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Continuity Constrained Modeling of Multi-molecular Transformations

for

Integrated Multi-scale Assessment of the Environment

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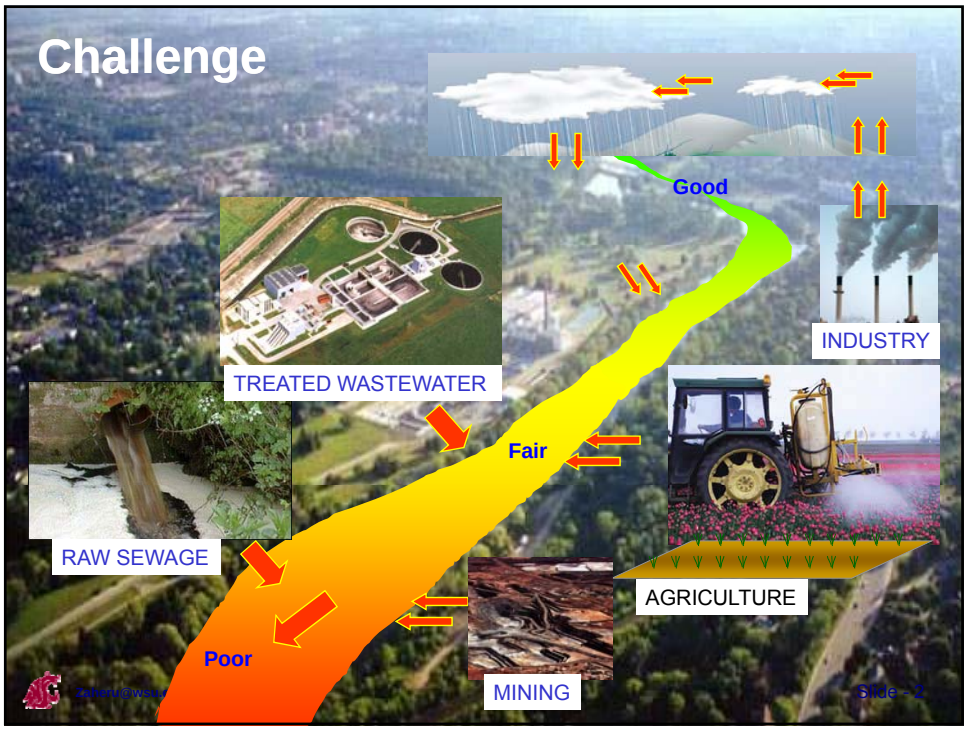
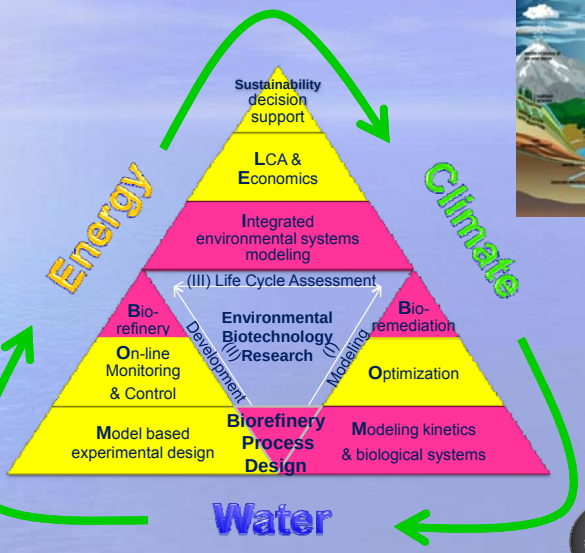
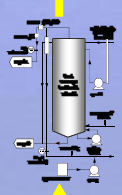
ACS NORM/RMRM, June 21, 2010, Pullman, WA

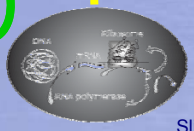
Challenge



Outline







Presentation's methodology focus

Highlighted results

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Classical Biological Model Formulation

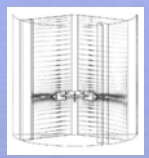
Petersen matrix of a Model A					
j \ k	X_1	X_2	…	X_P	Rate
Conv. 1	$\nu_{1,1}$	$\nu_{1,2}$	…	$\nu_{1,P}$	ρ_1
:	:	:	:	:	:
Conv. n	$\nu_{n,1}$	$\nu_{n,2}$	…	$\nu_{n,P}$	ρ_n
ThOD	$i_{ThOD,1}$	$i_{ThOD,2}$	…	$i_{ThOD,P}$	

Theoretical Chemical Oxygen Demand

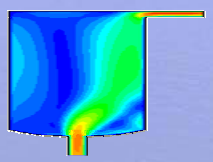
Transport

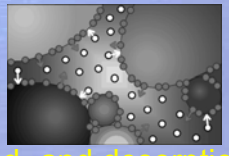
CSTR

$$\frac{dx_k}{dt} = Q/V\,(x_{k,in} - x_k) + \sum_j^n \nu_{j,k}\,\rho_j$$

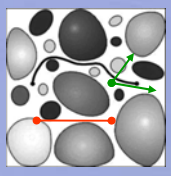


CFD





ad- and desorption



Diffusion

Advection

Dispersion

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Continuity Constrained Modeling

Biochemical
Chemical
Physical

	X_1	X_2	…	X_P	Rate
Conv. 1	$\nu_{1,1}$	$\nu_{1,2}$	…	$\nu_{1,P}$	ρ_1
:	:	:	:	:	:
Conv. n	$\nu_{n,1}$	$\nu_{n,2}$	…	$\nu_{n,P}$	ρ_n

Composition matrix of Model A

ThOD	$i_{ThOD,1}$	$i_{ThOD,2}$	…	$i_{ThOD,P}$
C	$i_{C,1}$	$i_{C,2}$	…	$i_{C,P}$
N	$i_{N,1}$	$i_{N,2}$	…	$i_{N,P}$
H	:	:	:	:
O	:	:	:	:
P	:	:	:	:
charge	$i_{e,1}$	$i_{e,2}$	…	$i_{e,P}$

$$\sum_k \nu_{j,k}\, i_{j,Comp} = 0$$

with $Comp = Thod, C, N, H, O, e$

& other elements

$\Delta G < 0$

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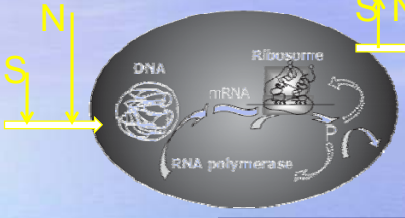
On the Cell Scale: Why continuity of nutrients !?

In Vivo



In Vitro

Particulate X_0

Nutrients release

Hydrolysis

Soluble COD S_1

X_1 Acidogenesis

VFA S_2

H_2

X_2

CO_2

Methanogenesis

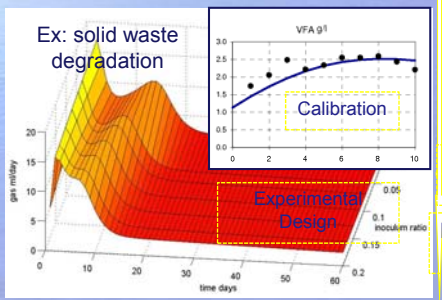
Nutrients uptake

CH_4

X_3

Nutrients recovery

Ex: solid waste degradation



Larger Scale

Zaher *et al.*, Applied Mathematical Modelling (2009), 33 (9), 3553–3564.

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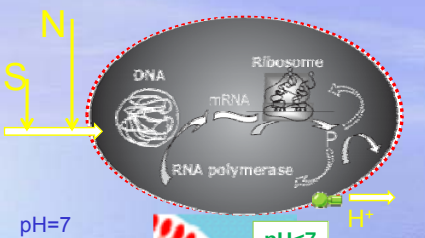
Why continuity of charge ?



pH=7

$CO_2 + H_2$

$Ac^- + H^+ \leftrightarrow HAc$

ATP

2ATP

ADP + Pi

pH<7

$HAc \leftrightarrow Ac^- + H^+$

½ mol Glucose Fermentation

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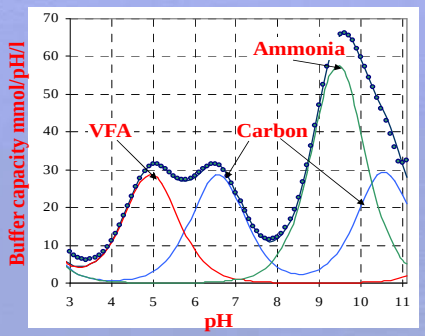
Mono-protic Di-protic

$$\beta = 2.303[H^+]\left(1+\sum_{i=1}^{n} C_i\left(K_a\frac{1}{([H^+]+K_a)^2}\right)_i+\sum_{j=1}^{m} C_j\left(K_{a1}\frac{[H^+]^2+4K_{a2}[H^+]+K_{a1}K_{a2}}{([H^+]^2+K_{a1}[H^+]+K_{a1}K_{a2})^2}\right)_j+\sum_{k=1}^{n} C_k\left(K_{a1}\frac{[H^+]^4+4K_{a2}[H^+]^3+(K_{a1}+9K_{a3})K_{a2}[H^+]^2+(4[H^+]+K_{a2})K_{a1}K_{a2}K_{a3}}{([H^+]^3+K_{a1}[H^+]^2+K_{a1}K_{a2}[H^+]+K_{a1}K_{a2}K_{a3})^2}\right)_k\right)$$

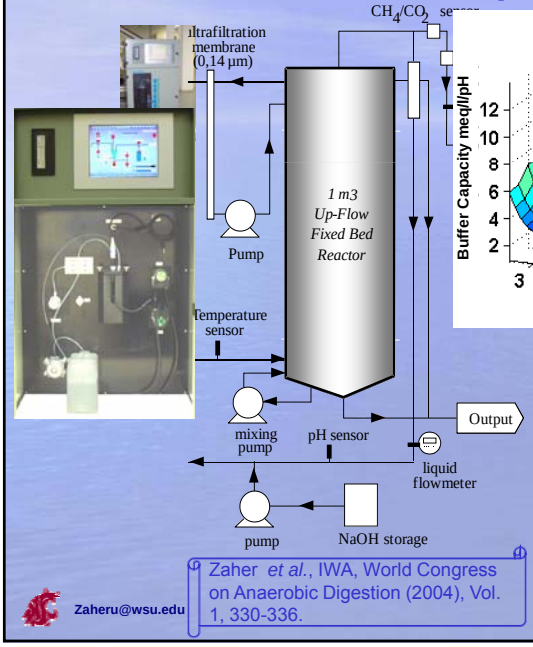
Tri-protic

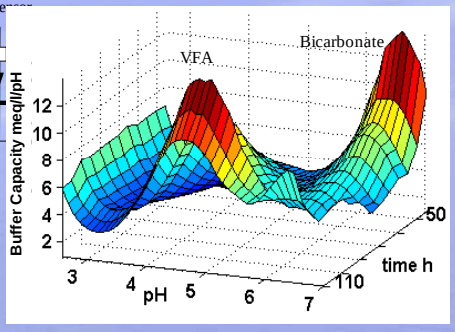


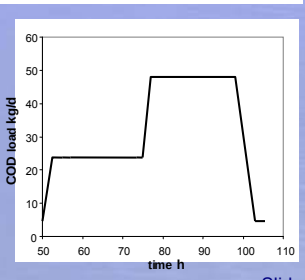
Zaher & Vanrolleghem, Analytical and Bioanalytical Chemistry, (2005) , 383(4), 605-618.

Slide - 7

On the Pilot Scale: *Example from Wine Industry*







Zaher *et al.*, IWA, World Congress on Anaerobic Digestion (2004), Vol. 1, 330-336.

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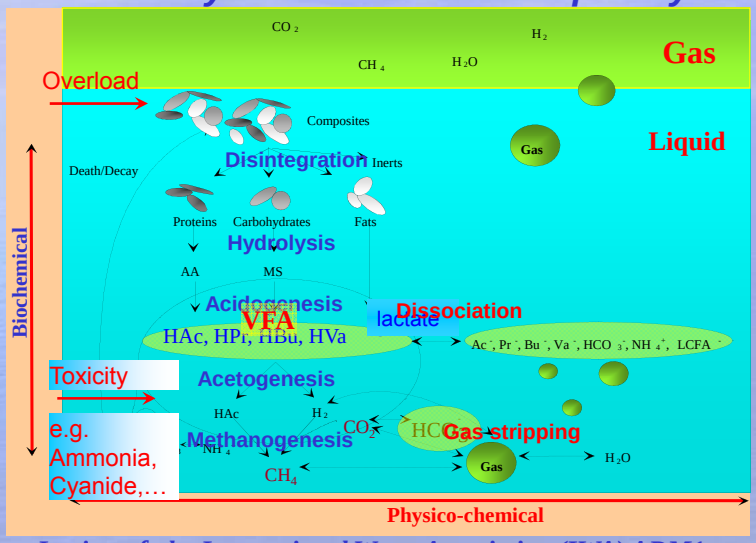
On the Full Reactor Scale
Bio-Physico-Chemical Complexity



In view of the International Water Association (IWA) ADM1

Continuity Resolves the Complexity
Maintaining the Bio-Physico-Chemical Cascade

24 components

S_{va} S_{bu} S_{pro} S_{ac} S_{h2} S_{ch4} S_{IC} S_{IN}

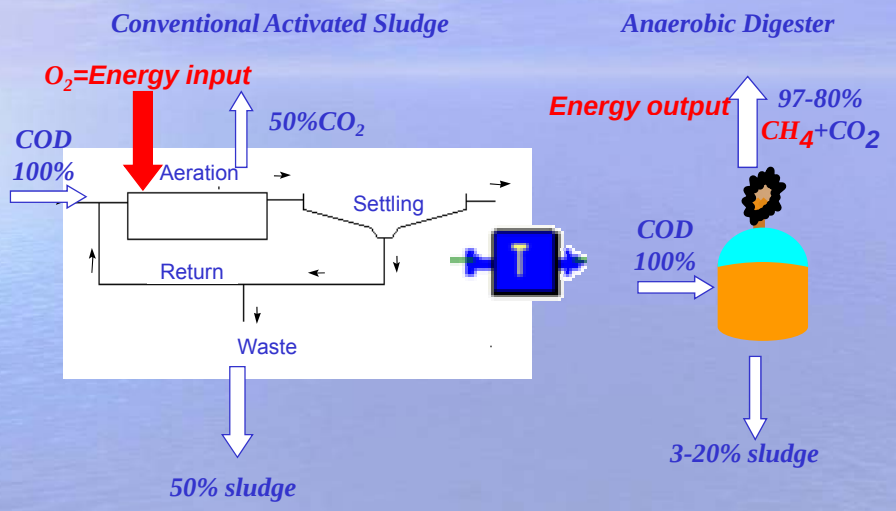
19 reactions

j	Component i → / process ↓	4b S_{va^-}	5b S_{bu^-}	6b S_{pro^-}	7b S_{ac^-}	10b S_{hco3^-}	11b S_{nh3}	Rate (ρ_j, all in kg COD.m^{-3}.d^{-1} except inorganic carbon and nitrogen in kmole.m^{-3}.d^{-1})
A1	Valerate acid-base							
A2	Butyrate acid-base							
A3	Propionate acid-base							
A4	Acetate acid-base							
A5	Inorganic carbon acid-base							
A6	Inorganic nitrogen acid-base							

i	Component →	S_{h2}	S_{ch4}	S_{IC}	$S_{gas,h2}$	$S_{gas,ch4}$	$S_{gas,co2}$	Rate (ρ_j)
j	Process ↓	Liquid-phase			Gas-Phase			
G1	H_2 Transfer	-1			1			$K_L a(S_{h2} - R \cdot T_{op} \cdot K_{H,h2} S_{gas,h2})$
G2	CH_4 Transfer		-1			1		$K_L a(S_{ch4} - R \cdot T_{op} \cdot K_{H,ch4} S_{gas,ch4})$
G3	CO_2 Transfer			-1			1	$K_L a(S_{co2} - R \cdot T_{op} \cdot K_{H,co2} S_{gas,co2})$
		Hydrogen (kg COD m^{-3})	Methane (kg COD m^{-3})	Inorganic carbon (kmole C m^{-3})	Hydrogen (kg COD m^{-3})	Methane (kg COD m^{-3})	Carbon dioxide (kmole C m^{-3})	Gas flow: $q_{gas} = \frac{RT_{opt}}{P_{atm} - p_{H2O}} \cdot V_{liq} \cdot \left(\frac{\rho_{h2}}{16} + \frac{\rho_{ch4}}{64} + \rho_{CO2}\right)$

Valerate (kgCOD) | Butyrat (kgCOD) | Propion (kgCOD) | Acetate (kgCOD) | Bicarbo (kmole) | Ammor (kmole)

On the Scale of Process Chain



Transformer models: *Continuity for integrated assessment*

Influx

Outflux

Petersen matrix section Model 1 ("origin")					Petersen matrix section Model 2 ("destination")				
j \ k	X_1	X_2	...	X_P	X_{P+1}	X_{P+2}	...	X_{P+Q}	Rate
Conv. 1	$\nu_{1,1}$	$\nu_{1,2}$	...	$\nu_{1,P}$	$\nu_{1,P+1}$	$\nu_{1,P+2}$	...	$\nu_{1,P+Q}$	ρ_1
:	:	:	:	:	:	:	:	:	:
Conv. n	$\nu_{n,1}$	$\nu_{n,2}$	...	$\nu_{n,P}$	$\nu_{n,P+1}$	$\nu_{n,P+2}$	...	$\nu_{n,P+Q}$	ρ_n
Composition matrix section Model 1					**Composition matrix section Model 2**				
ThOD	$i_{ThOD,1}$	$i_{ThOD,2}$	...	$i_{ThOD,P}$	$i_{ThOD,P+1}$	$i_{ThOD,P+2}$	...	$i_{ThOD,P+Q}$	
C	$i_{C,1}$	$i_{C,2}$	...	$i_{C,P}$	$i_{C,P+1}$	$i_{C,P+2}$	...	$i_{C,P+Q}$	
N	$i_{N,1}$	$i_{N,2}$	...	$i_{N,P}$	$i_{N,P+1}$	$i_{N,P+2}$	...	$i_{N,P+Q}$	
H	:	:	:	:	:	:	:	:	
O	:	:	:	:	:	:	:	:	
P	:	:	:	:	:	:	:	:	
charge	$i_{e,1}$	$i_{e,2}$	...	$i_{e,P}$	$i_{e,P+1}$	$i_{e,P+2}$	...	$i_{e,P+Q}$	

$$\sum_k \nu_{j,k} i_{j,Comp} = 0 \quad with\ Comp = Thod, C, N, H, O, e$$

$$\sum_{j=1}^{n} \nu_{j,k} \rho_j = Influx_k \quad for\ k = 1,P$$

$$Outflux_k = \sum_{j=1}^{n} \nu_{j,k} \rho_j \quad for\ k = P+1, P+Q$$

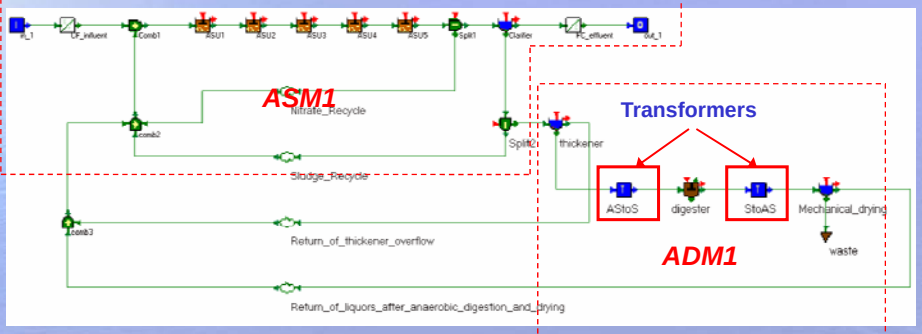
Developed at UGENT
Upgraded at WSU
Applications:
UGENT : Plant-wide modeling
WSU : High solids digestion

On the Plant-Wide scale

IWA taskgroup on benchmarking WWT control strategies

The Activated Sludge Benchmark Simulation Model No.1

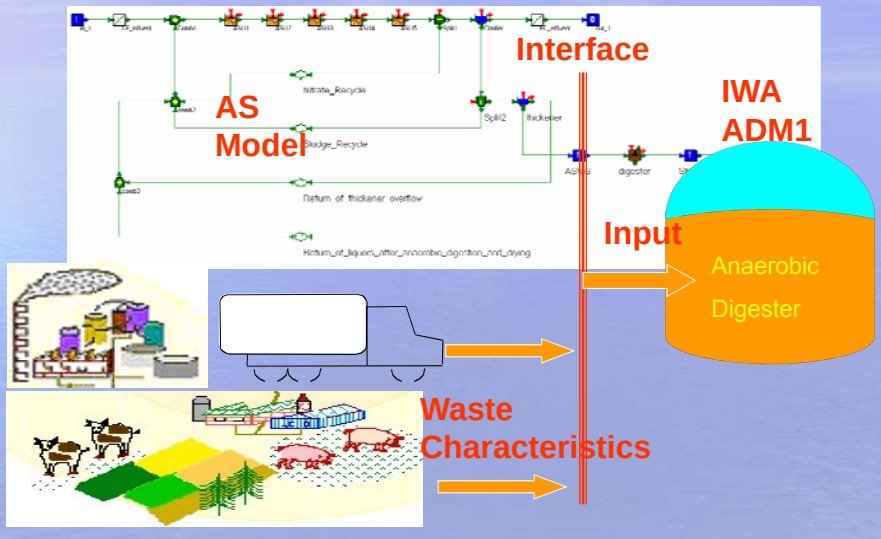
European project COST action 624



Sludge treatment facilities

Developed at UGENT

On the treatment centers' scale
Co-digestion in Biogas plant



Transformer: general ADM1 interface

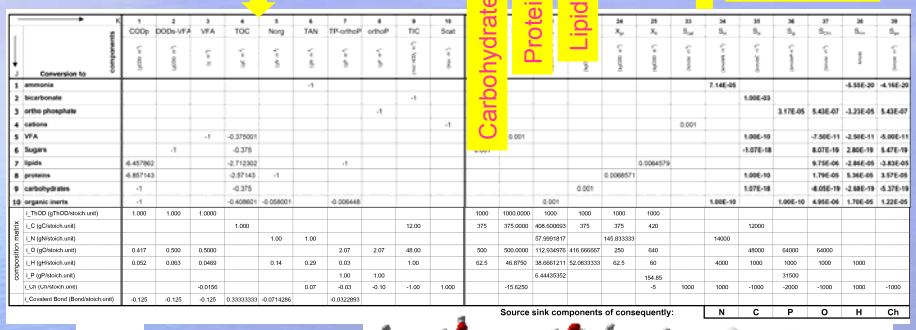
Waste practical characteristics

Carbohydrates

Proteins

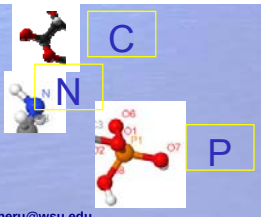
Lipids

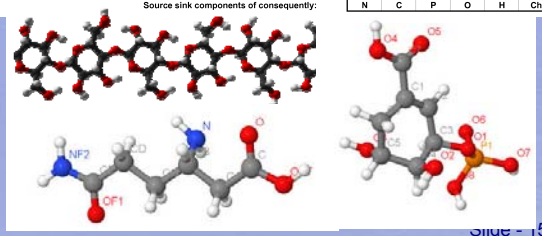
ADM1 Input



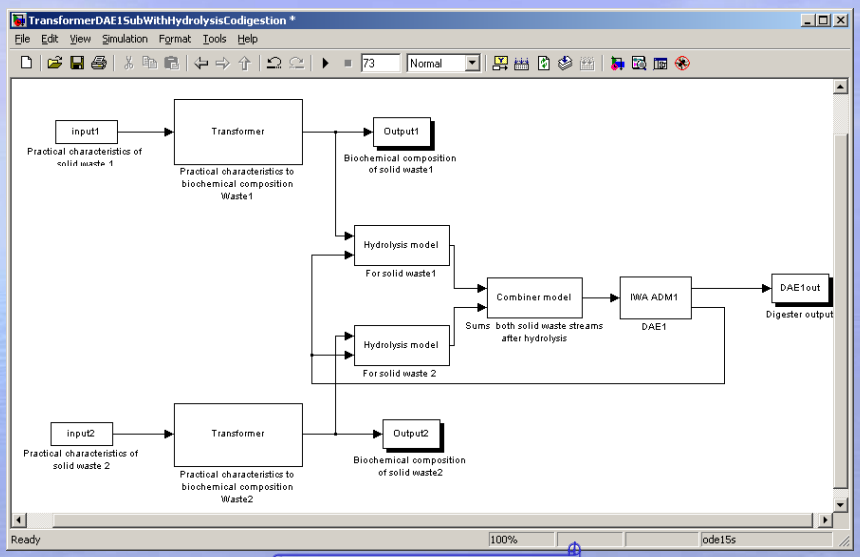
Source sink components of consequently:

N	C	P	O	H	Ch





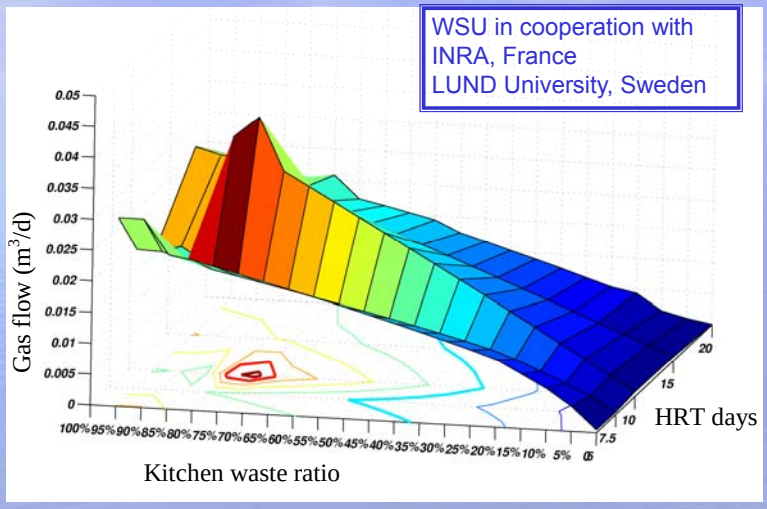
Co-digestion Model for Biogas Plants



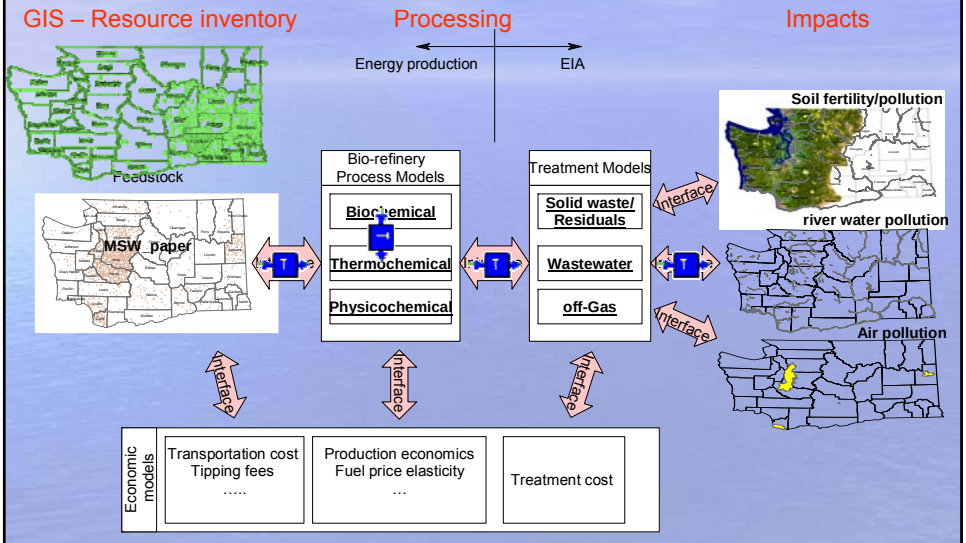
Zaher et al., IWA Publishing, Water Research (2009), 43(10), 2717-2727

Co-digestion optimization

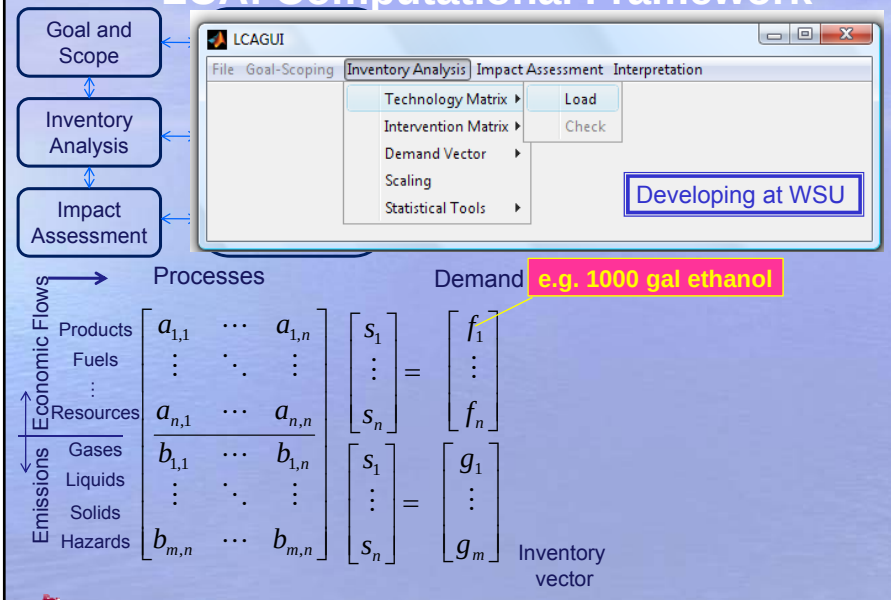
WSU in cooperation with
INRA, France
LUND University, Sweden



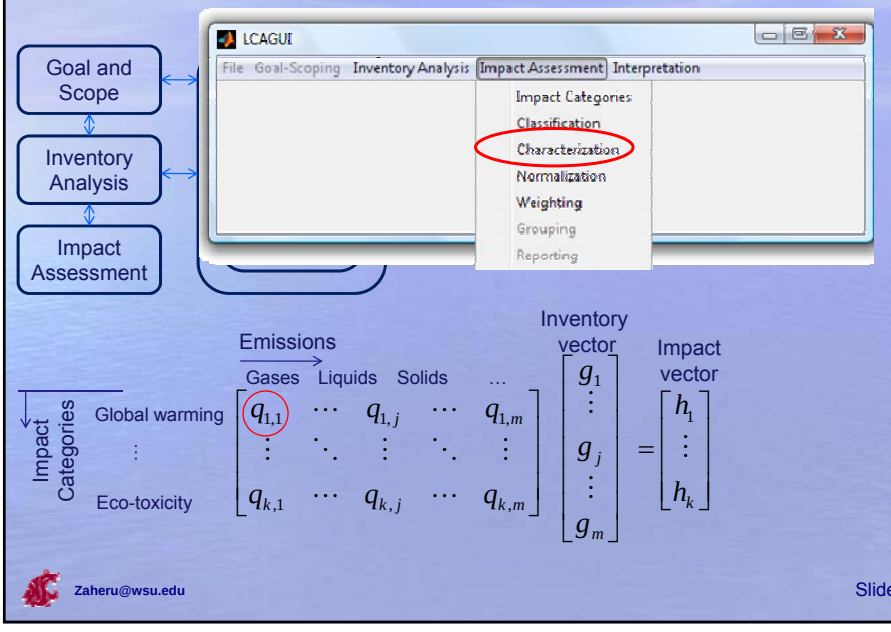
On the Eco-System Scale
Life Cycle Assessment



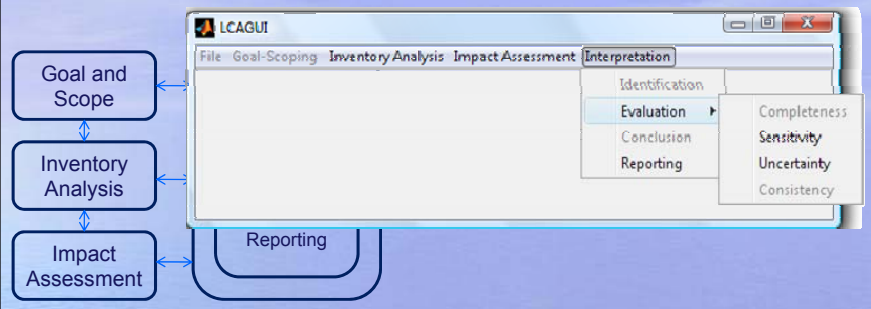
LCA: Computational Framework

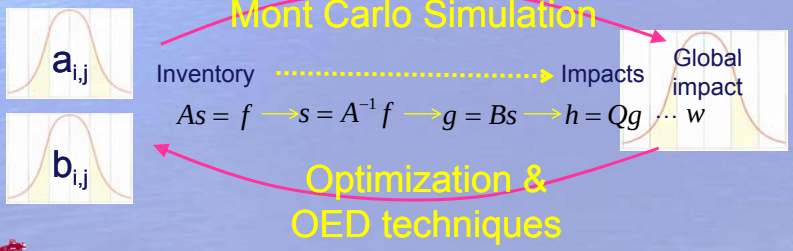


LCA: Computational Framework



LCA Uncertainties ←→ Optimization





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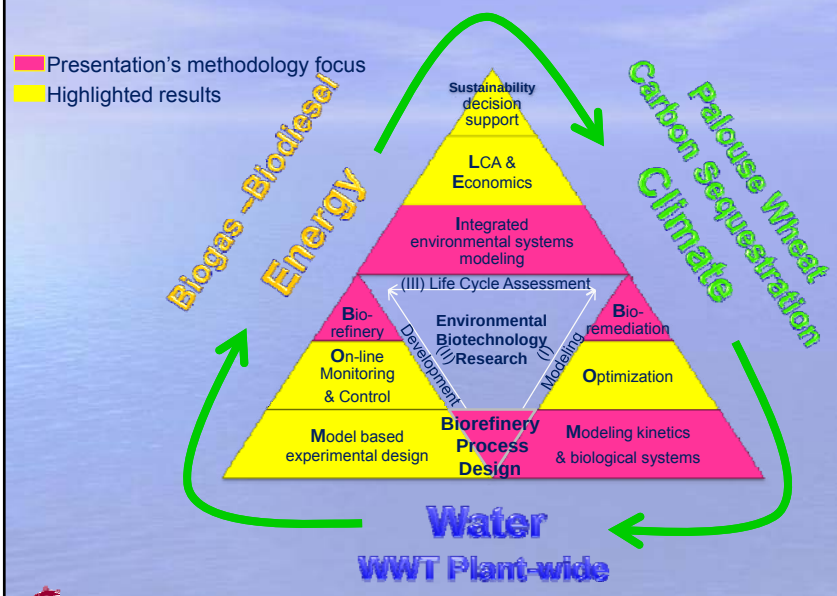

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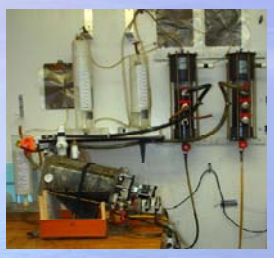
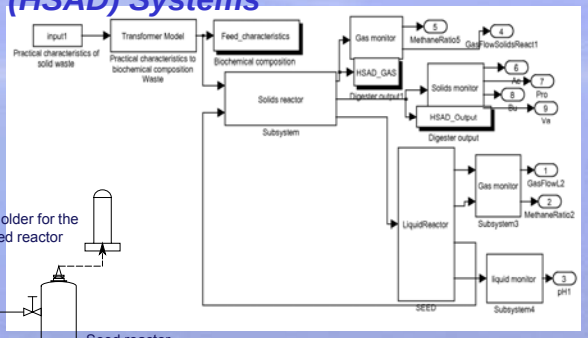
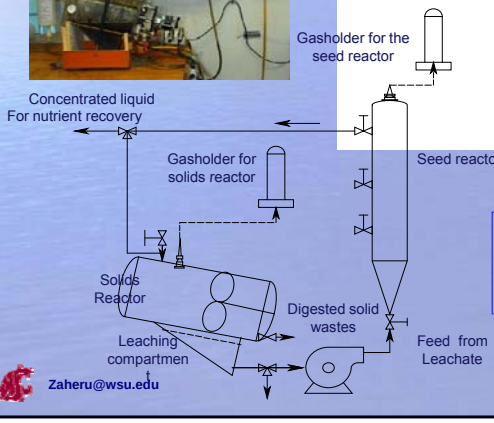
ENERGY(Biogas)

Development of High Solids Anerobic Digestion (HSAD) Systems







California Energy Commission – WSU High Solids Anaerobic Digestion

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HSAD System Design Criteria

Threshold Optimization for process design

Design/performance parameter	Optimization		Typical HSAD system installation with solid waste recycle using Kompogas design
	(1) New HSAD system with augmentation	(2) Conventional HSAD system with solid waste recycle	
Total COD g/L	200	200	
Optimization Threshold m^3 CH_4/ton/day	39.7	39.7	
Optimization results for feed rate of 1 ton/day:			
Methane production efficiency	96%	96%	
Solids reactor volume m^3	17	25	38.3*
Performance			
Solids digester loading rate ton/m^3/day (lb/ft^3/day)	0.06 (3.75)	0.04 (2.50)	0.026 (1.63)*
Biogas production rate m^3/ m^3/day	4.62	3	2.8*
Methane production rate m^3/ m^3/day	2.28	1.52	
Potential fertilizer:			
kgN/ton waste	2.10	--	--
kgP/ton waste	3.72	--	--
capital cost $/ton including post composting	18.9	27.8	48.6

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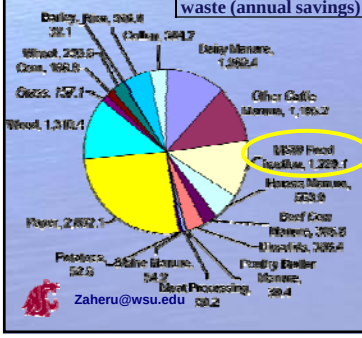
HSAD Systems Economic Analysis

California

Cost and economic benchmarks	(1) New HSAD system with augmentation	(2) Conventional HSAD system with solids recycle	Annual Savings of the new HSAD system	
			US$	%
Total cost production $/kWh	**1.0750517**	**1.5538188**	**0.4787671**	**31%**
kWh from food waste in California	1,229,000,000	1,229,000,000		
Total cost utilizing all food waste in California (annual savings)	**$1,321,238,572**	**$1,909,643,305**	**$588,404,732**	**31%**
kWh from all digestible waste in California	5,130,000,000	5,130,000,000		
Total cost utilizing all digestible waste (annual savings)	**$5,515,015,359**	**$7,971,090,442**	**$2,456,075,083**	**31%**



η_r : relative efficiency ~ 0.8 Mixing is 75% of the cost

SG: specific gravity 1.2

μ: viscosity

G: mixing intensity

$$\frac{W_L}{W_S}=\frac{\eta_S \rho_L}{\eta_L \rho_S}=\frac{\eta_r}{SG}$$

$$W_{mixing}=G^2 \cdot \mu \cdot Vol$$

$$\text{Capital cost \$/ton}=\frac{(A/P,i\%,n)P}{Q}$$

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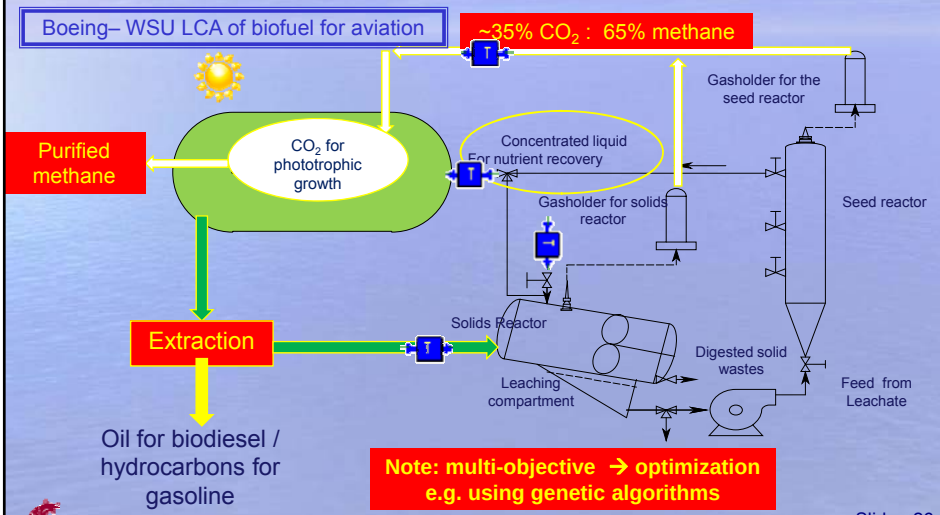
ENERGY(Biogas-Biodiesel)

California Energy Commission – WSU High Solids Anaerobic Digestion

Washington State Ecology dept.– WSU Energy and Fertilizers from Solids Waste

Boeing– WSU LCA of biofuel for aviation



Note: multi-objective → optimization e.g. using genetic algorithms

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Water
WWT Plant → Biorefinery

Gabal El-Asfar WWT/Biorefinery Plant (GEAWWTP), Cairo, Egypt

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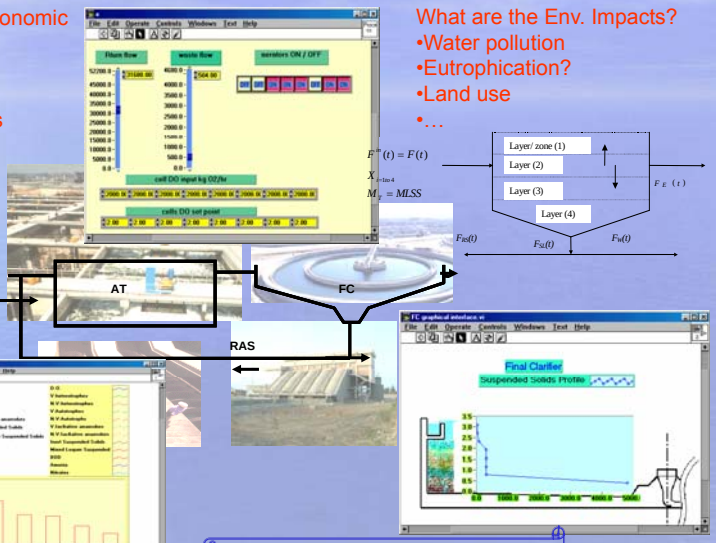
GEAWWTP Optimization

Nitrify or NOT?

What are the Economic Impacts?
- Energy in/out
- Capital cost
- Operation costs
- Tariffs / profit
- Sustainability



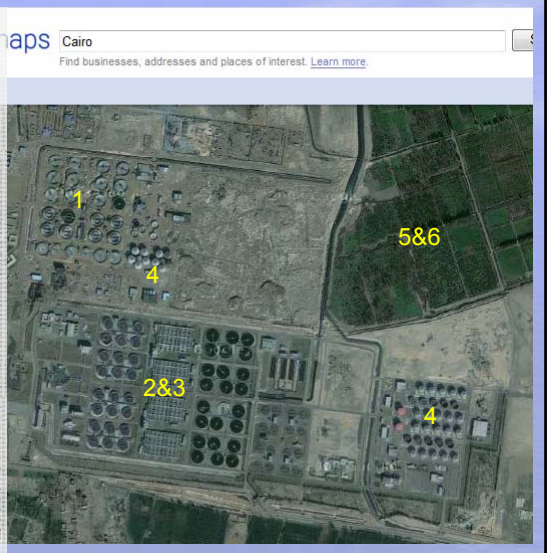
What are the Env. Impacts?
- Water pollution
- Eutrophication?
- Land use
- …

- M.Sc. (2000), Cairo University, Egypt
- Water Intelligence (2004), IWA publishing (on-line)

GEAWWTP Improvements

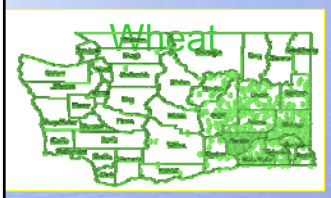
1. Capital cost savings on plant extension
2. Operation cost saving due to not nitrifying
3. Saving > 50 GWh/year
4. Biogas increase due to no NO_3^-
5. Improved land use desert reclamation
6. Biodiesel from oil-plants BOT contract
7. ….

A biorefinery…, indeed,



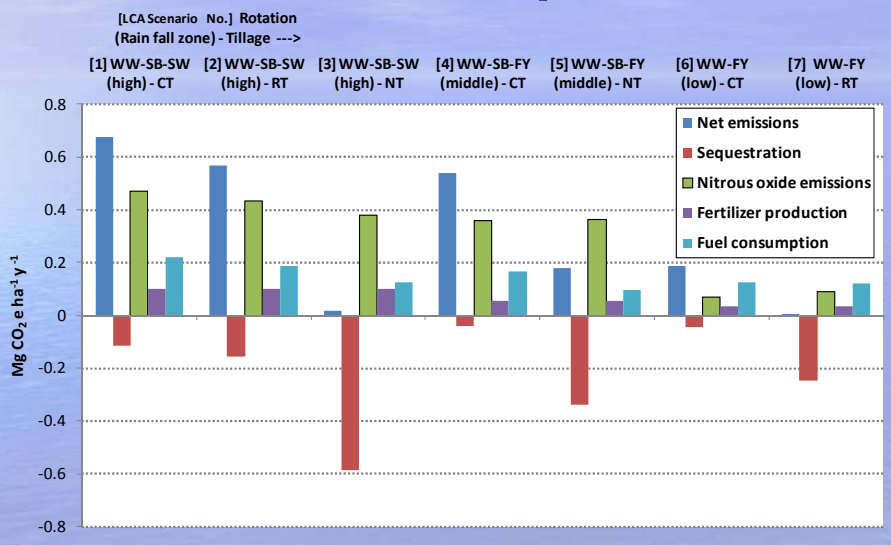
Climate

From Built to Natural Environment



Using the CropSyst® model

Palouse Wheat
LCA & Carbon Sequestration



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Main Messages

- Considering continuity of elemental mass, charge and energy advances modeling of biochemical multi-molecular transformation
- Applying the continuity constraints expands mechanistic modeling to multi-scales from the cell level to the ecosystem
- Integrated modeling on these multi-scales lead to sustainable environmental solutions
- Tackling water, energy and climate challenges in such integrated manner is the tripod that supports sustainable environmental decisions

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Questions