

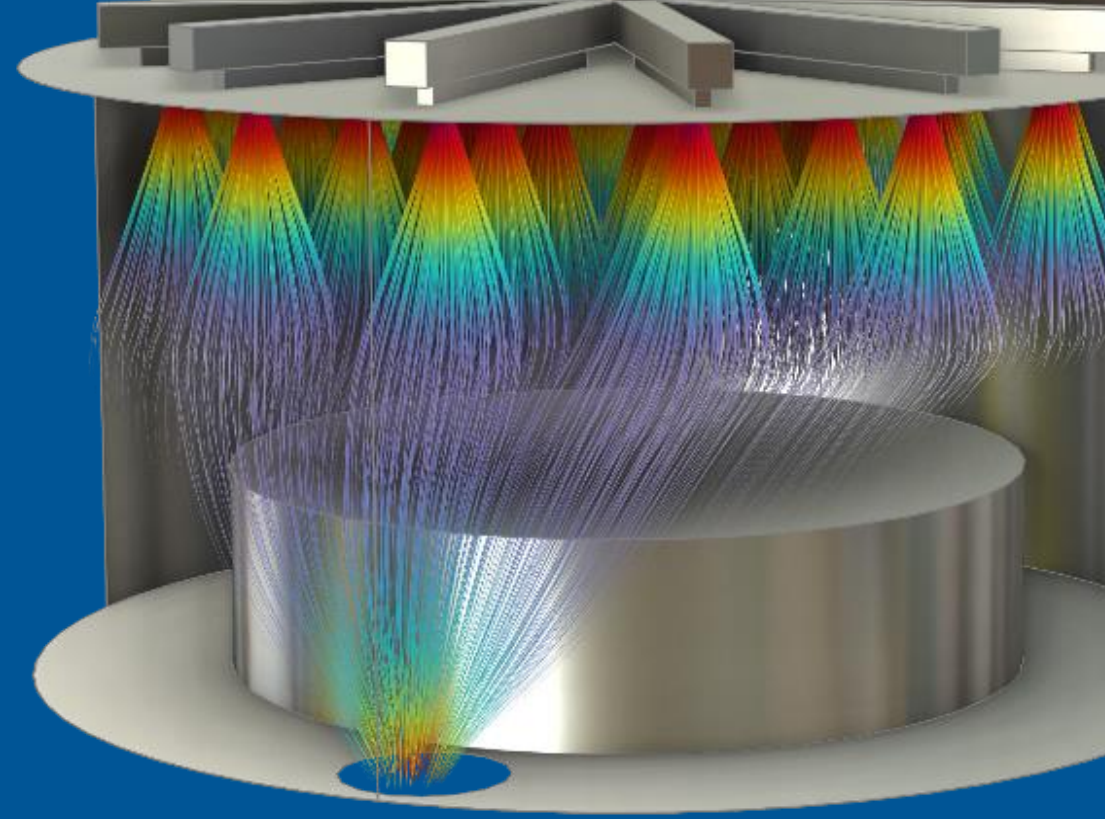
# Humusoft Collaboration: CFD Simulation for the Efficient H<sub>2</sub>S Removal



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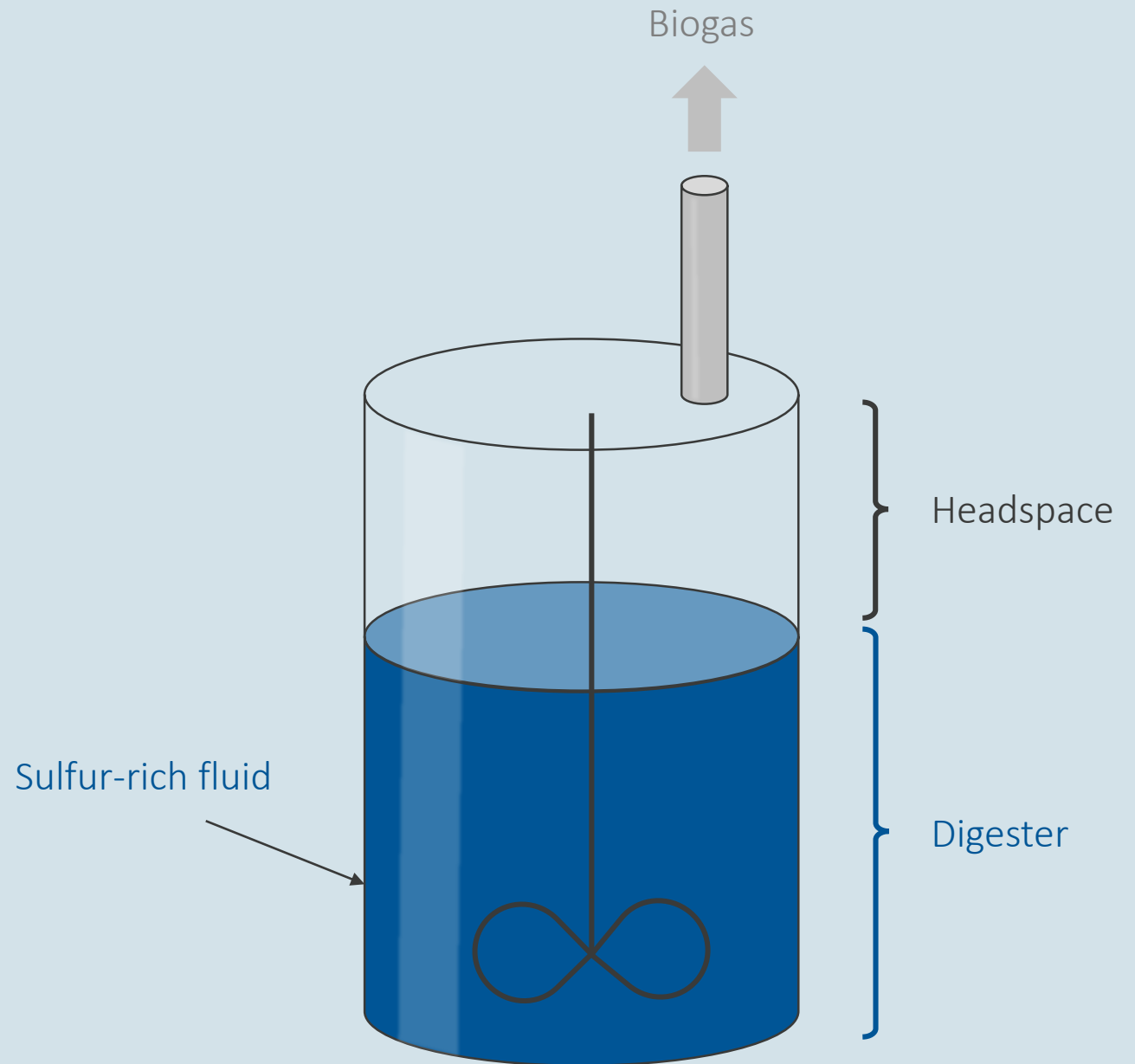
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*Department of Water Technology and Environmental Engineering  
University of Chemistry and Technology Prague*



# The Biogas Production Challenge

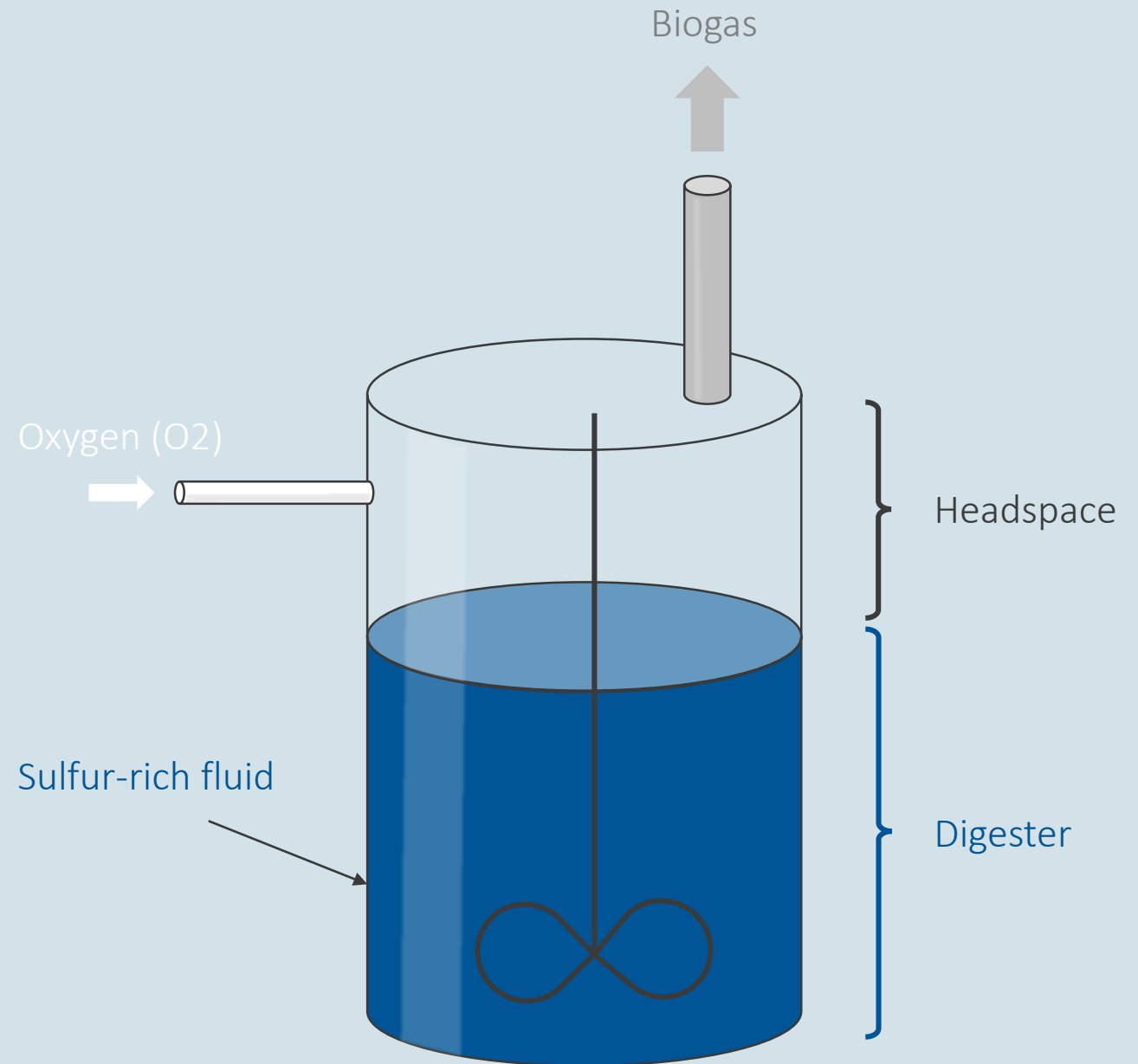
# The Biogas Production Challenge

- Anaerobic digestion of organic matter
  - Sludges from urban wastewater treatment plants, agricultural resources or animal waste
  - Biogas contains a small amount of Hydrogen Sulfide (H<sub>2</sub>S) which is toxic and corrosive



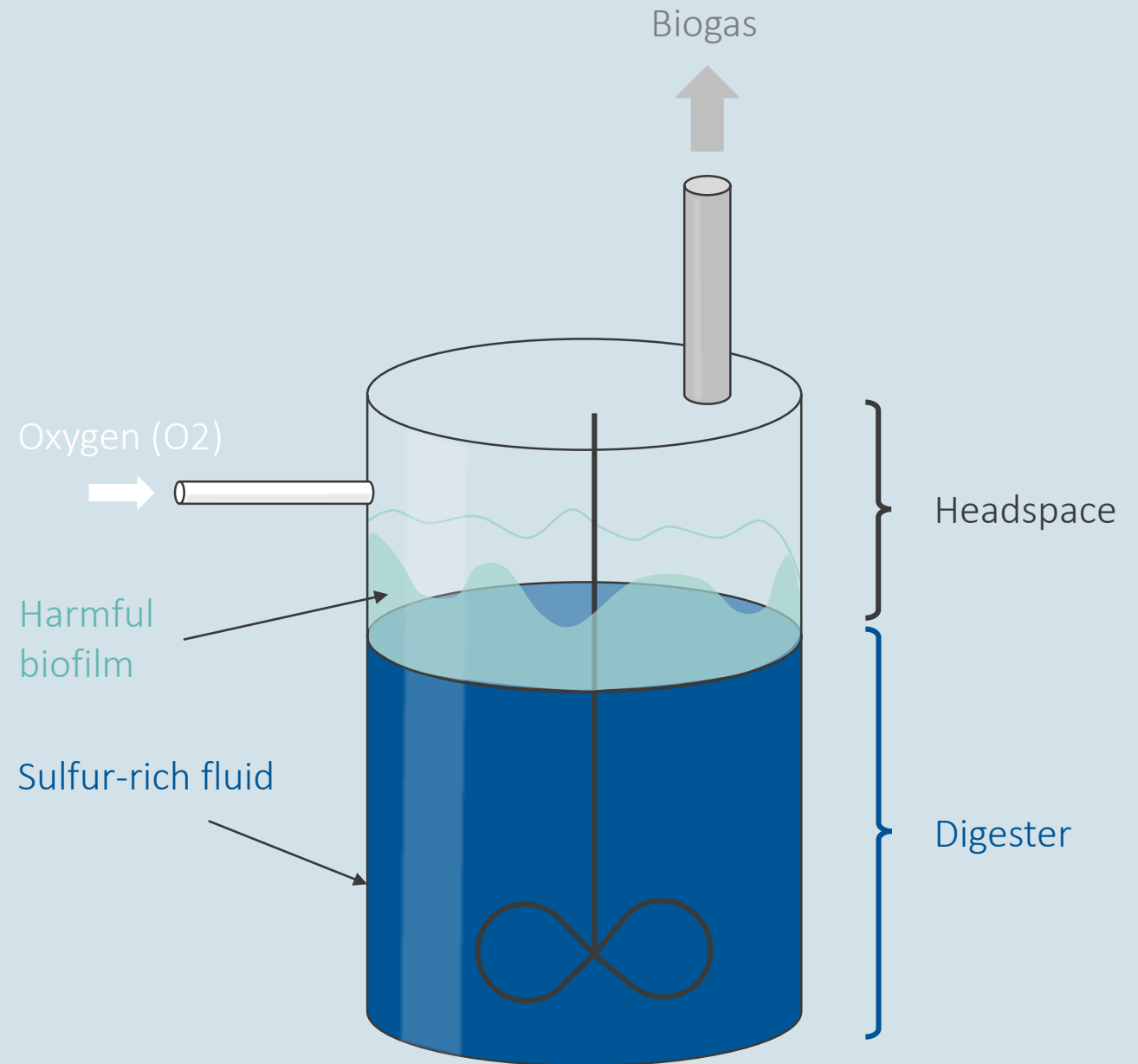
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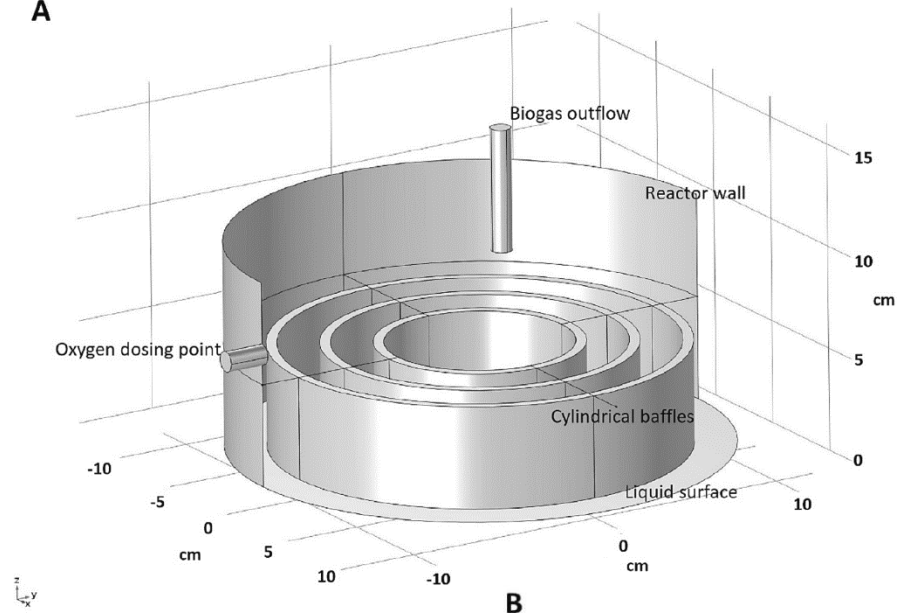
# How to Protect Digester's Headspace?

„By modifying headspace geometry biofilm growth can be directed to designated areas, reducing harmful effects on the reactor“

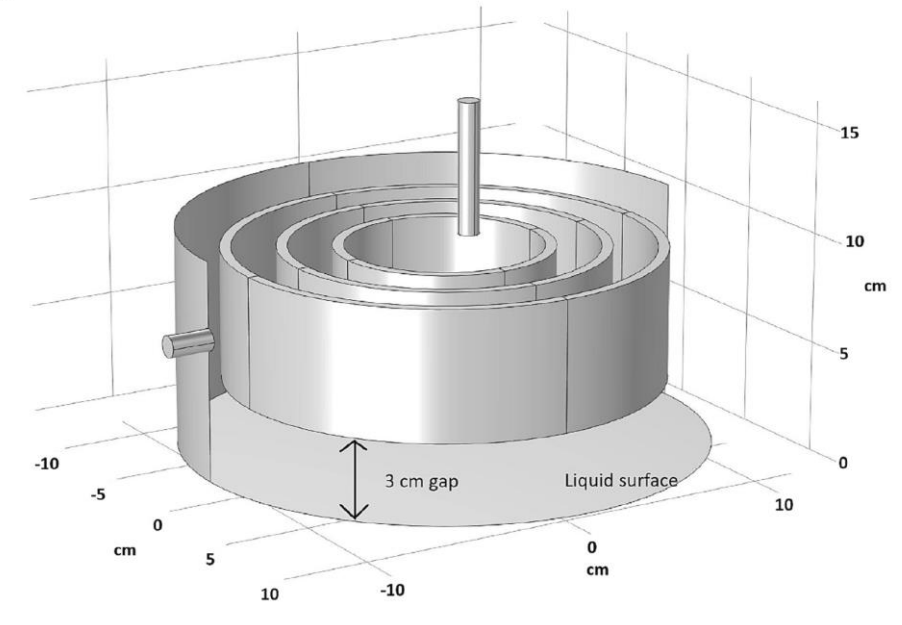
– UCT team

- Installation of cylindrical baffles serving as a surface for biofilm growth
- 360 days experimental setup:
  - Digester with empty headspace
  - Digester with variable headspace
- Surprising result. Walls were protected, but only up to the height of cylinders. Why? What is the process behind?

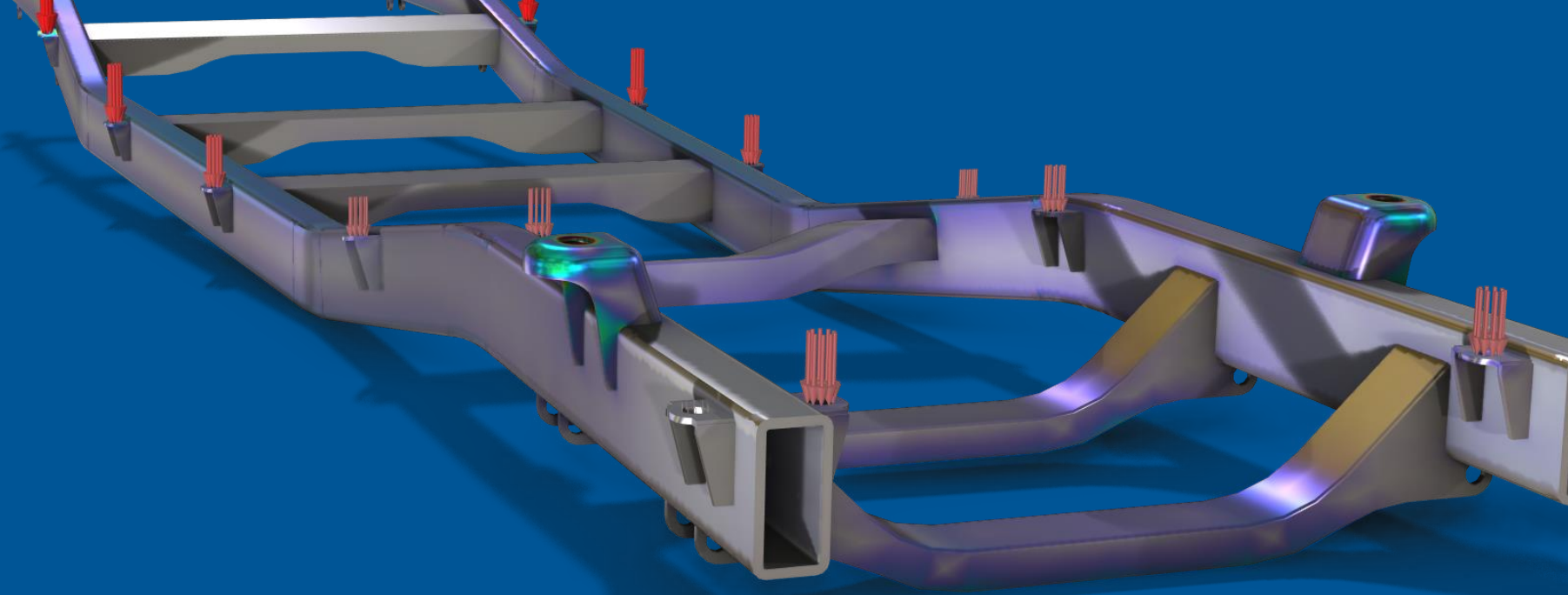
A



B



The variable headspace geometry and surprising results: A – Cylinders immersed in the liquid phase protected digester's wall, B – Cylinders were suspended 3 cm above the surface and biofilm growth up to 3 cm height.



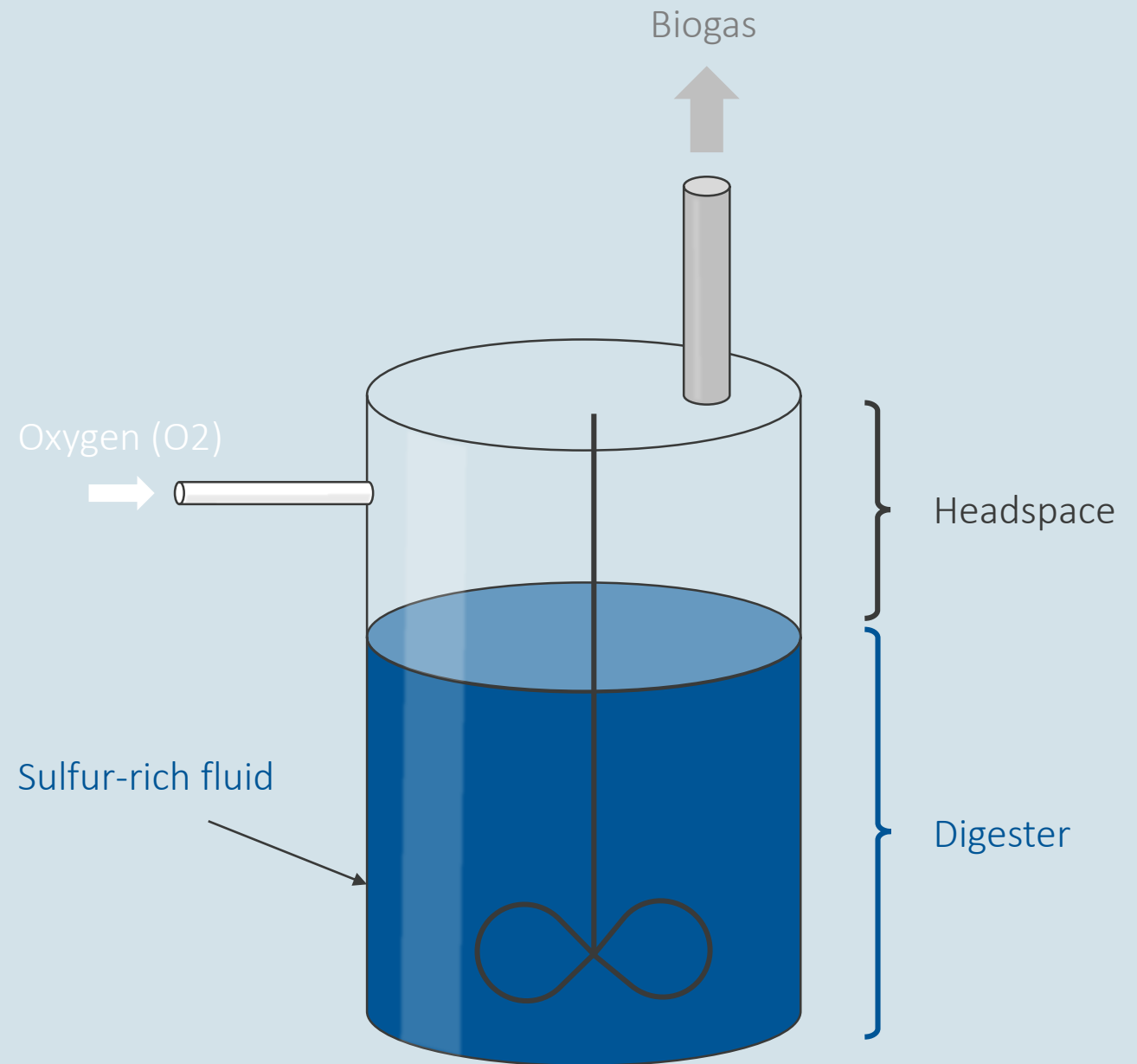
Time for COMSOL Multiphysics®



# Time for COMSOL Multiphysics

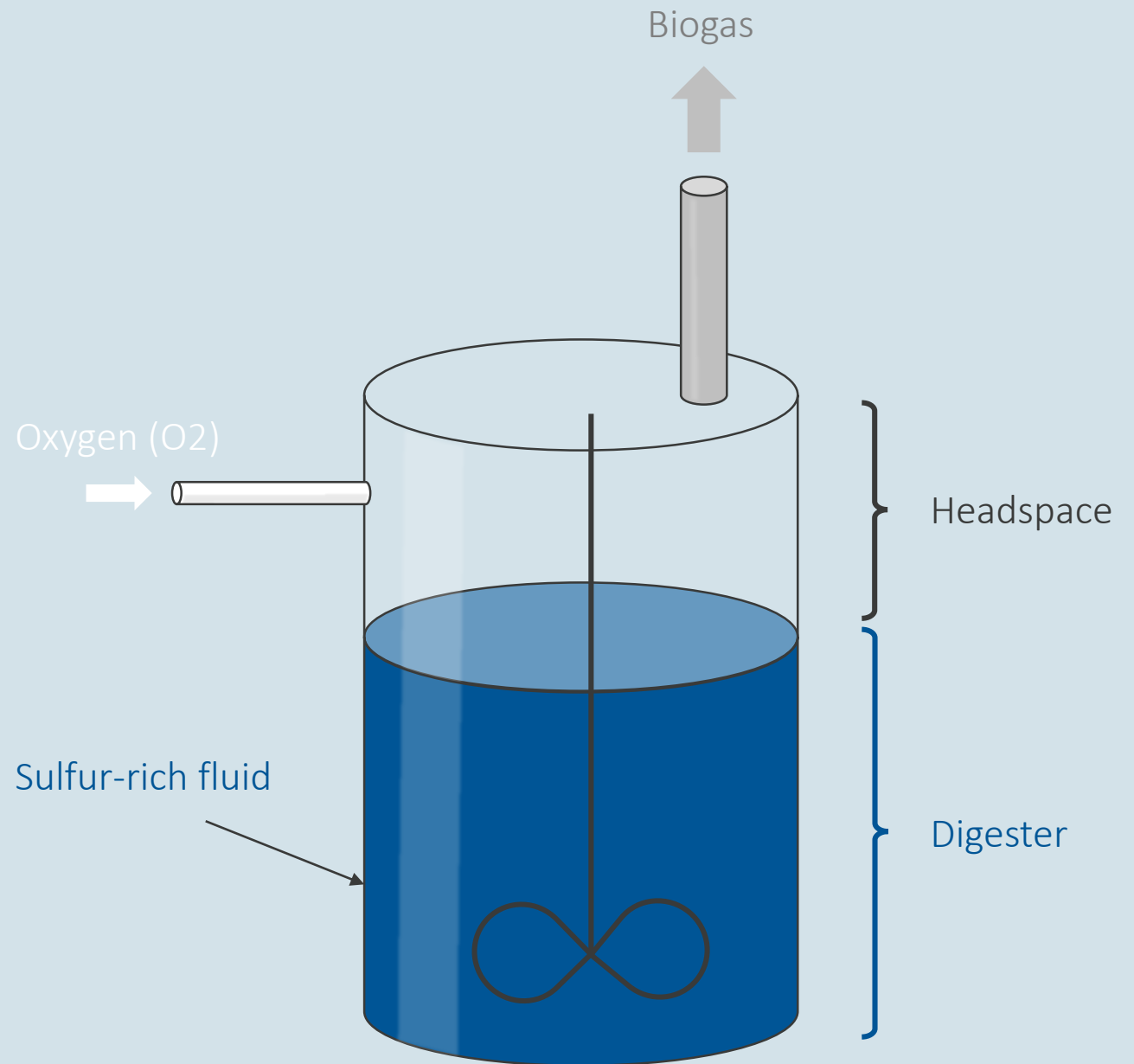
*CFD simulation on demand for the university team*

- Physics Interface
  - Mixture Model, Laminar Flow (continuous phase biogas, dispersed phase oxygen)
- Modelling challenges:
  - Stirring of the sulfur-rich fluid (60 RPM)
  - Three geometry scenarios



# Modelling Challenges: Simulation of Stirring

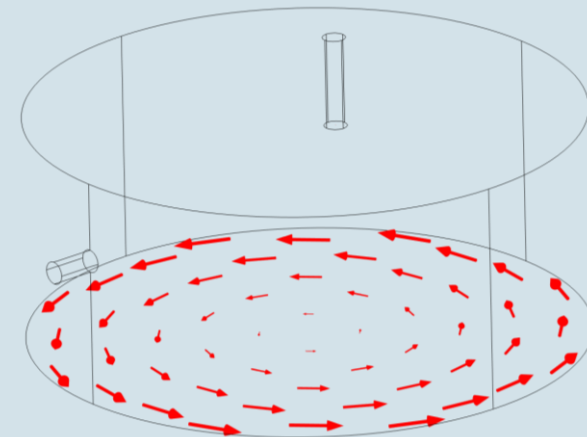
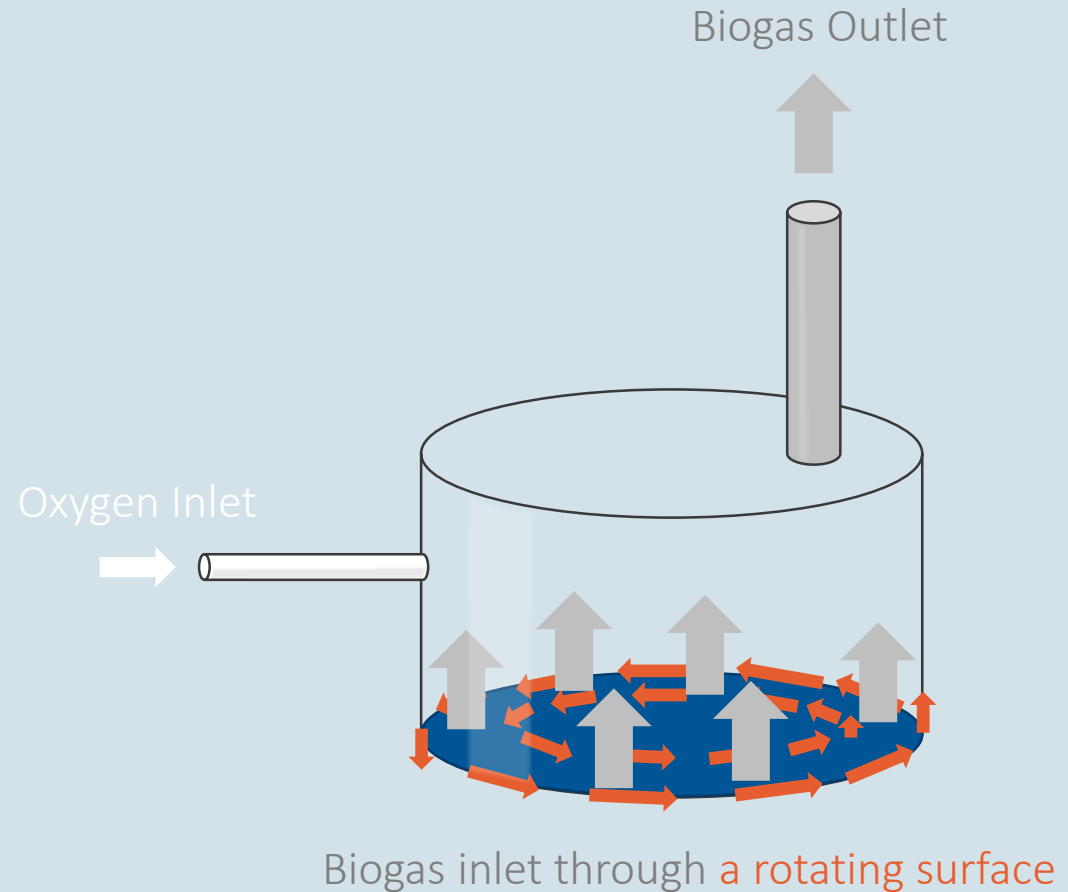
*Important simplification: Computational domain made only from digester's headspace*



# Modelling Challenges: Simulation of Stirring

*Important simplification: Computational domain made only from digester's headspace*

- Assumption 1: Biogas uniformly inflows through rotated fluid surface
- Assumption 2: Fluid surface rotates with the same RPM as the stirrer
- Assumption 3: We neglected shape of rotated fluid surface – paraboloid (we computed with planar boundary instead)



# Modelling Challenges: Simulation of Stirring

*Important simplification: Computational domain made only from digester's headspace*

## Model Settings:

- Cylindrical Coordinate System defined
- Biogas laminar inlet with user-defined velocity field (transformation between Cartesian system 1 and cylindrical 2 used)
- Oxygen normal inflow velocity
- Biogas constant pressure outlet
- Gravity included

The screenshot displays the COMSOL Multiphysics interface for a simulation titled "CFD\_Skruže\_3D\_mixture\_model.mph (root)". The Model Builder window shows the following structure:

- CFD\_Skruže\_3D\_mixture\_model.mph (root)
  - Global Definitions
  - Component 1 (comp1)
    - Definitions
      - Variables 1 - vypocet vstupni rychlosti w
      - Selections
      - Integration 1 (intop1)
      - Boundary System 1 (sys1)
      - Cylindrical System 2 (sys2)
      - View 1
    - Geometry 1
    - Materials
    - Mixture Model, Laminar Flow (mm)
      - Mixture Properties 1
      - Initial Values 1
      - Wall 1
      - Inlet 1 - bioplyn
      - Inlet 2 - kyslik
      - Outlet 1
      - Gravity 1
      - Equation View
    - Meshes
    - Study 1 - bez skruží (O2 included)
    - Study 2 - skruže vysunuté (O2 included)
    - Study 3 - skruže zasunuté
    - Results

The Settings window for "Inlet 1 - bioplyn" shows the following configuration:

- Label: Inlet 1 - bioplyn
- Boundary Selection: Cylinder 1 - vstupni plocha
- Selection: 3
- Override and Contribution: (empty)
- Equation: (empty)
- Mixture Boundary Condition: Velocity
- Velocity:
  - Normal inflow velocity
  - Velocity field
- Velocity field:
 

Component	Equation	Unit
$j_0$	$(\text{sys2.r} * \omega) * \text{sys2.T21}$	x
	$(\text{sys2.r} * \omega) * \text{sys2.T22}$	y
	vstupni_rychlost	z
- Dispersed Phase Boundary Condition: No dispersed phase flux

The Graphics window shows a 3D wireframe model of a cylindrical vessel with a central stirrer. The velocity field is visualized as a blue flow entering from the top. The coordinate system is cylindrical, with the z-axis pointing downwards. The vessel has a radius of 10 and a height of 10. The stirrer is located at the bottom of the vessel.

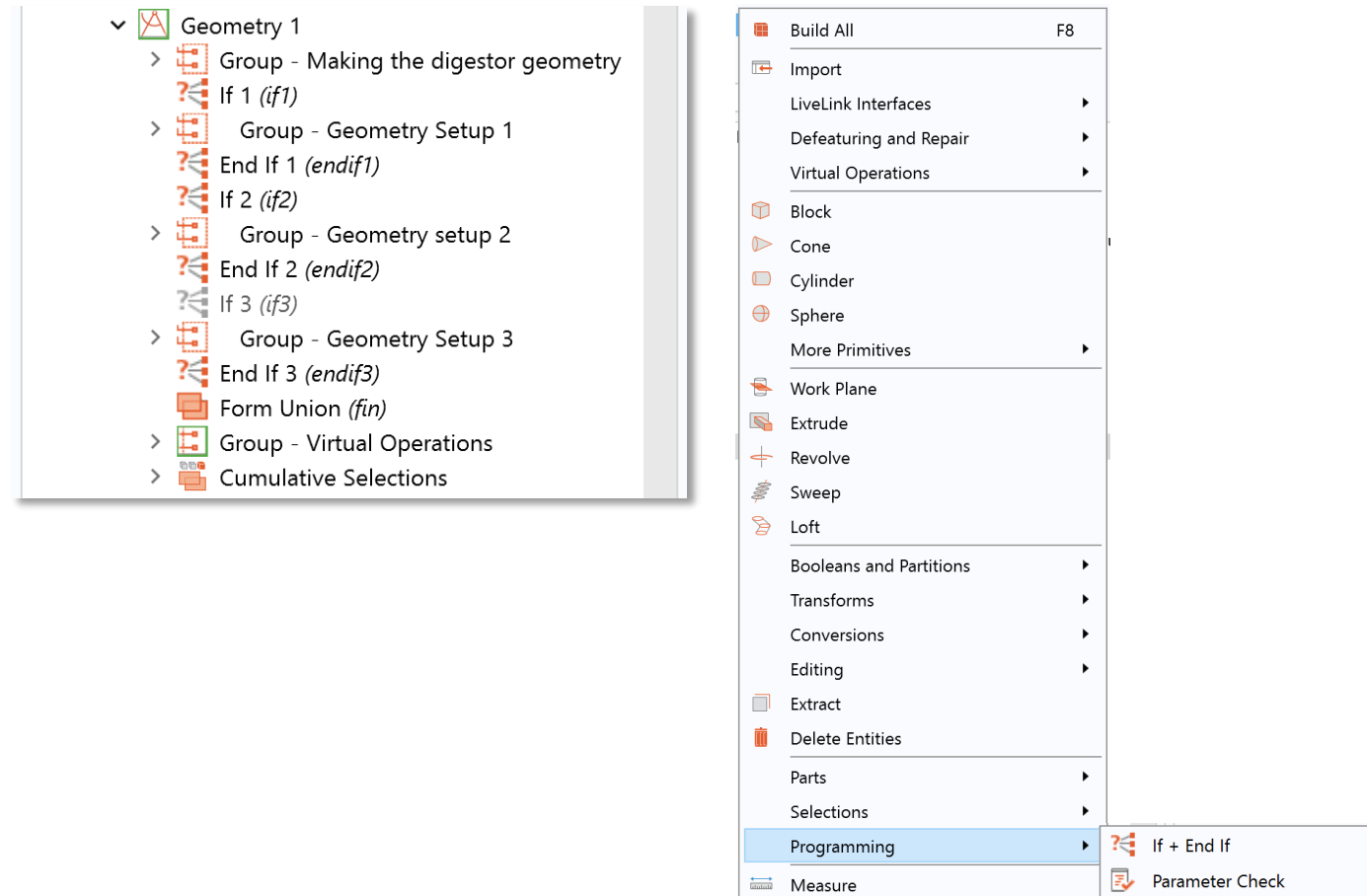
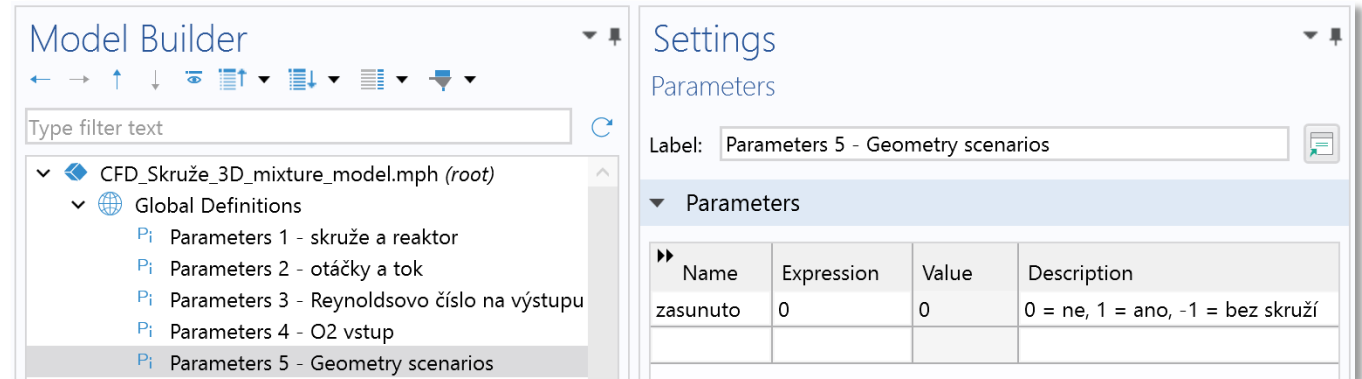
Two pop-up windows are visible in the bottom right corner, showing the transformation of the velocity field from the global Cartesian system to the local cylindrical system:

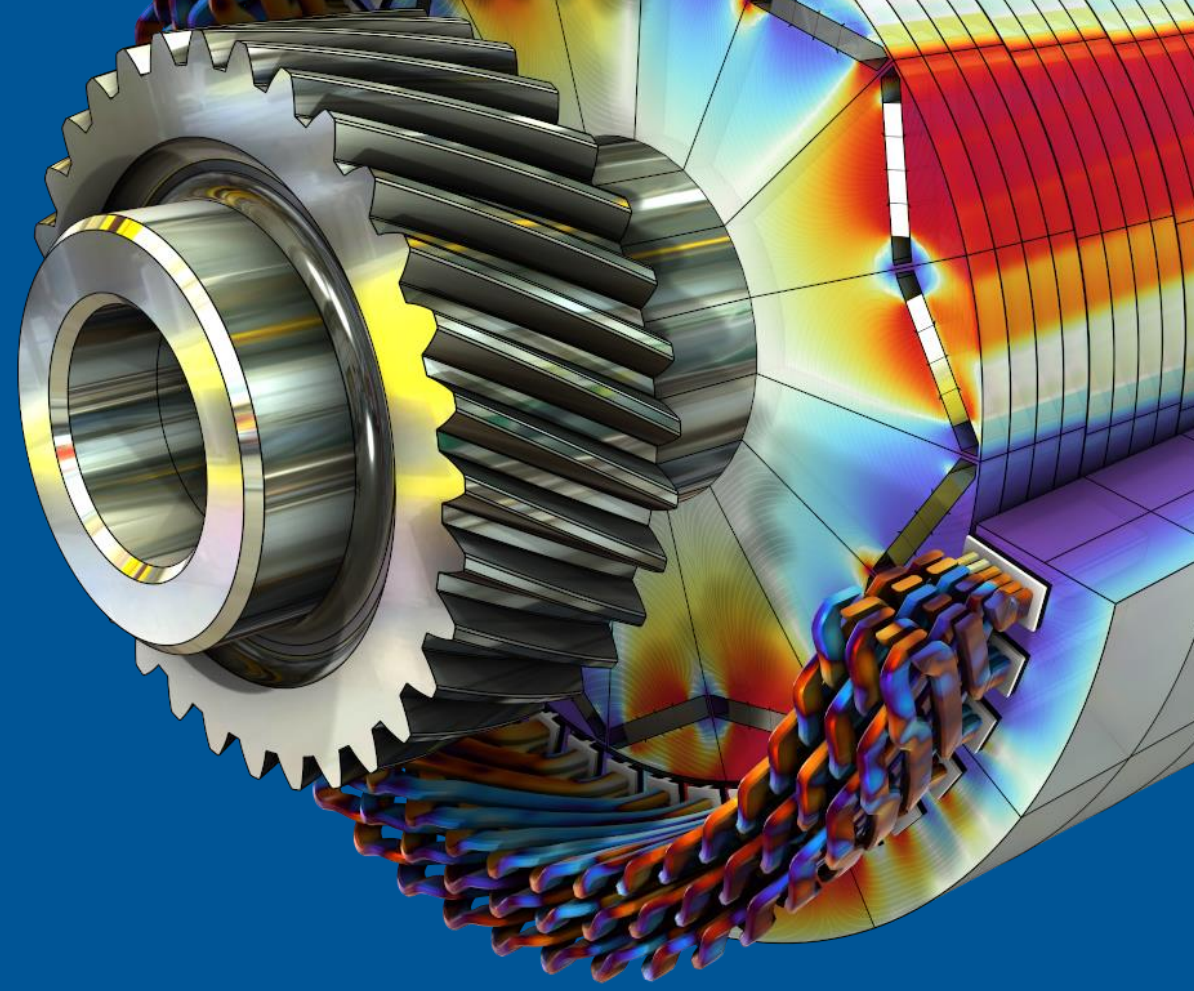
- Component 1 (comp1)
  - Definitions
    - Cylindrical System 2
      - Transform to global system (sys2)
        - sys2.T21 - Transform to global system (sys2), phi-x-component

- Component 1 (comp1)
- Definitions
  - Cylindrical System 2
    - Transform to global system (sys2)
      - sys2.T22 - Transform to global system (sys2), phi-y-component

# Modelling Challenges: 3 Geometry Scenarios

- Scenarios have different topology
- User changes a global parameter value:
  - 0 = cylindrical baffles 3 cm above
  - 1 = cylindrical baffles immersed in fluid
  - 1 = without baffles
- Less known functionality of programming the geometry reads parameter and changes geometry setup accordingly.
- Another possible solution would be making three different components.



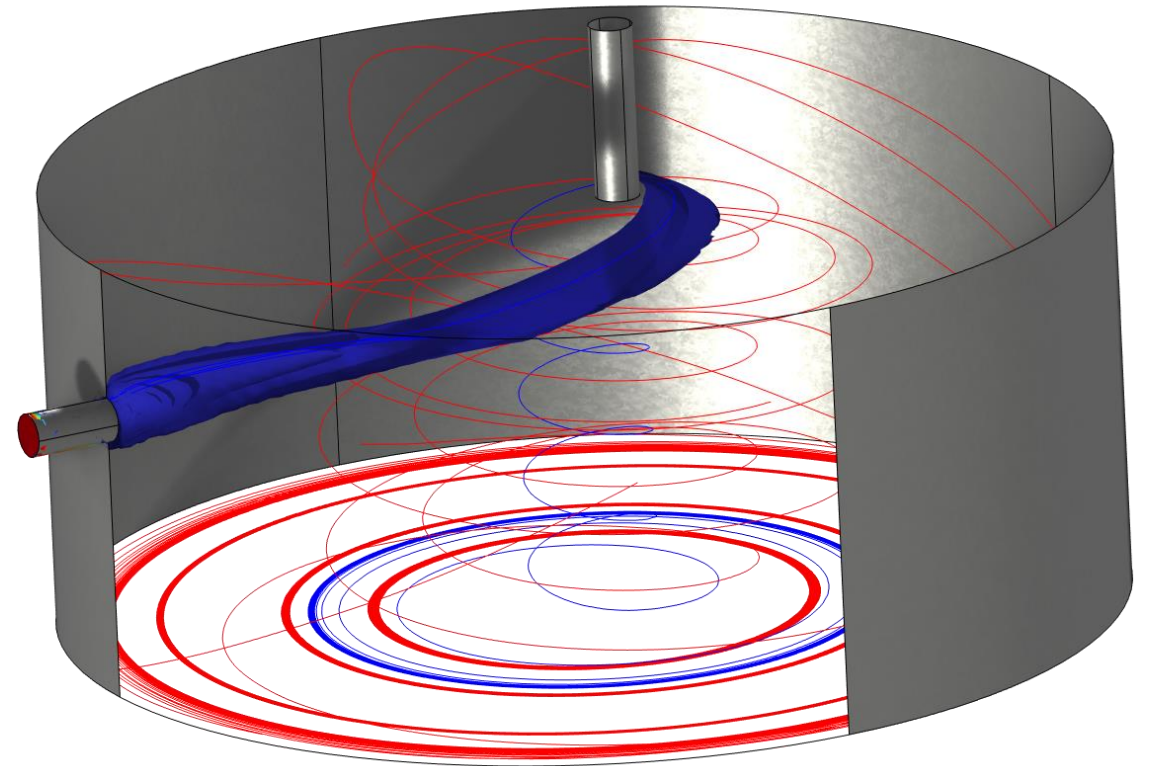
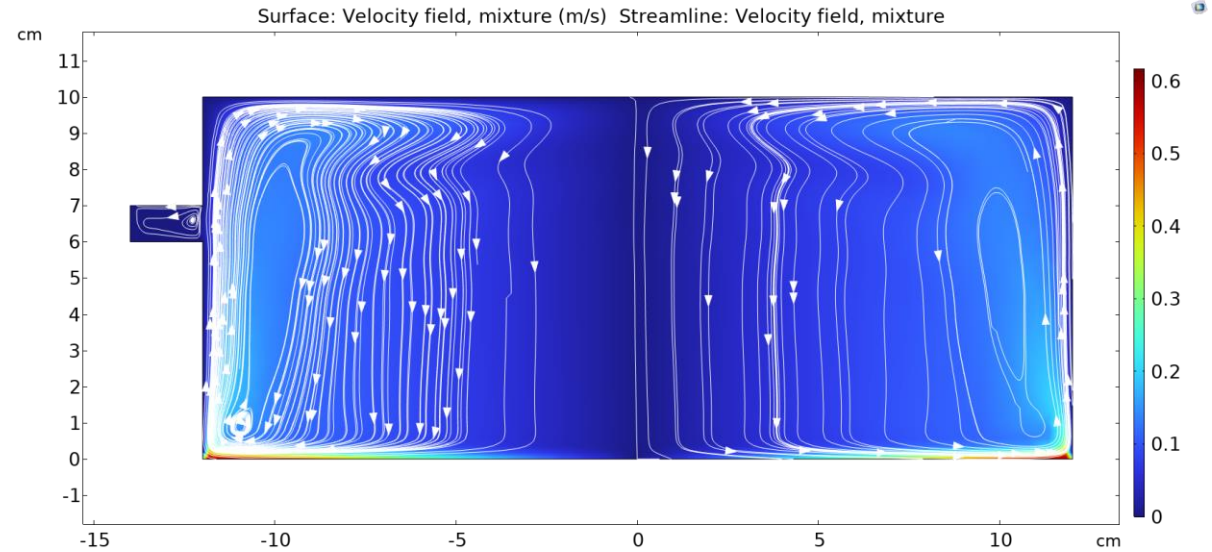


Simulation Results

## Without the Cylindrical Baffles

- Mesh consists of 133410 elements
- Results are independent on the mesh
- Red Streamlines: continuous phase
- Blue Streamlines: dispersed phase
- Isosurface: Dispersed phase volume fraction
- Conclusion:

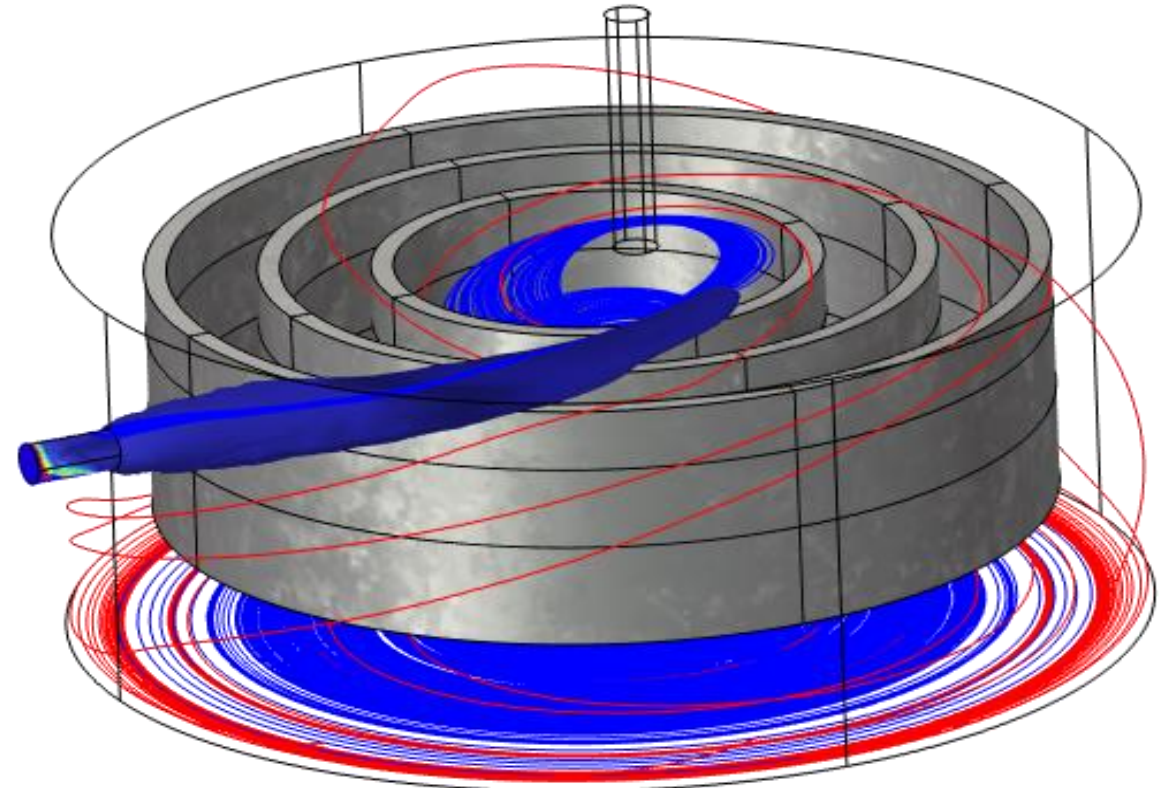
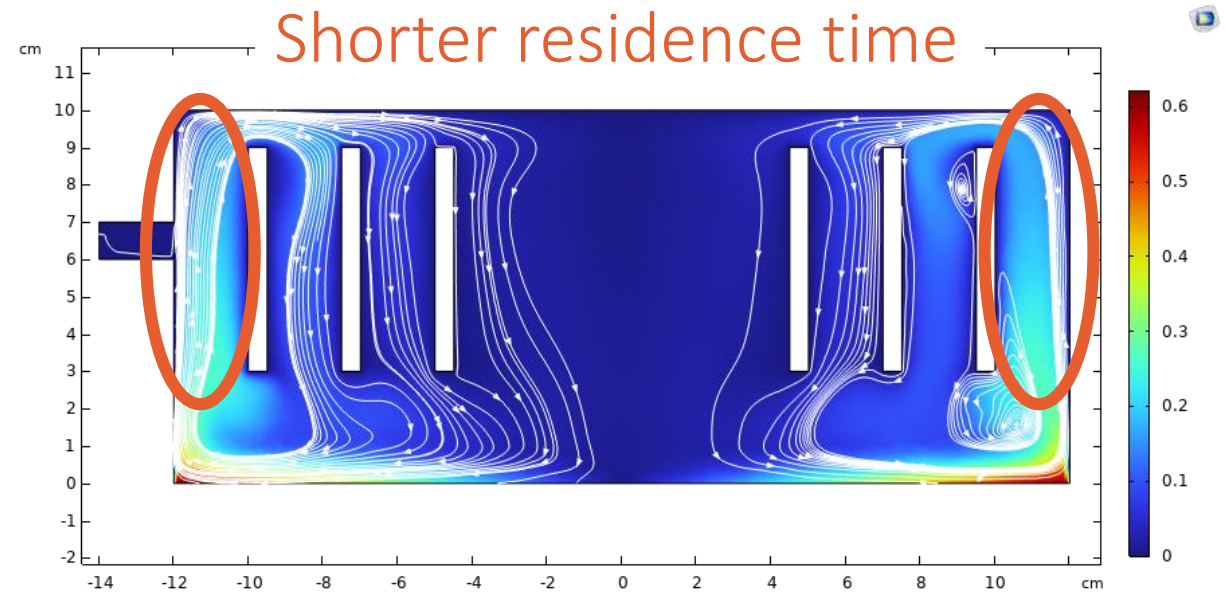
*„In the experiment with empty headspace, the biogas coming from the liquid was carried to the walls by centrifugal force together with oxygen. The gas mixture was evenly distributed throughout the headspace.“*



## Cylindrical Baffles Up

- Mesh consists of 1290048 elements
- Results are independent on the mesh
- Red Streamlines: continuous phase
- Blue Streamlines: dispersed phase
- Isosurface: Dispersed phase volume fraction
- Conclusion:

*„The biogas coming from the liquid was carried to the walls by centrifugal force together with oxygen. However, the velocity between the last cylinder and the wall is much higher because of a cross-section reduction. It leads to shorter residence time in the area.“*

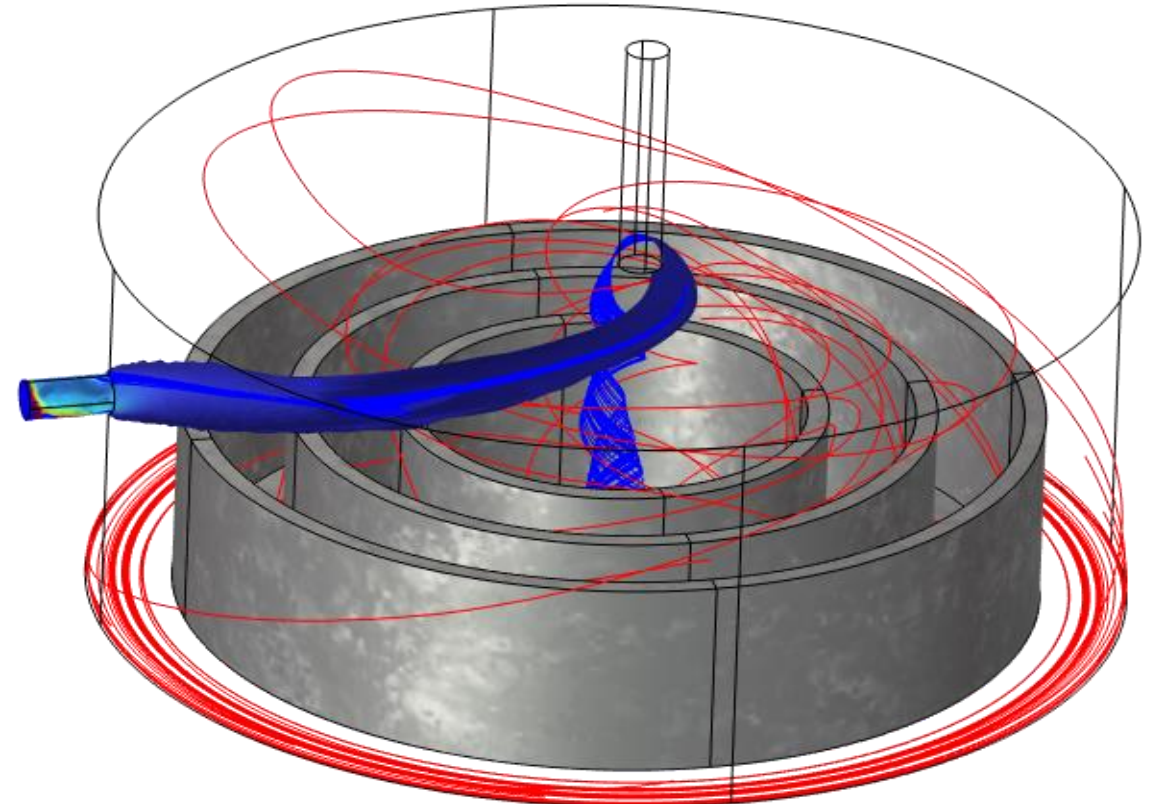
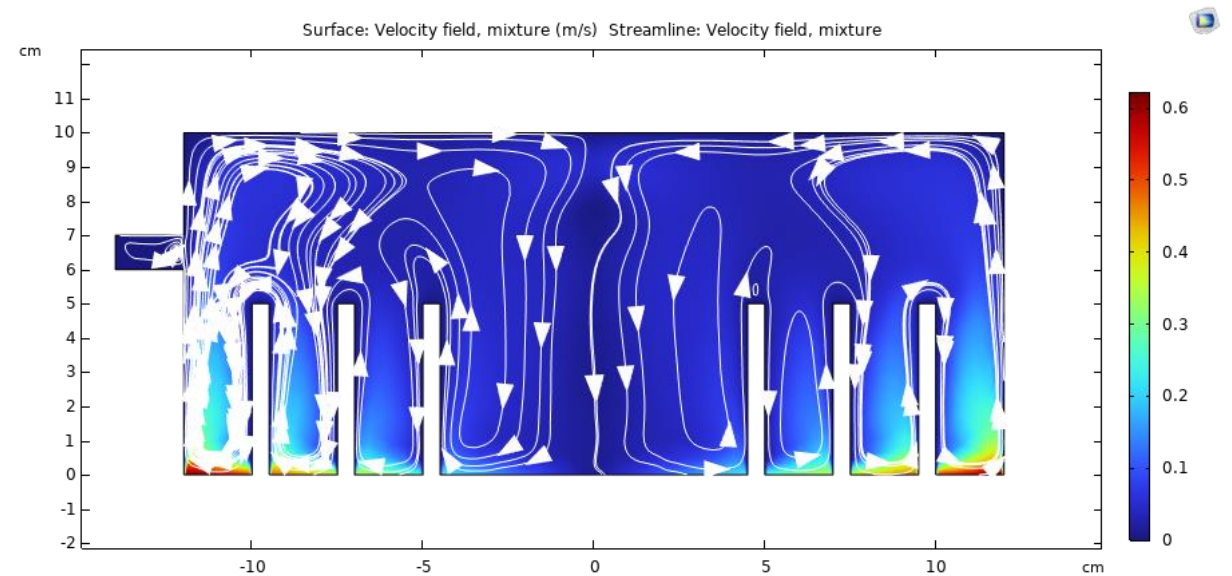




# Cylindrical Baffles Immersed

- Mesh consists of 1168122 elements
- Results are independent on the mesh
- Red Streamlines: continuous phase
- Blue Streamlines: dispersed phase
- Isosurface: Dispersed phase volume fraction
- Conclusion:

*„The gas mixture could not be directly pushed to the walls since the cylinders interrupted the flow. The mixture flows from the center from one gap to another. The residence time of the mixture between the cylinders could have caused all oxygen was entirely consumed.“*



# Results Were Published in Prestigious Journal FUEL

Fuel 362 (2024) 130900



Contents lists available at [ScienceDirect](#)

Fuel

journal homepage: [www.elsevier.com/locate/fuel](http://www.elsevier.com/locate/fuel)



Full Length Article

## Importance of digester's headspace geometry for the efficient H<sub>2</sub>S removal through microaeration; experimental and simulation study

Markéta Andreides<sup>\*</sup>, Lucie Pokorná-Krayzelová, Jan Bartáček

*Department of Water Technology and Environmental Engineering, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic*

### ARTICLE INFO

#### Keywords:

Anaerobic digestion

CFD model

### ABSTRACT

Microaeration for biogas desulfurization occurs mainly in the headspace of anaerobic digesters where the biofilm growth is mainly reported; however, no study has been focused on the effect of headspace geometry on



There is a Space for Improvements

## There is a Space for Improvements

- The model explained the experimental results, but...
- Boundary condition **Internal Wall** for the baffles would spare plenty of DOFs
- **Particle Tracing** would help to visualize and compute the Residence Time Factor
- The **Optimization Module** could find the optimal design of cylindrical baffles

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