Advanced Computational Methods for Modelling, Sensitivity Analysis, and Optimization of VOC Emissions in Cargo Tank Systems

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(1) – Introduction

- Methane and other Volatile Organic Compounds (VOC) [4] emitted during storage, loading, and transport of crude oil and condensate represent a growing environmental and operational concern.
- Industry faces tightening regulations in terms of reporting to be able to operate. They also require capable tools to aid in decision making and planning process operation in order to increase efficiency while lowering emissions.
- Existing tools are not feasible to extend to meet all current and future needs of the industry.
- A new modelling and analysis tool is needed in order to satisfy these demands.

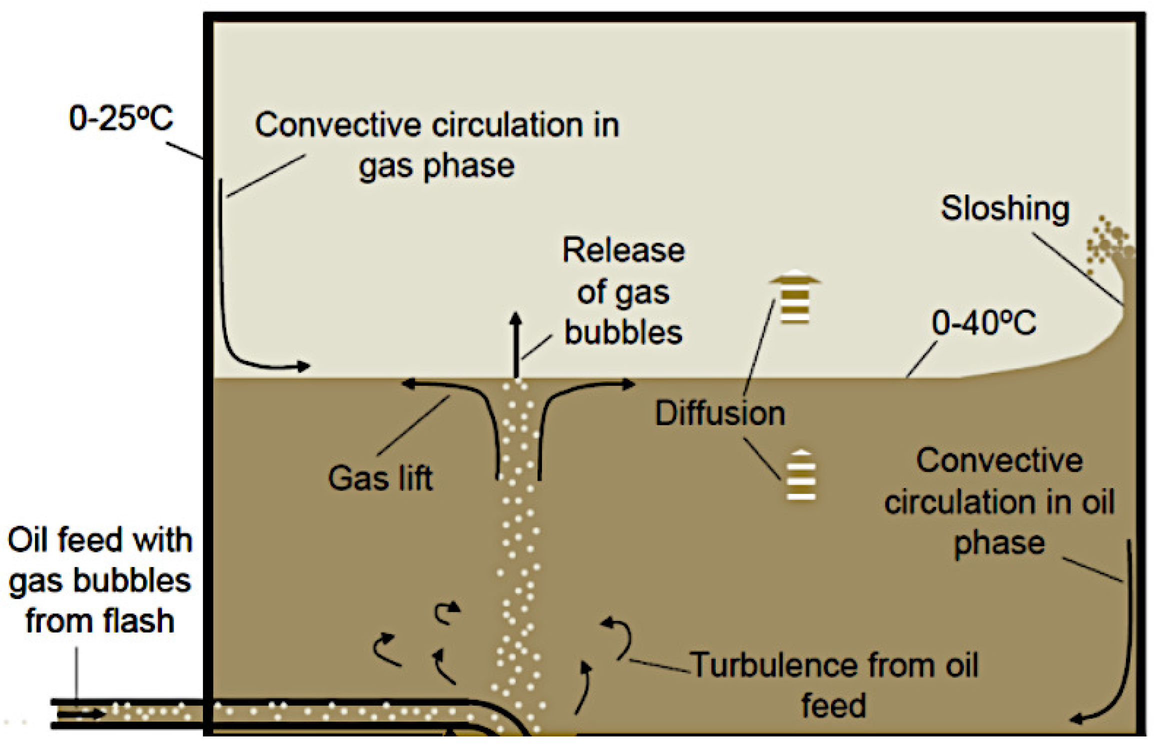


Figure: Illustration of VOC transport mechanisms (figure from [2])

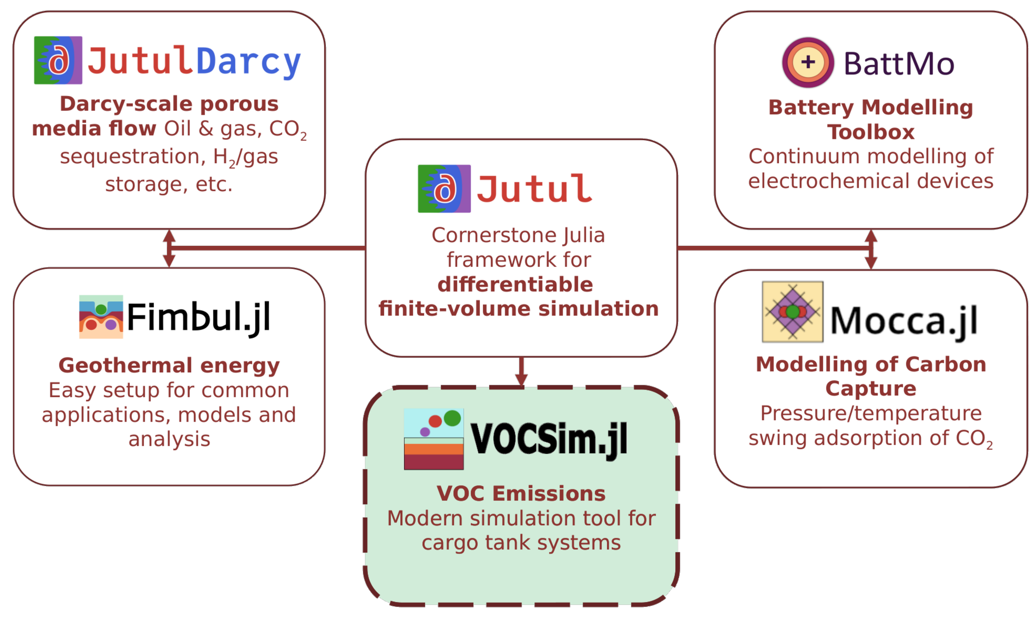
(2) – VOCSim.jl

The solution – VOCSim.jl

- VOCSim.jl will be a modern simulation tool made from the ground up to solve both current and future problems faced by industry.
- It should be accurate, easy to extend with new modelling, sufficiently performant, and be able to perform complex optimization tasks and sensitivity analysis. It should also be capable of leveraging available data to improve modelling capabilities.
- VOCSim.jl will be written in Julia, a modern programming language aimed at computational science. Julia has a rich ecosystem of libraries which are openly available. While being performant, it also provides scripting capabilities which makes rapid prototyping simple.
- Further, VOCSim.jl will be based on Jutul.jl, which provides a lot of powerful functionalities for developing numerical simulators.

(3) – The Jutul.jl Framework

- Jutul.jl [5] is an open-source Julia framework for high-performance, fully implicit finite-volume simulation, designed from the ground up to be fully differentiable.
- It leverages automatic differentiation (AD) [1] to enable end-to-end differentiation of complex implicit finite-volume multiphysics simulations. Adjoint [3] (backward) simulations allow for computation of sensitivities of simulator outputs with respect to inputs.
- Several Jutul-based simulators have been (and are currently being) developed for a range of different application areas, e.g., for simulation of reservoirs, geothermal energy, batteries, and carbon capture.



(4) – Physical Modelling

There are many physical processes involved in the modelling problem, including, but not limited to:

- Transport of components in the cargo tanks
- Mixing due to sloshing of the liquid
- Phase-change on the liquid-vapour interface
- Coupling between tanks through pipes and valves
- Inflow of liquid and outflow of gas
- Heating from tank walls

It is unfeasible to resolve the full 3D problem with multiple tanks and time scales potentially on the order of days for industrially relevant cases. We first need to simplify the problem to solve it.
→ We make the assumption that we can model transport of fluid in the tank as a vertical 1D problem, and that unresolved effects can be modelled using effective parameters.

Equations

Advection-diffusion transport equations for the different components in 1D can be written as

$$\frac{\partial C_i}{\partial t} + \frac{\partial (C_i v)}{\partial z} = \frac{\partial}{\partial z}\left(D_i \frac{\partial C_i}{\partial z}\right) + q_i, \tag{1}$$

which are solved within both the liquid and vapour phases. The height of the liquid/vapour interface can be tracked using conservation of mass, considering varying liquid density. A separate equation needs to be solved in each phase to calculate fluid temperature, i.e.,

$$\frac{\partial (\rho c T)}{\partial t} + \frac{\partial}{\partial z}(\rho c v T) = \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right) + Q. \tag{2}$$

We can use an equation of state, e.g., The Soave-Redlich-Kwong (SRK) given by

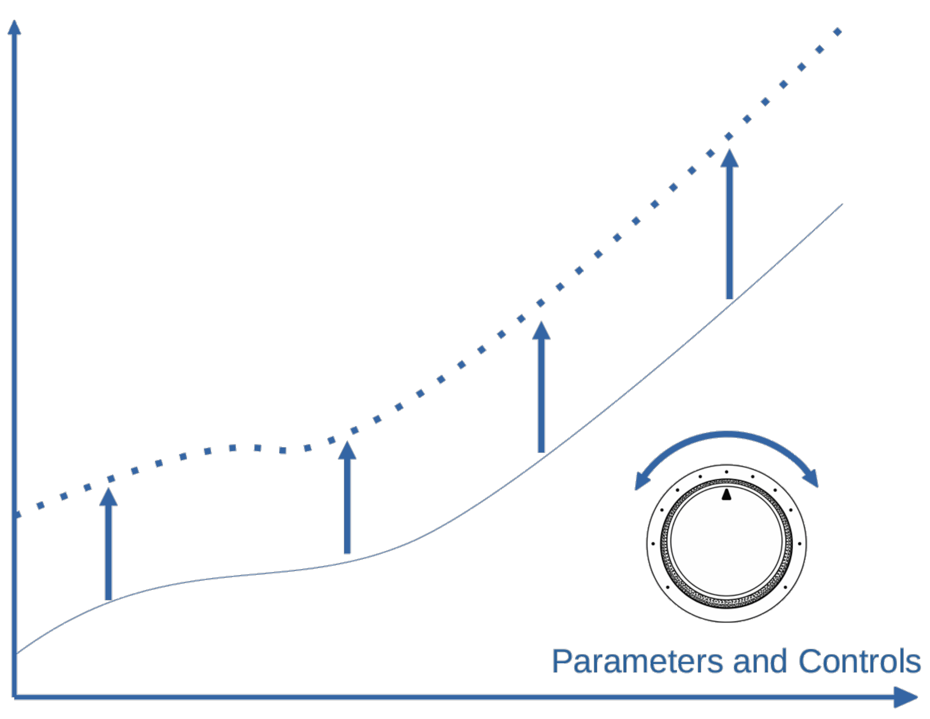
$$p = \frac{RT}{V_m - b} - \frac{a\alpha}{V_m (V_m + b)}, \tag{3}$$

to calculate the vapour-liquid equilibrium at the interface.

C_i	– Concentration of component i
v	– Bulk flow velocity
t	– Time
z	– Vertical coordinate
D_i	– Effective diffusivity
q_i	– Inflow & outflow
c	– Mixture specific heat capacity
ρ	– Mixture density
T	– Fluid temperature
k	– Mixture thermal conductivity
Q	– Heat source from surroundings
p	– Pressure
R	– Universal gas constant
V_m	– Molar volume
α	– SRK Correction factor
a, b	– SRK parameters

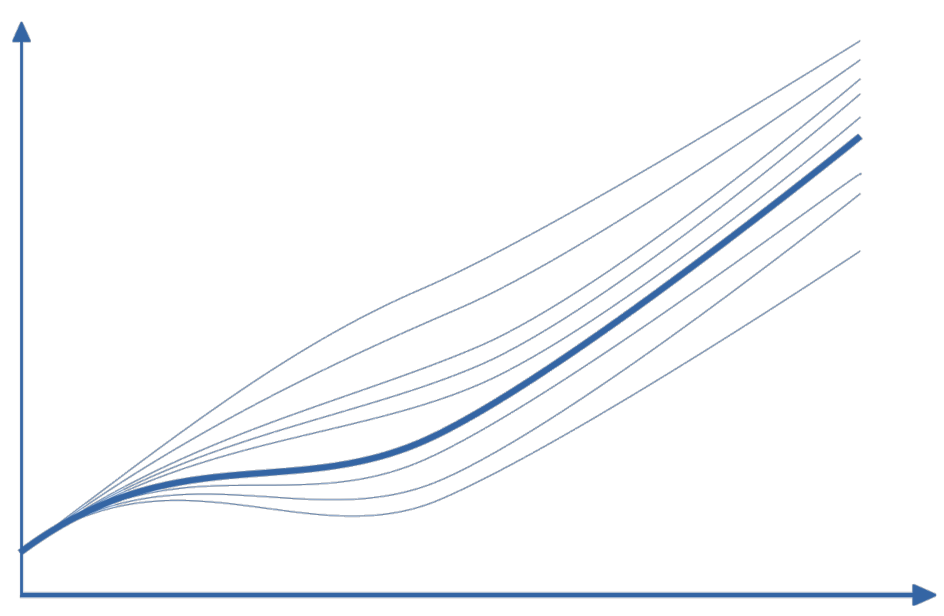
(5) – Optimization and Calibration

- We are able to leverage AD and adjoints to do efficient Gradient-based optimization.
- This means that we can tune simulation parameters and process controls in order to maximize/minimize some objective.
- The optimization framework provided by Jutul.jl is highly flexible, allowing for optimization of any simulator input parameter using fully customizable objective functions.
- Calibrating the simulator parameters using available measurement data is also available through history matching.



(6) – Uncertainty Quantification

- There are several uncertainties when modelling this complex system. Many of the physical parameters are difficult to measure exactly, and small changes in them may significantly change the system response. In addition, the system needs to be simplified to a point where we are able to solve it with reasonable time and computational resources. This introduces modelling uncertainties which also affect our simulation results.
- Uncertainty quantification (UQ) techniques will be employed in VOCSim.jl in order to study and quantify how the problem uncertainties affect the simulation results. This will aid in decision-making processes where it is important to know the degree of trust that can reasonably be placed on the results.



(7) – Hybrid Modelling

- VOCSim.jl will integrate machine-learning (ML) models into the computational pipeline. We refer to hybrid modelling as combining data-driven models with more conventional computational techniques, e.g., numerical solutions of PDEs.
- Examples of where ML models can be relevant are when physical relations are unknown, or when the relations are known but expensive to compute.
- We have access to existing relevant measurement data from real operational processes, which we can use for training and validating the ML models. Additional data will also be collected throughout the project.

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