Environmental Biotechnology Network (EBNet)

Report of the workshop on:

Sludge modelling: best practice, challenges and opportunities

Hosted by the EBNet Engineering/Biology theme

Novotel Hotel, York, 4 - 5 December 2024

Workshop participants

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All delegates are grateful for the financial and logistical support provided by the Environmental Biotechnology Network in relation to this event.

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Executive Summary

Recent years have seen an increase in the development of approaches to modelling the flow and mixing of sludge amongst a relatively small group of academic researchers.

The modelling of sludge flow is complex, being a non-Newtonian fluid phase with an entrained solid phase, often mixed by injected gas bubbles over time periods of days. Recent developments have extended the modelling techniques which now encompass lattice Boltzmann approaches as well as finite volume computational fluid dynamics (CFD). The challenge of coupling a biokinetic model with a hydrodynamic model to optimise mixing remains an open question. Other challenges include the heterogeneity and spatial and temporal variations in sludge quality, and the multiscale nature of mechanisms and processes at play.

Sponsored by the Environmental Biotechnology Network and falling within the remit of its Engineering / Biology theme which considers interactions between microbial and engineering factors, this two-day workshop brought together sludge flow modellers with microbiologists and end users to discuss best practice, challenges and opportunities in sludge predictive behaviour from both a flow and biogas generation perspective. Specifically, the workshop considered the following questions:

1. Who is doing what, where and what are the recent innovations?
2. What are the challenges? What is preventing developments in certain areas?
3. What is, or might be, the role of AI / ML / NN in sludge modelling?
4. What does the industrial community want from sludge predictive behaviour?
5. How can we develop, drive and sustain a national or international sludge predictive behaviour network?

The key R&D priorities arising from the workshop are summarised as:

Modelling:

- The need to link microbiology and CFD with an improved understanding of the biology of AD systems
- Consideration of AD as a system comprising: operations, storage, emissions, varying electricity prices, energy usage.
- AI-enabled individual models
- Parameterising the biology to apply to a CFD model – i.e. achieve a 6% feed and 3% product in a model
- Compartmentalise mixing in reactors – how achievable is this in practice?

Operations:

- Asset optimisation with limited budget and reduced staffing levels.
- Reducing secondary emissions
- Maximising gas production and minimising energy use
- Addressing the feedstock – *i.e.* tailoring the feedstock to maximise gas production

Data:

- Accurate sludge characterisation to drive change in sludge management – which parameters?
- Quick and accurate sampling techniques

Sludge modelling: best practice, challenges and opportunities

Introduction

This report presents a summary of a workshop on sludge modelling run by the Environmental Biotechnology Network (EBNet, www.ebnet.ac.uk). The goal was to discuss best practice, chal- lenges and opportunities in sludge predictive behaviour from both a flow and biogas generation perspective and then to identify key questions and areas for further research activity which would be of most value to industry.

The workshop drew delegates from academia and industry whose expertise covered biological sciences and microbial ecology, slurry mixing, decision-making, multiphase computational mod- elling, reactor design and operation, and sludge management.

EBNet's proposal for a workshop on sludge modelling came from its Engineering / Biology theme which seeks to develop and improve technology for pollution control, resource recovery and bioenergy generation.

Workshop process

The workshop took place over two days on 4th and 5th December 2024 at the Novotel hotel, York. Delegates were invited to participate based on discussions and recommendations from the two work- shop co-convenors.

The event started with introductions and brief descriptions of experiences and motivations for attending the workshop in order that all delegates became acquainted with one another.

There followed a session led by Dai and Taylor on **current issues with anaerobic digestion in the water industry**. Key points identified:

- Sludge to land is always at risk, a risk heightened by issues such as PFAS, AMR and microplastics.
- Improvements need to be made in technology to improve sludge digestability.
- Hydrolysis is the rate-limiting step in anaerobic digestion (AD), and thermal hydrolysis is ex- pensive.
- Sufficient, reliable mixing is a major issue for AD performance. Historically, mechanical mixing has been avoided in Yorkshire Water (and elsewhere in the UK) because of the hostile environment in which impellers are required to operate.
- Grit accumulation detrimentally affects digestion and biogas production whilst also causing wear to pumps and heat exchangers.
- Management of primary and secondary sludge in combination or separately is challenging.
- The production and presence of vivianite and struvite hinder gas production and cause scaling issues, respectively.
- From a research perspective, digestion reactors do not appear to scale from laboratory to site.
- The Industrial Emissions Directive places additional burden on the operation of digesters, par- ticularly with regard to methane and ammonia.
- Data requirements for enhanced AD performance remain unknown or unachievable.

Following this, Wicks and Dapelo gave presentations on **current computational fluid dynamics (CFD), Lattice Boltzmann Modelling (LBM) and microbiological modelling approaches for the water industry**. Key points identified:

Current position:

- Liquid phase: Non-Newtonian fluid
  - Power-law
  - Herschel-Bulkley
- Bubbly phase: Lagrangian particles
  - Two-way coupling
  - Bubbles modelled as pointwise spheres
- Assumes ‘complete mixing’ is the target (CoV ¡ 0.05)
- Ignore thixotropy, sedimentation and variation within the digestion process
- No chemistry
- Mostly compares the efficiency of mechanical or gas mixing options, or the benefits of intermit- tent (or dynamic mixing)
- Tracer residence time distribution (RTD) curves provide insight, but not flow patterns

Challenges:

- Multiphase modelling (liquid, solid, gas)
- Recirculation of gas bubbles
- How best to model the non-Newtonian sludge?
- How best to model the thixotropic sludge?
- How do geometry and mixing strategy influence the details of the flow patterns?
- Dead zone locations
- Dimensional analysis / scaling is tricky:
  - Flow in full-scale vessels is transitional
  - No-mix full-scale digestion fails; lab-scale does not
- Lab-scale for numerical validation only
- Sludge is opaque, making flow visualisation challenging

State-of-the-art:

- ADM1: Batstone et al, Wat Sci Tech, 45, 65-73 (2002) – the generalised anaerobic digestion model created by the IWA Digestion Modelling Task Group [1]
- Some limited progress including these in CFD, but yet to see the same impact as ASM1 and ASM2 in CFD models of Activated Sludge plants.

In a presentation on his **experiences and modelling approaches beyond the water industry**, Dogbe described the challenges in the scaling of battery slurry mixing processes. Dogbe highlighted the issues associated with the prediction of mixing time in small scale processes and provoked an interesting debate around the transition from laminar to turbulent flow characteristics at small scale.

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This was followed by presentations from Chong and Curtis in which they reflected on **approaches to, and limitations of, modelling engineered biological systems**. Here, Curtis provided a helpful introduction to multi-scale modelling of microbial communities, ranging from genomes (nm), cells (μm), mechanistic Individual-based model of microbial communities at the mm scale to CFD modelling at the scale of metres.

Curtis introduced the work of Sloan et al, 2006 [2], in which it was shown that show, for a wide range of prokaryotic communities, the relative abundance and frequency with which different taxa are observed in samples can be explained by a stochastic, birth–death immigration process and that in a community of N_T bacteria within which dead individuals are replaced by immigrants from a source community with probability, m, $N_T m$ must be approximately constant. Curtis also discussed the effective community size, (N_{EC}), this being the size of community to explain the diversity held by the system, which is actually very small in comparison to the actual community size. Curtis emphasised that diversity does not scale with the size of reactor.

Curtis also discussed the use of multivariate dynamic emulators, and, quoting the work of Coughtrie [3] (in which a new photosynthesis-nutrient model was coupled with a CFD gas-lift bioreactor model), described how modelling can be taken from Individual-based (IB) modelling, through emulation to large scale modelling, and the clear benefits that emulators offer (e.g. 1000x increase in speed).

Using data obtained from full scale sites, Chong demonstrated that there remains much about the microbiology of anaerobic digestion plants which is poorly understood but nevertheless, if the en- vironment is controlled, then the outcome is often predictable. Chong also described the challenges faced in the development of an effective synthetic anaerobic digestion community – *e.g.* How many species?, Does the community survive? Is frozen as good as fresh? What grows? What's required?, Is synthetic as good as natural? Is synthetic resilient? What about phage? On the subject of frozen vs unfrozen, Chong showed interesting data indicating enhanced cumulative gas production for fresh vs frozen communities over 40 days, but they converged thereafter. Interestingly, although commu- nities subject to a freeze-thaw process had an initial gas production rate that was lower than fresh over the first 25 days, the two rates became approximately equal thereafter until 35 days at which point the fresh rate plateaued. Concerning abundance and resilience, Chong made the point that multiple organisms can achieve the same level of performance in a reactor, and showed several im- ages conveying the variation in species abundance.

End of day 1

Following a discussion on key points arising from the previous day, Day 2 began with a session from Short and Dapelo who provided presentations on **the role of AI, ML and NN in anaerobic di- gestion**. Of particular note was Short's description of his group's work on the development of mathematical optimisation tools to create software for automated optimal sustainable, process design. Specifically focussing on AD, Short described non-confidential outputs from the EPSRC 'Artificial Intelligence Enabling Future Optimal Flexible Biogas Production for Net-Zero' project undertaken by the Universities of Surrey, Southampton, Manchester, and Nottingham to create digital solutions for anaerobic digestion using artificial intelligence, site-wide optimisation, experimental programmes, life cycle assessment, and microbial community characterisation. Short also described the work of Koksal et al (2024) [4] in which standard and physics-informed neural networks were used to predict dissolved oxygen concentration in activated sludge, recognising the importance of physics-informed modelling when standard modelling is insufficient, but equally recognising that it may not be necessary when standard modelling produces an adequate result.

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Dai, Taylor and Wicks then all contributed to a session on **what does industry want from modelling?**

It was agreed that the primary goal for the water industry is to maximise biogas production alongside a reduction in energy costs for its production; that is, improve mixing strategies and design to decrease input energy mixing whilst maintaining, or even enhancing the digestate quality and biogas yield. There followed a discussion on the need for mixing in AD and how it might be achieved. Key points arising:

To Mix Or Not To Mix?

- Mixing brings substrates in contact with microbial communities
- Without mixing, the process fails (in full-scale; not necessarily in lab-scale)
- Energy-consuming (17-73% of overall digester consumption)
- Inconsistency in operational practice, *e.g.* some plants mix for 10 min per hour, some plants mix continuously
- Attempting to achieve perfect mixing conditions is a costly exercise. Is it necessary?
- AD reactors exhibit a shear distribution which affects nutrient and substrate concentration gradients and their contact time.
- Fermentation processes require a period of local quiescence, therefore are intermediate levels of mixing required. If so, what does that mean?
- Modelling requirements: non-Newtonian viscosity, nutrient chemistry and biogas production calculations from first principles.

Working from the premise that industry requires an accurate, first principles, biogas production prediction model, Wicks proposed that the flagship AD mixing model would include:

- Incorporation of an ADM1 (or ADM1-lite) model (including nutrient chemistry, methanogens and biogas formation)
- Non-Newtonian viscosity/shear relationship changing over time during a digestion cycle (in- corporating a first principles determination of rheology and the viscosity/shear curve from dry solids/substrate content) to be delivered via a three-stage approach:

i ADM1 inclusion (initially assuming non-Newtonian properties remain unchanged during diges- tion)

ii Development of a first principles viscosity-shear relationship for a two-phase sludge system

iii Combination of (i) and (ii) and subsequent comparison of mixing options vs biogas production at full scale from first principles.

Following the conclusion of the presentations, there followed an extended discussion on where the research opportunities lay, what the funding opportunities may be, and what the experimental needs to support modelling were. These are summarised inn the key priorities section below.

End of day 2

Summary of key R&D priorities

Modelling:

- The need to link microbiology and CFD with an improved understanding of the biology of AD systems
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Further work and planned outputs

Delegates agreed on the need for the following:

1. A position statement reflecting the delegates' views on current state of the art in modelling sludge predictive behaviour from the perspectives of the modelling and practitioner communities, and areas for research focus to offer maximum benefit and advantage to industry.

Action: Bridgeman to provide initial draft for comment and editing by all delegates.

2. Further consideration of the need for, and benefits arising from, a fully coupled biokinetic / hydrodynamic model of an anaerobic digester, which accounts for, inter alia, changes to sludge thickness in the digestion process.

Action: Bridgeman to provide initial scope for delegates to assess feasibility of approach.

3. A review of the measurement and characterisation of sludge. Work possibly suitable for UG final year or MSc dissertation topic.

Action: Volunteer sought from one of the universities represented.

4. Proactive positioning for identification of appropriate research call.

Action: Activities 1 & 2 above go some way to achieving this.

5. Proposal for development of network.

Action: Concept subject to ongoing discussion. amongst delegates.

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