# Mini-Project: Mathematical modeling and simulation of Methane gas production.

## Mathematical Model

We have the following model to simulate the production of methane and carbon dioxide:

$$\frac{d\mathbf{u}}{dt} = \mathbf{F}(\mathbf{u}, \mathbf{X}) \qquad \text{on } [0, T], \tag{1}$$

eq:Math_Model

where

- $\mathbf{u} = (u_0, u_2, ..., u_7)$ are the states. In particular, the last two states represent the methane and carbon dioxide concentration levels.
- $\mathbf{X}$ are the parameters such as moisture, decay rate. More details of the parameters can be found in Table 2 of [1].
- Details of $\mathbf{F}$ can be also be found in [1].

## The Algorithm

**Algorithm 1:** The general algorithm to numerically solve (1)

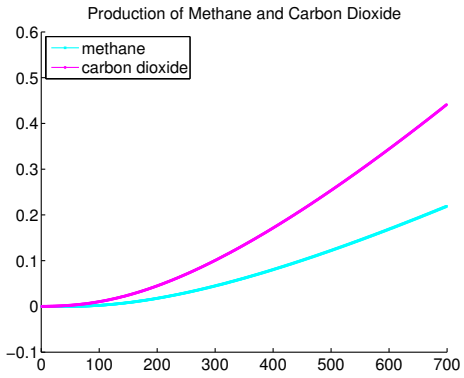
Set $t_m = t_0$
Compute $\mathbf{u}(t_m)$
Precompute the time independent parameters $X$
Fix the time stepsize $\tau_m = \tau_0$
**while** $t_m < T$ **do**
    Compute $\mathbf{F}(\mathbf{u}(t_m), X)$
    $t_{m+1} = t_m + \tau_m$
    Solve ODE at $t_{m+1}$ for $\mathbf{u}(t_{m+1})$
**end**

The step Solve ODE involves replacing the derivative $\frac{d\mathbf{u}}{dt}$ in (1) with an approximation for example a finite difference approximation.

## Parameters chosen

We start with the initial conditions provided from the actual experiments [1] for reactor R1. We document the results for time domain $t_0 = 0$ and final time $T = 700$ days with the timestep size $\tau_m = 1$.

## Results




## References

### Tasks for this week

1. One of the main goals of this class is to model a scientific process through a mathematical model. Please consider the provided code `ode_solver_0.cpp`. The main goal of this program is to convert the data of the problem into arrays. Your first task is to initialize the concentrations of $\mathbf{u} = [\mathbf{6.25},\ \mathbf{0.4},\ \mathbf{0.4},\ \mathbf{0.4},\ \mathbf{0},\ \mathbf{0},\ \mathbf{0}, \mathbf{0}]$ and set up the right hand side function $\mathbf{F}$.
   At every stage you are cautioned to be a careful / defensive programmer. So please, keep testing your code for robustness.
2. Once we have initialized $\mathbf{u}$ and set up the right hand side function $\mathbf{F}$, we need to put the **Algorithm 1** in the code.

`math_model_ref`

[1] Sandeep Pareek, Saburo Matsui, Seog Ku Kim and Yoshihisa Shimizu *Mathematical modeling and simulation of methane gas production in simulated landfill column reactors under sulfidogenic and methanogenic environments*. Water Science and Technology, Volume 39, Issue 7, 1999.