MOABS/DT: Methane Odor Abatement Simulator with Digital Twins

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Abstract— **Digital twins (DT) are quickly being realized in many different applications for improving performance and adding intelligence. Depending on the application, the specific details of the DT may vary. For DT's of fluid systems, such as with fugitive methane emissions (containing millions of degrees of freedom), different numerical and reduced order modeling approaches are required for implementation. In practice, weather conditions and repeatability become an issue when evaluating detection and quantification strategies. This paper outlines a virtual evaluation center DT based on the Methane Emission Technology Evaluation Center (METEC) that aims to test quantification strategies under controlled virtual conditions, namely, the methane odor abatement simulator (MOABS/DT).**

Index Terms— **digital twins, methane emission, methane abatement, mobile sensing, simulator.**

I. INTRODUCTION

Methane emissions are important to care about for several reasons, namely, it is a powerful greenhouse gas (GHG) as compared to carbon dioxide, and the atmospheric lifespan of methane is much shorter than that of carbon dioxide. Therefore, reducing methane can yield significant short term benefits. The first step in the mitigation process, is making emissions measurements. There are, broadly speaking, two approaches: top-down (inventory based) or bottom up (site level). It has been shown that underestimation from top-down approaches vs bottom up [1], [2] can happen. There has also been global effort to reduce methane emissions by the Global Methane Initiative called the Global Methane Challenge. Other methane mitigation techniques have been explored through simulation, which rely on early detection and repair of larger leaks to achieve maximum reduction [3].

Traditional methods of methane detection in oil and gas are done on foot, such as with a flame ionization detector (FID), remote methane leak detector (RMLD) or optical gas imaging (OGI). Quantification of individual gas leaks typically can be done by bagging the leaking equipment and measuring the volume obtained in a specified time. This requires a full or partial shutdown of plant/equipment. Non-invasive approaches, static or using mobile vehicles, have shown great promise in detecting and grading leaks. For example, quantification of entire sites can be calculated using the tracer correlation method (TCM) or mobile TCM taken from measurements downwind of the source [4]–[6]. Drones have also been used to quantify emissions using mass balance based approaches from oil and gas sites [7]–[9], natural ecosystem emissions [10], [11], and from landfills [12]. Other drone-based quantification approaches, such as the near-field Gaussian plume inversion (NGI) [13] have shown promise. In a study at a landfill site, surface emissions monitoring (SEM), drone emission monitoring (DEM), and downwind plume emission monitoring (DWPEM) were compared to a GA-based estimation approach by [14]. A controlled release test site has been developed, as a part of ARPA-E funded effort, to evaluate new methane emission technologies, called methane emission technology evaluation center (METEC). In a recent single-blind study, drone-based technology performed quite well, with a detection limit of 1 SCFH [15].

Digital twins (DT) could be used to further improve some of these methodologies by providing smart insight and analytics [16]. This work introduces a conceptual framework for applying detection and quantification of fugitive gas emissions with digital twins. The paper is organized as follows: section II discusses the general details and implementation of the framework; section III gives a case study example of the digital twin for methane detection and quantification strategies; and section IV gives concluding remarks and future work.

II. THE DIGITAL TWIN FRAMEWORK

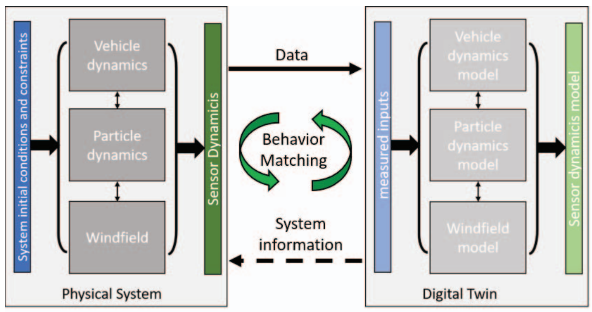

Fig. 1: The DT framework for environmental sensing [?].

What is a DT? In 2003 it showed up in a product lifecycle management course at the University of Michigan, taught by Michael Grieves [17]. His definition at the time was, "A digital twin is a virtual, digital equivalent to a physical product." The idea of having twins can be seen as far back as the NASA Apollo missions and their hardware twin of the rover. Alternatively, sometimes their can be a mixture of hardware and software, such as the 'Iron Bird' (e.g. flight simulator). The DT used here could be more general and we therefore use the definition from [18]: "A Digital Twin is the

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combination of multiple, individual, and detailed simulation models (continuous, discrete, hybrid), where its interconnection represents the dynamics of a complex system, which is updated periodically (windowed or real time) with the system information in order to reflect the system current status as well as predict its future behavior and possible faults."

Examples of DT used can be seen in industrial automation and process control engineering [19], [20], smart cities [21], discrete dynamics systems [22], and more. There are four basic levels of DT development. **Level 1 (L1)**: DT environment with no physical system. The systems do not interact and smart capabilities do not apply. Provides a preliminary design. **Level 2 (L2)**: DT environment is built based on physical system, with the physical system operating standalone. Systems interact in non-real time for data acquisition and do not have smart capabilities. Provides performance analysis and system status. **Level 3 (L3)**: DT environment with a monitoring interface and physical system operating in standalone with supervisory systems. Systems can interact with real time data acquisition and have limited smart capabilities. Provides data analytics, fault detection and prognosis. **Level 4 (L4)**: DT environment with a monitoring interface and physical system operating in closed loop with the DT virtual environment. Systems interact with real time data acquisition and have smart control. Provides data analytics, fault detection and prognosis as well as automated recommendations and actions for the physical system.

Generally, there are three main challenges with implementing a DT. The first, is subsystem modeling, which, includes: model fidelity (level of detail), numerical schemes (e.g. finite elements), multi-physics systems, multi-component systems and degradation of system components. The second, is sensor integration and data fusion. Challenges include: real time data acquisition for multi-physics and component level modeling, high computational cost, and varying communication protocols. Lastly, is behavioral matching, which makes the DT update parameters based on the physical system's behavior or feedback. This can be quite difficult if there is lack of system knowledge (e.g. mathematical realizations) and or problems are ill-posed.

There are five steps to constructing the DT. (1) Target system definition, which defines: simulation requirements, desired DT Level, controller requirements, system purpose and desired outcomes. (2) System documentation, which includes: control algorithms, sensor/actuator specifications, common problems/troubleshooting, data streams, types of signal processing and analysis. (3) Multi-domain simulation of: data-driven models, stochastic and probabilistic models, deterministic physics models, or some combination thereof (e.g. hybrid modeling). (4) DT assembly and behavior matching (choosing parameters for each DT subsystem in order to match its complete system dynamics and behavior with the real state of the physical system) (see Fig. 1), including: input and output communication between the DT and physical system; behavior matching in open or closed loop configuration; and choose suitable optimization strategies, constraints and cost functions. (5) DT validation and deployment by: validating behavior of digital twin in offline setting with multiple data sets; developing supervisory system for real time data management and visualization; real time parallel operation of DT and physical system in online setting; and online behavior matching deployment for smart DT capabilities (e.g. fault diagnosis and prognosis).

III. MOABS/DT CASE STUDY

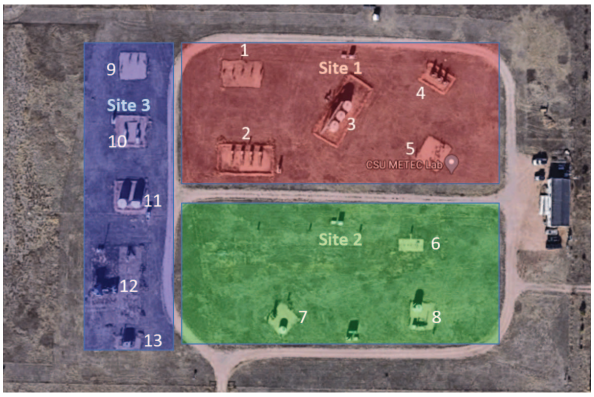

Fig. 2: A satellite image of the Colorado State University methane emission technology evaluation center (METEC), sub-divided into sites and equipment pads are numbered for simplicity in topology modeling.

In this section we outline a Digital Twin for use in reducing fugitive gas emissions by early detection and quantification, namely, methane odor abatement simulator (MOABS/DT). The real world site we choose to focus on is METEC (see Fig. 2), as it was designed for testing and evaluating new technologies as well as provides a benchmark for future research efforts.

The first step is the target system definition. We want the simulation requirements to be: create a digital representation of METEC that can simulate short time-scale behavior of emission dynamics and provide real-time or near real-time operation; create a L2 DT for analyzing performance of detection and quantification strategies; and conduct offline control of DT for studying how environmental variables impact behavior of the DT (such as source location, atmospheric stability, and surface topology). The overall purpose of the system is to connect a DT representation of a physical asset (i.e. METEC) for running virtual controlled release experiments.

The second step is to gather all the system documentation and known problems. Since direct feedback from the L2 DT is not applicable in this case study, control algorithms seek to perform analysis, in an offline sense. For example, the source location using measured data from sparse sensors throughout the field [23] and perform behavior matching using synthetic and real timeseries data [24]. The sensor used in this application is a tunable diode laser absorption spectrometer (TDLAS). This sensor makes point based measurements at 5Hz with sensitivities in the 10 ppb s^{-1} [25]. It is mounted out front of a multi-rotor aircraft (or drone) that actuates the location in space and time. The full state of the drone can be realized using the vehicle dynamics and motor inputs or treated as a subsystem in guided control mode with single or double integrator dynamics. One of the common problems with methane emissions is detection itself. Having good measurements of the local wind field is not generally possible, so in situ wind or static wind measurements are used to inform the operator of where to search (e.g. downwind and around equipment). Flying upwind and downwind of the source can be used to isolate leaking equipment or sections of a site. Multiple point source emissions are often difficult to distinguish using point based measurements, which include sources from adjacent sites that may drift into the measurement region through variable wind conditions. Utilizing on-board computers and WiFi based communication systems, data can be streamed to a local computer for feedback of the real system. Upon completion of physical data gathering process, the DT can be used to behavior match the system and exploit new methods of detection and quantification performance.

The third step in the construction is the multi-domain simulation. For this case study, there is a need to model diffusion and transport of the methane gas, as well as the model the dynamics of the wind field. Since these domains are governed by partial differential equations, namely, the advection diffusion equation and viscous Burger's equation, the computational cost can be quite high depending on numerical strategy. For these reasons, we adopted the 2D small time-scale filament model by [26], which stochastically treats the chemical transport at different length scales. The wind field is solved using an implicit finite differences approach [27]. The dynamics of the chemical sensor can be modeled with an effective sensor area and a low pass filter. The dynamics of the actuator (e.g. multi-rotor drone) can be modeled using single or double integrator dynamics as well. To extend the model to 3D power law scaling of the wind is applied [28]. The site topology can be modeled using simple geometric shapes defined at locations specified by the equipment pads (see Fig. 2). The interaction between topology and gas filaments can be implemented with a filament collision model.

The fourth step is the DT assembly and behavior matching. The DT is assembled by first connecting wind field model with the chemical filament dynamics and the collision model defined by the topology. Next, the interaction with the sensor and actuator models for measuring observations in space and time. Once the DT is assembled, the behavior matching to the physical system of interest can be done by calibrating simulation leak rates with observed timeseries concentration signals [24] (see Fig. 1). This is done with a training data set (a subset of the overall data gathered) that captures rich measurement data and knowledge of meteorological conditions (e.g. atmospheric stability [29]). These data sets have been gathered, in this example, through a series of survey flights that include: initial perimeter sweeps for detection of leaks, and mass balance flights for quantification of emissions (see Fig. 3).

The fifth and last step in the construction process, is the DT validation and deployment. The validation can be done by comparing the quantification results (previously unseen data) to the behavior matched DT (from step 4) in an offline setting. A well defined/trained DT will produce results suitable for prediction defined within the purpose of the DT. The DT can then be deployed to run in parallel with the physical system (see Fig. 4) gathering system wide data in the process (from static sensors or other mobile systems deployed). This opens up the possibility to perform online behavior matching of parameters, ultimately, providing estimates to key parameters (such as source location [23]) for smarter path planning as well as improving quantification efforts [30].

IV. Conclusions

As we continue to use energy sources such as natural gas in our homes and methane emission reduction continues to be an focus in society, there will always be a need to detect and quantify emissions for repair and validation. This work proposes the use of DT's for improving and testing the limitations of advance leak detection and quantification techniques. Improving accuracy and frequency of surveys that can lead to reductions in overall emissions. The DT provides a way to cost effectively test techniques and optimize approaches. The DT can also provide an added layer of intelligence for site performance and smarter path planning. Additionally, if component level DT's are incorporated within the site equipment (valves, tanks, etc.), prognosis features such as remaining useful life (RUL) can be applied. Using analytics such as RUL, the frequency of surveys can be prescriptively increased for areas near the failure limit.

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(a) (b) (c)

Fig. 3: (a) Site level emission survey and quantification from METEC using TDLAS equipped drone. (b) The survey begins with a perimeter flight to identify leaking equipment. (c) Once a leak is identified the quantification can be done using downwind and upwind mass balance flights.

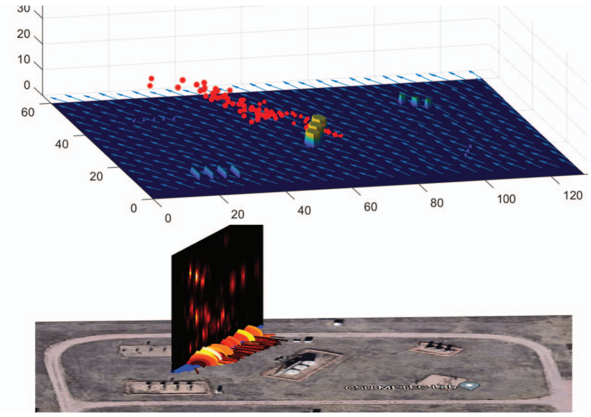

Fig. 4: Running the DT in parallel with the physical system, the dynamics of the gas filaments are being lofted into the air due to the cylinders on equipment pad 3 at site 1 (top). The physical observations seen from experiment and calculated with the mass balance (bottom) reflect those in the DT.

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