BIOCOMEM

H2020 GRANT AGREEMENT NUMBER: 887075

Start date of project: 01/06/2020 **Duration: 3 years**

[WP2 – Industrial Specifications, Process design]

D2.1
MODA for the membrane modelling

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v0.1	26-07-2020	First Release	TUE	F.Gallucci
V0.2	24-09-2020	After comments from partners	TUE	F.Gallucci

Project funded by European Union's Horizon 2020 research and innovation programme (2014-2020)		
Dissemination Level		
PU	Public	
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	X
CON	Confidential, only for members of the Consortium	

(*) for generating such code please refer to the Quality Management Plan, also to be included in the header of the following pages

(**) indicate the acronym of the partner that prepared the document

Content

1. EXECUTIVE SUMMARY

1.1. Description of the deliverable content and purpose

In the framework of BIOCOMEM project, the key objective is the scale-up and manufacturing of advanced biobased materials for membrane production and their demonstration in CO_2 separation processes.

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The particular aim of this deliverable is to present the MODA for the modelling of bio-based membrane separation for CO_2 separation from different mixtures (biogas, post-combustion and natural gas).

1.2. Brief description of the state of the art and the innovation brought

N/A

1.3. Deviation from objectives

N/A

1.4. If relevant: corrective actions

N/A

1.5. If relevant: Intellectual property rights

N/A

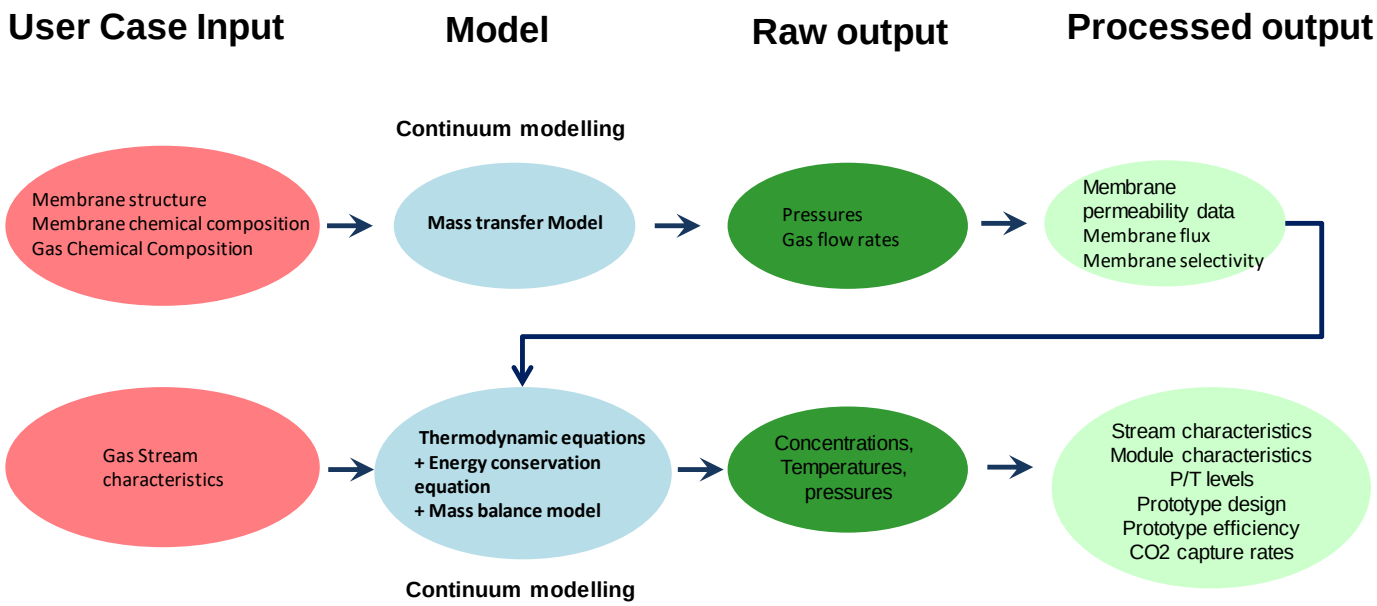
2. The MODAs

2.1. MOdelling DAta providing a description for <Membranes> simulated in project <BIOCOMEM>

OVERVIEW of the SIMULATION			
1	USER CASE	The user wants to model the CO_2 capture process in polymeric membranes	
2	CHAIN OF MODELS	MODEL 1	Continuum model: Mass transfer Model based on thermodynamics (dusty gas model)
		MODEL 2	Tightly coupled Continuum model: Thermodynamic equations + Energy conservation equation + Mass balance model
3	PUBLICATION PEER-REVIEWING THIS DATA		
4	ACCESS CONDITIONS	Model 1: implementation using commercial software Matlab/Simulink (mathworks.com) and Excel (www.microsoft.com). Will be made available for other users Model 2: implementation of custom models in commercial software ASPEN (http://home.aspentech.com/products/engineering/aspen-plus) and SImSci Pro/II (http://software.schneider-electric.com/products/simsci/design/pro-ii/) and self-developed software. Except for the confidential parts it will be made available for other users.	
5	WORKFLOW AND ITS RATIONALE	First the permeation characteristics of the membranes should be computed (Model 1) to obtain the permeability and the permselectivity to be used in Model 2. Model 2 calculates the flow through the selected membrane under operational conditions. Model 2 is a tightly coupled set of Thermodynamic models and mass and heat balance models embedded in a typical simulator used in the process engineering and for the computation of heat/material balances and efficiency calculation of the system.	

Workflow picture

Workflow materials models: Membranes



BIOCOMEM

2.1.1. MODA: Physics-based Model

2.1.1.1. Simulation with MODEL 1

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	To determine the permeability of a membrane Via performing detailed mass transfer simulation of (ultra-thin/porous) polymeric membranes. To analyze and understand the permeation behavior, to generate input for the overall process scheme simulators. To propose optimal membrane characteristics to enhance membrane flux and selectivity.
1.2	MATERIAL	Membrane material: Bio-based polymers Characteristics of the membranes and compositions measured during the project. Gas composition
1.3	GEOMETRY	Flat sheet membranes and hollow fibers. Geometry optimized during the project
1.4	TIME LAPSE	Not applicable. Only steady state conditions
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Pressure
1.6	PUBLICATION ON THIS DATA	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum Model: Mass transfer Model based on thermodynamics	
2.1	MODEL ENTITY	finite volumes	
2.2	MODEL PHYSICS / CHEMISTRY EQUATION PE	**Equation**	PE: Dusty Gas Model $\frac{1}{RT}\frac{\partial}{\partial t}(\varepsilon p_i) = -\nabla \cdot \vec{N}_i + R_i$ for *i*=1, … *N what is Ri?* $\nabla p_i = -\frac{p_i}{RT}\left(\frac{RT}{p} - \frac{M_i}{\rho}\right)\nabla p + \sum_{\substack{j\neq i \\ j\neq s}} \frac{RT}{pD_{i,j}^{eff}}\left(p_i\vec{N}_j - p_j\vec{N}_i\right) - \frac{RT}{D_{K,i}^{eff}}\vec{N}_i$ for *i*=1, … *N*-1

			$RT\frac{\sum_{i\neq s} M_i \vec{N}_i}{\sum_{i\neq s} M_i p_i} = -\frac{k}{\mu}\nabla p$ $p = \sum_{i=1}^{N} p_i$
		Physical quantities	*T = Temperature* *p = Partial Pressure* *D = Diffusivity* *N = molar flow* *M = molar mass*
2.3	**MATERIALS RELATIONS**	**Relation**	– Effective molecular binary diffusivities: $D_{i,j}^{eff} = \frac{\varepsilon}{\tau} D_{i,j}$ with $D_{i,j} = 1.013\cdot 10^{-2} \frac{T^{1.75}}{p} \frac{\sqrt{\frac{1}{M_i}+\frac{1}{M_j}}}{\left(\sqrt[3]{V_i}+\sqrt[3]{V_j}\right)^2}$ (Fuller et al., 1966, 1969). where *T* in K, *p* in Pa, M_i in g/mol and V_i the diffusional volume of species *i* – Effective Knudsen diffusivities: $D_{K,i}^{eff} = \frac{\varepsilon}{\tau} D_{K,i}$ with $D_{K,i} = \frac{d_{pore}}{3}\sqrt{\frac{8RT}{\pi M_i}}$
		Physical quantities/ descriptors for each MR	*T = Temperature* *p = Partial Pressure* *D = Diffusivity* *N = molar flow* *M = molar mass*
2.4	**PHYSICS FORMULATION OF THE CONDITIONS**		
2.5	**SIMULATED INPUT**		

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	finite volumes	
3.2	SOFTWARE TOOL	*Solved in Matlab and/or Excel*	
3.3	TIME STEP	Variable time step	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	
3.5	COMPUTATIONAL BOUNDARY CONDITIONS		
3.6	ADDITIONAL SOLVER PARAMETERS	• *Specific tolerances, 10^{-6} on mols* *Grid, adaptive*	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	Membrane permeability Membrane flux Membrane selectivity
4.2	METHODOLOGIES	Use of ideal gas law to change from pressures to moles and masses and concentrations. Calculation of the separation factor based on the following formula $S_F(AB) = \left(X_A/X_B\right)\Big\|_{permeate} \Big/ \left(X_A/X_B\right)\Big\|_{retentate}$ Rejection factors $R=1-C_{i,p}/Ci,r$
4.3	MARGIN OF ERROR	numerical error < 0.1 % in post-processing

2.1.1.2. Simulation with MODEL 2

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	To perform detailed Thermodynamic calculation and Energy conservation and Mass balance calculation for the optimal process scheme. To calculate the process efficiency and performance
1.2	MATERIAL	Membrane characteristics from Model 1
1.3	GEOMETRY	Hollow fiber
1.4	TIME LAPSE	Not applicable steady state simulation
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Gas flow, Temperature composition and pressure
1.6	PUBLICATION ON THIS DATA	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum Model: Thermodynamic equations + Energy conservation equation + Mass balance model	
2.1	MODEL ENTITY	finite volumes	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	System of Conservation equations of mass and Energy, Thermodynamics relations
		Physical quantities	*T = Temperature* *p = Partial Pressure* *N = molar flow* *M = molar mass* *m = mass flow*
2.3	MATERIALS RELATIONS	**Relation**	
		Physical quantities/ descriptors for each MR	*T = Temperature* *p = Partial Pressure* *D = Diffusivity* *N = molar flow* *M = molar mass*
2.4	PHYSICS FORMULATION OF THE CONDITIONS		

2.5	**SIMULATED INPUT**	Permeability (function of T) of the membrane calculated with model 1.

3	**SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS**		
3.1	**NUMERICAL SOLVER**	Iterative solver	
3.2	**SOFTWARE TOOL**	*Solved in Aspen or Pro/II*	
3.3	**TIME STEP**	N/A	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	Conservation equations of mass and Energy, Thermodynamics relations. MR: connections between D, T, P, m and M via permeability
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**		
3.6	**ADDITIONAL SOLVER PARAMETERS**	• *Specific tolerances, 10^{-4} on molar flow (absolute value - mol/s)*	

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT**	Stream characteristics Module characteristics P/T levels Prototype design Prototype efficiency CO_2 capture rates
4.2	**METHODOLOGIES**	CO_2 capture $E_{CO_2} = \frac{\dot{m}_{CO_2,capt}}{\dot{m}_{NG} \cdot LHV_{NG} \cdot E_{NG}} \left[\frac{g_{CO_2}}{MJ_{H2}}\right]$ Equivalent CO_2 Emission $E_{CO_2,eq} = \frac{\dot{m}_{CO_2,capt} - Q_{th} \cdot E_{th,ref} - W_{el} \cdot E_{el,ref}}{\dot{m}_{NG} \cdot LHV_{NG} \cdot E_{NG}} \left[\frac{g_{CO_2}}{MJ_{H2}}\right]$ Equivalent specific primary energy consumption for CO2 avoided $SPECCA_{eq} = \frac{\frac{1}{\eta_{H_2,eq}} - \frac{1}{\eta_{H_2,eq,ref}}}{E_{CO_2,ref} - E_{CO_2,eq,ref}} \cdot 1000 \left[\frac{MJ_{th}}{kg_{CO_2}}\right]$ (to be adapted for the different schemes)
***4.3**	**MARGIN OF ERROR**	numerical error < 1 % in post-processing