

# A novel Versatile reaction scheme for modeling Anaerobic Digestion with Elemental balance Rigor (vADer)

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## 1 Context

- The Interreg OBIWAN Project: convert organic waste streams into advanced chemicals (solvent, aviation fuel, solid carbon) through anaerobic digestion
- Project funding: Interreg France-Wallonie-Vlaanderen, total budget of 2.59 M€ (1.56 M€ through European Region Development Fund (ERDF))
- A consortium of Academic & industrial partners: Ghent University, Université de technologie de Compiègne (UTC) – UniLaSalle Beauvais, CNRS Lille, Certech
- End goal: Material valorization of CH<sub>4</sub> and CO<sub>2</sub>, moving up the value chain (advanced products), mitigating climate change (closed carbon cycle)
- Seasonal/regional variability of feedstock: production volatility, downstream operational inefficiency, & destabilization of process
- Doctoral work: stabilize biogas composition and flow rate: need a novel reaction scheme for precise modeling of biogas production and emission of impurities

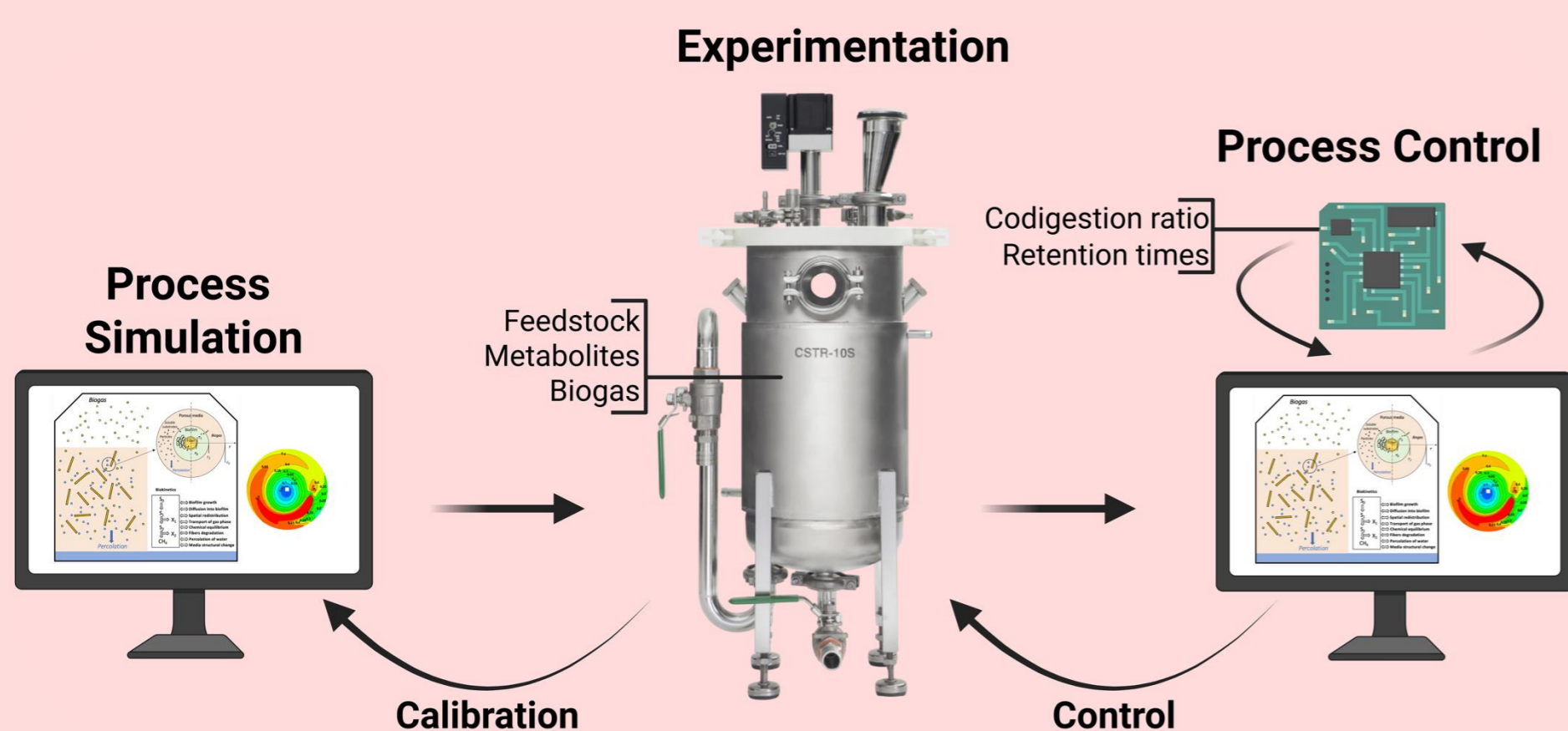


Figure 1: The scope of the doctoral project

## 2 Framework

### Modeled outputs:

- Modeling of biogas (CH<sub>4</sub>, CO<sub>2</sub>) production ⇒ integrating Carbon & chemical oxygen demand (COD)
- Catalytic downstream ⇒ needs to eliminate sulfur and nitrogen: modeling their emission during anaerobic digestion to minimize release and to scale purification

### Reaction scheme design principles:

- Control oriented modeling ⇒ parsimonious choice of state variables and biochemical processes, excluding chemical species with low concentration under process conditions
- Precision despite variability ⇒ determination of stoichiometric coefficients for mass and energy balance closure (elements, charge, COD)
- More Constraints than variables ⇒ prioritizing, quadratic optimization
- Operational realism: reconciling practical industrial measures and the ambitious added-value targets ⇒ elemental composition, COD, ammonium, biomethane potential
- The reaction scheme: Disintegration of composite feedstock, Sugar-lipid degradation, Protein degradation, acetoclastic methanogenesis, and sulfate reduction

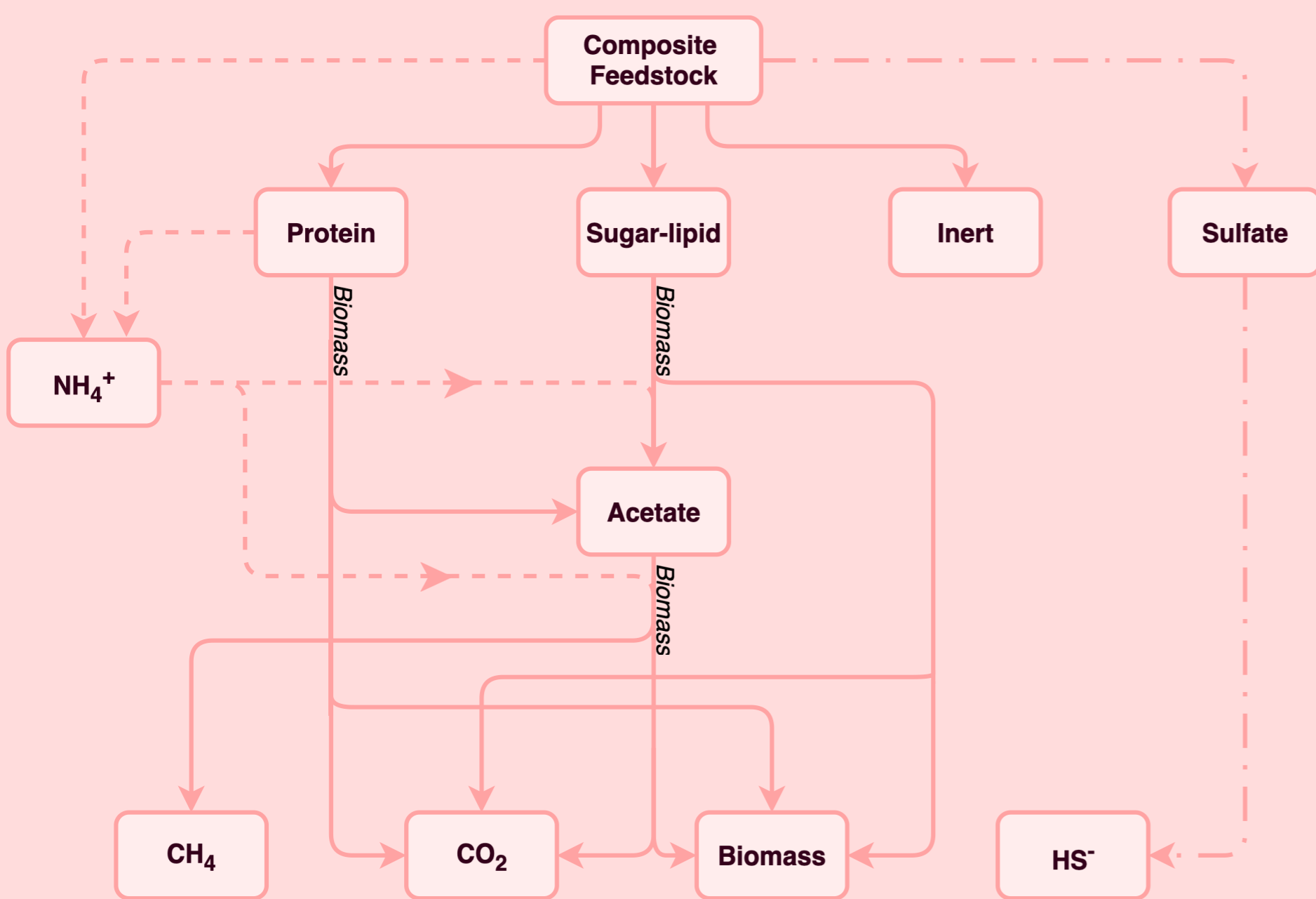


Figure 2: the vADer reaction scheme

## 4 Conclusion

- A novel reaction scheme is proposed for anaerobic digestion based on stoichiometry for balance closure to ensure precision.
- Key features: Parsimony (control oriented), adaptability (level of information), & practical alignment
- Comparison with the literature: better overall balance closure, performance for various feedstocks and model structures
- Limit reached: lipid & protein rich feedstock
- Experimental validation of the reaction scheme in progress
- Next step: developing the kinetic framework, deployment, experimental calibration & validation

## 3 Results

### About Figure 3:

- Balance = products ÷ reactants
- The Bigger the Bar, the Better the Balance
- Left: literature, Right: vADer balance closure

### Choice of articles:

- Acetate representing VFA
- Only acetoclastic methanogenesis
- Stoichiometric coefficients and required measures provided, inferable, or available elsewhere

### Comparison pipeline:

1. Obtain / estimate measures from literature
2. Convert stoichiometrics & measures to molar values
3. Compute balance (Scilab)
4. Plot balance closure (Python)

### Bernard et al (2001):

- No stoichiometric coefficient calculation: unclosed balance
- Model fit ⇒ compensation by other parameters (kinetic)

### Donoso-Bravo et al (2014):

- No stoichiometric coefficient calculation: unclosed balance
- COD-focused model: perfect COD closure, to the detriment of carbon balance (65.5%)

### Fedorovich et al (2003):

- Acetate-based reactions selected
- Sulfate reduction is not COD balanced (3.4%)

### Mairet et al (2011):

- Deviation of calculated balanced from ones reported in article
- Balancing COD to the expense of carbon and nitrogen
- Underperformance of vADer in sugar-lipid degradation: limit of vADer for lipidic feedstock

### Discussion:

- Better overall balance closure ([79%, 100%]) than literature
- Versatility of vADer: functions with varying levels of information
- protein degradation: no silver bullet, prioritization or optimization
- Limit reached for protein or lipid-rich feedstock

For more detail about vADer reaction scheme and the comparison with the literature:

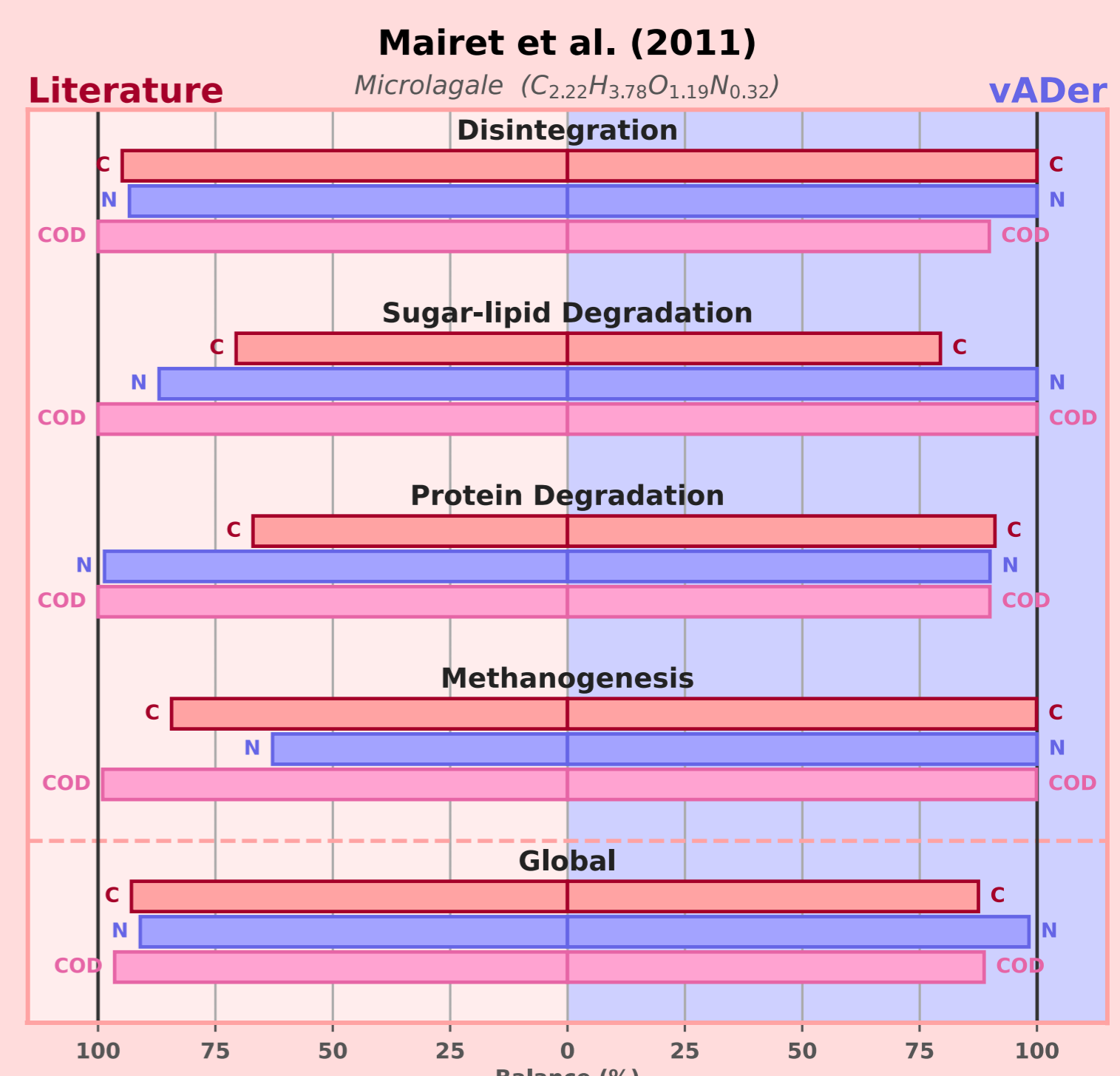
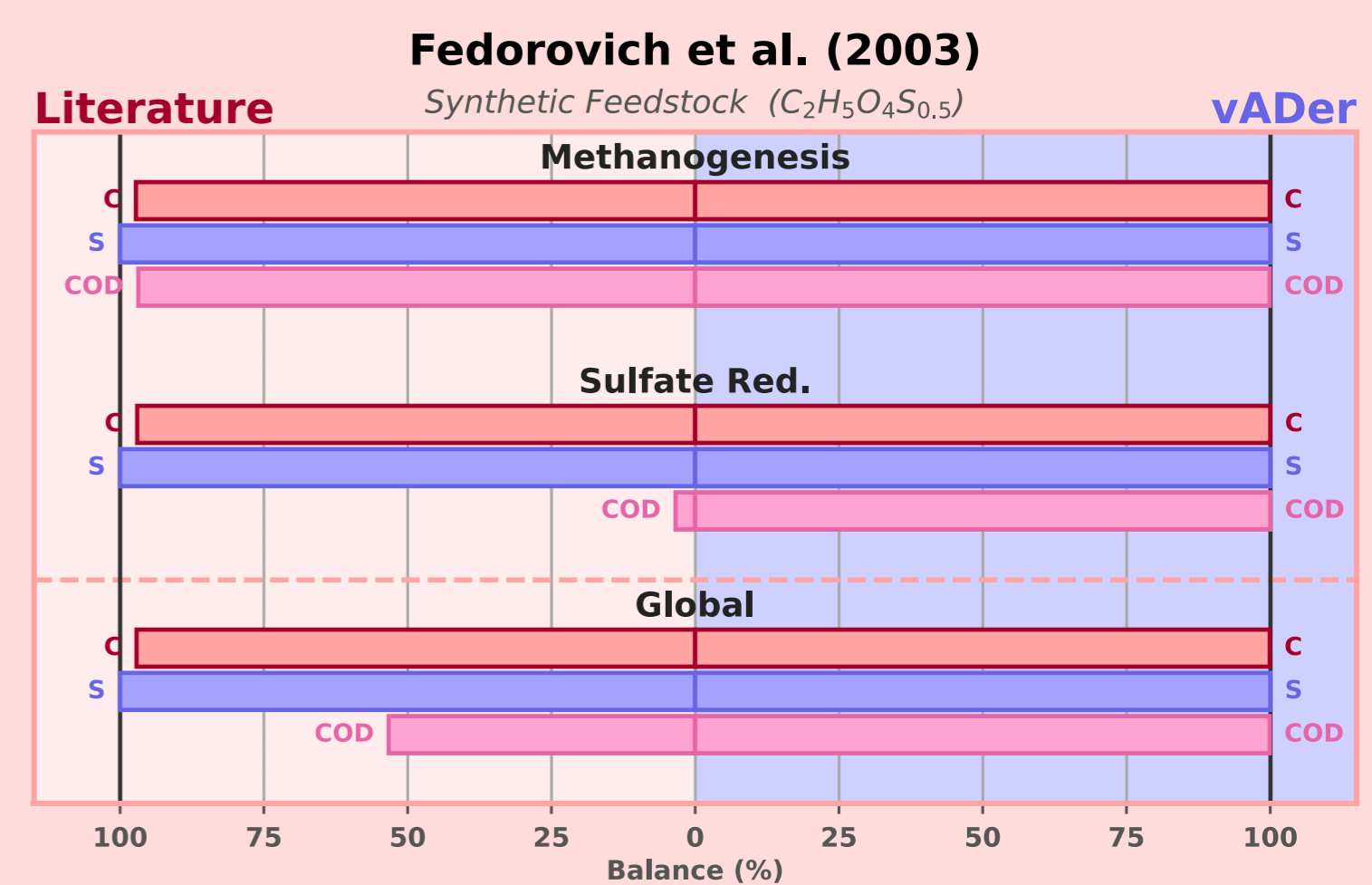
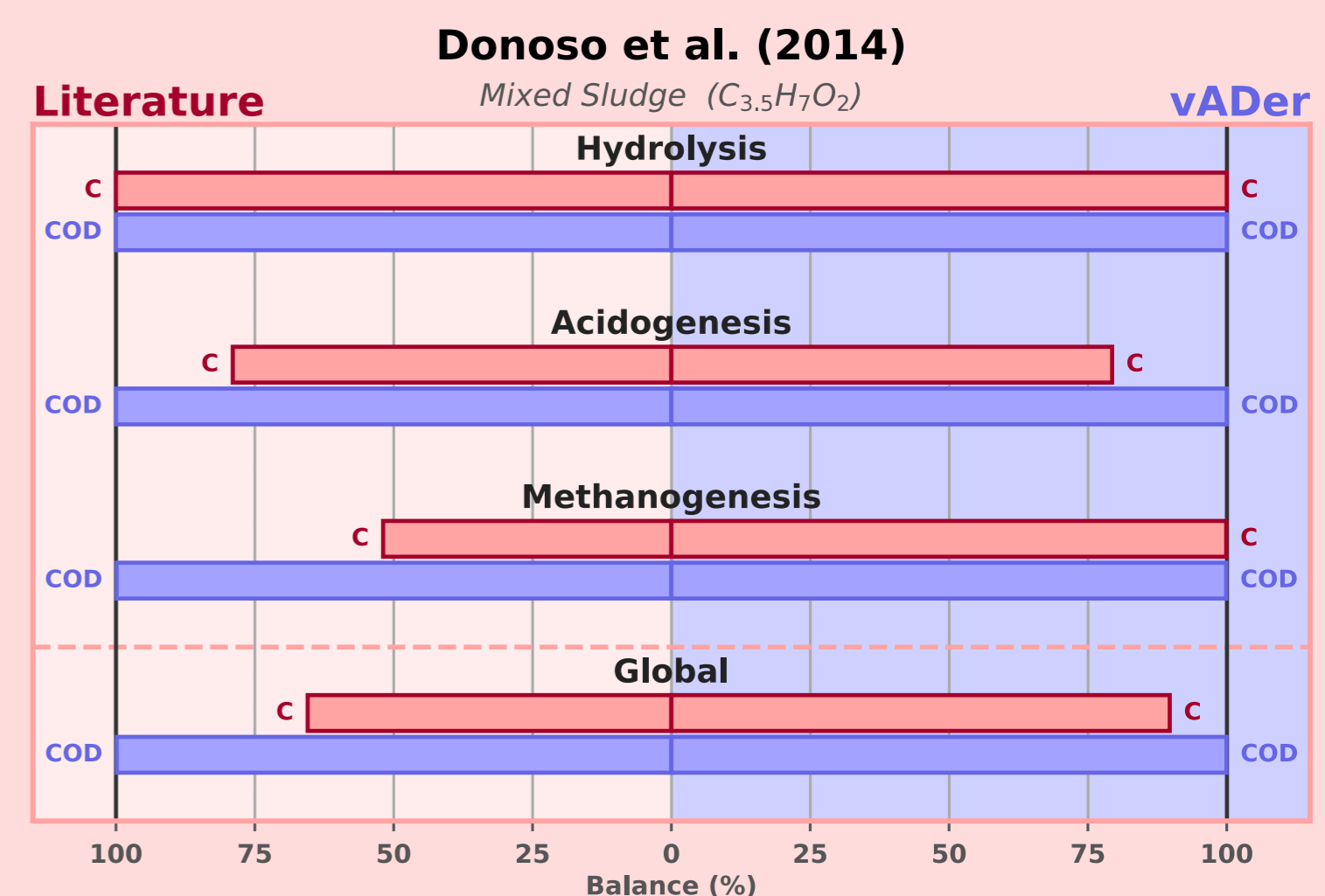
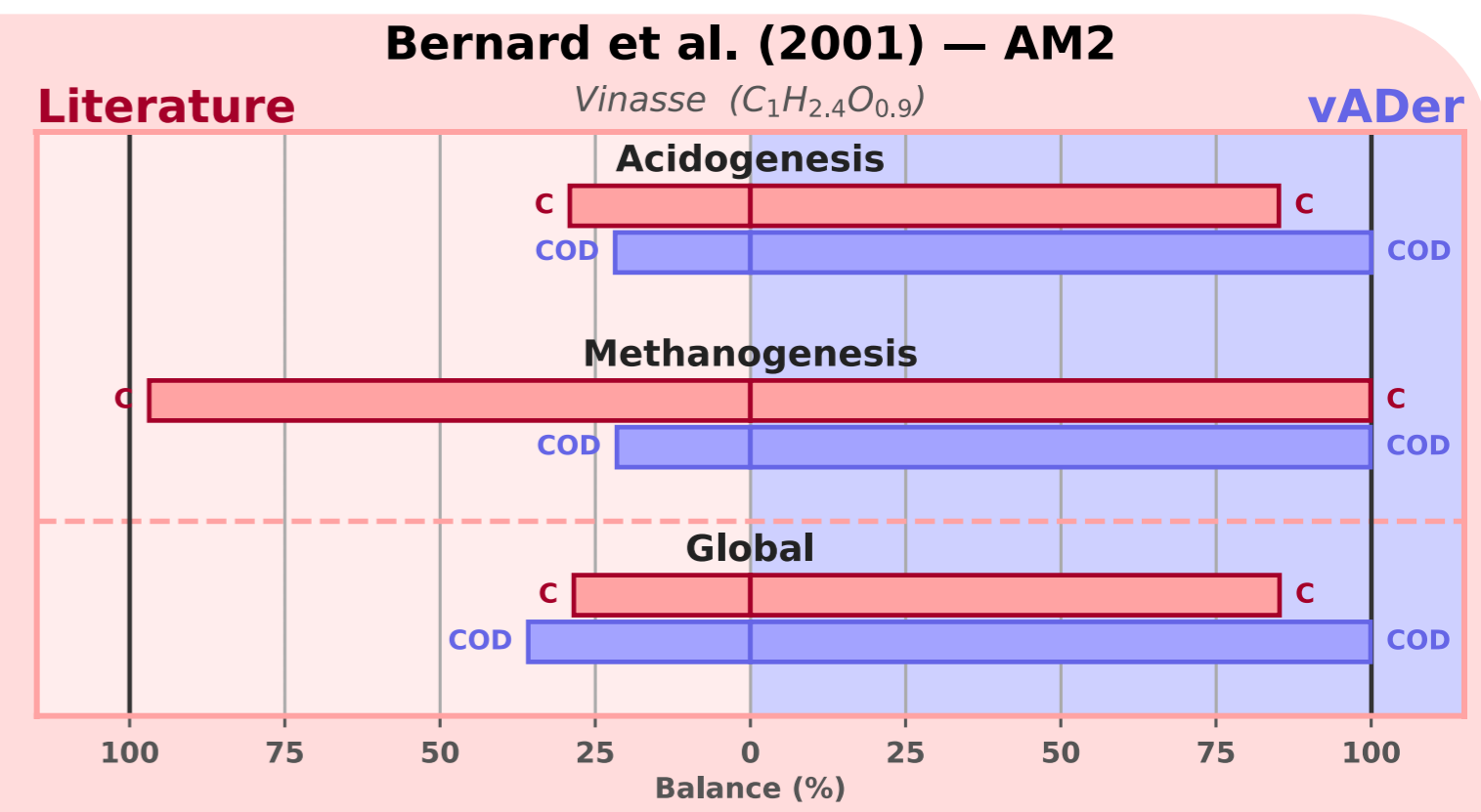


Figure 3: Percentage of elemental balance closure

## 5 References

- D. J. Batstone et al. Anaerobic Digestion Model No. 1 (ADM1) (IWA Publishing, London, 2002), Scientific and Technical Report Ser.  
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## Acknowledgement

