Prediction of turbulent reactive flows by means of numerical simulations applied to anaerobic digesters

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Anaerobic digestion

- Organic matter degradation, in the absence of O₂, to obtain biogas
- Feed: sludge (from WWTP) or manure/waste from agriculture activities
  - Stabilisation of sludge
  - High energetic product value
  - Reduction in sludge volume
  - Destruction of pathogens
  - Odour reduction
  - Economic benefits
  - Slow reaction rates
  - Vulnerable to various inhibitors
  - Low COD removal
  - Tight process control

Role of mixing

- Good Mixing = homogeneous properties
- Currently, there is no consensus about the role of mixing and its effect on the anaerobic digestion performance

PhD Roadmap

1. Methodology
   - Use of Computational Fluid Dynamics (CFD) to obtain spatio-temporal knowledge
     - Complex fluid matrix → Challenging modelling
     - Select proper models to describe accurately the system

2. How do we model turbulence/mixing inside the bioreactor?
   - Test different turbulence models and select the best one in terms of accuracy/computational cost
     - RANS: Standard, RNG, realizable k-ε, standard k-ω, RSM, ...
     - LES (Large Eddy Simulation)
   - Validation:
     - Compare to experimental and/or benchmark data

3. How do we model the sludge rheological behaviour?
   - Sludge behaves as a non-Newtonian fluid → Apparent viscosity
     \[ \tau = \eta \cdot \dot{\gamma} \]
   - Select model which is valid for the shear rate range inside the bioreactor

4. How do we model the conversion from substrates to products?
   - Select simple models and increase in complexity
     - Empirical correlations to obtain CH₄ yield
     - AMD1 model (most complex model)
   - Test the influence of the hydrodynamics on the biokinetic performance

Biochemistry

- Sludge (complex particulate waste)
- Hydrolysis
- Soluble organics (sugars, amino acids, LCFA)
- Acidogenesis
- Acetogenic
- Methanogenesis
- CH₄ + CO₂

Problems

- Complex microbiology: different optimum working conditions
- Inhibition: pH, alkalinity, NH₃, H₂, VFAs, etc.
- Disruption of methanogenic activity!
- Non-ideal hydrodynamics:
  - Short-circuits (lower SRT)
  - Dead zones (lower Volume)
  - Mass/heat local gradients
  - Stratification (different densities)