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Current Project Overview

Mechanistic Air Emissions Simulator (MAES) is a software tool to estimate emissions at oil and gas facilities. Earlier versions of the toolbox were called Methane Emission Estimation Tool (MEET) [1], [2]. Current GHG inventories provide a yearly aggregated emissions rates of emissions at the facilities, while assuming all the facilities are similar. MAES is a toolkit that provides variation in emissions and produces a timeseries of emission estimates. Each piece of equipment at a facility has its own mechanistic model along with relevant corresponding emission models. Mechanistic models are stochastic in nature and provide causality effects within and between models. To model mechanistically, we follow a specific series of steps. First, we understand the physical processes in an equipment, and second, we translate them into finite state machines. These state machines represent equipment on facilities, and the states represent major processes of the equipment. Discrete Event Simulation (DES) is the method we use to simulate these state machines through a specified amount of time. Emission models are separate models that represent the emissions occurring on the equipment at a particular state. These models utilize inventory available emission and activity factors to estimate emissions in a timeseries. Some of the emissions are modelled mechanistically. For example, when there is a stuck dump valve in a separator, some gas slips into tanks and creates an overpressure situation in tanks leading to a pressure relief valve popping open. These emissions can be traced back to production from wellpads. This causality of processes in MAES is the main feature of mechanistic modeling.

Research Progress

Five modelling tasks have been completed since Summer 2023. They include:

1. Compressor overloads and throughput dependent exhaust emissions: Compressor load in MAES used to be calculated by rated power which is defined in the input study sheet. This is not appropriate because the loads on the compressor vary depending on the throughput vapor flows. To solve this issue, we developed an update in the compressor model to determine the fuel consumption in the compressor. First, we calculate the load which is a function of throughput flow, compressor efficiency, and change in enthalpy between compressor and separator. If this load is greater than compressor rated power, we have an overload state. Second, we get the fuel consumption which is a function of the calculated load and power equations. Power equations are a derived from compressor data sheets that contain the transformation of load to fuel consumption. Mercy Ngulat, another graduate student in the Zimmerle group, worked on developing the power equations.

2. Switching tank emissions from mechanistic to emission factors: For midstream facilities, we may choose to switch to emission factor models for tanks. For the mechanistic model, we need separators to be stuck so that we get overpressure vents.

3. Rearrangement of emissions factors by facility type: The curated data directory has been rearranged to classify factors based on facility type: Production, Midstream and Common. Common refers to facilities where both production and midstream factors are used.

4. A new continuous separator model with multiple phases: A new model has been developed that contains asynchronous dump valves on a continuous separator. To model this, we designed three separate models each for condensate, water, and vapor phases. This will allow the fluid flows to be flexible to individual dump valves. Each of the phases have their own sub-state machines that will be logged in the output event list. These three models are wrapped by main separator model that will allocate state change and state duration calculations to phase models. The main separator model has its own state machine that is dependent on sub-states from the phases. If we have at least one STUCK-DUMP-VALVE state, the main state will be STUCK-DUMP-VAVLE. Appropriate fluid flows will also be logged in the event list.

Modelling tasks completed in Spring 23:

1. Heaters model: Heaters are modeled with combustion emissions based on inlet vapor flows. This model can be inserted between any equipment where heaters are used. Heaters do not have any derived flows except for combustion emissions.

2. Continuous and Intermittent Pneumatics: Two new models have been developed for pneumatics. These can also be inserted between equipment with no derived flows. To develop this model, we determined the behavior of pneumatics from the Gathering Emission Factor (GEF) field study [3]. This behavior has been translated to two separate state machines for continuous and intermittent pneumatics.

Continuous pneumatics will always be emitting. Some will be low bleed and others will be high bleed. Here, low bleed refers to pneumatics emissions with low emission rates, and high bleed refers to pneumatic emissions with relatively higher emission rates. The emission factors for low and high bleed have been developed from GEF data. The behaviors modeled in continuous pneumatics are normal emissions, abnormal emissions, and not operating. Each of these behaviors have their own emission models that switch based on Mean-Time-To-Repair (MTTR) determined in the input study sheet.

For intermittent pneumatics, the behaviors modelled are intermittent vent, abnormal venting, waiting for actuations, and not operating. Abnormal venting in intermittent pneumatics is defined by the U.S. EPA as any intermittent emissions that last longer than 3 minutes. The durations and pLeak of these emissions are determined in the input study sheet, where pLeak is the probability of a component leaking at any time. This model also has an appropriate factor tag that is used in switching between emissions in each state. Intermittent pneumatics act intermittently, i.e., depending on actuations (state change) in upstream equipment. Thus, the emission factors must also have a distinction between 'waiting' emissions and 'vent' emissions. Crude emission factors for this purpose have been developed using GEF data, but more work is needed to develop these factors.

MAES also can add pneumatic counts for each of these models. They will behave like individual equipment models rather than emission models when logging-in event lists. We can allocate fluid flows to any of the pneumatics from the pneumatic count. MAES uses mechanistic causality when using fluid flows for pneumatics.

Research Plans

1. Compressor model lacks the scaling of rod packing and blowdown emission factors based on the size of the compressors. The scaling is done offline currently, which creates a lot of derived emission factor files. To reduce the file sizes of these factors and to make MAES more capable of handling sizing requirements, a new update must be developed to scale these factors online.
2. Implementing a new dehydrators model that will have scaled emission factor calculations.
3. An implementation of screw compressors with dry and wet seal types.
4. Heaters that have mechanistic emissions based on weather.
5. Develop better emission factors for intermittent behavior of the intermittent pneumatics.

Publications

Currently writing my first paper.

Literature cited

[1] David T. Allen, Felipe J. Cardoso-Saldaña, Yosuke Kimura, Qining Chen, Zhanhong Xiang, Daniel Zimmerle, Clay Bell, Chris Lute, Jerry Duggan, Matthew Harrison, A Methane Emission Estimation Tool (MEET) for predictions of emissions from upstream oil and gas well sites with fine scale temporal and spatial resolution: Model structure and applications, Science of The Total Environment, Volume 829, 2022, 154277, ISSN 0048-9697, https://doi.org/10.1016/j.scitotenv.2022.154277.

[2] Daniel Zimmerle, Gerald Duggan, Timothy Vaughn, Clay Bell, Christopher Lute, Kristine Bennett, Yosuke Kimura, Felipe J. Cardoso-Saldaña, David T. Allen, Modeling air emissions from complex facilities at detailed temporal and spatial resolution: The Methane Emission Estimation Tool (MEET), Science of The Total Environment, Volume 824, 2022, 153653, ISSN 0048-9697, https://doi.org/10.1016/j.scitotenv.2022.153653.

[3] Luck, Ben & Zimmerle, Daniel & Vaughn, Timothy & Lauderdale, Terri & Keen, Kindal & Harrison, Matthew & Marchese, Anthony & Williams, Laurie & Allen, David, (2019), Multi-day Measurements of Pneumatic Controller Emissions Reveal Frequency of Abnormal Emissions Behavior at Natural Gas Gathering Stations, Environmental Science & Technology Letters, 2019, 6, 6, 348–352, https://doi.org/10.1021/acs.estlett.9b00158.

[4] Picture credit – Prajay Vora, Compressor at METEC facility.