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# *Smart Sensing with Digital Twins: Methane Emission Source Determination with sUAS*

*To Elvira, my family & mentors,*
*without your support this accomplishment would not have been possible.*

*To Dalia,*
*through smart thinking, hard work and persistent effort,*
*anything is possible.*

*To my readers,*
*I hope this book helps you implement smart sensing systems to make the world a better place.*

*— D.H.*

*To my mentors and family.*

*— Y.C.*

# Contents

# Preface

During our time as a graduate student, when it came to topics of research, we have always been tasked with solving the problem of "so what, who cares, and why you", Therefore our research into the use of small unmanned aircraft systems (sUAS – also referred to as drones) with the methane emission source determination problem has been largely motivated by climate change and the warming of our planet. Methane is a very potent greenhouse gas when compared to carbon dioxide, and methane has more potential to bring change to global warming effects due to its decreased atmospheric lifespan – i.e. our 'control' knob for near-term change. However, tn turns out, methane is seemingly challenging to measure. It is a colorless and odorless gas that is requires special sensors to detect. Therefore, we focused our efforts on solving this problem because it had the potential of real-world impact and is difficult to solve. However, before we can achieve this goal, we need to master our understanding of the measurement problem. This will ultimately provide pathways for detecting leaks, locating their sources, and quantifying the emissions but more importantly it provides pathways in measurement, verification (i.e. confirming that they have been fixed), and reporting programs. As Peter Drucker said, "what gets measured, gets managed."

In the literature, in the context of applications, there has been discrepancies between the top-down (or direct measurements) and the bottom-up (or inventory-based) approaches. Often the bottom-up approach under-estimates the emission source, which prompts investigation into improving the emission factors associated with these kind of methods. There are also issues with minimum detection limit and how industry is looking towards probability of detection to help understand how 'well' we can measure in all environments and scenarios - not just 'ideal' cases. Understanding how different sensing technologies and how the different modes of measuring methane (in situ, path-integrate, imaging-based) are effective in localization and quantification tasks are key to addressing this issue.

In the past decade, we have seen the integration of Digital Twins (DT) into key research areas (such as manufacturing, smart cities, etc.), improving the way we provide solutions. Currently, DTs have not been applied to environmental systems research, especially in the source determination problem. Benefits of DT technology success in other industries, give insights on how they may be useful in this problem. Furthermore, advances in industry 4.0 thinking or advances in IoT and edge devices with DTs, provide the potential for making methane sensing smarter within all sorts of applications – Oil & Gas, Agriculture, Dairy, Landfill, and even permafrost. Within the DT framework, a vision can be formed for how these measurements can be automated for more robust sensing, early detection, and faster repairs.

Many of the techniques employed by practitioners, rely on satellite, manned aircraft, foot-based measurements, or by installing many fixed sensors (also referred to as continuous emission monitoring). However, it is wrong to say that one approach is a ‘one size fits all’ and better than the others. A much better approach is to provide a holistic view of the measurement problem by providing complementary sensing at different measurement scales. And, there just so happens to be a gap between ground measurements and manned aircraft that is suitable for drone-based sensing – from 400 feet above ground level (AGL) to the surface. Drones also offer a unique capability for being able to be rapidly deployed, they have the ability to be re-configured with different sensors, they can access areas between the ground and manned aircraft that traditional vehicles or personnel on foot cannot travel (e.g. over bodies of water or tree-lines, next to flares or tanks, etc.), they can provide faster and more frequent surveys with finer spatial resolutions, and they can be relatively more cost effective than traditional surveys.

The atmospheric turbulence and weather pose challenges within the use of DTs and drone systems, both for flight capabilities and for solving the emission source determination in general. For example, strong winds and extreme cold / hot, can prevent or reduce flight times. Or, specific weather conditions may prohibit a sensor from use (e.g. in rain or high humidity conditions). Additionally, as the terrain becomes more complex, the air flow around that terrain also becomes more complex, requiring more sophisticated DT modelling to capture higher levels of detail (or fidelity). This higher fidelity results in an increase in the dimensionality of the modeling problem. Since environmental modeling can already be costly to undertake – high-dimensionality – added complexities from terrain and weather further increases the computational expense for the DT, limiting and or preventing the useful real-time capabilities. Of which is a core goal of smart sensing and this book.

This book offers a new way to look at the environmental sensing problem with sUAS by incorporating DTs and smart sensing frameworks. First, we integrate hybrid style modeling, allowing for near real-time computation, with advanced leak detection and quantification methods. Second, we investigate ‘where to sense’ through integrating multiple sUAS and quantified observability concepts. The combination of the two, enables smarter measurements and even allows for more simulation based testing to avoid unnecessary field work and controlled release testing (speeding up the development iteration cycle).

This book is designed and written for graduate students, researchers, scientists, field operators/drone specialists, industry experts, and policy makers in an introductory fashion. The book contains both high-level explanations and examples, as well as mathematical details for a general understanding. For the interested reader, the references included therein, are sufficient to fully understand and implement the techniques. To help foster the use of the topics covered in this book, a Github repository will be included, such that the reader can explore and play with the proposed DT framework. Unfortunately, due to non-disclosure agreements, not all of the data used to produce the results of this manuscript will be made publicly available. However, some of the controlled release data will be made available for use and reference.

The book is divided into two major sections or parts. The first major section will cover an introduction to the methane sensing problem, and the detection, localization, and quantification of methane emission sources with sUAS. The aim is to provide a general overview of these topics and give the important aspects related to each subproblem. Within each chapter, a 'Pause and Reflect' is included to help the reader think about how these topics can be expanded and also prompts the readers thinking for the next chapter section or chapter. A series of case studies are showcased at the end of the first major section, highlighting the experiments done, but more importantly, the observations made and lessons learned during the field experiments. The second major section will introduce the concepts of DTs and their use cases (include some case studies), as well as build up the concept of smart sensing, sensor placement and steering problem. The goal of this major section is to highlight how DTs can be leveraged to expand sUAS-based source determination problem method developments, but also embed smartness into the 'how to best sense' questions, with respect to observability or solving the inverse problem. At the end, we highlight some case studies on the topic of smart sensing before concluding with a summary of the book's takeaways, lessons learned, and the MOABS/DT code breakdown.

We wish to thank the funding support by the Center for Methane Emission Research and Innovation (CMERI) through the Climate Action Seed Funds grant (2023-2026) at the University of California, Merced. We also wish to thank MESA Lab members and many undergraduate researchers involved in various field campaigns. We wish to thank Dr. Lance Christensen of JPL for jointly starting methane drone detection project in 2014. This book grows out of the first author's 2023 Ph.D. dissertation with some new yet systematic developments included.

Last but not least, the authors would like to thank Ms Xiaoyin Feng, Books Editorial Assistant, Routledge & CRC Press, Taylor & Francis Group, for her professional coordination of the book project; Ms. Lian Sun, Publisher, Head of China Books Publishing and International Cooperation Taylor & Francis Advanced Learning for her professional vision and help in the peer review process.

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# List of Acronyms

| | |
|---|---|
| **ADE** | Advection diffusion equation |
| **ADMM** | Alternating direction method of multipliers |
| **AGL** | Above ground level |
| **AMFC** | Alberta Methane Field Challenge |
| **APEX** | Alaskan Peatland Experiment |
| **APRA-E** | Advanced Research Projects Agency-Energy |
| **AVIRIS** | Airborne Visible/Infrared Imaging Spectrometer |
| **AVIRIS-NG** | Next Generation AVIRIS |
| **BFGS** | Broyden-Fletcher-Goldfarb-Shanno |
| **bLS** | Backwards Lagrangian stochastic |
| **Bm** | Brownian motion |
| **CARB** | California Air Resources Board |
| **CFD** | Computational fluid dynamics |
| **CFL** | Courant-Friedrichs-Lewy |
| **CFP** | Cylindrical flux plane |
| **CFR** | Code of Federal Regulations |
| **CMERI** | Center for Methane Emission Research and Innovation |
| **CMI** | Concentration measurement instrument |
| **CRDS** | Cavity ring-down spectrometer |
| **CRF** | Controlled release facility |
| **CRLB** | Cramer Rao lower bound |
| **CVT** | Centroidal Voronoi tessellations |
| **D-CVT** | Density CVT |

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|---|---|
| **DE-CVT** | Density and entropy CVT |
| **DMD** | Dynamic mode decomposition |
| **DM+V** | Distribution modeling with variance |
| **DM+V/W** | Distribution modeling with variance and wind |
| **DT** | Digital twin |
| **EC** | Eddy covariance |
| **ECMWF** | European Centre for Medium-Range Weather Forecasts |
| **EDF** | Environmental Defense Fund |
| **EMI** | Electromagnetic interference |
| **EPA** | Environmental Protection Agency |
| **ESC** | Extremum seeking control |
| **fBm** | Fractional Brownian motion |
| **FFT** | Fast Fourier transform |
| **fGn** | Fractional Gaussian noise |
| **FID** | Flame ionization detector |
| **FIM** | Fisher information matrix |
| **FISTA** | Fast iterative shrinking-threshold algorithm |
| **FNO** | Fourier neural operators |
| **FOM** | Figures of merit |
| **FTIR** | Fourier transformed infrared |
| **GCS** | Ground control station |
| **GCV** | Generalized cross-validation |
| **GDT** | Gauss divergence theorem |
| **GHG** | Greenhouse gas |
| **GLM-VFP** | general linear model VFP |
| **Gn** | Gaussian noise |
| **GPM** | Gaussian plume model |
| **GPS** | Global positioning system |

| | |
|---|---|
| **GWP** | Global warming potential |
| **HOT** | High operating temperature |
| **IDW** | Inverse distance weighting |
| **IMAP-DOAS** | Iterative maximum a posterior differential optical absorption spectroscopy method |
| **IME** | Integrated mass enhancement |
| **IoT** | Internet of things |
| **IR** | Infrared |
| **ISTA** | Iterative shrinking-threshold algorithm |
| **JPL** | Jet Propulsion Lab |
| **LASSO** | Least absolute shrinkage and selection operator |
| **LDAQ** | Leak detection and quantification |
| **LDAR** | Leak detection and repair |
| **LGD** | Laser gas detection |
| **LGR** | Los Gatos Research |
| **LiDAR** | Light detection and ranging |
| **LTA** | Lighter than air |
| **LWIR** | Long-wave infrared |
| **MB** | Mass balance |
| **MCMC** | Markov chain monte carlo |
| **MCRWM** | Merced County Regional Waste Management |
| **METEC** | Methane emission technology evaluation center |
| **MGGA** | micro-portable greenhouse gas analyzer |
| **MLE** | Maximum likelihood estimator |
| **MMC** | Mobile Monitoring Challenge |
| **MMD** | Micrometeorological mass difference |
| **MMF** | Modeled mass flux |
| **MOABS/DT** | Methane Odor Abatement Simulator Digital Twin |

**MONITOR** Methane Observation Networks with Innovative Technology to Obtain Reductions

**MOS** Metal oxide sensors

**MOST** Monin-Obukhov similarity theory

**MSWL** Municipal solid waste landfill

**MUST** Mock Urban Setting Test

**MVPGR** Merced Vernal Pools and Grassland Reserve

**MWIR** Mid-wave infrared

**NASA** National Aeronautics and Space Administration

**NGI** Near-field Gaussian plume inversion

**NIR** Near infrared

**NSF** National Science Foundation

**ODE** Ordinary differential equation

**OGI** Optical gas imaging

**OGMP** Oil and Gas Methane Partnership

**OPLS** Open path laser spectrometer

**OTM** Other test method

**PD** proportional derivative

**PDE** Partial differential equation

**PE** Persistence of excitation

**PFP** Perimeter flight plan

**PG** Pasquill-Gifford

**PG&E** Pacific Gas & Electric

**PIML** Physics-informed machine learning

**PINN** Physics-informed neural network

**PI-RNN** Physics-informed recurrent neural network

**PI-VFP** Path integrated VFP

**pMGGA** prototype micro-portable greenhouse gas analyzer

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|---|---|
| **POD** | Probability of detection |
| **PSG** | Point source Gaussian |
| **PSG-CS** | Conditionally sampled PSG |
| **PSG-RB** | Recursive Bayesian PSG |
| **PSG-SBM** | Sequential Bayesian MCMC PSG |
| **PSI** | pounds per square inch |
| **QCLS** | Quantum cascade laser spectrometer |
| **QOGI** | Quantitative OGI |
| **QUIC** | Quick Urban and Industrial Complex |
| **RBF** | Radial basis function |
| **RF** | Radio frequency |
| **RMLD** | Remote methane leak detector |
| **RNN** | Recurrent neural networks |
| **SCFH** | Standard cubic feet per hour |
| **SciML** | Scientific machine learning |
| **SDE** | Stochastic differential equation |
| **SDK** | Software development kit |
| **SEM** | Surface emission monitoring |
| **SOTA** | State-of-the-art |
| **SPSA** | Simultaneous perturbation and stochastic approximation |
| **SR** | Sufficient richness |
| **STILT** | Stochastic time inverted Lagrangian transport |
| **sUAS** | small unmanned aircraft system |
| **SVD** | Singular value decomposition |
| **TCM** | Tracer correlation method |
| **TDLAS** | Tunable diode laser absorption spectrometer |
| **TI** | Turbulence intensity |
| **TVA** | Toxic vapor analyzers |

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|---|---|
| **UGGA** | Ultra-portable greenhouse gas analyzer |
| **UNEP** | United Nations Environment Programme |
| **USR** | Upwind survey region |
| **VFP** | Vertical flux plane |
| **VOC** | Volatile organic compounds |
| **VRPM** | Vertical radial plume mapping |
| **VTOL** | Vertical takeoff and landing |
| **WRF** | Weather research and forecasting |

# I

## From Detection to Quantification: sUAS-based Methane Sensing Techniques