INTRODUCTION TO
MODELLING & SIMULATION

Hydromantis, Inc.
Objectives

- Introduction to modelling and simulation
  - Important modelling issues
- Overview of IWA activated sludge models
- Example wastewater applications:
  - design
  - training
  - analysis
  - operation and control
Outline

● What is modelling? Simulation?
● Dynamic-mechanistic models
● Modelling wastewater treatment systems
● Example applications
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- What is modelling? Simulation?
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What Is Modelling?

- **What is a model?**
  - A representation of a system that can predict *some* system behaviour

- **Why model a system?**
  - Stand in for the real system (system doesn’t exist, not feasible to “test” the system)
A Few Useful Terms

- **Model** - representation of a system
  - for this week - mathematical equations

- **Simulator** - implementation of a model
  - e.g., a computer program

- **Simulation** - application of a simulator
What’s in a Model?

● Series of Process Equations
  • main guts of the model

\[
\frac{dC}{dt} = -kC
\]

● Parameter Values
  • allow the model to calibrated

● Initial Conditions
  • starting point

● Boundary Conditions
What’s in a Simulator?

\[ \frac{dC}{dt} = -kC \]
Numerical Integration

● Simulator takes the model, and executes it:
  • solves (integrates) the equations to give values over a simulated period of time
What’s in a Simulator?

Integration Methods:

Initial Condition
What’s in a Simulator?

● Integration Methods:

\[ \frac{dC}{dt} \]
What’s in a Simulator?

- Integration Methods:
What’s in a Simulator?

Integration Methods:

\[ \frac{dC}{dt} \]
What’s in a Simulator?

Integration Methods:

\[ \frac{dC}{dt} \]
What’s in a Simulator?

- Integration Methods:
  
  \[
  \int dt
  \]
What’s in a Simulator?

- Integration Methods:
  - fixed-step/variable-step methods

- Trade-off: Resolution/Stability vs. Time

- GPS-X handles all this automatically, but you need to be aware of the implications.
Implementation

- Programming languages (e.g., C/C++, VB)
  - write your own simulator
- Specialty Languages (e.g., ACSL)
- Generic simulators (e.g., SimuLink)
- Specialty simulators (e.g., GPS-X)
Simulator
Outline

● What is modelling? Simulation?
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Dynamic-Mechanistic Models

- **Dynamic models** - are used to predict the time-varying performance of a process (vs. steady-state)
- **Mechanistic models** - are developed from a fundamental knowledge of the process (vs. empirical)
- also ... deterministic versus stochastic
Dynamic-Mechanistic Models

- Not new!

- Has become more accessible through:
  - Increases in fundamental knowledge
  - Ongoing model development
  - Improvements in simulation power (CPU)
Why Use Modelling?

- Predictive power provides better insight
- Reduce risk of failure:
  - lost production, fines, loss of public confidence, environmental degradation
- Improve operations
  - O&M costs, capital upgrades, better effluent
Modelling Complexity

- How complex a model should I use?
  - More complex models are not always better.
Complexity Considerations

- Complexity Issues
  - Data Requirements
  - Flexibility
  - Uncertainty
    - Sensitivity
    - Error
Some Simple Complexity Rules

- Make it as simple as possible - but not simpler! (Albert Einstein)
- Do not fall in love with your models
- Know the limits of your model and do not extrapolate ... too far
Outline

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Modelling Wastewater Treatment

- Individual processes to whole facilities

- Types of Models:
  - Physical: bench to pilot
  - Mathematical: single explicit equation to inter-related differential equations requiring implicit solutions
Typical Wastewater Model

- **Variables**
  - $Q$ - flow
  - $X$ - biomass concentration
  - $S$ - substrate
  - $V$ - aeration tank volume

- **Subscripts**
  - $i$ - influent
  - $e$ - effluent
  - $w$ - waste
  - $r$ - recycle
  - $m$ - mixed liquor

- Gasses (CO$_2$, N$_2$, excess O$_2$)
Typical Model Form (Biomass)

ACCUMULATION = INPUT - OUTPUT + REACTION

(Rate of accumulation of biomass in the system)
(Mass flow of biomass into the system)
(Mass flow of biomass out of the system)
(Growth of biomass in the system)

MASS BALANCE
ACCUMULATION = INPUT - OUTPUT + REACTION

\[ \frac{dX_m}{dt} V = Q_i X_i - \left[ Q_w X_w + Q_e X_e \right] + r_x V \]

\[ r_x = \left( \frac{\mu_m S}{K_s + S} - k_d \right) X \]
Steady-State Simplifications

- Constant flow rate \( \frac{dQ}{dt} = 0 \)
- Constant influent substrate \( \frac{dS}{dt} = 0 \)
- No change in solids storage in clarifier or aeration basin \( \frac{dX}{dt} = 0 \)
What is Missing?

- Dynamic behaviour
  - influent quality and quantity changes
  - operational changes, automatic control

- Other important reactions
  - multiple biomass types (e.g., autotrophs)
  - other important components (e.g., multiple substrates)
Traditional Design Model

● States:
  ➢ biomass (measured as suspended solids)
  ➢ substrate (measured as BOD$_5$ or COD)
  ➢ oxygen (or assumed)

● Bio-chemical processes:
  ➢ aerobic growth of biomass on substrate
### ASM1 States

<table>
<thead>
<tr>
<th>Inert soluble organics</th>
<th>Cell decay products</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inert solid organics</td>
<td>Oxygen</td>
</tr>
<tr>
<td>Soluble substrate</td>
<td>Nitrate/Nitrite</td>
</tr>
<tr>
<td>Particulate substrate</td>
<td>Ammonia/Ammonium</td>
</tr>
<tr>
<td>Heterotrophic biomass</td>
<td>Soluble organic N</td>
</tr>
<tr>
<td>Autotrophic biomass</td>
<td>Particulate organic N</td>
</tr>
</tbody>
</table>

- Alkalinity
ASM1 Processes

- Aerobic growth of heterotrophs
- Anoxic growth of heterotrophs
- Aerobic growth of autotrophs
- Decay of heterotrophs and autotrophs
- Ammonification of soluble organic N
- Hydrolysis of entrapped organics
- Hydrolysis of entrapped organic N
ASM1 Processes

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Cell Growth
Cell Death
Transformation of Nitrogen
Transformation of Carbon
ASM1 Parameters

- Kinetic rates:
  - Growth rates (maximum specific, half saturation)
  - Decay rates
  - Switching function parameters (aerobic?, anoxic?, etc.)
  - Hydrolysis rates

- Stoichiometric
  - e.g., yield
IWA ASM Family

- ASM1 - carbon/nitrogen model
- ASM2 - carbon/nitrogen/phosphorus
  - excess biological phosphorus removal (EBPR)
- ASM2d - ASM2 + anoxic EBPR
- ASM3 - most recent C,N model
Other Models

- Other published models and modified version of IWA ASM models
- Industrial modifications (multiple biomass populations and substrates)
- Fixed film, complex hydraulics
- Other models: clarifiers, solids handling etc.
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Applications

- Design and Retrofit
- Analysis
- Operation
- Training
Application Notes

● **Effort**: tens of person-hours to thousands
● **Modelled Layout**: simple to complete
● **Data**: existing to extensive monitoring
● **Calibration**: default data to complex
● **Model Evaluation**: none to formal
● **Analysis**: specific to wide-ranging
Design and Retrofit

- How to make the most efficient design? – taking into account influent characterization
- How to make the most of the existing plant?
- Will the plant be able to meet future effluent guidelines?
Design Application Example

- Gabal el Asfar WWTP - Cairo, Egypt
Design Application Results

- Stage 1 Capacity:
  - 1400 ML/d for liquid train (vs. 1000 design)
  - 1100 ML/d for solids train
- Pre-thickening configuration limits the solids train capacity
- Recommend change to operating plan to minimize nitrification
Anticipation of New Effluent Requirements

- WWTP in the Niagara Region, Ontario, Canada
Anticipation of New Effluent Requirements

- Current compliance criteria for BOD and TSS
- Nitrification required soon
- Plant currently has mechanical aerators
- Will it be able to make it?
Anticipation of New Effluent Requirements

- Current OC not sufficient for nitrification
- Upgrade to more efficient aeration system needed
Analysis Application

- Hamilton Woodward STP - 400 ML/d
- New effluent guidelines (Great Lakes RAP)
- Simulate effects of proposed upgrades
- Upgrades:
  - pre-treatment
  - convert CSTRs to plug flow
  - step-feed
Analysis Application

![Graph showing Oxygen Transfer (1/d) vs. Distance Through Tank (%). The graph includes lines for Required kLa, Available kLa, and Ammonia (mg-N/L). The Anoxic Zone is indicated.](image-url)
Analysis Results

- Step feed: reduce effluent TSS by 10 to 35% during peak storm events

- Overall savings: retrofits and changes in operation save $5 to 10 million versus capital upgrades
Final Comments

- Confluence of:
  - Fundamental Process knowledge
  - Synthesis of knowledge into models
  - Implementation of the model in a simulator

- Use for process design, analysis, operation, and training

- Applications demonstrate better operation or cost savings