  $f_L$ ) and the Doppler (Gaussian lineshape,  $f_D$ ) broadening. Figure 4.4 shows a Voigt profile assuming equal HWHM for the Gaussian and Lorentz profiles. The Voigt lineshape is typically used for high-pressure combustion applications where due to relatively higher pressure and temperature conditions, the effects of Doppler broadening cannot be ignored. The Voigt lineshape can be implemented according to the following expression provided by Gharavi and Buckley [94]

$$f_v = \sigma_0 \left\{ (1 - x_v) \exp(-0.693 y_v^2) + \frac{x_v}{1 + y_v^2} + 0.016(1 - x_v) x_v \left[ \exp(-0.084 y_v^{2.25}) - \frac{1}{1 + 0.0210 y_v^{2.25}} \right] \right\} \quad (4.5)$$

where  $x_v = \gamma_L/\gamma_v$  is the ratio between Lorentz lineshape HWHM and Voigt lineshape HWHM, denoted by  $y_v = |\eta - \eta_{ij}|/\gamma_v$ . The Voigt lineshape HWHM can be obtained from the following expression

$$\gamma_v = 0.5346\gamma_L + \left(0.2166\gamma_L^2 + \gamma_D^2\right)^{0.5} \quad (4.6)$$

where  $\gamma_D$  is Doppler lineshape HWHM. The normalized center line strength in Eq. (4.5) is given by

$$\sigma_0 = \frac{1}{2\gamma_v \left(1.065 + 0.447x_v + 0.058x_v^2\right)} \quad (4.7)$$

The parameters required for calculating the absorption coefficients of  $\text{CH}_4$ ,  $\text{CO}_2$ ,  $\text{CO}$ , and  $\text{H}_2\text{O}$ , including line intensity, lineshape HWHM, and line position, are available in the HITRAN database [93]. Each line is generated independently, and the gas spectral absorption coefficient is computed as the summation of the absorption coefficients of each spectral line. This approach, as demonstrated in Figure 4.5, is known as the line-by-line (LBL) and can be expressed via

$$\kappa_{\eta,m} = \sum_{ij} \kappa_{\eta,ij} \quad (4.8)$$

in which the transition-specific absorption coefficient can be denoted by

$$\kappa_{\eta,ij}(s) = S_{ij} [T(s)] f_v [\eta, \eta_{ij}, T(s), p] \frac{\chi(s) p}{k_B T(s)} \quad (4.9)$$

where  $S_{ij}$  and  $k_B$  are the spectral line intensity of the  $ij^{\text{th}}$  transition ( $\text{cm}^{-1}/(\text{molecules} \cdot \text{cm}^{-2})$ ) and the Boltzmann constant, respectively.

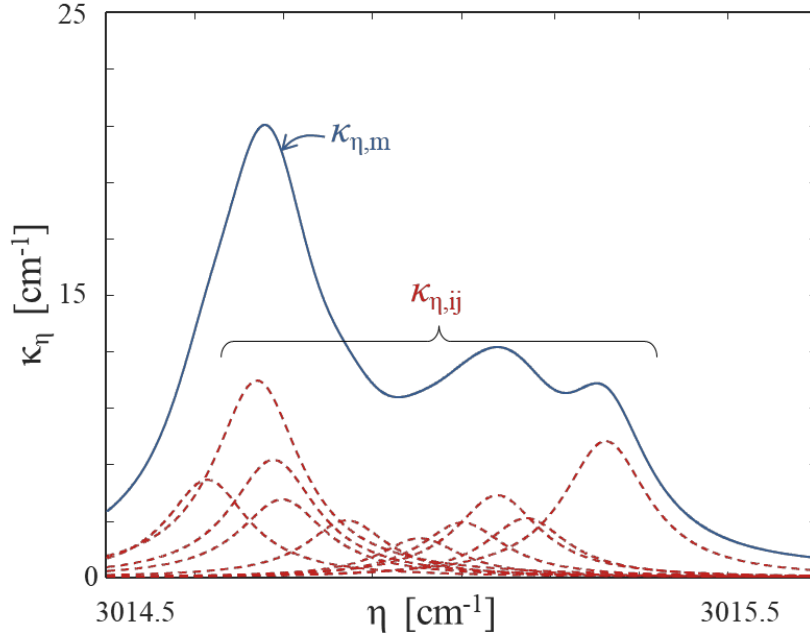


Figure 4.5 CH<sub>4</sub> absorption lines and absorption coefficient. Adapted from Ref. [92].

In this work, lookup tables for the gas absorption coefficient, obtained based on the LBL model, were created for each species as a function of wavenumber, temperature, volume fraction, and pressure, in order to make the computational procedure more convenient and less time-consuming,

Different species in a gas mixture can absorb and emit simultaneously over the same spectral region. Since the spectra of distinct species and their absorption coefficients can be modelled independently, the spectral absorption coefficient of a mixture may be expressed as the summation of distinct species absorption coefficient at any given wavenumber,  $\eta$ ,

$$\kappa_{\eta,mix} = \sum_{m=1}^N \kappa_{\eta,m} \quad (4.10)$$

where  $\kappa_{\eta,m}$  and  $\kappa_{\eta,mix}$  are the absorption coefficient of arbitrary species  $m$  and the gas mixture, with a total of  $N$  participating species. This assumption means that the collision broadening between two species in the gas mixture is approximated as collisions between one species and air. Although recent

updates on the HITRAN database contain collision broadening caused by  $\text{H}_2\text{O}$  for different species [93], this effect is expected to be small and is excluded from this analysis. The used lookup tables approach is only possible, assuming that the gas mixture absorption coefficient is the sum of individual species' absorption coefficients. Knowledge of the gas state makes it straightforward to obtain the gas mixture's absorption coefficient, which is required to model the spectral irradiation incident on the optical instrument aperture.

## 4.2 VISR Broadband Multispectral Radiometric Model

The incident intensity entering the camera aperture along each pixel LOS is spectrally integrated, e.g., by capturing the scene through a series of spectral broadband filters and then imaging it onto an IR sensor. Assuming idealized “top hat” filters that are perfectly transparent over the corresponding detection spectrum, the signal of the  $k$ th channel for the  $j$ th pixel is given by

$$S_{k,j}^{\text{exact}} = C_{cal,k} \int_{\Delta\eta_k} I_{\eta,L} d\eta \quad (4.11)$$

where  $C_{cal,k}$  is a calibration constant that accounts for the detector sensitivity, pixel spatial resolution, integration time, and pixel solid angle, and  $I_{\eta}$  is the spectral intensity, obtained by applying Eq. (4.2) to the  $j$ th pixel LOS. In this work, calibration constants are assumed to be perfectly known and taken as unity.

Following the descriptions provided by Zeng et al. [95], the selected spectral channels are broadly aligned with spectral absorption features of  $\text{CH}_4$  (Channel 1, 3.2–3.4  $\mu\text{m}$ ),  $\text{CO}_2$  (Channel 2, 4.2–4.4  $\mu\text{m}$ ), and  $\text{CO}$  (Channel 3, 4.5–4.9  $\mu\text{m}$ ), while the fourth transparent channel is excluded from the analysis. Note that the chosen broadband windows in this study are slightly narrower than the ones originally proposed by Zeng et al. [48] solely for computational efficiency purposes. Figure 4.6 Incident intensity spectrum along the line-of-sight of a sample pixel, along with the filter windows used to generate the measurement channels. Spectral lines (normalized for each species) are plotted at the top. shows a simulated emission spectrum made using the CFD-simulated flare plume described in the next section and the alignment of the bandpass filters. The VISR method, as defined by Zeng et al. [95], assumes that the flare fuel is composed entirely of  $\text{CH}_4$ , which may seem to be reasonable for upstream flaring cases but is less certain in other flaring scenarios, such as petrochemical refining. Figure 4.6 Incident intensity spectrum along the line-of-sight of a sample pixel, along with the filter windows used

to generate the measurement channels. Spectral lines (normalized for each species) are plotted at the top. also reveals very few H<sub>2</sub>O lines over the detection spectrum, which is a key attribute of MWIR imaging. While one would expect a stronger HC signal in the LWIR, the presence of overlapping H<sub>2</sub>O and HC lines would be far more challenging to detangle, particularly when using an instrument having limited spectral resolution.

Computing the governing equations of the VISR radiometric model, defined by Eqs. (4.2), (4.3) and (4.11), can be extremely computationally demanding and complex to be inverted directly for the unknown temperature and species column densities needed to compute the local CE, particularly if the goal is to provide near real-time feedback on flare performance. To this end, Zeng et al. [48] developed an explicit formula for the local CE by assuming: (i) a uniform temperature profile along each pixel LOS (isothermal medium); (ii) an optically thin plume medium (i.e., no self-absorption); (iii) the  $k$ th channel intensity only corresponds to contributions from the corresponding  $k$ th carbon-containing species spectral absorption features; and (iv) negligible background intensity. Following these assumptions, Eq. (4.2) may be rearranged into

$$I_{\eta} \approx I_{\eta,B}(T) \tau_{\eta,L}(T) \quad (4.12)$$

where the optical thickness,  $\tau_{\eta,L}$ , is defined according to the Beer-Lambert law,

$$\tau_{\eta,L}(T) = \frac{1}{L} \int_0^L \kappa_{\eta,k} s \, ds = \frac{1}{L} \int_0^L \alpha_{\eta,k}(T) s \, ds = \alpha_{\eta,k}(T) \sigma_k \quad (4.13)$$

Substituting Eq. (4.13) into Eq. (4.12) yields the final expression for the VISR spectral intensity

$$I_{\eta} \approx I_{\eta,B}(T) \alpha_{\eta,k}(T) \sigma_k \quad (4.14)$$

By approximating the blackbody intensity as spectrally-uniform over each filter window, the broadband pixel intensity (pixel brightness) for the  $k$ th channel of the  $j$ th pixel is expressed by

$$S_{k,j} \approx C_k \Delta \eta_k \left\langle I_{\eta_k,b}(T_j) \alpha_{\eta,k}(T_j) \right\rangle_{\eta_k} \sigma_{k,j} \quad (4.15)$$

Rearranging for the species column density and substituting the result into local CE, Eq. (2.9), yields

$$CE_{local,j} \approx \frac{S_{CO_2,j} / \left[ C_{CO_2} \Delta \eta_{CO_2} \left\langle I_{\eta_{CO_2},b}(T_j) \alpha_{\eta,CO_2}(T) \right\rangle_{\eta_{CO_2}} / n_{C,CO_2} \right]}{\sum_{k=1}^3 S_{k,j} / \left[ C_k \Delta \eta_k \left\langle I_{\eta_k,b}(T_j) \alpha_{\eta,k}(T) \right\rangle_{\eta_k} / n_{C,k} \right]} \quad (4.16)$$

where the effective pixel plume temperature,  $T_j$ , influences the flare CE estimates through both the absorption line strengths in  $\alpha_{\eta,k}$ , and the ratio of blackbody intensities of the spectral channels.

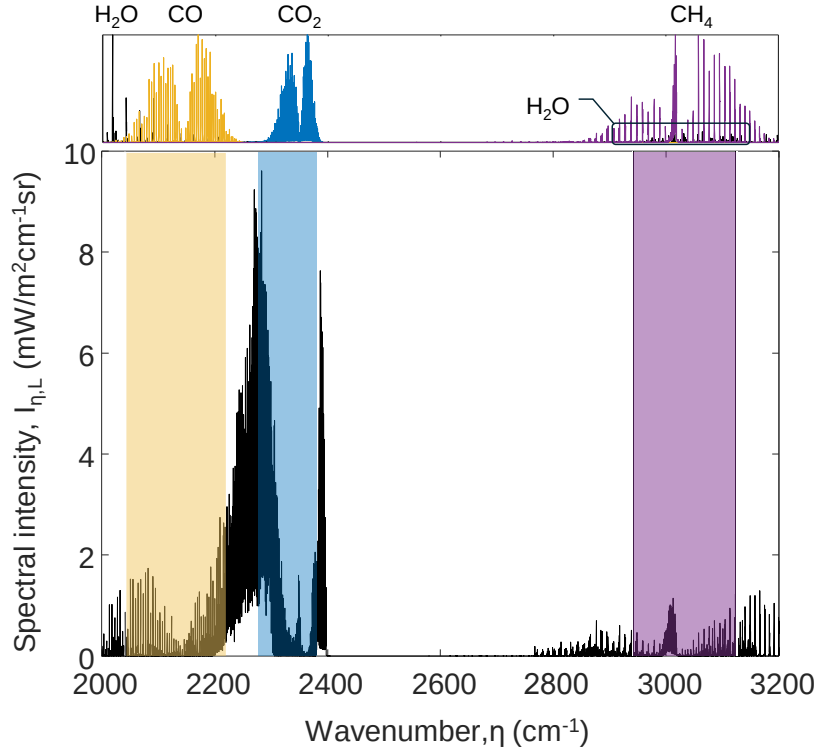


Figure 4.6 Incident intensity spectrum along the line-of-sight of a sample pixel, along with the filter windows used to generate the measurement channels. Spectral lines (normalized for each species) are plotted at the top.

#### 4.2.1 Global CE Inference Model

Finally, the inferred local (pixel-wise) CE values are averaged over the VISR region-of-interest (ROI), having an inner surface defined by the outer boundary of the flame envelope and an outer surface limited to the region where the observed spectral signal is detectable, above the camera noise threshold (NESR). In other words,

$$CE_{\text{VISR}} = \frac{1}{N_{\text{ROI}}} \sum_{j=1}^{N_{\text{ROI}}} CE_j = \sum_{j=1}^{N_{\text{ROI}}} \left( \frac{n_{\text{C,CO}_2} \sigma_{\text{CO}_2,j}}{\sum_k n_{\text{C,k}} \sigma_{k,j}} \right) \quad (4.17)$$

According to Zeng et al. [38], the inner region may also be approximated by an isotherm surrounding the visible flame boundary. The VISR region-of-interest (ROI) is bound within these two surfaces, as shown conceptually in Figure 4.7.

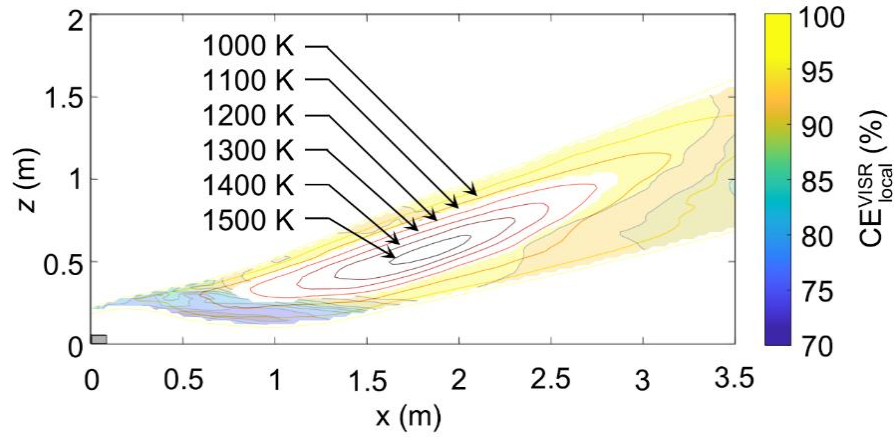


Figure 4.7 The VISR ROI is comprised of pixels outside the flame envelope. Isotherms are taken along the plume centerline. The flame envelope, shown as the white region within the VISR ROI, can be approximated by an isotherm confining the visible flame [38,48]. The vent gas exits the burner at the plane  $z = 0.14$  m from a jet centered on (0,0) in the (x, y) plane.

### 4.3 Simulated VISR Broadband Measurement

The performance of the VISR technique is assessed through a series of simulated broadband measurements using CFD-LES data of a steam-assisted flare operating in a crosswind. The CFD-LES simulations aim to replicate the experimental trials of flaring 100% Tulsa natural gas (TNG), conducted by Clean Air Engineering [80] on the John Zink SKEC<sup>®</sup> steam-assisted flare [14]. The CFD-LES simulations are based on tests conducted at the John Zink test facility as part of the Marathon Petroleum Company's Flare Consent Decree [80]. In these simulations, the flare stack has an outer diameter and height of 0.128 m and 0.5 m, respectively, and is terminated with a John Zink SKEC<sup>®</sup> flare tip [14]. The flare tip, shown in Figure 4.8, consists of eight arms with a steam jet exiting from each arm. The vent gas exits the burner from a central jet. The low vent gas flow rate, 7.6 g/s, used in all simulations represents a high turndown condition, the normal operating condition in a refinery unless waste gas must be flared. Injected natural gas (TNG), composed of 95% methane, 4.5% ethane, and 0.5% propane by volume, exits the flare tip with a velocity of 1.2 m/s at 298 K and reacts with a crosswind with uniform velocity. Table 4.1 summarizes the crosswind and steam-assist rates and the associated net heating value of the combustion zone ( $NHV_{cz}$ ) considered in this analysis. These cases are a subset of



Figure 4.8 John Zink SKEC<sup>®</sup> flare tip. Adapted from Ref. [97].

20 cases within the two-dimensional design space defined by the range of crosswind velocities (measured = 0.22-6.8 (m/s), design space = 0-8 m/s) and steam-assist flow rates (measured = 13.9-145 g/s, design space = 0-200 g/s) experienced during a four-day testing period of the SKEC<sup>®</sup> burner. Four of these cases were selected for spectroscopic analysis.

The one parameter that was tested outside of “normal” operating ranges was the steam-assist flow rate. Of the four cases listed in Table 4.1, only Cases 1 and 2 are in the range that conforms to a  $NHV_{cz} \geq 270$  BTU/scf ( $\sim 10$  MJ/sm<sup>3</sup>), which is required by the US Environmental Protection Agency (EPA) for proper operation of a flare [96]. Cases 3 and 4 illustrate what happens to combustion efficiency if the flare is over-steamed.

The governing transport equations are solved using the Uintah-Arches LES solver [97], which incorporates a two-step modelling strategy for the turbulent CH<sub>4</sub> combustion based on the rate-controlled constrained equilibrium (RCCE) method [98,99]: a slow step utilizing the Westbrook and Dryer single-step mechanism [100] that is computed using LES-filtered quantities, and an infinitely fast step at the LES sub-grid scale that yields chemical equilibrium. The combustion module also includes the Dryer and Glassman reduced-order model [101] to account for nonequilibrium CO oxidation kinetics. Radiative heat transfer is modelled using the discrete ordinates method (DOM) with S<sub>2</sub> quadrature [102]. To initiate the combustion reactions, the simulation uses a pilot ignition source at the exit plane of the flare tip where the fuel enters the computational domain.

The CFD-LES cases are summarized in Table 4.1. Each domain is discretized into  $8 \times 8 \times 8$  mm<sup>3</sup> cube elements. The computational domain for all four cases extends from  $x$  (downwind direction) = - 0.5 m to varying lengths (determined by the length/direction of the flare plume),  $y$  (crosswise direction) = varying widths centered on 0 m (wide enough to encompass reaction zone),  $z$  (vertical direction) = - 0.5 m to varying lengths (depending on the length/direction of the plume). In Figure 4.7 and subsequent

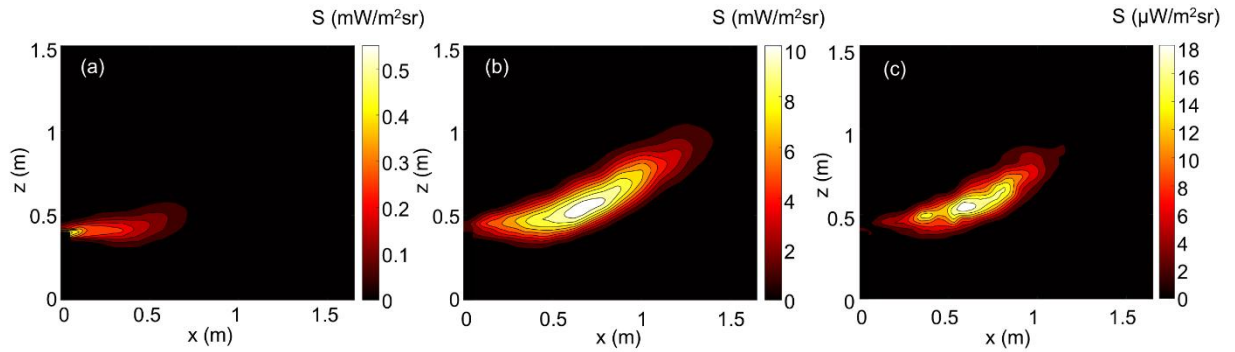


Figure 4.9 Exact time-averaged broadband images of the VISR camera for Case 2, illustrated for spectral channels corresponding to: (a) CH<sub>4</sub> (3.2-3.4  $\mu\text{m}$ ), (b) CO<sub>2</sub> (4.2-4.4  $\mu\text{m}$ ), and (c) CO (4.5-4.9  $\mu\text{m}$ ).

figures, the vent gas exits the flare tip at  $z = 0.14$  m centered around point (0,0) in  $x$ - $y$  space. To fully capture the transient behaviour of the plume, the CFD-LES cases were run for a minimum of 10 s of simulation time with timesteps on the order of  $10^{-5}$  (s). For additional information regarding the CFD-LES configurations, including images of the simulated temperature, velocity, and species concentration field, refer to Appendix A, CFD-LES Supplementary Information.

Table 4.1: CFD-LES simulation case studies.

| Case | Crosswind uniform velocity at 298 K (m/s) | Assist steam mass flow rate at 373 K (g/s) | Total number of cubic elements | CFD-LES domain size ( $\text{m} \times \text{m} \times \text{m}$ ) | NHV <sub>cv</sub> (MJ/sm <sup>3</sup> )* |
|------|-------------------------------------------|--------------------------------------------|--------------------------------|--------------------------------------------------------------------|------------------------------------------|
| 1    | 2.2352                                    | 16.38                                      | 37,687,500                     | $4.0 \times 1.8 \times 2.68$                                       | 11.18                                    |
| 2    | 4.2448                                    | 10.694                                     | 23,500,400                     | $3.92 \times 1.76 \times 1.75$                                     | 14.61                                    |
| 3    | 5.0232                                    | 70.539                                     | 11,704,000                     | $3.04 \times 1.12 \times 1.76$                                     | 3.47                                     |
| 4    | 6.174                                     | 160.8                                      | 7,087,500                      | $2.0 \times 1.08 \times 1.68$                                      | 1.60                                     |

The simulated temperature and species concentration profiles are substituted into Eq. (4.2) to generate spectral intensity, which is then transformed into vectors of the exact broadband data,  $\mathbf{b}^{\text{exact}} =$

\* sm<sup>3</sup> = standard cubic meters

$[S_1^{\text{exact}}, S_2^{\text{exact}}, S_3^{\text{exact}}]$  via Eq. (4.11). Figure 4.9 shows simulated time-averaged broadband intensity images of the three VISR-specified spectral channels corresponding to Case 2.

Finally, the simulated broadband intensities are contaminated with artificial white noise sampled from an unbiased Gaussian distribution derived from a noise equivalent temperature difference (NETD) of 0.035 (m.K), typical of the SOC750 used by Zeng et al. [38] for VISR

$$\mathbf{b}^{\text{meas}} = \mathbf{b}^{\text{exact}} + \delta\mathbf{b}^{\text{noise}}, \quad \delta\mathbf{b}^{\text{noise}} \sim \mathcal{N}(0, \Gamma_{\text{NETD}}) \quad (4.18)$$

Crucially, the NETD defines the outer detection envelope and limits the camera's ability to resolve pixels containing unoxidized fuel that has been aerodynamically stripped from the combustion zone and carried downwind of the flare stack.

In their experimental analysis, Zeng et al. [38] temporally averaged 325 data cubes to reduce the number of data sets that would need to be processed analytically, although this also improved the signal-to-noise (S/N) ratio. We explore this effect by averaging temporally resolved synthetic images over approximately five seconds, resulting in an extended region of detected intensity across all the VISR spectral bins.

A noise threshold is introduced to the simulated broadband images, based on the overall net equivalent spectral radiance (NESR) value. The implemented noise threshold filters out the pixels with a S/N ratio below 0.05, depicted by the white region in Figure 4.10 Synthetic time-averaged broadband images corresponding to the spectral bins of the VISR camera for Case 2: (a) CH<sub>4</sub> (3.2–3.4  $\mu\text{m}$ ), (b) CO<sub>2</sub> (4.2–4.4  $\mu\text{m}$ ), and (c) CO (4.5–4.9  $\mu\text{m}$ ). The white region represents pixels with undetectable signals reaching over the noise threshold/ below the NESR value.. This effect is most pronounced for the CH<sub>4</sub> and CO channels at high and low flare CE, respectively, since these scenarios coincide with the lowest abundance, temperature, and concentrations of those species in the flare plume. In principle,

the finite dynamic range of the camera likely means that some pixels in the combustion zone may also be saturated, although this effect is not considered here.

Finally, while the CFD simulations have been validated against experimental measurements conducted within a wind tunnel [97], it is important to note that the veracity of the CFD measurements is not crucial to this procedure. This is because both the local and global combustion efficiencies and the radiance measured by the camera are obtained from the same CFD data that acts as a “ground truth”. This is a key advantage of conducting measurements *in silico*, versus experimental validation procedures that can be confounded by unavoidable artifacts, including, e.g., the location of the gas sampler (hood).

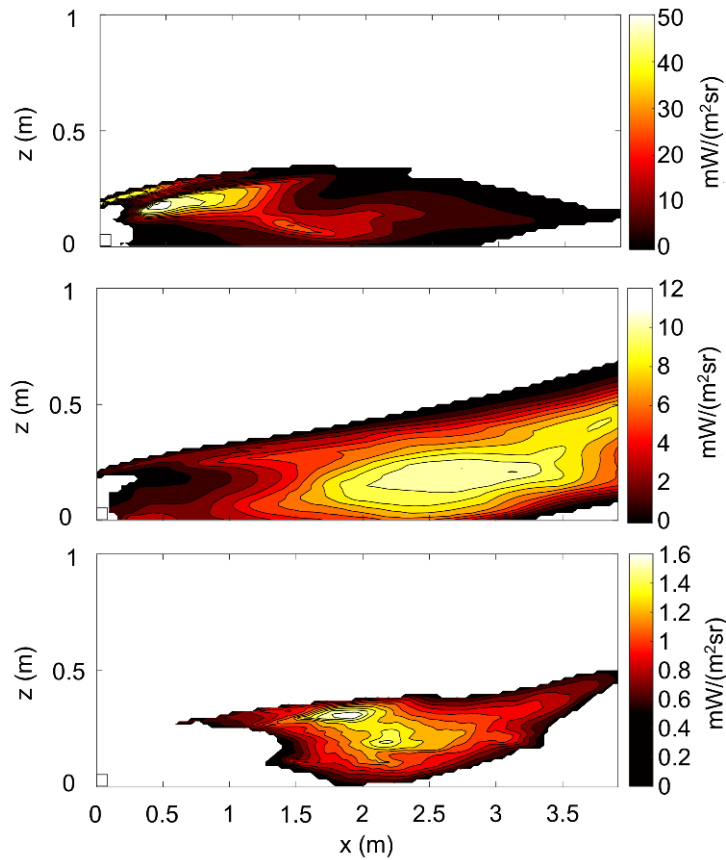


Figure 4.10 Synthetic time-averaged broadband images corresponding to the spectral bins of the VISR camera for Case 2: (a)  $\text{CH}_4$  (3.2–3.4  $\mu\text{m}$ ), (b)  $\text{CO}_2$  (4.2–4.4  $\mu\text{m}$ ), and (c)  $\text{CO}$  (4.5–4.9  $\mu\text{m}$ ). The white region represents pixels with undetectable signals reaching over the noise threshold/ below the NESR value.

## Chapter 5

### Results and Discussion<sup>\*</sup>

This chapter provides an assessment of the veracity of the simplified VISR method, presented in Chapter 4, for remote flare CE quantification applications. The presented numerical assessment utilizes the simulated temperature and species concentration datasets of the CFD-LES cases, discussed in Table 4.1, to analyze the performance of the VISR method in three distinct categories.

The first section discusses the evaluation of the VISR-inferred local CE, particularly for pixels located within the VISR ROI, and investigates the potential causes of discrepancy between estimated and ground truth (CFD-driven) local CE, primarily the optically-thin and isothermal plume approximations applied in the VISR radiometric model, as discussed in Section 4.2, for pixels within the VISR ROI. The second section provides an assessment of the veracity of the VISR flare CE inference model, discussed in Section 4.2.1, which infers flare CE as the average VISR local CE estimates of the pixels within the ROI. This is followed by a section on the last aspect of VISR method assessment, the capabilities and limitation of VISR imaging instrument for detection of unburned (cold) methane downwind of the flare plume and its potential impact on VISR flare CE estimates.

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<sup>\*</sup> This chapter is adapted from the following Ref:

Kaveh, A., Spinti, J., Lapeyre, P., Bonarens, M., & Daun, K. J. (2025). Viability of video imaging spectro-radiometry (VISR) for quantifying flare combustion efficiency. *Journal of the Air & Waste Management Association*. <https://doi.org/10.1080/10962247.2025.2495026>

## 5.1 Veracity of Inferred Local CE

We first investigate the impact of the optically thin and uniform temperature assumptions made to transform the non-scattering RTE, Eq. (4.2), into local (pixel-wise) CE estimates using the VISR radiometric model, Eq. (4.15). Figure 5.1 shows sample 2D contours of the VISR-inferred and ground-truth local CE for simulation Case 1 (see Table 4.1), the latter obtained by substituting LES-computed species column number densities into Eq. (2.9). Figure 5.1 also shows the relative error (RE) associated with the inferred local CE quantities for pixels within the VISR ROI at an arbitrary timestep. Figure 5.3 plots the relative error in the local CE as a function of the VISR-inferred estimate for all pixels and all timesteps within the VISR ROI. For pixels within the ROI, the VISR-inferred local CE values are typically within 3% of the true values across all simulation cases, although the errors are significantly higher within the visible flame region. Figure 5.3 shows that, in general, the relative error for pixels having higher local CE tends to be lower, which one would expect given that these pixels correspond to low  $\text{CH}_4$  column densities and are thus inherently insensitive to any uncertainty in the column density ratio estimation.

A key advantage of using CFD data is the ability to distinguish between the influence of the two underlying RTE simplifications on the model error. First, we consider the impact of the optically thin approximation, which assumes negligible self-absorption across gas species within the plume, by comparing the ground-truth broadband intensities, Eq. (4.11), obtained with and without considering the self-absorption term in the non-scattering RTE, Eq. (4.2). Figure 5.2 shows the RE associated with the optically thin approximation for pixels residing inside the VISR ROI over all three spectral bands at an arbitrary timestep for Case 1 (see Table 4.1). Generally, the observed intensity RE values for pixels within the VISR ROI may be as large as 10%, particularly in the case of the broadband channel representing methane in the vicinity of the flare exhaust, suggesting that modelling spectral intensity

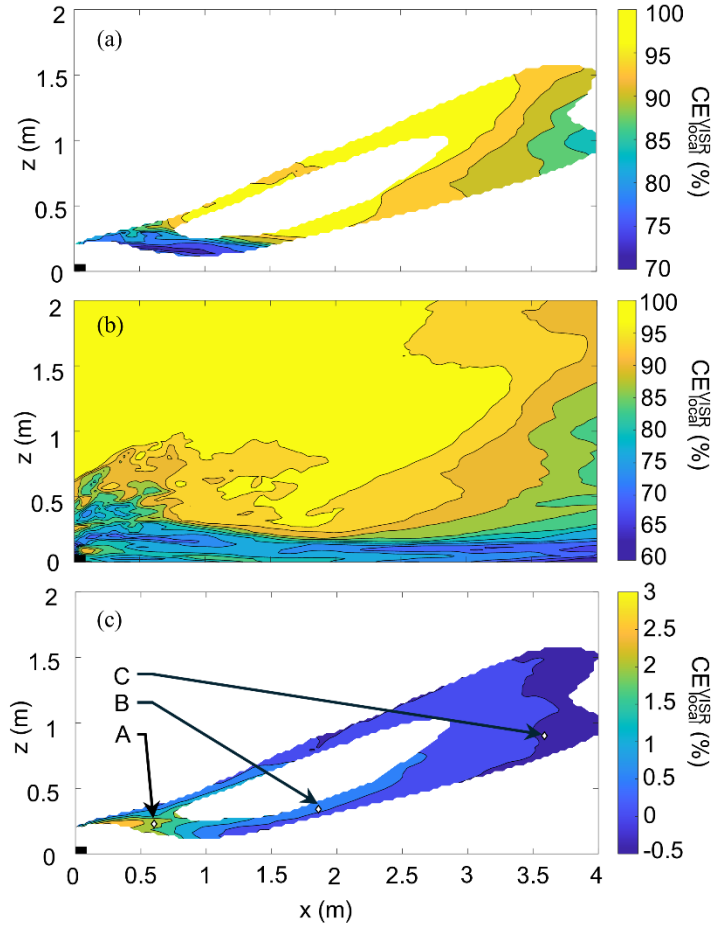


Figure 5.1 Sample 2D contours of: (a) VISR-inferred local CE, (b) ground-truth local CE and (c) relative error associated with VISR-inferred local CE for Case 1 at an arbitrary timestep. Points A, B, and C correspond to profiles shown in Figure 5.7.

as optically thin should be applied cautiously to this segment of the image. Additionally, for the other two broadband channels representing CO and CO<sub>2</sub>, negligible bias, up to 3% intensity RE, was reported across all 4 CFD-LES cases, shown in Table 4.1, showing the assumed optically-thin plume approximation for these channels to be reasonable.

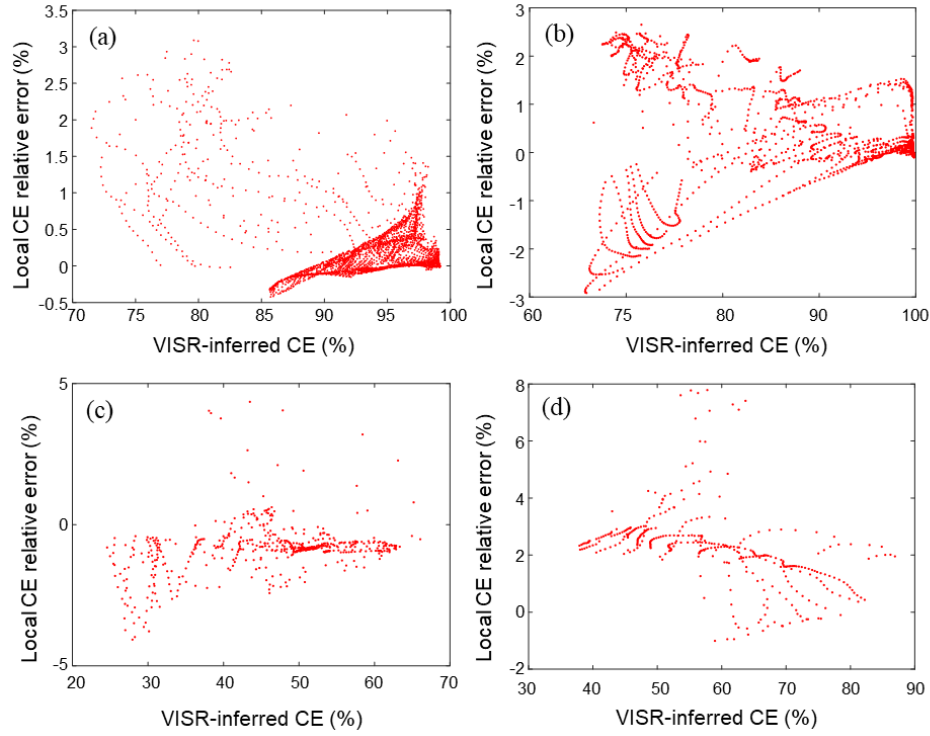


Figure 5.3 Correlation between inferred local CE using the VISR technique and its corresponding relative error for the pixels located within the VISR ROI for (a) Case 1, (b) Case 2, (c) Case 3, and (d) Case 4.

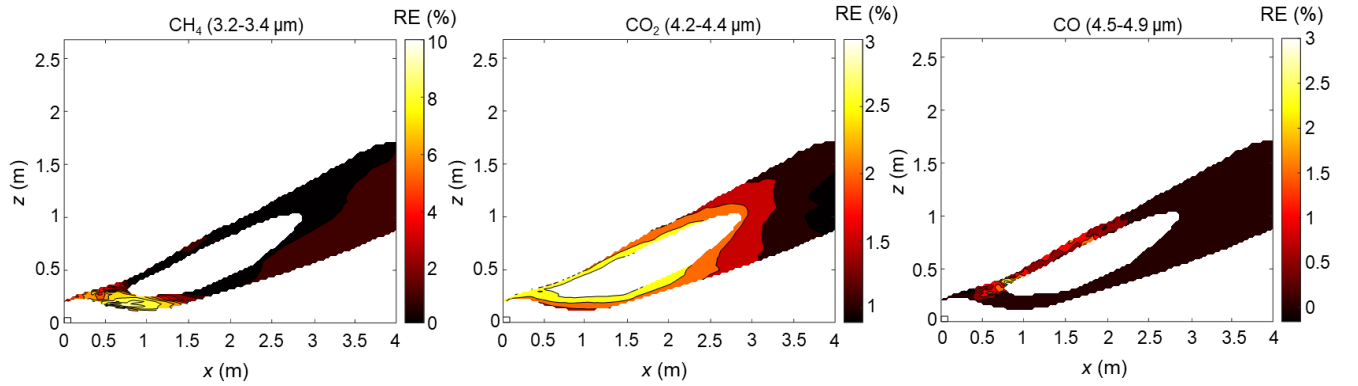


Figure 5.2 Simulated broadband intensity relative error (RE) associated with the “optically-thin” plume approximation, Eq. (4.11) excluding the self-absorption term in the non-scattering RTE, Eq. (4.2), demonstrated for the pixels located within the VISR ROI at an arbitrary time step for CFD-LES Case 1, presented in Table 4.1.

Secondly, due to the turbulent nature of the flare plume, the isothermal plume simplification, assuming a uniform temperature profile along each pixel's LOS inside the VISR ROI within the plume region, can have a potentially much larger impact on the accuracy of the modelled VISR broadband images. Figure 5.4 shows the temperature and species concentration profiles along the LOS of three sample pixels, identified in Figure 5.1 (c), paired with the corresponding RE between the true and predicted values. According to this figure, in contrast to the underlying isothermal plume assumption, the gas temperature profile along the plume resembles a Gaussian distribution, where it reaches the peak temperature within the combustion zone and cools down closer to the atmospheric temperature near the ends. Therefore, one would expect large temperature and species concentration variations along the LOS of pixels located within the visible flame domain, which contains both combustion products and unburned reactants, resulting in significant discrepancies from the uniform distribution assumption. Figure 5.5 shows the sample broadband intensity RE associated with the isothermal plume assumption for pixels located within the VISR ROI, for simulation Case 1, presented in Table 4.1. Generally, broadband intensity RE values of less than 2% were observed downstream of the flare plume across all simulation cases, presented in Table 4.1, showing reasonable agreement with the isothermal plume assumption, suggesting a sufficiently well-mixed gas plume downwind of the flare stack. Additionally, for pixels within the VISR ROI closer to the combustion zone, where there are more pronounced gradients in temperature and species concentration, the broadband intensity RE approaches closer to 20%, particularly for the broadband channel representing CO<sub>2</sub>.

Overall, despite the discrepancies reported above, a comparison between the VISR-inferred and CFD ground-truth local CE supports the RTE simplifications applied to the VISR radiometric model, for the pixels contained within the flame envelope.

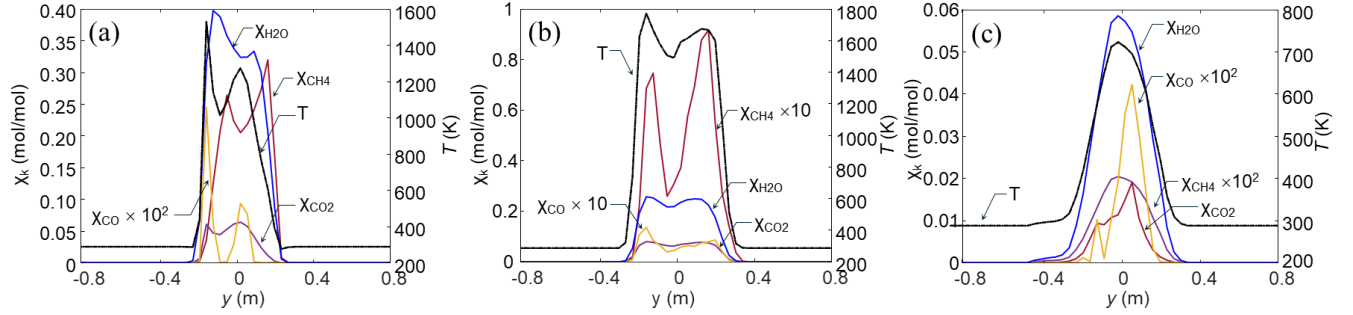


Figure 5.4 Plume gas mixture temperature and carbon-containing species concentration profiles along the LOS for sample pixels (a) “A”, (b) “B”, and (c) “C” shown in Figure 5.1 (c). The relative differences between the true and VISR-predicted CEs are 2.2%, 0.59%, and -0.08%, respectively.

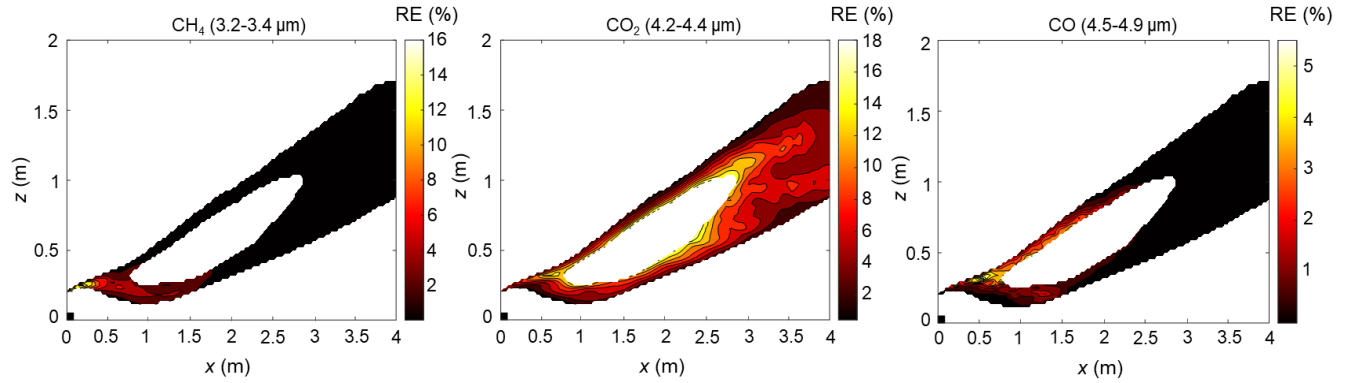


Figure 5.5 Simulated broadband intensity relative error (RE) associated with the isothermal plume approximation, uniform plume temperature distribution along each pixel LOS, demonstrated for the pixels located within the VISR ROI at an arbitrary time step for CFD-LES case 1, presented in Table 4.1.

## 5.2 Viability of the Global CE Estimates

Zeng et al. [38,48], propose that the global CE may be estimated from the local CE by averaging the local CE of the pixels within the VISR ROI. This definition differs from Eq. (2.7), which is based on the total mass flow rates of the species crossing a control volume leaving the flare plume. Specifically, Eq. (2.7) may be written as

$$CE = \frac{\oint_{CV} \sigma_{C,CO_2} \mathbf{u} \cdot \hat{\mathbf{n}} ds}{\sum_k \oint_{CV} n_{C,k} \sigma_{C,k} \mathbf{u} \cdot \hat{\mathbf{n}} ds} = \frac{\oint_{CV} \sigma_{C,CO_2} \mathbf{u} \cdot \hat{\mathbf{n}} ds}{\oint_{CV} \sum_k n_{C,k} \sigma_{C,k} \mathbf{u} \cdot \hat{\mathbf{n}} ds} \quad (5.1)$$

where  $ds$  is an infinitesimal arc length along the ROI boundary, and  $\mathbf{u}$  and  $\hat{\mathbf{n}}$  are the local mass-weighted velocity and unit normal vector, respectively. The summation in the denominator of Eq. (5.1) may be incorporated into the integral since all species have the same projected velocity at a given plume location. The integrals in Eq. (5.1) may be approximated by the summation of pixels located along the boundary,

$$CE \approx \frac{\sum_{j=1}^N \sigma_{C,CO_2,j} (\mathbf{u} \cdot \hat{\mathbf{n}})_j \Delta s_j}{\sum_{j=1}^N \sum_k n_{C,k} \sigma_{C,k,j} (\mathbf{u} \cdot \hat{\mathbf{n}})_j \Delta s_j} \quad (5.2)$$

This approximation differs from Eq. (4.17) in two important ways: (i) Eq. (5.2) explicitly considers the advection of species into and out of the control volume, while Eq. (4.17) does not; and (ii) the summation in the denominator of Eq. (5.2) is applied over the entire boundary, while in Eq. (4.17) the carbon column number density affixed to the  $CO_2$  of each pixel is normalized by the total carbon column number density of the corresponding pixel and not the overall value within the ROI. Coupled with the fact that the combustion products should be concentrated downwind of the combustion zone, and not upwind, the velocity terms give more weight to pixels located on the downwind surface of the

control boundary, while in the VISR approach, all pixels in the ROI have equal influence on the CE estimate. As a result, pixels containing lower concentrations of combustion byproducts (either as unburned HCs, CO<sub>2</sub>, or CO) will have an outsized influence on the average CE.

Figure 5.6 Comparison between instantaneous (temporally resolved) VISR-inferred and ground truth values of global CE for 72 timesteps for (a) Case 1, (b) Case 2, (c) Case 3, and (d) Case 4. Horizontal lines indicate the corresponding time-averaged values. compares the instantaneous VISR global CE estimates found using Eq. (4.17) and those from the CFD “ground truth” found in Eq. (5.2), for the four simulation cases. In all cases, the VISR-inferred CEs differ by as much as 25% from the CFD-LES ground truth. In contrast, Zeng et al. [38] found the average difference between  $CE_{\text{VISR}}$  and the value inferred by extractive sampling to be 0.5% (absolute difference in CE, not relative error). There are two possible reasons for this disparity. First, for all but five of the 28 comparative cases considered by Zeng et al. [38], the flares were operated at CEs greater than 99%. Considering the lower CE cases alone, the difference between  $CE_{\text{VISR}}$  and the extractive sampling values is more typical of the differences observed here. Second, the inferred CE from extractive sampling is subject to its own uncertainties, as described at the beginning of this paper, and may not reflect the flare CE represented by Eq. (2.6).

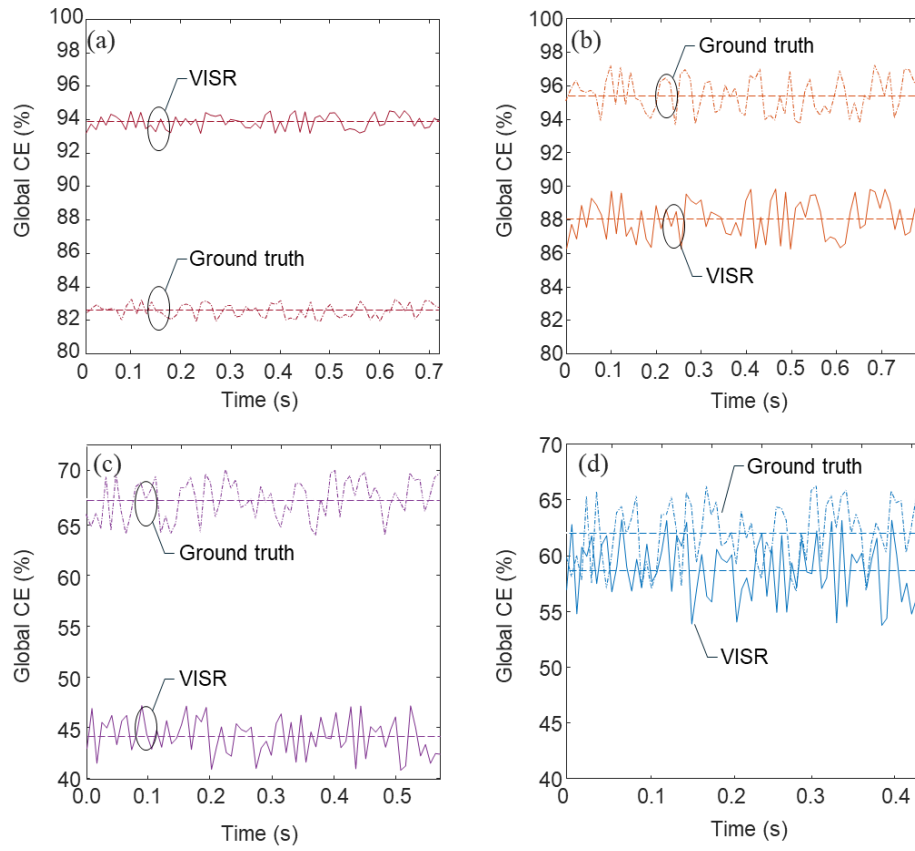


Figure 5.6 Comparison between instantaneous (temporally resolved) VISR-inferred and ground truth values of global CE for 72 timesteps for (a) Case 1, (b) Case 2, (c) Case 3, and (d) Case 4. Horizontal lines indicate the corresponding time-averaged values.

### 5.3 Stripped Methane Detection: Implications and Shortcomings

In the case of strong crosswinds, vortices that form in the wake of the flare stack may extract localized pockets of unburned fuel from the flare tip and strip them away from the combustion zone. In contrast to the hot combustion by-products, the cold unburned  $\text{CH}_4$  tends to sink, resulting in a segregated, fuel-rich region beneath the visible flame [5,30], with much lower local CE, e.g., Figure 5.1 (b). Emissions from the stripped, unheated hydrocarbons are much harder to detect than partially combusted plumes using MWIR imagers, particularly in the presence of hot gases, due to the limited dynamic range of the instrument.

This detection issue is illustrated in Figure 5.7. The lower part of the figure superimposes the  $\text{CH}_4$  column density and isotherms at the centerline, while  $\text{CH}_4$  mass flux ( $\text{kg}\cdot\text{m}^{-1}\text{s}^{-1}$ ) and centerline temperature profiles for three sample transects are plotted at the top. A significant portion of the unburned  $\text{CH}_4$  leaving the computational domain through the downwind face comes from the stripping mechanism. Most of this  $\text{CH}_4$  stream exists outside the VISR ROI and at temperatures that would be very difficult to detect using MWIR sensors.

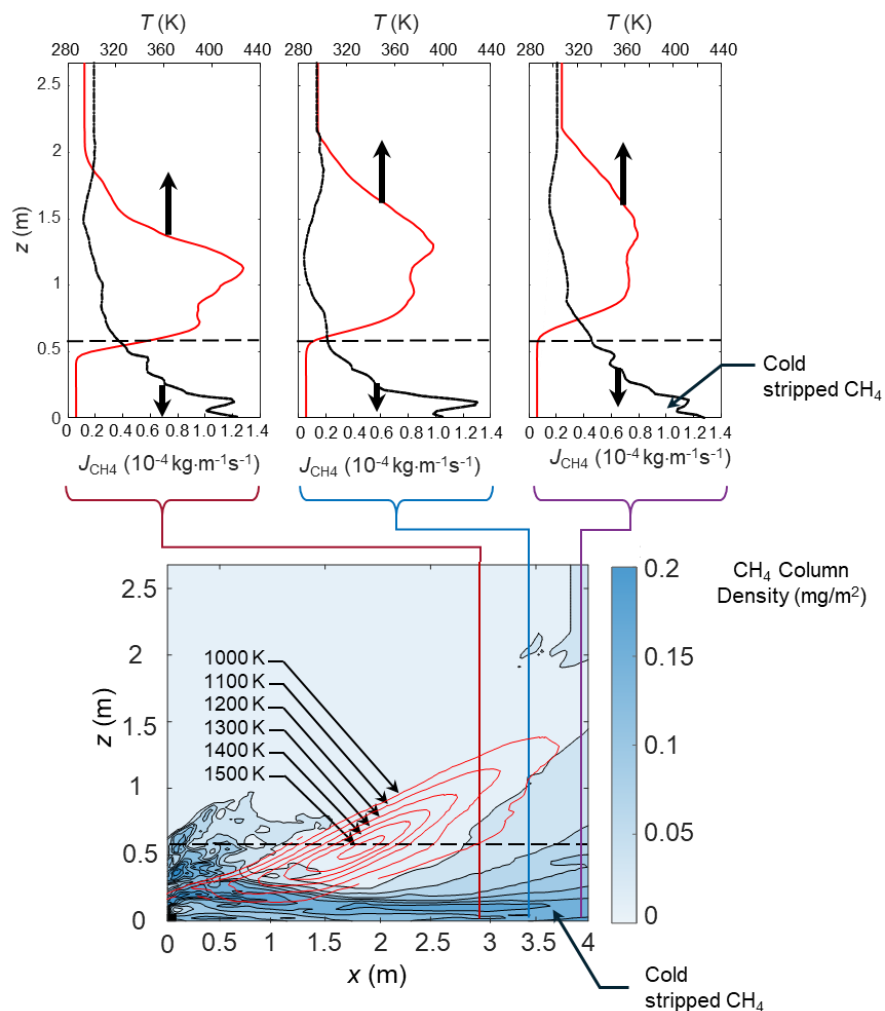


Figure 5.7 Maps of  $\text{CH}_4$  mass fluxes and centerline temperature contours at three cross-sections, along with the isotherms and column densities of  $\text{CH}_4$  for an arbitrary timestep of Case 1. The fuel-rich region beneath the flare plume is unlikely to be detected using MWIR imaging, due to the limited dynamic range of the instrument.

Table 5.1 summarizes the fraction of methane that could potentially be detected by the VISR mechanism for the four scenarios considered here, indicating that a considerable amount of the CH<sub>4</sub> emissions from the flare would be unaccounted for using the VISR method. It is important to note that this is not a shortcoming of the VISR technique per se, but a limitation common to all remote sensing technologies based on MWIR imaging. In this table, the second and third columns report the overall proportion of the fugitive methane comprised of cold methane, generated through the aerodynamic-stripping mechanism, and the portion of stripped (cold) methane detectable by the VISR MWIR imager, respectively. The amount of cold methane is calculated by tracking the methane mass flux through multiple vertical transects, and identifying the region that remains below 100°C, the temperature at which steam and methane are mixed and exit the flare stack. The fraction of methane that can be imaged is estimated from the methane mass flux corresponding to pixels having a broadband intensity greater than the cutoff signal-to-noise ratio.

Table 5.1: VISR stripped (cold) CH<sub>4</sub> detection: limitations and capabilities

| CFD-LES case ID | Stripped methane mass flow rate (g/s) | Contribution of stripped methane to the overall unburned methane | Proportion of stripped methane, detected by the VISR instrument | Ground truth (CFD-driven) flare global CE |
|-----------------|---------------------------------------|------------------------------------------------------------------|-----------------------------------------------------------------|-------------------------------------------|
| 1               | 4.4                                   | 32 %                                                             | 20 %                                                            | 83.00 %                                   |
| 2               | 1.4                                   | 25 %                                                             | 22 %                                                            | 95.41 %                                   |
| 3               | 2.8                                   | 46 %                                                             | 15 %                                                            | 67.11%                                    |
| 4               | 2.5                                   | 37 %                                                             | 12 %                                                            | 61.48 %                                   |

## 5.4 Conclusions

Given the large discrepancies observed between modelled and ground truth broadband intensities, for both isothermal and optically-thin plume approximations, as high as 20% reported bias for specific broadband channels, the results show that the presented simplified VISR model can provide accurate local CE estimates for pixels located within the VISR ROI.

However, the VISR flare CE model lacks any physical grounding, and the MWIR instrument's limited sensitivity to detect unburned fugitive methane, downwind of the plume, further compromises the reliability of VISR-derived flare CE values.

Moreover, despite the results showing fairly accurate local CE estimates for pixels located within the VISR ROI; to address any concerns regarding the veracity of VISR method, it is crucial to conduct a detailed uncertainty analysis. Chapter 6 provide a hierarchical Bayesian framework, utilized for the uncertainty analysis of VISR-inferred local CE values.

## Chapter 6

### VISR local CE uncertainty analysis

A CE estimate for a pixel may be computed by substituting the radiometric data, recorded by the camera broadband channels, into Eq. (4.16). In this Chapter, we focus on developing a statistical inference model utilizing a Bayesian framework to quantify the uncertainty associated with this estimate. The parameters involved in this statistical model include the inferred (post-processed) measurement data,  $\mathbf{b}$ , quantities-of-interest (QoI),  $\mathbf{x}$ , along with some auxiliary parameters, all characterized as independent and identically distributed (IID) random variables, each distributed according to a corresponding probability density function (pdf). This statistical data-driven model ultimately aims to infer the probability distribution of the VISR-estimated flare CE, as the mean local CE of pixels residing within the VISR ROI, Eq. (4.17), using the inferred posterior pdfs associated with the QoI model parameters, hence updating our knowledge regarding the flare CE target distribution.

The Bayesian framework uses a two-stage hierarchical Bayesian inference model, in which the QoI parameters in the primary stage are comprised of select gas state parameters, the species column number densities and effective plume temperature, denoted by  $\mathbf{x} = [\sigma_{\text{CH}_4,j}, \sigma_{\text{CO}_2,j}, \sigma_{\text{CH}_4,j}, T]$ , which can be inferred from applying the VISR instrument model to the VISR broadband camera measurements, denoted by  $\mathbf{b}^{\text{meas}}$ , for pixels located within the VISR ROI. Noted that the inferred QoI parameters for a sample pixel  $j$  within the VISR ROI are utilized in the VISR instrument model, Subsection 4.2, to compute an estimate for the local (pixel-wise) CE, denoted by  $\text{CE}_j$  in Eq. (4.16). The measured broadband data can be linked to the primary QoIs according to

$$\mathbf{b}^{\text{meas}} = \mathbf{b}^{\text{model}}(\mathbf{x}) + \delta\mathbf{b}^{\text{model}}, \quad \delta\mathbf{b}^{\text{model}} \sim p(\mathbf{b}^{\text{exact}}) \quad (6.1)$$

where  $\delta \mathbf{b}^{\text{model}}$  is the difference between ground truth incident broadband signal,  $\mathbf{b}^{\text{exact}}$ , governed by Eqs. (4.2) and (4.11), and the post-processed camera broadband measurement,  $\mathbf{b}^{\text{model}}$ , computed by Eq. (4.15), for the same QoI parameters,  $\mathbf{x}$ . This bias mainly represents the error due to the simplifications and assumptions applied to RTE in the VISR radiometric model, to obtain an explicit linear relation between the local CE estimate for pixel  $j$ th,  $\text{CE}_j$ , and the measured broadband data, as expressed by Eq. (4.15). In contrast to the magnitude of the model error, other forms of uncertainty originating from optical and electrical interferences while operating the instrument, commonly known as the measurement error, are considered to be negligible.

While the model error,  $\delta \mathbf{b}^{\text{model}}$ , is theoretically deterministic, it should be considered as a random variable from an experimentalist's perspective since calculating this parameter requires an exhaustive knowledge of the unknown target distributions of primary stage QoIs along the LOS of each pixel residing within the VISR ROI. In this analysis, the effective plume temperature along the  $j$ th pixel,  $T_j$ , is taken as the temperature that minimizes the corresponding model error. Figure 6.1 shows histograms of the sampled model errors, which are highly skewed. As previously discussed in Section 5.1, Much of the model error arises from the difference between the incompatibility of the RTE assuming an isothermal plume, a uniform temperature along each pixel's LOS, Eq. (4.14), and the non-scattering RTE, Eq. (4.2). This is the well-known turbulence-radiation interaction (TRI) [103,104] originating from the difference between  $\langle I_{\eta,b} \cdot \kappa_{\eta} \rangle_s$  and  $\langle I_{\eta,b} \rangle_s \cdot \langle \kappa_{\eta} \rangle_s$ , due to partially-correlated fluctuations in the species concentration and temperature fields. The target probability density functions (pdfs) of the VISR broadband signals are expected to be represented by the family of Gaussian (normal) distributions close to the combustion zone but become progressively skewed due to increasing turbulent mixing, as more ambient air is entrained into the plume further downstream [105]. To reduce the complexity of the model and acquire a conservative estimate for the uncertainty associated with the

inferred flare CE, broadband channel model errors, Eq. (6.1), are assumed to be uncorrelated, despite the evidence showing highly correlated or anticorrelated behaviour across various spectral channels.

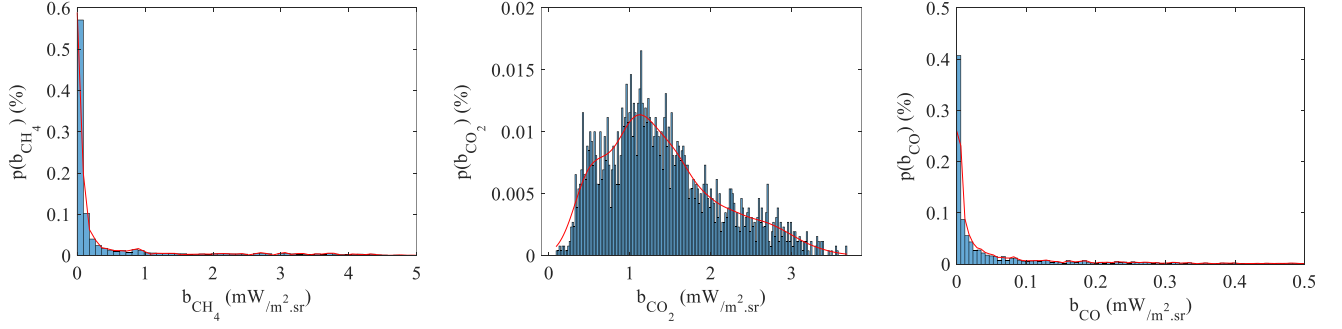


Figure 6.1 Histograms of the sample model errors for pixels located within the VISR ROI, paired with the fitted pdf based on the generalized kernel density maximum entropy method [107], for CFD-LES Case 1, presented in Table 4.1.

The fact that the target distributions of the measurement noise,  $\delta \mathbf{b}^{\text{noise}}$ , and model error,  $\delta \mathbf{b}^{\text{model}}$ , parameters are bounded within finite domains, guarantees that any data from a set of sample measurements has a finite probability of being observed. The likelihood of observing the data for a hypothetical set of QoI random variables,  $\mathbf{x}$ , is characterized by the joint likelihood pdf. In the Bayesian framework, the inferred probability density of a set of QoI parameters,  $\mathbf{x}$ , given a set of observations (measured data),  $\mathbf{b}^{\text{meas}}$ , is referred to as the joint posterior pdf, denoted by  $p(\mathbf{x}|\mathbf{b})$ , which is related to the joint likelihood pdf, denoted by  $p(\mathbf{b} = \mathbf{b}^{\text{meas}}|\mathbf{x})$ , and prior distributions, denoted by  $p_{\text{pr}}(\mathbf{x})$  according to the Bayes' equation

$$p(\mathbf{x}|\mathbf{b}) = \frac{p(\mathbf{b} = \mathbf{b}^{\text{meas}}|\mathbf{x}) p_{\text{pr}}(\mathbf{x})}{p(\mathbf{b})} \propto p(\mathbf{b}|\mathbf{x}) p_{\text{pr}}(\mathbf{x}) \quad (6.2)$$

where  $p_{\text{pr}}(\mathbf{x})$  is the joint prior pdf that encodes the preliminary knowledge of the QoIs,  $\mathbf{x}$ , before conducting the measurements, and  $p(\mathbf{b})$  is the marginal pdf of observing the specified measured data,  $\mathbf{b}$ , commonly referred to as the probability of the evidence, which is a normalization of the numerator

on the right side of the Eq. (6.2), hence resulting in the posterior pdf satisfying the Law of Total Probability.

There are four unknown QoI parameters consisting of three species column number densities and the effective plume temperature, and three measurement (observation) random variables, each corresponding to broadband irradiation along the three spectral bins spectrums. It is important to ensure that the prior pdfs for the QoI variables accurately reflect what is known about them so as to minimize the uncertainty in the CE estimate while avoiding biasing the outcome of the inference. Accordingly, a robust method for defining prior distributions based on past and current knowledge of the measured parameters, without compromising the inference outcome, is utilized based on the Principle of Maximum Entropy, which approximates the probability density function of the random variable target distribution by maximizing the Shannon entropy (minimizing the information contained by the pdf), subject to testable information [106]. In this framework, the prior distributions are estimated utilizing a version of this non-parametric model, applied to the bootstrapped resampling dataset of the inferred species column number density and effective plume temperature along the LOS of the pixels confined within the VISR ROI, to resemble the priors target distribution. This non-parametric inference method, referred to as the generalized kernel density maximum entropy (GKDME) method [107], operates by adopting kernel density representation of the target distribution while determining its free parameters using the principle of maximum entropy (ME) [108,109]. Figure 6.2 shows a set of histograms representing the informative prior pdfs used in the current Bayesian framework, at an arbitrary timestep for Case 1, presented in Table 4.1.

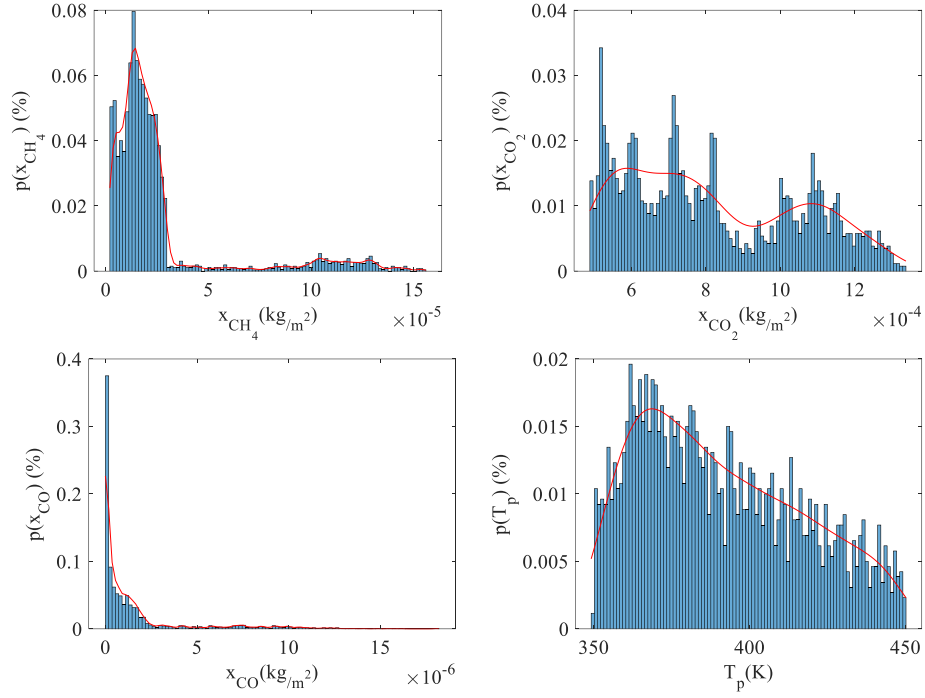


Figure 6.2 Prior distributions computed using a nonparametric inference approach, referred to as the generalized kernel density maximum entropy method [107], representing the target distributions as the kernel density function (KDF) applied to the bootstrap resampled evidence (post-processed measurements), for CFD-LES Case 1, presented in Table 4.1.

While in many problems the model error and measurement noise are distributed according to a convenient class of pdf (e.g., Gaussian, lognormal, Gamma), Figure 6.1 shows this not to be the case, and in the absence of such a distribution, it is impossible to write a closed-form expression for the joint likelihood pdf using common distribution families. Instead, the joint likelihood conditional probability function for a given set of  $\mathbf{x}$  is estimated by obtaining  $\delta \mathbf{b} = \mathbf{b}^{\text{exact}}(\mathbf{x}) - \mathbf{b}^{\text{meas}}(\mathbf{x})$  and then substituting each error component into a corresponding nonparametric pdf, derived from the distributions shown in Figure 6.1. Since all the measured data, synthetic VISR broadband images, can be assumed to be

independent and identically distributed (IID), the unscaled posterior pdf, comprised of the product of joint likelihood and prior probabilities, in Bayes' Law, Eq. (6.2), can be expressed as

$$p(\mathbf{x}|\mathbf{b}) \propto \prod_{k=1}^3 p_k(\delta b_k|\mathbf{x}) p_{pr,k}(\mathbf{x}) \quad (6.3)$$

Samples from the unknown posterior probability density are then generated using a Markov-chain Monte Carlo (MCMC) simulation; starting from an initial set of QoIs,  $\mathbf{x}^0$ , the proposed MCMC algorithm generates a sequence of QoIs,  $\{\mathbf{x}^0, \mathbf{x}^1, \mathbf{x}^2, \dots\}$ , for a given measurement (observation) dataset. In the  $(k+1)$ th step of the MCMC approach, a candidate set of QoI values,  $\mathbf{x}^{k+1,c}$ , is sampled using the previously generated set of QoIs in step  $k$ th,  $\mathbf{x}^k$ , followed by an acceptance or rejection process based on the relative value of its corresponding unscaled posterior pdf. After ignoring a pre-specified initial set of the  $m$  generated QoI parameters, known as the “burn-in” period, the resulting set of simulated QoIs,  $\{\mathbf{x}^m, \mathbf{x}^{m+1}, \mathbf{x}^{m+2}, \dots, \mathbf{x}^n\}$ , becomes ergodic to the joint target posterior probability distribution,  $p(\mathbf{x}|\mathbf{b})$ , satisfying the requirements to be considered as a Markov Chain.

In this work, the Bayesian inference model was carried out using the generalized slice sampler technique [110], a unique classification of the auxiliary variable MCMC models, to infer posterior distributions of the primary stage QoI parameters, utilizing the pre-built slice sampler algorithm in MATLAB software [111]. The advantage of the slice sampling approach, compared to other conventional MCMC algorithms, such as Metropolis-Hastings [112], lies in its inherent ability to sample from any target distribution that might be impossible to directly draw a sample from using conventional sampling techniques, yet it can potentially suffer from intractability issues of generating uniformly distributed samples from all plausible sections within a horizontal slice of the target distribution at each step. Figure 6.3 shows the histograms of the inferred primary QoIs marginalized posterior pdfs, using an MCMC technique, the slice sampler method, for CFD-LES Case 1, presented

in Table 4.1. The red lines in this figure represent the kernel probability density functions (pdfs), fitted on the marginalized posterior histograms according to the prescribed GKDME model.

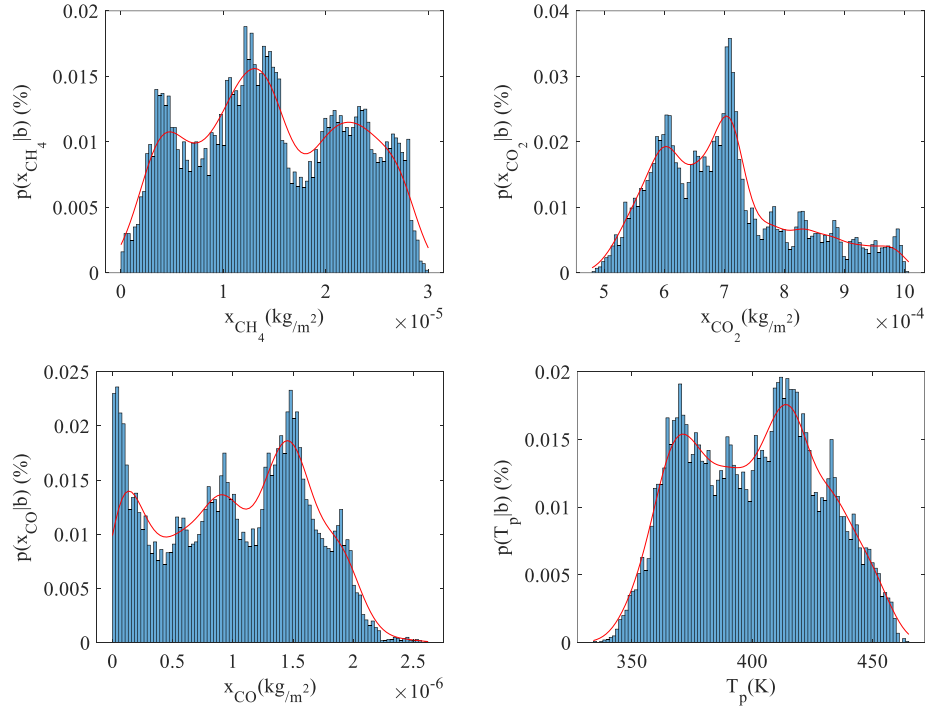


Figure 6.3 Posterior distributions of the primary QoIs, obtained using Slice sampler, a Markov Chain Monte Carlo algorithm [110], for CFD-LES Case 1, presented in Table 4.1.

Finally, to infer the ultimate posterior pdf,  $p(\text{CE}_{\text{VISR}}|\mathbf{b})$ , representing the target distribution of the secondary QoI parameter, the VISR-estimated local CE, the primary QoI parameters, mainly the species column number densities, are sampled from their corresponding marginalized posterior pdf, denoted by  $p(x_k|\mathbf{b})$ , and their corresponding local CE is estimated based on Eq. (2.9). Applying the GKDME model on the bootstrapped resampling of the sampled local CE dataset, yields the “expected” probability distribution of the VISR-inferred local CE based on the inferred posterior distributions of the primary QoI parameters. Figure 6.4 compares the prior and posterior probability density distributions of the estimated local CE, utilizing the VISR approach, as described in Section 4.2, at an

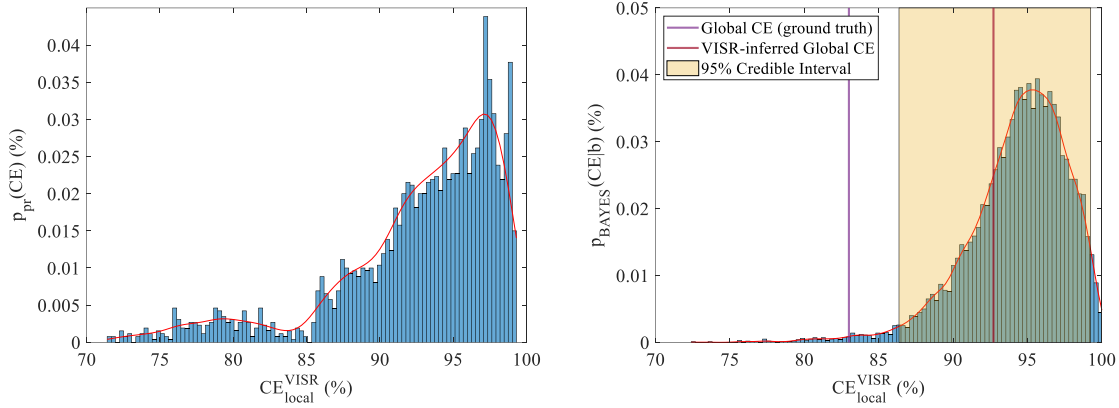


Figure 6.4 VISR-inferred local CE a) Prior distribution, obtained based on the Maximum Information Entropy Principle [108,109], by fitting nonparametric kernel density functions, b) Expected posterior distribution derived from the quantities-of-interest (QoIs) pdfs, Figure 6.1 Histograms of the sample model errors for pixels located within

the VISR ROI, paired with the fitted pdf based on the generalized kernel density

maximum entropy method [107], for CFD-LES Case 1, presented in Table 4.1., obtained arbitrary timestep for CFD-LES Case 1, presented in Table 4.1. The red curvature in both figures represents the best-fitted kernel density function, based on the GKDME model, for the prior and posterior pdfs.

Figure 6.5 shows the posterior (expected) pdf of the secondary QoI, local CE, for all CFD-LES cases, presented in Table 4.1. The estimated local CE prior pdfs, shown in Figure 6.4, are assigned utilizing the prescribed non-parametric approach for estimating the informative prior distributions, on the bootstrapped resamples of the dataset of local CE, inferred along the LOS of the pixels located within the VISR ROI. The global CE sensitivity analysis is conducted, assuming that the local CE target distribution, posterior pdf, potentially provides the basis for determining an uncertainty for the estimated global CE by the VISR model, Eq. (4.17). The proposed uncertainty can be determined according to the credible bounds of the local CE posterior pdf. This uncertainty, 95% credible interval

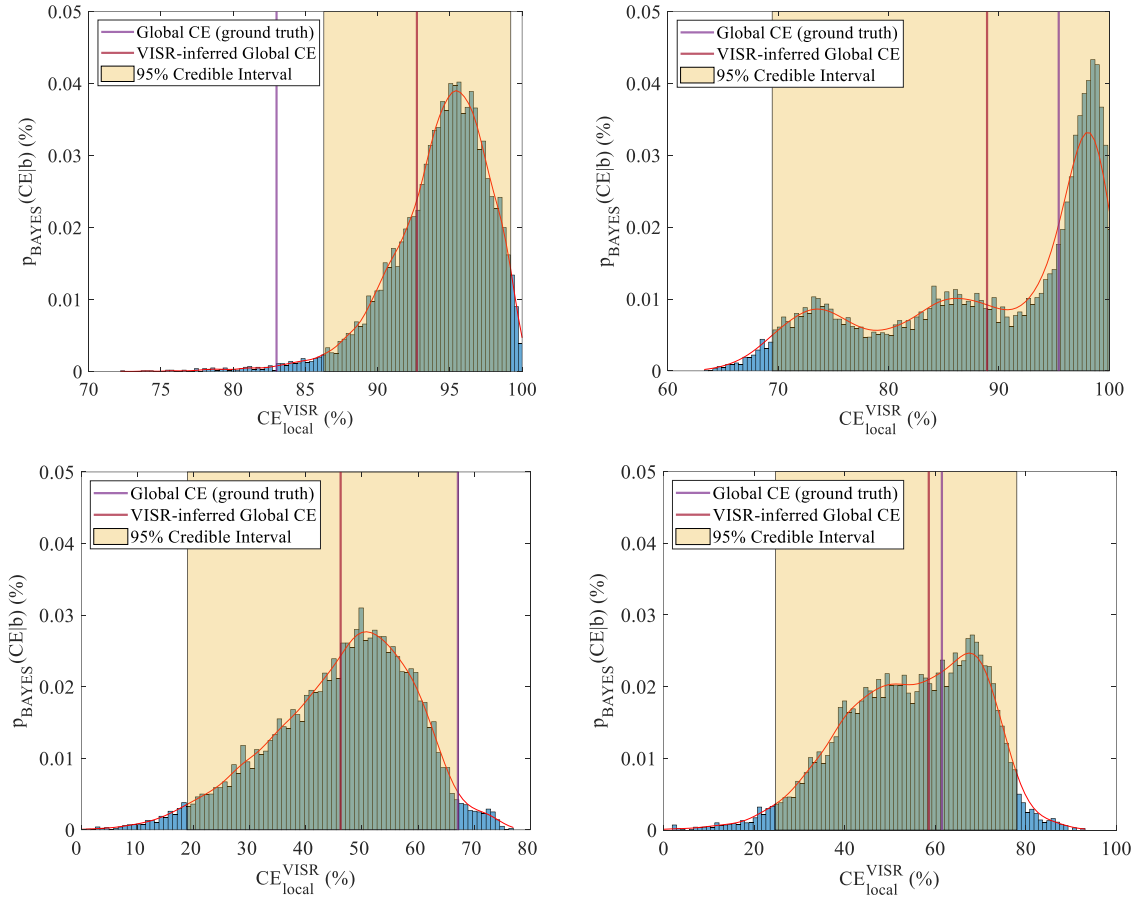


Figure 6.5 Expected posterior pdfs of the VISR-inferred local CE, secondary QoI, derived from the posterior pdfs of primary QoIs, Fig. 10, for LES-CFD a) case 1, b) case 2, c) case 3, d) case 4, presented in Table 4.1.

(CI) based on the highest posterior density (HPD) region along with the VISR-inferred and ground-truth flare CE is illustrated in Figure 6.5, for all the CFD-LES cases in Table 4.1. In addition to the uncertainty sources in the VISR radiometric model, there are uncertainty associated with inherent flaws of the VISR method including the VISR flare CE averaging model, with no physical grounds, and dismissal of undetected unburned fugitive methane, downwind of the plume, which are unaccounted for in this analysis. Considering all the mentioned sources of uncertainty, it can be expected to observe the ground truth flare CE to fall outside the 95% credible intervals.

## 6.1 Optimized VISR flare CE inference model

In an attempt to improve the accuracy of the overall flare CE predicted by the proposed VISR model [38], an optimized statistical-based version of this model is introduced here. The new model incorporates the “predicted” posterior probability of the inferred local CE, shown in Figure 6.5, as scaling factors for their corresponding CE value, in the VISR weighted averaging scheme to deliver a more robust and statistically-backed estimate of the flare overall CE.

The following expression represents the modified VISR global CE inference model

$$CE_{\text{VISR,modified}} = \frac{1}{N_{\text{ROI}}} \sum_{j=1}^{N_{\text{ROI}}} \left( p(CE_j | \mathbf{b}) CE_j \right) = \frac{1}{N_{\text{ROI}}} \sum_{j=1}^{N_{\text{ROI}}} \left( p(CE_j | \mathbf{b}) \frac{n_{\text{C,CO}_2} \sigma_{\text{CO}_2,j}}{\sum_k n_{\text{C,k}} \sigma_{k,j}} \right) \quad (6.4)$$

An essential outcome of this optimized model is that all the estimates are data-driven, where our prior knowledge of the primary QoI parameters,  $\mathbf{x}$ , is updated at each iteration of the flare CE measurement using the previously inferred posterior pdfs of the primary QoIs, expected to resemble the target distributions more accurately by incorporating the potential impact of the time-dependent physical aspects of the flaring process such as the fluctuating crosswind conditions and steam and air assistance on reducing the overall flare CE. Note that the modified VISR model is developed to improve the accuracy of the VISR flare CE estimates, despite all the shortcomings and lack of physical relevance in the original simplified VISR flare CE inference model, which predicts the flare CE as the average local CE of the pixels located within the VISR ROI, as discussed in 4.2.1.

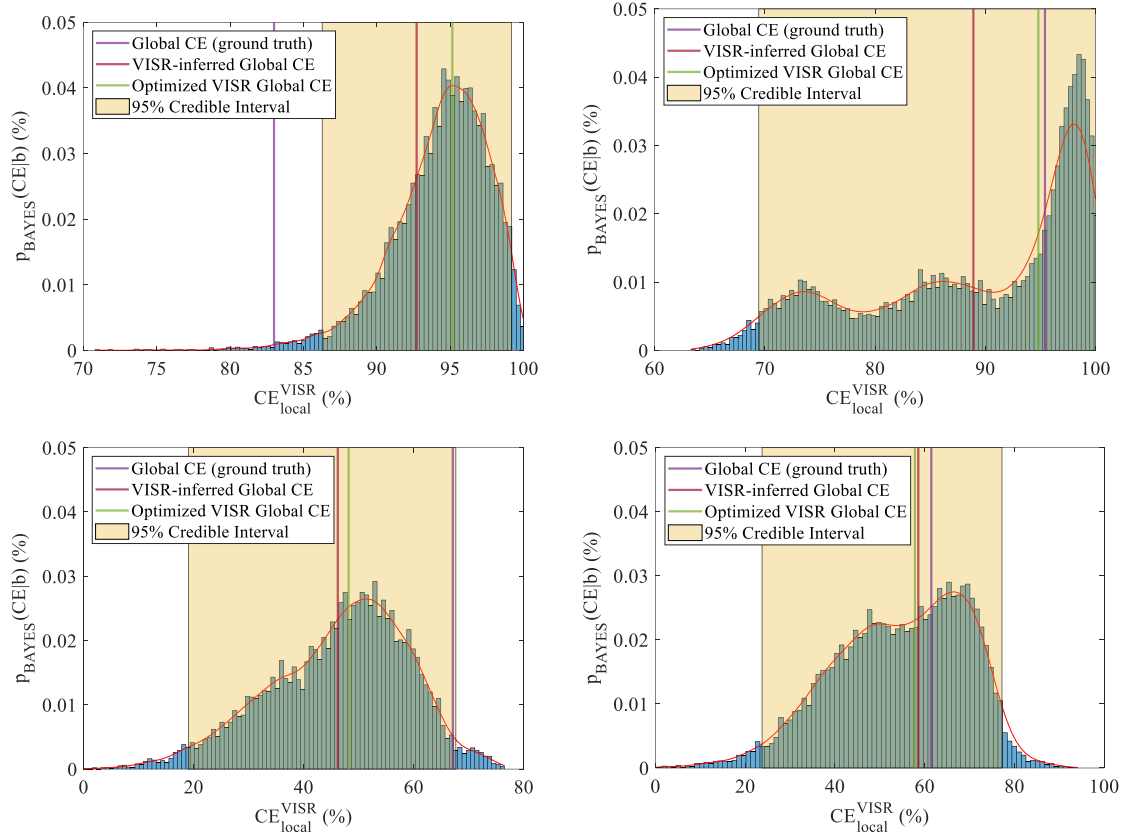


Figure 6.6 Comparison of the ground truth and estimated flare CE by the modified VISR model, after 5 iterations of updating the local CE posterior pdf according to the proposed Bayesian inference model, paired with the 95% credible interval for LES-CFD: a) case 1, b) case 2, c) case 3, d) case 4, presented in Table 4.1.

Figure 6.6 shows the estimated flare global CE using both original and modified VISR models along with their corresponding 95% CI associated with the flare CE posterior pdf HPD, for all CFD-LES cases presented in Table 4.1. According to this figure, for CFD-LES cases where the ground truth flare CE falls within the plausible uncertainty region, the 95% constructed CI based on the local CE posterior pdf HPD, the modified VISR model is generally capable of providing a reasonably more accurate estimate, in comparison to the previously proposed VISR model by Zeng et al. [38]. For flaring

conditions with undesirable flare CE estimates by the VISR approach, where the ground truth lies outside the acceptable uncertainty bounds, similar to the original VISR model, the modified data-driven VISR model is unable to provide acceptable results. It is crucial to consider that in real-world scenarios, checking whether this condition was satisfied would be much more difficult due to the lack of benchmark flare CE values.

To fully assess the capabilities of the modified VISR model, in terms of providing more accurate flare CE estimates, an additional analysis is conducted to estimate the optimized number of iterations required for updating the local CE posterior pdf and to determine whether the proposed modified model could accurately predict flare CE, particularly for flaring facilities operating under crosswind and steam and air assistance conditions. Figure 6.7 shows the progression of error associated with the estimated flare CE using the modified VISR model for CFD-LES cases 2 and 4, presented in Table 4.1, for seven consecutive iterations, within a 5-second period. In each iteration, the local CE posterior pdf is updated, assuming the posterior pdf from the previous iteration as the local CE prior pdf. Since updating local CE posterior pdf involves an extensive dataset and is considered to be a computationally intensive process, each iteration, shown in Figure 6.7, represents the average error associated with the flare CE estimates, in contrast to the ground truth (CFD-driven) flare CE values, for ten successive timesteps. According to this figure, the modified VISR model may be promising given the local CE posterior pdf, used as the scaling factors in the averaging process of the original VISR model, is sufficiently updated to resemble the true local CE target distribution, in which the estimated flare CE could potentially provide a more accurate prediction of the flare CE.

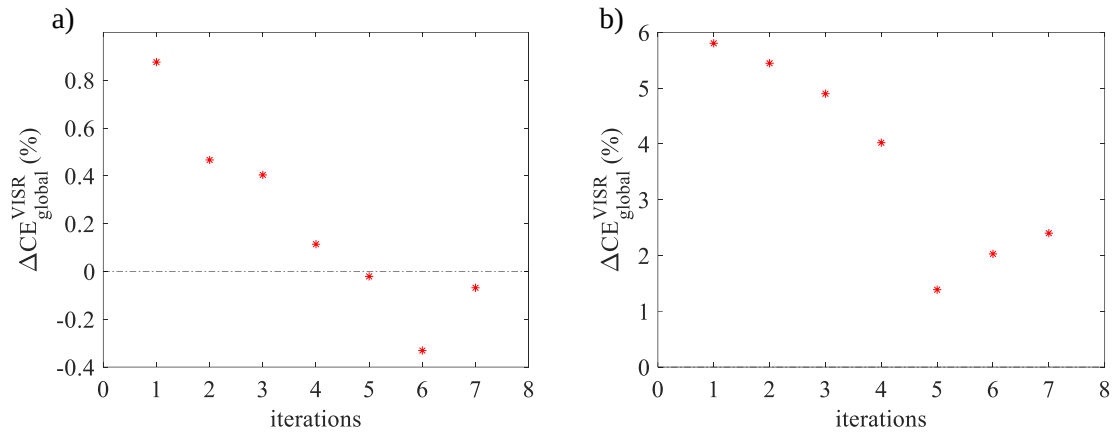


Figure 6.7 Flare CE uncertainty progression for seven consecutive iterations of updating the expected local CE posterior pdf, defined in the modified VISR model, for CFD-LES: a) case 2, b) case 4, presented in Table 4.1. The flare CE uncertainties shows the difference between modified VISR estimate and the ground truth for each iteration.

## 6.2 Conclusions

The results show a general trend of VISR model under-estimating the flare CE, in which for most CFD-LES cases, both the VISR-estimated and ground truth flare CE lie within the 95% credible intervals. As expected, these credible intervals cover a vast range of flare CE values, showing large uncertainties associated with VISR flare CE inference.

On the other hand, in contrast to the original method, the modified VISR model can provide more accurate flare CE estimate with less bias; yet this model also suffers from inherent characteristics of the original simplified VISR model, including the lack of physical relevance for flare CE inference model and the unaccounted unburned fugitive methane presence downstream of the flare stack, in the VISR flare CE calculations.

## Chapter 7

### Conclusions

Optical gas imaging is a powerful tool for detecting and potentially quantifying various types of gaseous emissions from flaring processes. Video imaging spectro-radiometry (VISR) is one of the proposed approaches, developed for real-time remote quantification of flare CE. This work presents a numerical evaluation of a simplified version of the VISR technique for estimating the flare CE. This version of the VISR approach is based on hyperspectral imaging through three detection spectral bands aligned with key absorption features of  $\text{CO}_2$  (4.2–4.4  $\mu\text{m}$ ),  $\text{CO}$  (4.5–4.9  $\mu\text{m}$ ), and  $\text{CH}_4$  (3.2–3.4  $\mu\text{m}$ ). Synthetic broadband images corresponding to the VISR spectral channels are generated using species concentration and temperature datasets, obtained from several CFD-LES simulation cases replicating the operational conditions of a crosswind steam-assisted industrial flare. These CFD-LES simulation datasets are also utilized as a benchmark (ground truth) to assess the performance of the simplified VISR method and evaluate the accuracy of VISR-inferred parameters, including local and global flare CE values.

Additionally, to improve the accuracy of the VISR radiometric model, an uncertainty analysis is conducted on the estimated local CE using a two-level hierarchical Bayesian model, which facilitates the development of a modified VISR spectroscopic model that can potentially obtain better robustness and higher accuracy, compared to the original VISR model.

## 7.1 Summary and Key Findings

This study focused on the assessment of the performance of the simplified VISR model in terms of computing two primary metrics, local CE of the pixels located within the VISR ROI and the flare global CE, in addition to investigating the capabilities and limitations of the VISR instrument for the detection of unburned fuel components, mainly methane, downwind of the plume.

Current analysis of the inferred local CE supports the RTE simplifications applied to the underlying VISR radiometric model for pixels located within the VISR region-of-interest (ROI), with an error typically less than 3% of the corresponding ground truth value. However, the assessment of the VISR instrument model performance for flare global CE quantification demonstrates a considerable bias from their respective ground truth, resulting in the overestimation of flare CE in most flare processing conditions. This can be linked to the dubious nature of the local CE averaging technique and the lack of physical relevance in the VISR flare CE model. The VISR instrument also demonstrated poor detection capabilities of fugitive cold methane, due to the stripping mechanism occurring in the presence of crosswind over the flare stack, and limited distinction from fugitive hot methane mass flux.

Our results suggest that the VISR approach can potentially yield accurate local CE estimates for pixels located within the VISR ROI, although the averaging technique used to estimate global CE does not reflect the underlying transport phenomena in the flare plume and may result in large biases compared to ground-truth CE. Additionally, due to the limited dynamic range of the sensor, a significant portion of stripped flare gas is likely to remain undetected, leading to a significant overestimation of flare CE in high crosswind scenarios.

Moreover, conducting a Bayesian uncertainty analysis on the VISR-inferred local CE datasets, suggests that for cases where the difference between ground truth (CFD-driven) and VISR-estimated

flare CE is significant, it is likely that the ground truth flare CE value lies outside the acceptable uncertainty 95% credible intervals of the local CE posterior pdf.

Finally, the proposed modified VISR model, based on the VISR-inferred local CE Bayesian uncertainty analysis, shows more accurate results; whereas for the cases with acceptable VISR flare CE estimates, the modified VISR approach can provide a more accurate estimate of the flare CE, compared to ground truth. Further analysis shows that updating the expected local CE posterior pdf through several iterations can improve the accuracy of the flare CE estimate, however it is crucial to consider that this model still suffers from the underlying drawbacks of the original VISR model, including the lack of physical relevance in the VISR flare CE model, estimating flare CE as the mean local CE of the pixels within the VISR ROI, and the undetected unburned (cold) methane downwind of the flare plume; hence, despite the improved flare CE estimates, this modified approach is more likely to not provide an accurate estimate for flare CE.

## 7.2 Future Work

Considering the characteristic drawbacks and limitations of the VISR radiometric model, as proposed in Section 4.2, the simplified VISR approach can benefit from several improvements including: (1) incorporating a long-wavelength infrared (LWIR) hyperspectral camera, which could theoretically enhance the detection capability for stripped (cold) methane, resulting in more robust flare CE estimates; (2) refining the definition of the flame envelope, representing the active combustion zone; along with (3) updating the VISR flare CE inference model, from a simple averaging of the local CE values for pixels located within the VISR ROI to a more complex and physical model, which incorporate the projected velocity field and the dynamic nature of the VISR ROI into calculations, potentially resulting in robust flare CE estimates. Note that these suggestions are specifically for the VISR version presented in this work, based on Zeng et al. 2012 patent and 2016 paper [38,48], and does not apply to the several advancements in VISR technology in the past couple of years.

Besides improving on the VISR spectroscopic model and instrumentation, more simulated and experimental field trials are required to better assess the full capabilities and shortcomings of the VISR approach in real-time applications. To improve and expand the simulated experiments, other than testing more complex fuel streams in both steam and air assisted conditions, more in-depth knowledge of the newer variations of the VISR technique, both on the incorporated radiometric models and instruments, is also required. As for the field trials, the estimated flare CE estimates by the VISR approach should be verified against a ground truth value, which can be acquired using more robust and tested IFTS methods, e.g., MWIR and LWIR hyperspectral cameras, or a classic near-field sampling technique, as used by Zeng et al. [38]. Note that both of these measurement methods have their distinct advantages and suffer from their own drawbacks, which should be considered when choosing one as the ground truth.

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## Appendix A

### CFD-LES Supplementary Information\*

This appendix provides additional information showcasing the results for the CFD-LES simulation cases used in this research, presented in Table 4.1, highlighting the quantities-of-interest for quantifying the flare performance, including how the CO, CO<sub>2</sub>, CH<sub>4</sub>, and H<sub>2</sub>O are distributed within the plume region, as well as plume gas temperature and the velocity field. Instantaneous images were created according to the simulation outcomes for the four cases listed in T, at the timestep of  $t = 10$  s. Complete simulation results are available in the Federated Research Data Repository (Canada):

(<https://doi.org/10.20383/103.01079>).

Figure A1 shows CO mass fraction, a consequence of inefficient combustion. Higher crosswind velocities and steam assistance, particularly for Cases 3 and 4, lower the mass fraction of post-combustion CO within the plume region. Both high crosswinds and steam assistance intensify fuel-air mixing in the combustion zone, leading to lower equivalence ratios and complete combustion. The CO<sub>2</sub> mass fraction distribution is plotted in Figure A2. Higher crosswind velocities and steam assistance lead to lower CO<sub>2</sub> mass fractions downstream of the plume region.

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\* This appendix is adapted from the supplementary document provided with the following Ref:  
Kaveh, A., Spinti, J., Lapeyre, P., Bonarens, M., & Daun, K. J. (2025). Viability of video imaging spectro-radiometry (VISR) for quantifying flare combustion efficiency. *Journal of the Air & Waste Management Association*. <https://doi.org/10.1080/10962247.2025.2495026>

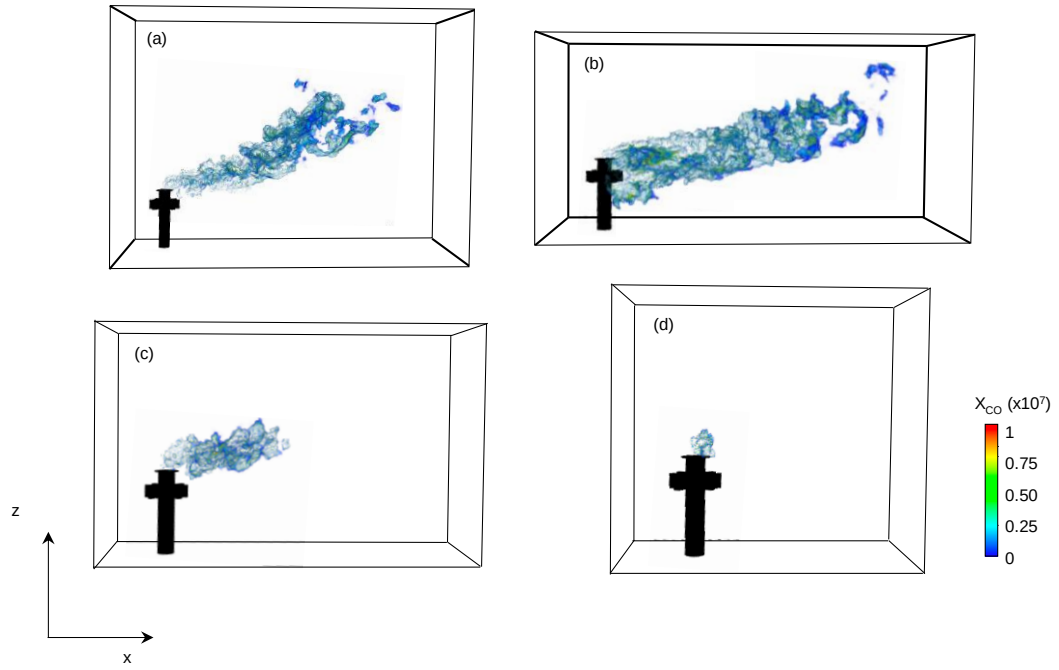


Figure A1 CO mass fraction within the flare plume at  $t = 10$ s: (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.

Figure A3 shows the  $H_2O$  vapor mass fraction within the simulation domain. Higher crosswind velocities and steam assistance, specifically in Cases 3 and 4, result in higher concentrations of steam downstream of the plume region.

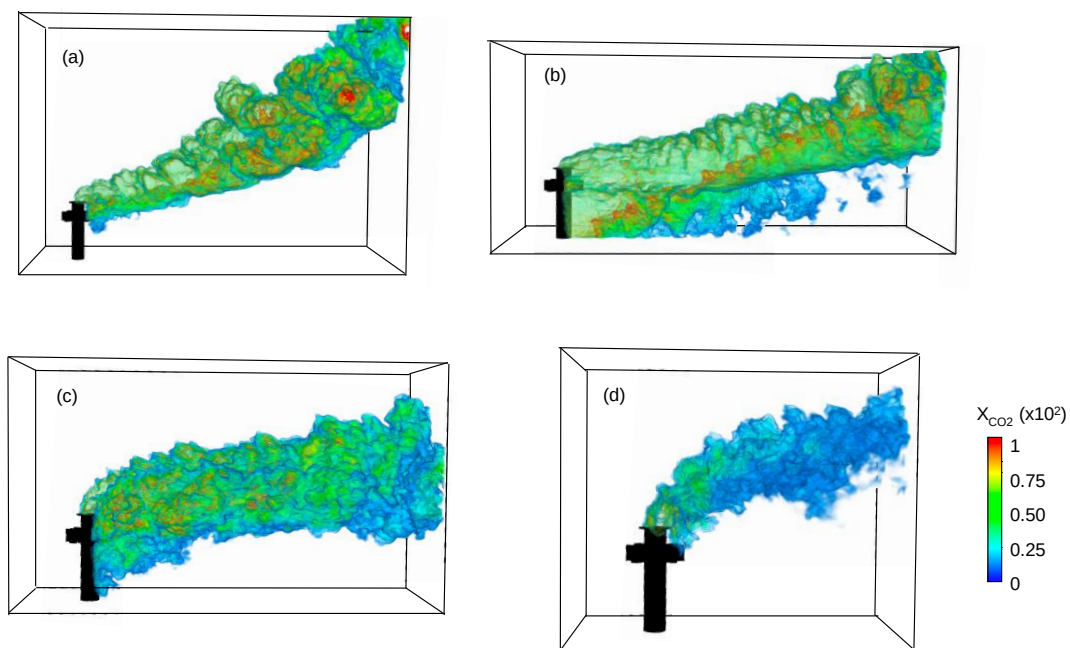


Figure A2 CO<sub>2</sub> mass fraction within the flare plume at  $t = 10$ s: (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.

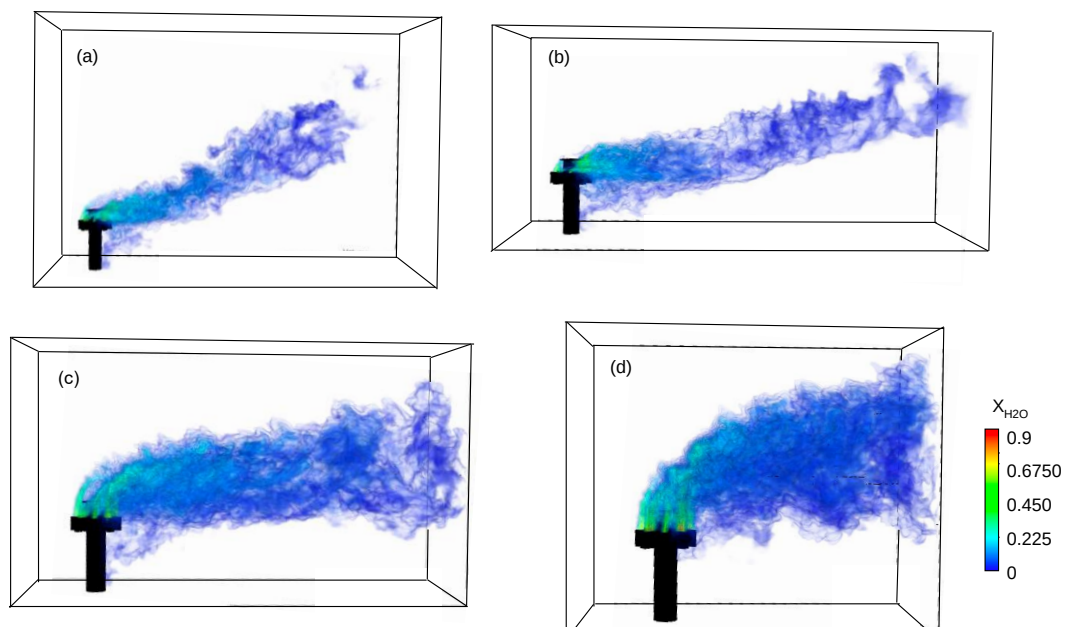


Figure A3 H<sub>2</sub>O mass fraction within the flare plume at  $t = 10$ s: (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.

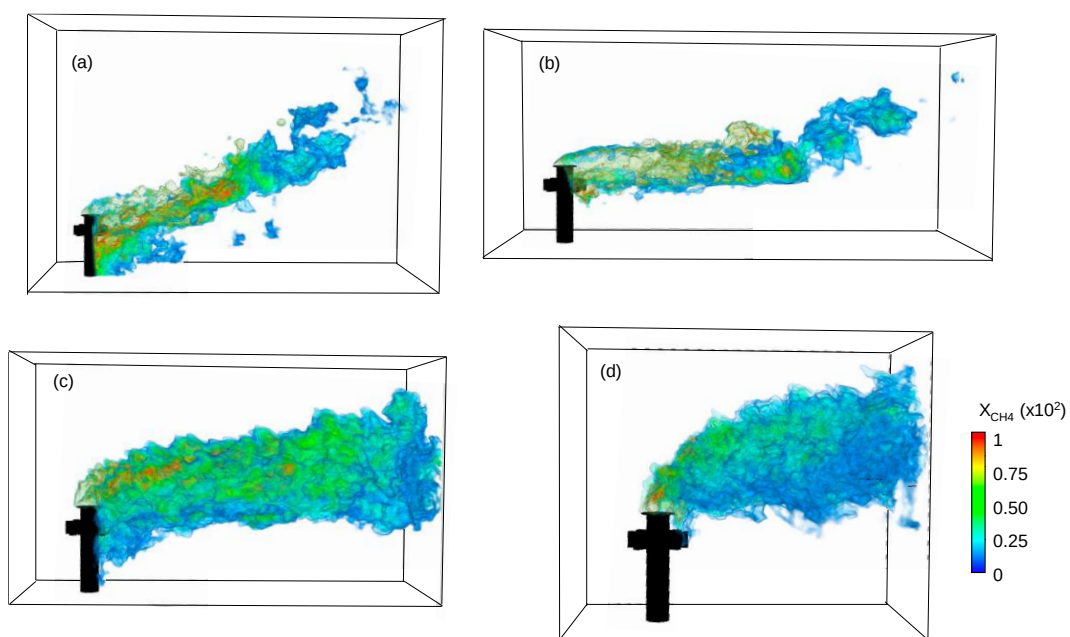


Figure A4 CH<sub>4</sub> mass fraction within the flare plume at t = 10s: (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.

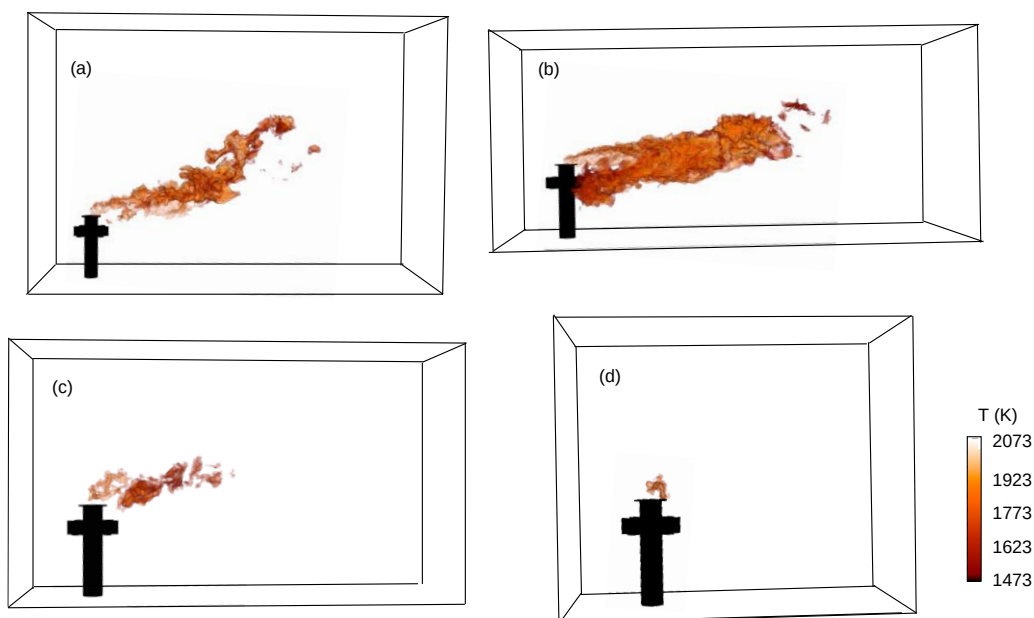


Figure A5 Temperature distribution within the plume at t = 10s: (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.

Figure A4 shows the distribution of unburned fuel ( $\text{CH}_4$ ) within the simulation domains. Some  $\text{CH}_4$  stripping is visible beneath the combustion zone, particularly in Cases 1 and 3. Large quantities of  $\text{CH}_4$  are also evident within the flare plumes for Cases 3 and 4, which are over-assisted.

The plume gas temperature is plotted in Figure A5. These contours correspond approximately to the visible flame. Comparing Cases 1 and 2, increasing crosswind velocity and steam injection flow rate could enlarge the combustion region to a point. However, in the case of high crosswinds and over-assistance (Cases 3 and 4) the combustion zone is confined close to the flare tip.

Figure A6 shows the sample velocity field within the simulation domain at transects of  $y = 0$  (midplane),  $z = 0.18 \text{ m}$  (stack height) and  $x = 0.5 \text{ m}$  (immediately downwind of the flare tip.) Cases 3 and 4 show higher degrees of turbulent intensity. Note the recirculation area in the wake of the flare stack, which is responsible for aerodynamic fuel stripping.

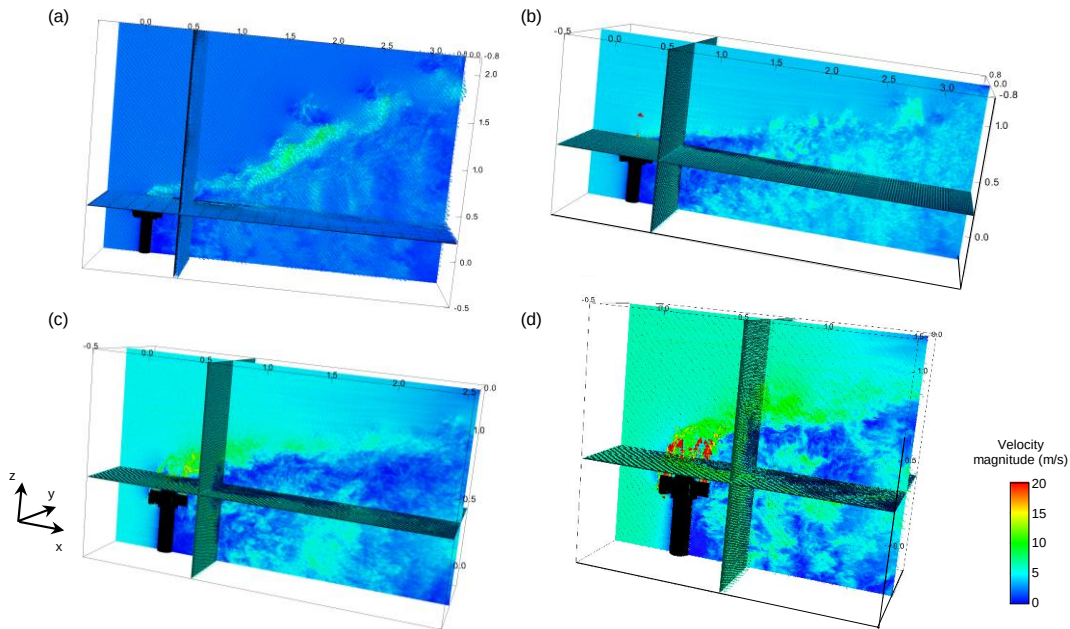


Figure A6 Instantaneous velocity field within the plume at  $t = 10\text{s}$ : (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.