Waste biorefinery technologies for accelerating sustainable energy processes

A Surrogate Approach for the Modelling of Thermal Treatment of Waste Streams

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The Surrogate Concept

Waste wood with chemical pollution

Food waste mixed with packaging

Sewage Sludge

Why?

- Quantify the impact of fuel flexibility
- Optimization of processes
- Deliver input data for system analysis

How?

- Chemical and numerical representation of various (bio)originated waste streams
- Thermal treatment units with focus on volatile products (tar and gas)
- Focus on representation of key characteristics

Chemical Model

Lignocellulosic components

- CELL
- HCE
- LIG_C
- LIG_H
- LIG_O
- SUGAR

Proteins

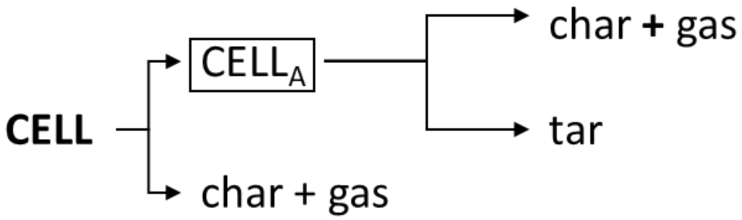
- $PROT_H$
- $PROT_C$
- $PROT_O$

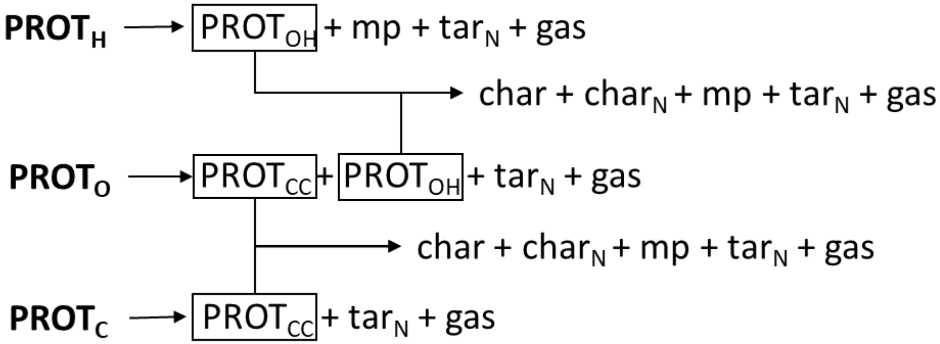
Products from inorganics

- $(NH_3)I$
- $(CO_2)I$
- $(H_2S\ SO_2\ COS)I$

Plastic / fat

- PA
- PP
- PVC
- PS
- PE
- LIPID





Woody Biomass: Ranzi et al., Energ. Fuel. 25 (2011), 4195–4205.
Algae: Debiagi et al. J. Anal. Appl. Pyrol. 128 (2017), 423 – 436.
Municipal Solid Waste (MSW): Netzer et al., Energ. Fuel. 35 (2021).
Sewage Sludge (SS): Netzer and Løvås, ChemEngineering 6(1) (2022), 16.

Chemical Model

WIRE

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Gas phase chemistry
188 species and 3200 reactions

Tar
Max C_{11}
Nitrogen-containing
Aromatic

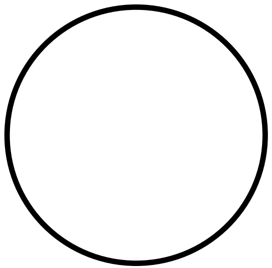
Emission models
NO_x
SO_x
HCl

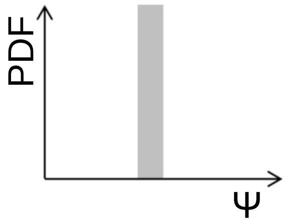
Hydrocarbon chemistry Ranzi et al., Energ. Fuel 25 (2011), 4195–4205;
Nitrogen chemistry Glarborg et al., Prog. Energy Combust. Sci. 67 (2018), 31– 68; Alzueta et al., Combust. Sci. Technol. 174 (2002), 151– 169; Wu et al., Combust. Flame 202 (2019), 394– 404.
Chlorine chemistry Pelucchi et al., Combust. Flame 162 (2015), 2693– 2704; Roesler et al. Combust. Flame 100 (1995), 495– 504.
Sulfur chemistry Glarborg and Marshall, Int. J. Chem. Kinet. 45 (2013), 429– 439; Glarborg et al., Int. J. Chem. Kinet. 28 (1996), 773– 790.
Compilation Netzer et al., Energ. Fuel. 35 (2021).

Stochastic Reactor Model

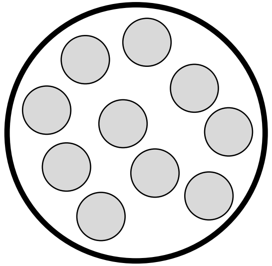
WIRE

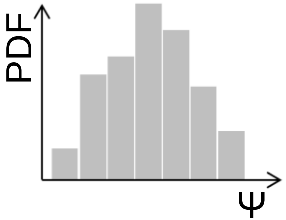
Homogeneous Reactor



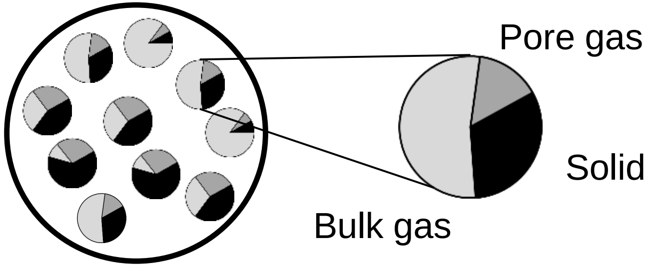


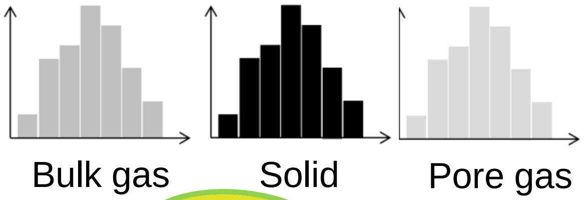
Stochastic Reactor





Stochastic Reactor – Gasification





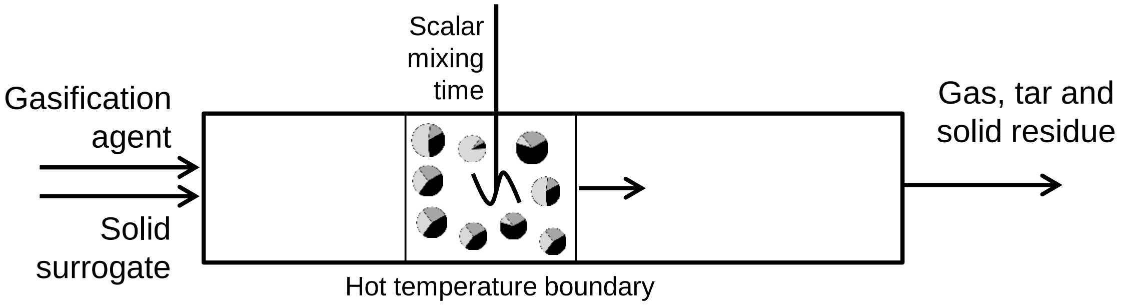
When to use?

- Inhomogeneity
- Incomplete mixed inflow
- Species f(local conditions)

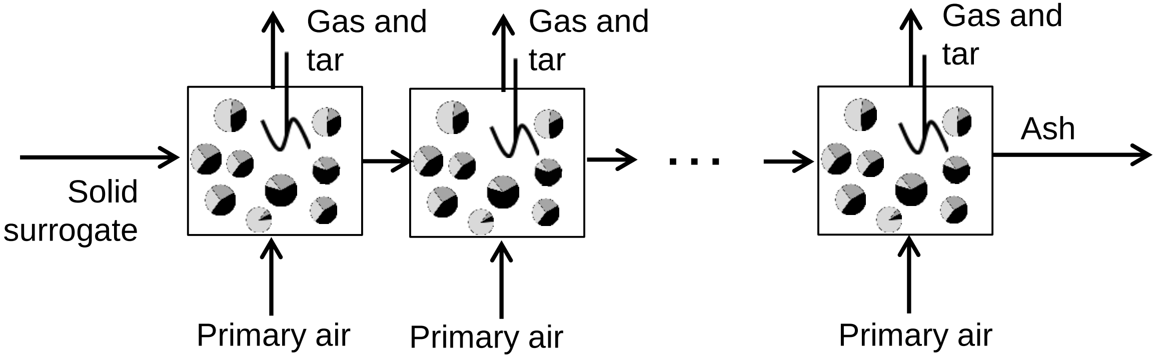
LOGEsoft v1.10, 2018. http://www.logesoft.com.
Weber et al., J. Anal. Appl. Pyrolysis 124 (2017), 592– 601.

Numerical Model

Plug flow reactor configuration



Reactor Network

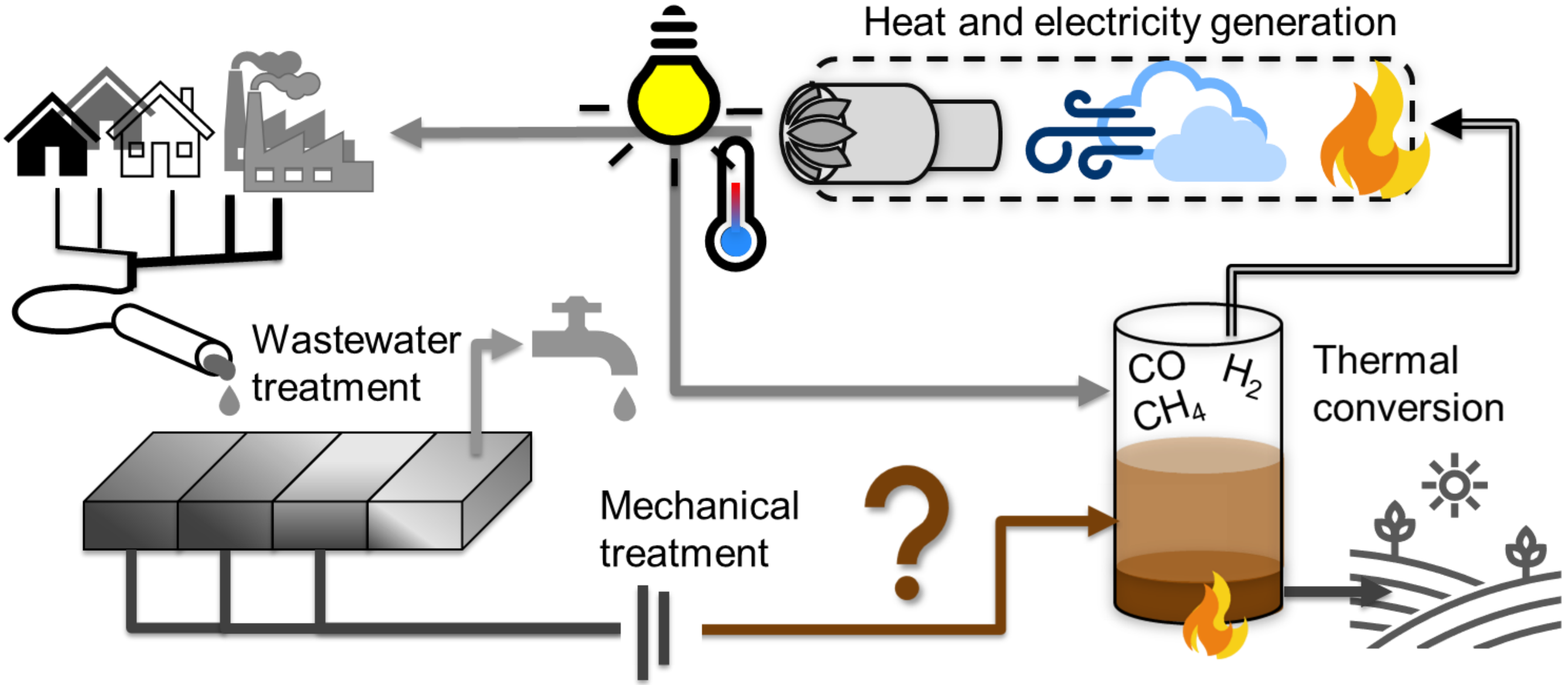


Crucial input parameter
- Amount of oxygen
- Temperature boundary
- Mixing time
- Residence time

Application
- Thermogravimetric analysis (TGA)
- Entrainment flow reactors
- Rotary kilns
- Grate-fired furnaces

Netzer et al., Energ. Fuel. 34 (2021), 12, 16599–16612.
Netzer et al., Energ. Fuel. 35 (2021), 9, 7030–7049.

Example Sewage Sludge



Example Sewage Sludge

Surrogate Formulation

Surrogate species

- **Proteins (20-40%*)**
  $PROT_H$ $PROT_C$ $PROT_O$
- **Lignocellulosic species**
  LIG_C LIG_H LIG_O (23-30%*)
  CELL(10%*) HCE (5%*)
- **Others (<5%)**
  LIPID SUGAR
- **Inorganic representation**
  CO_2I NH_3I (H_2S SO_2 COS)I
- **Ash content** ASH
- **Moisture** H2O(S)

* Mass weight dry ash free

Linear least-squares fit

- Target: UCA
- Conditions, e.g., ratio CELL/HCE
- Ash and moisture from experiment

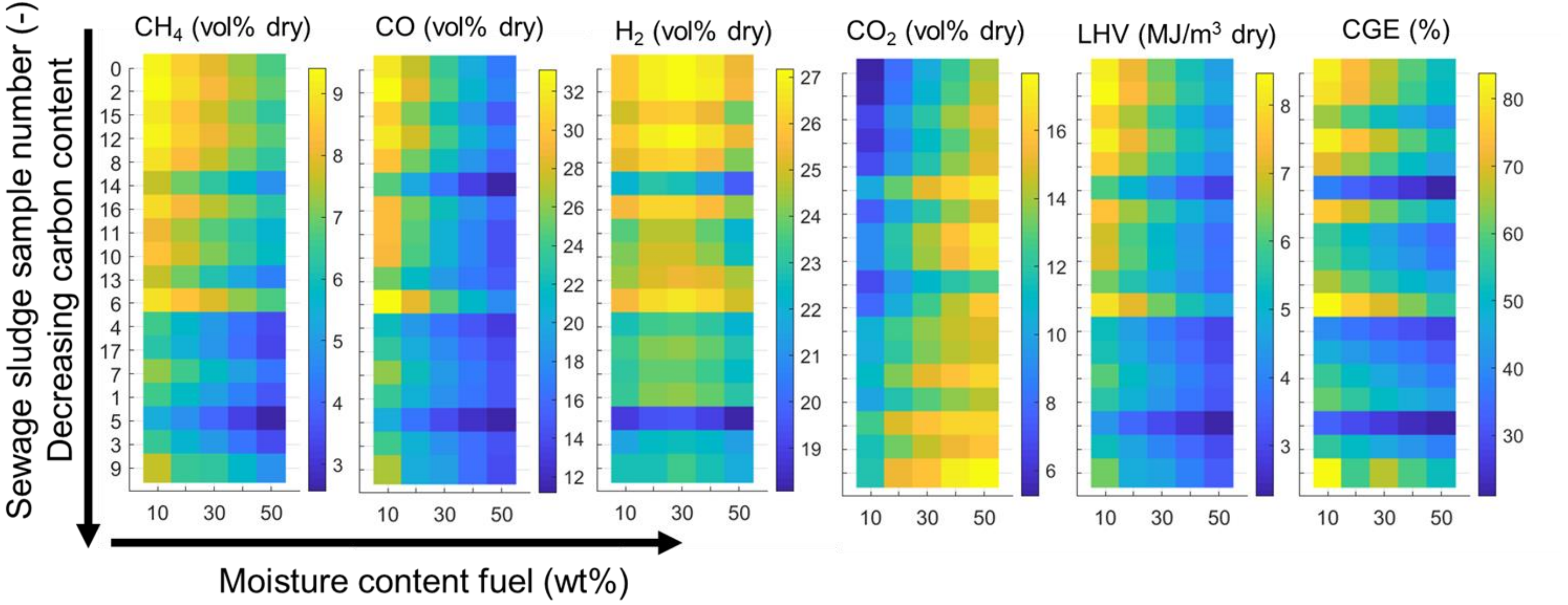
	C (wt%)	H (wt%)	N (wt%)	S (wt%)	Ash (wt%)
Sludge	41.2	6.1	3.6	0.83	24
Surrogate	40.8	5.75	3.7	0.8	24

Sewage Sludge (SS): Netzer and Løvås, ChemEngineering 6(1) (2022), 16.

Example Sewage Sludge

Rotary kiln gasification

$$CGE = \frac{LHV_{product\ gas} \times gas\ yield}{LHV_{sewage\ sludge}} \times 100$$

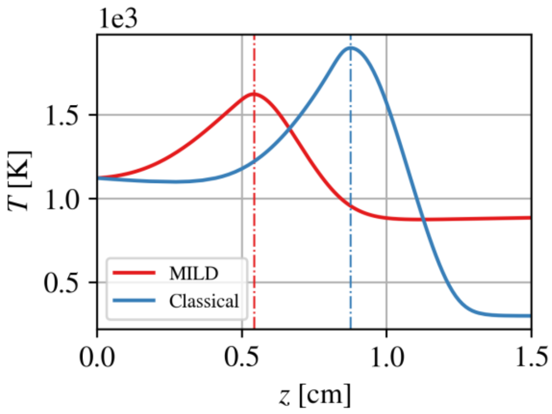


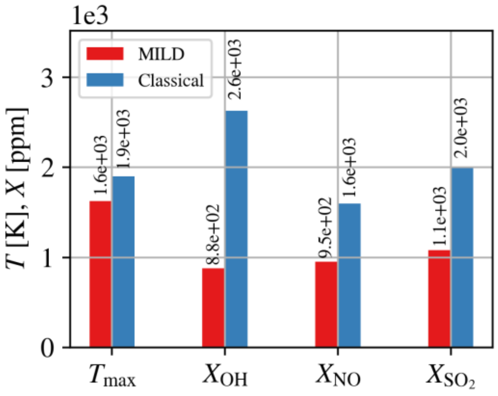
Experiments UCA sewage sludge: Gómez-Rico et al., J Anal Appl Pyrol, 74(1), 421–428, 2005.
Experiments rotary kiln: Freda et al., Fuel, 212, 88–94, 2018.
Numerical results: Netzer et al., INFUB 13, Algarve, Portugal, 19-22 April 2022.

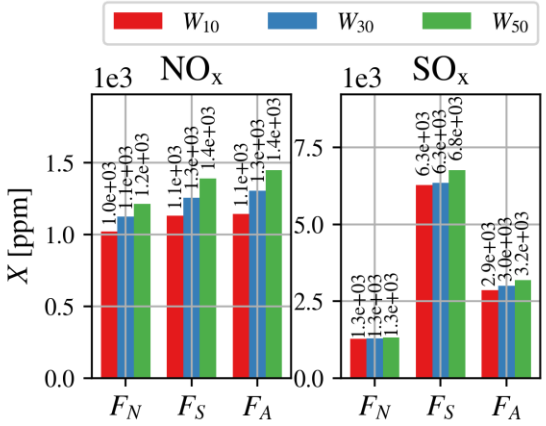
Example Sewage Sludge

Producer Gas Combustion

Fuel:







Numerical results: Guo et al., Fuel 2022, under review.

Summary

WIRE

- Combination of detailed chemistry and stochastic reactor model to predict thermal conversion of (bio-originated) waste streams
- Yield = f(fuel elementary composition, moisture content)
- Predicted gas composition, CGE efficiency and emission precursors relevant for energy supply unit and exergetic analysis of conversion process

Acknowledgement

WIRE

Collaborators

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GASPRO, Fundamental insight into biomass gasification using experiments and mathematical modeling, no 267916

Norway Grants - Negative CO2 emission gas power plant, NOR/POLNORCCS/NEGATIVE-CO2-PP/0009/2019-00