Delivery date: 14-9-2014

Authors:

Patrick Anderson
TU/e
E-mail : pda@tue.nl

Javier LLorca
IMDEA
Email : javier.llorca@imdea.org

Jaraj Kosek
VSCHT
Email : Juraj.Kosek@vscht.cz

Daniele Marchisio
POLITO
E-mail :
daniele.marchisio@polito.it

Andreas Daiss
BASF
E-mail : andreas.daiss@basf.com

MODENA

Deliverable 3.1

Layout of macro-tools, their interfaces to other tools and an initial set of computational recipes

WP's leader: TU/e

Principal investigator:
Patrick D. Anderson, TU/e (NL)

Project's coordinator:
Heinz Preisig, NTNU (N)

1. Description of deliverable

This deliverable contains the results of task 3.1 which objective was to define the layout of macro-scale tools that will be the blueprint of activities in this Work Package 3. This layout contains a review of the existing software that will be used for the macro-scale computations and are suitable for the protocols to be developed. In conjunction with the protocols, diverse reference recipe(s) will be developed the manufacturing of PU foams describing reactants, initial mixture composition, process configuration, conditions and constraints, typical meso-scale morphology of resulting foam(s). The equivalent virtual recipe is constructed as the algorithmic flow sheet describing the flow of information within this WP and interfaces to other WPs. Furthermore, a detailed description of the interfaces and communication protocols required for the design of software adaptors (coupling between scales) is developed.

With these components into place, inputs from WP1 and WP2 (including physical properties, property methods, reaction kinetics and equations of state) can be processed as well. Furthermore, a description of concepts in macro-tools for initial dispersion of reactants, bubble initiation, solidification of cell walls and cell coalescence/wall drainage can be completed, as well as descriptions of suitable validation procedures. Moreover, tools for simulation of application mechanical and transport properties including their deterioration will be adopted or developed.

2. Summary of contribution of involved partners to deliverable

VSCHT, POLITO and IMDEA will develop 5 macro-scopic modelling tools. They contain models for thermal insulting properties (VSCHT), acoustic insulating properties (VSCHT), foam reconstruction (VSCHT), mechanical properties (IMDEA) and fluid dynamics (POLITO)

VSCHT, BASF, IMDEA and POLITO have provided a review of existing software, (information) protocols and interface and algortihm flow sheet for each of these tools or for the whole macro-scopic scale. In addition, BASF provided reference recipe(s) for the manufacturing of PU foams describing reactants, initial mixture composition, process configuration, conditions and constraints and typical meso-scale morphology of resulting foam(s). They are however in D2.1

3. Macro-scopic tools in flowchart of all tools

The macro-scopic tools receive inputs and produce outputs for modelling tools at nano-scale and meso-scale. This is shown in the flow chart figure in the Appendix.

The macro-scopic tools are explained below with some information about their interfaces and protocols, such as input and output names. More details including operating ranges, data types and dimensions of all inputs and outputs are in the Appendix.

4. Tool for foam thermal insulating properties

4.1 Introduction

The primary goal of the tool is to predict the thermal insulating properties of the final foam. The thermal insulating properties will be characterized by the equivalent conductivity.

Results of this tool will be validated together by measurement of equivalent conductivity in WP6.

4.2 Review of existing software

Currently, no software is available that is able to predict thermal insulating properties of high porosity polymeric foams. The state-of-the-art models describe both important heat transfer modes: conduction and radiation. Convection can be safely neglected when the cell size is below 1 mm. These models either use “homogeneous approach” (Coquard et al., 2009) or “multi-phase approach” (Ferkl et al., 2014) to coupled heat transfer. VSCHT will develop this software containing the latter model for estimation of heat transfer properties.

The mathematical model will describe coupled conductive-radiative heat transfer in spatially three-dimensional two-phase domain (Ferkl et al., 2014). This model accounts for the absorption and emission of radiation both in the solid and in the gas phase, partial reflection of radiation on phase interfaces (including the interference effects) and the effect of complex foam morphology on the thermal insulating properties of polymer foams. The model will be extended to account for the non-Fourier conduction occurring in foams with very small cells.

The first version of the tool will be coded in Fortran.

4.3 Interface and Protocols

Inputs and outputs will be communicated through ASCII text files.

Here we list input variables for the tool and its connection to other work packages:

- Thermal conductivity of gas and solid phase (user or literature)
- Absorption coefficient of gas and solid phase (user or literature)
- Foam thickness (user)
- Voxel-based foam morphology (WP3)
- Foam porosity and average cell size and average wall thickness (WP3)

The results/outputs of the tool are following:

- Equivalent foam conductivity

The results of this tool will be validated by experimental measurements of equivalent conductivity for various foam samples in WP6, specifically in T6.1.

5. Tool for foam acoustic insulating properties

5.1 Introduction

The primary goal of the tool is to predict the acoustic insulating properties of the final foam. The acoustic insulating properties will be characterized by the characteristic impedance and the wavenumber of the foam at audible frequencies. The second output can be the acoustic absorption coefficient of a layer of the foam.

Results of this tool will be validated together by measurement of equivalent conductivity in WP6.

5.2 Review of existing software

Currently, only commercial software exists that is able to predict acoustic insulating properties of polymer foams. The list of the commercial software includes: Acoustic module for COMSOL, ZORBA, NOVA, SAM Predictor_MAA. To promote the idea of open source VSCHT will develop this software in Fortran. It will contain simple predictive models for the estimation of acoustic properties.

Open cell polymer foams can be used as sound absorbing materials. The acoustic properties of a porous material can be characterized by the characteristic impedance and the wavenumber (Allard and Atalla, 2009). The acoustic absorption is dependent on the overall foam geometry and expresses the ratio of the absorbed energy to the energy of the incident sound wave.

The first version of the tool will be based on laws of Delany and Bazley (Delany and Bazley, 1970). In these laws, acoustic properties are determined by the foam flow resistivity. Flow resistivity is inversely proportional to permeability, which is known from the Darcy's law. The flow resistivity will be determined from the simulation of the steady-state Stokes flow through the inner structure of the open-cell foam.

The extended version of the tool will use the Johnson-Champoux-Allard model. This model utilizes more information about the foam morphology.

5.3 Interface and Protocols

The first version of the tool will be coded in Fortran. Inputs and outputs will be communicated through ASCII text files.

Here we list input variables for the tool and its connection to other work packages:

- Voxel-based foam morphology (WP3)
- Air thermal diffusivity (literature)

The results/outputs of the tool are following:

- Characteristic impedance
- Wavenumber
- Acoustic absorption coefficient

The validation of this tool can be done in WP6 by direct measurement of acoustic absorption coefficient for various foam samples.

6. Tool for foam reconstruction

6.1 Introduction

The primary goal of the tool is to provide spatially three-dimensional image of foam morphology. Results of this tool will be validated together by measurement of equivalent conductivity in WP6.

6.2 Review of existing software

Currently, no software is available that is able to create representative three-dimensional foam morphology from morphology descriptors like porosity, average cell size, strut content, etc. However, procedures how to accomplish that are described in scientific literature. Thus, VSCHT will develop this software.

The inner structure of polymer foams constitutes from polyhedral cells separated by polymer struts and walls. In polyurethane foams, large portion of polymer mass is located in the struts (in open cell foams, all polymer is in the struts). The basic requirement on the reconstructed foam is, that it will resemble the real foam as much as possible, while preserving foam porosity, cell size, wall thickness etc.

The foam image will be based on Voronoi tessellation. The struts will be created as tetrahedrons and triangular prisms located in the cell corners and along cell edges, respectively.

6.3 Interface and Protocols

The first version of the tool will be coded in Fortran. Inputs and outputs will be communicated through ASCII text files.

Here we list input variables for the tool and its connection to other work packages:

- Porosity (WP3)
- Average cell size (WP3)
- Strut content (WP2)
- Wall thickness (WP2)

The results/outputs of the tool are following:

- Voxel-based foam morphology (WP3)

The results of this tool will be validated by measurements of foam samples morphology using micro-tomography in WP6.

7. Tool for fluid dynamics

7.1 Introduction

The primary goal of the tool is to predict the fluid dynamic behavior of the PU foam, while expanding under the action of the various chemical reactions involved. Since these foams are mainly used in mold filling processes, it is of paramount importance to accurately track the evolution of the interface between the foam and the surrounding air, as currently done in the volume-of-fluid (VOF) method.

7.2 Review of existing software

The CFD tool is founded on the well-known OpenFOAM CFD code. Amongst various solvers implemented in OpenFOAM, solvers in which the VOF approach is utilized, have been selected for further investigations and modifications. As the complex multiphase system is considered to be constituted by two immiscible fluids, the VOF approach is able to capture the interface between the expanding PU foam and its surroundings. It is worth mentioning that most of the work carried out in the past with the VOF method to describe expanding PU foams was done with the commercial CFD code Fluent (Geier et al., 2009).
Some modifications are however required to the existing software in order to account for the size distribution of the disperse gas bubbles in the PU foam. A Population Balance Equation (PBE) is integrated into the solver to assess the evolution of the bubble size distribution (BSD) within the foam. This method also takes into consideration the influence of the continuous and discontinuous phenomena such as bubble growth and coalescence. The PBE is implemented in openFOAM through a well-established method, the Quadrature-Based Method of Moment, that allows us to track the moments of BSD (Marchisio and Fox, 2013). Eventually the BSD can be reconstructed using a summation of basis functions such as Dirac delta or log-normal distribution. As a case in point, the BSD can be reconstructed using Eq. 1 as follow:

$$n(v) = \sum_{i=1}^{n} w_i \delta(v - v_i) \tag{1}$$

where v is the bubble volume and w_i is the number density (weights) of the gas bubbles of volume v_i and n is the number of nodes. This information about the bubble size distribution can be passed to the related work packages in a backward manner. On the other hand, the PBE model should be augmented by the description of the gas bubbles' interactions including the bubble growth rate and coalescence rate. The required theoretical or experimental models can be forwarded into the CFD-PBE model from other work packages, for instance WP2.

7.3 Interface and Protocols

OpenFOAM is developed in C++ and does not have a GUI. All the required information to setup, start and run a simulation is provided to the code in standard ASCII text files. As a consequence all the inputs and outputs will be communicated through ASCII text files.

The following flow chart looks at the CFD model as an individual modeling unit and simplifies the inputs (i.e., the required theoretical, experimental, or analytical formulations to be implemented in the CFD model) and outputs (i.e., the CFD results to be passed to the other WPs) of the macro-scale CFD model. More details are in Table 1.

Model validation can be performed by comparing predictions with experiments of various complexity. The simplest experiment is the quantification of the expansion of a PU foam into a cylindrical vessel. The properties to be measured and tracked in time are the foam height, density, temperature and the internal foam structure (notably the bubble size distribution).

More complex experiments involve the measurement of the foam expansion in more complicated geometries, such as actual molds employed in practical applications.

8. Tool for Mechanical properties

8.1 Introduction

The objective of the toolset is to predict the mechanical behaviour (stress-strain curve) of the PU foams having as inputs the foam morphology and the foam material (after foam growth) mechanical properties (elasticity and strength).

8.2 Review of existing software

The mechanical behaviour of the PU will be numerically simulated using the commercially-available Finite Element (FE) Method software Abaqus which implements a vast number of algorithms to solve highly-nonlinear problems by means of implicit or explicit integration schemes.
FE Representative Volume Element (RVE) models of the foams will be constructed having as inputs 1) the grown-foam material mechanical properties (elasticity is required; strength is of secondary importance), as predicted by molecular dynamic simulations or measured by means of nanoidentation experiments, and 2) foam morphology, as predicted by foam growth fluid dynamic computations or measured by Scanning Electron Microscope and Computerized X-Ray observation techniques. The translation of those properties, mainly foam morphology, into FE models will require specific pre-processing tools (e.g. the commercially-available GeoDict) or algorithms developed in Matlab. The efficient FE meshing of the RVE can be performed conveniently using the specific commercially-available meshing tool Hypermesh (Altair), since Abaqus own meshing algorithms are relatively poor.
With morphology, properties and mesh set, Abaqus will be used to calculate the tensile and compressive mechanical behaviour of the RVE of the PU in both raise and transverse directions, including the linear-elastic region, the plateau-like crushing region and, if possible, the densification region. The behaviour will be described in terms of stress-strain curves, specific mechanical properties (elasticity and strength) and failure mechanisms.

8.3 Interface and Protocols

The inputs required by the mechanical modelling strategy just outlined are 1) the foam morphology and 2) the foam material (after foam growth) mechanical properties (elasticity and strength). These inputs will made available by other partners in WP3.
While the mechanical properties are numerical values used in the Abaqus input deck, the foam morphology can be described in either of the two ways: 1) 3D geometrical model that is used for direct meshing (Hypermesh) followed by simulation (Abaqus), or 2) statistical descriptors of foam cell morphology that will be used to construct 3D geometrically, and statistically, representative RVE of the foams (e.g. GeoDict or Matlab), which are then meshed (Hypermesh) and simulated (Abaqus).

The prediction of the homogenized mechanical properties of the PU foams (elasticity and strength in the rise and transverse directions, under both tensile and compressive loads) is in the end of the multiscale simulation ladder proposed in MODENA.

The validation of the ‘virtual testing’ methodology described above will be done by correlation with actual mechanical test performed in WP6.

9. Conclusion and summary

Software for five macro-scopic tools, their connection with other tools at other scales, interfaces and communication protocols have been explained. These tools will predict thermal insulting properties, acoustic insulating properties, foam reconstruction, fluid dynamics and mechanical properties.

The material developed over the reporting period has two main domain of utilisation:
1. The described / selected tools are being used for the modelling of the PU-foam on the associated scale. Thus this part contributes the computations of scale-models towards the overall multi-scale framework.
2. It contributes towards the possible scenario of the overall multi-scale computation's workflow (see annex).
3. It provides the information of the connectivities between the various modelling tasks detailing the information to the extent it is presently known, thereby enabling the design of the data structures and the engine handling the workflow on a distributed computing environment (see annex).

10. Dissemination & exploitation

The flow chart and tables for the Inputs and Outputs of the CFD model as an individual modeling unit are ready to be disseminated at the MODENA website. During the progress of this project the evolution of the models, and possible corrections for input and output, will be updated.

11. Bibliography

Allard, J.F., Atalla, N., 2009. Propagation of Sound in Porous Media.

Delany, M.E., Bazley, E.N., 1970. Acoustical properties of fibrous absorbent materials. Appl. Acoust. 3, 105–116.

Ferkl, P., Pokorný, R., Kosek, J., 2014. Multiphase approach to coupled conduction–radiation heat transfer in reconstructed polymeric foams. Int. J. Therm. Sci. 83, 68–79.

Coquard, R., Baillis, D., Quenard, D., 2009. Radiative Properties of Expanded Polystyrene Foams. J. Heat Transfer 131, 012702.

Geier, S., Winkler, C., Piesche, M. 2009. Numerical simulation of mold filling processes with polyurethane foams, Chem. Eng. Tech., 32, 1438-1447.

Marchisio, D.L., Fox, R.O. 2013. Computational models for polydisperse particulate and multiphase systems, Cambridge University Press: Cambridge.

Delivery date: 21-07-2014

Authors:

Heinz Preisg
NTNU
E-mail:
heinz.presig@chemeng.ntnu.no

Misganaw Berhanu
NTNU
E-mail:
misganaw.b.addis@ntnu.no

MODENA

Appendix A

Principal investigators:

Heinz Preisig, NTNU (N)

Misganaw Berhanu, NTNU (N)

Non-permanent students and collaborators:

Ida Kragh, NTNU (N)

Project's coordinator:

Heinz Preisig, NTNU (N)

A list of tables that summarize the interaction between all MoDeNa tools is presented below. For every tool, three tables which are inputs, 'softwares and models' and outputs are provided. In the input and out tables, the name of the variables is listed down in the first column followed by symbol, operating range, data type and dimension entries. In the last column, it is specified from which WPs and tools the inputs are obtained from and the outputs are transfered. It is important to mention here that some tools are developed by more than one MoDeNa partner. For instance, the bubble growth tool is a task shared by TUE and VSCHT. In this tool, the activity of coalescence kernel and bubble growth rate will be performed by TUE and VSCHT, respectively. In addition, the kinetics tool is co-developed by VSCHT and BASF. The ‘softwares and models' table contains some information on the softwares (commercial or internal) and the type of equations the models have (Algebraic, PDE, ODE etc.). So far, it is possible to obtain a mathematical formulation of the models in CFD tool and for the other tools, it will be made available in the model development phase of the project.

Next to the tables, the overall work flow in MoDeNa is depicted in a single diagram. Each ellipse in the figure represents a tool and the data that is transferred between two tools is indicated on the forward (blue), backward (red) and sideway (black) arrows.

1 WP1 input/output data

1.1 Nano-scale tool (UNITS)

a) Inputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	Temperature		300-500 K	real	scalar	WP3 (CFD (POLITO))
2	Pressure		10^5-10^6 Pa	real	scalar	WP3 (CFD (POLITO))
3	Molecular weight		up to 10kDa	real	scalar	WP2 (Kinetics (BASF, VSCHT))
4	Sequence length		any	integer	scalar	WP2 (Kinetics (BASF, VSCHT))

b) Model

Software	Model type (s)	Type of equation
Materials studio	Molecular structure	Text file of real numbers

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Gas diffusivity in TPU polymer			real	scalar	Molecular structure	WP2 (Initial dispersion (POLITO, TUE), bubble growth (VSCHT,TUE))
2	Force Fields (COMPASS)			real	scalar	Molecular structure	WP1 (Thermodynamics (US))
3	Thermal conductivity of TPU polymer			real	scalar	Molecular structure	WP3 (HT (VSCHT))
4	Morphology data of TPU polymer			real	scalar	Molecular structure	WP2 (Polymer solidification (VSCHT))

1.2. Thermodynamics (EOS) tools (US)

1.2.1 Atomistic Simulations

a) Inputs

Variable Name	Symbol	Operating range	Data Type	Dimension	Obtained from (WPs)
Force Fields (COMPASS)			Real	Tupel	WP1, Task 1.2 (UNITS)

b) Model

Software	Model type	Type of Equation
In house FORTRAN code to perform Monte Carlo simulations (stand alone code)	Stochastic sampling of the systems' configurational phase space to obtain thermodynamic properties (vapor pressure).	Algebraic

c) Output

Variable name	Symbol	Operating range	Data Type	Dimension	Dependent On	Passed to (WPs)
Vapor pressure			Real	Scalar	Temperature	WP1, Task 1.5 (US)

1.2.2 Equation of State

a) Inputs

Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
PC-SAFT Parameters	m, ε, σ*		real	scalar	fitting to vapor pressures from atomistic simulations (WP 1 US) and experimental data (WP6)
Temperature	T	K	real	scalar	WP3 (POLITO (CFD))
Initial guesses of Bulk densities of phases	ρ	Kg/m^3	real	scalar	WP1 (US)

*ε (depth of pair potential), m (segment number per chain),σ (segment diameter)

b) Model

Software	Model type (s)	Type of equation
In house FORTRAN code (PC-SAFT equation of state) -stand alone	EOS (Thermodynamics) Helmholtz energy (F)= f (m, ε, σ, T, ρ) Note: vapor pressure, solubilities and general PvT	Algebraic

	behavior are obtained. Bulk density of coexisting phases (ρ_{bulk}) is calculated here by equating the chemical potentials since the phases are in equilibrium. The result will then be used as an input (boundary condition) for the DFT model below.	

c) Output

Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
Vapor pressures		Pa	real	scalar	Temperature	WP1(improve d dispersive force field parameters,(US)))
Solubilities		Mol/l	real	scalar		WP2 (initial dispersion, bubble growth, (VSCHT,TUE))
Bulk densities		kg/m^3	real	scalar		WP1(US)

1.2.3 Density Functional Theory

a) Inputs

Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
PC-SAFT Parameters	m, ε, σ*		real	scalar	fitting to vapor pressures from atomistic simulations(WP1 US) and experimental data (WP6)
Temperature	T	K	real	scalar	WP3 (POLITO (CFD))
Bulk density of phases	ρ	Kg/m^3	real	scalar	WP1 (US)

*ε (depth of pair potential), m (segment number per chain),σ (segment diameter)

b) Model

Software	Model type (s)	Type of equation
In house FORTRAN code - requires an interface to PETSc library (a solver package for systems of nonlinear equations).	DFT $\rho_{local}(r) = f(m,\varepsilon,\sigma, T, \rho_{bulk})$ Note: surface tension is obtained from local density	Variational problem

c) Outputs

Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
Interfacial Tension		J/m^2	real	scalar		WP2 (dispersion of reactants, bubble growth , wall drainage and rupture (VSCHT,TUE))

1.3. Quantum chemistry calculation tool (BASF)

a) Inputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Obtained from (WPs)
1	Assumed kinetic scheme	-	-	-	-		Literature, experiments or hypothesis

b) Models

Software	Model type (s)	Type of equation
Commercial quantum chemistry code Turbomole (could also be Gaussian)	DFT and higher ab-initio methods	Differential equation (Approximate molecular solution of Schrödinger equation)
Cosmos RS for solvatization effects	Chemistry independent parameterized solvation model	Partial differential equation

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Stoichiometric coefficients	ν	0-2 (typically)	integer	scalar	Inherent to considered elementary reactive step	WP2 (Kinetics (BASF, VSCHT))
2	Pre-exponential factor	A	10^4 - 10^{13} s^{-1} or $l \cdot mol^{-1} \cdot s^{-1}$ (typically)	real	scalar	Computed activation entropy (depends on stoichiometry)	WP2 (Kinetics (BASF, VSCHT))
3	Activation energy	E	0 – 150 kJ/mol	real	scalar	Direct result of computation	WP2 (Kinetics (BASF, VSCHT))

2. WP2 input/output data

2.1. Tool for initial dispersion of reactants (TUE, POLITO)

a) Inputs

No.	Variable Name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	Interfacial tension	σ	10-80 mN/m	real	scalar	WP1 (Thermodynamics (US))
2	Diffusion coefficients (in polymer solution)		10^{-15}-10^{-9} m^2/s	real	scalar	WPx()
3	Solubilities, f(T) (depends on the type of phase equilibria used			real	scalar	WP1 (Thermodynamics (US))
4	Energy of mixing			real	scalar	WP3(), recipe
5	Air bubble size		10^{-9}-10^{-5} m	real	scalar	WP3(CFD)
6	Air bubble volume fraction		0-0.1	real	scalar	WP3(CFD)
7	Type of deformation (shear, elongation)			real	Scalar/tensor	WPx()

b) Softwares and models

Software	Model type (s)	Type of equations
	Micro-mixing model	Algebraic and PDE
TFEM	FEM, Direct simulations with sharp interphase models	PDE

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Composition of all phases (fraction of each component in each phase)		0-1.0	real	scalar		WP2()
2	Characteristic size of phases		10^{-9}-10^{-4} m	real	scalar		WP2()
3	Orientation and deformation of the phases			real	tensor		WP2()

2.2. Tool for bubble growth (co-developed by VSCHT and TUE)

a) Inputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	Kinetic parameters (stoichiometric coefficients, pre-exponential factor, activation energy)	C-source code		C code ASCII	vector	WP2 (Kinetics (BASF, VSCHT))
2	Initial conc. of reactants (polyol, isocyanate,water, CO_2, physical blowing agent)		0-1000 Kg/m^3	real	scalar	WP2 (initial dispersion (TUE)), literature
3	Number density of initial bubbles		10^{15}-10^{24} m^{-3}	real	scalar	WP2 (initial dispersion (TUE)), literature
4	Size distribution of initial bubbles -mean		10^{-10}-10^{-7} m,	real	scalar	WP2 (initial dispersion (TUE)), literature
5	Size distribution of initial bubbles- standard deviation		0-100	real	scalar	WP2 (initial dispersion (TUE)), literature

6	Viscosity, f(T, conversion)	η	10^{-3}-10^{8} Pa.s	real	scalar	WP2 (polymer solidification (VSCHT))
7	Diffusion coefficients (of blowing agents in gas phase), f(T, conversion)		10^{-15}-10^{-9} m^2/s	real	scalar	literature
8	Solubilities of blowing agents, f(T,conversion)			real	scalar	WP1 (Thermodynamics (US)), WP6
9	Interfacial tension, f(T, conversion)	σ	10-80mN/m	real	scalar	WP1 (Thermodynamics (US))
10	Temperature	T	300-500 K	real	scalar	WP3 (CFD (POLITO))
11	Pressure	p	10^{5}-10^{6} Pa	real	scalar	WP3 (CFD (POLITO))
12	Conversion	X	0-1	real	scalar	WP3 (CFD (POLITO))
13	shear-rate	G	10^{-5}-10 s^{-1}	real	scalar	WP3 (CFD (POLITO))

b) Softwares and models

Software	Model type (s)	Type of equation
Software will be internal, written in Fortran with the use of some open source general mathematical libraries.	material balances, transport, phase equilibria, thermodynamics	PDE, ODE

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Bubble growth rate	G		real		Bubble radius, T,P,conversion	WP3 (CFD (POLITO))
2	Coalescence kernel	β		real		T, conversion, shear-rate	WP3 (CFD (POLITO))

2.3. Tool for wall drainage and rupture (1st stage and 2nd stage)

a) Inputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	Temperature , as a f(time)	T	300-500 K	real	scalar	WP3 (CFD (POLITO))
2	Pressure, as a f(time)	p	10^5-10^6 Pa	real	scalar	WP3 (CFD)
3	Conversion, as a f(time)	X	0-1	real	scalar	WP3 (CFD (POLITO))
4	Bubble size*, as a f(time)-1st stage		10^{-6}-10^{-3} m	real	scalar	WP3 (CFD (POLITO))
5	Surface tension, as a f(surfactant conc.)- 1st stage	σ	10-80 mN/m	real	scalar	WP1 (Thermodynamics (US))
6	Viscosity, as a f(T, conversion)- 1st stage	η	10^{-3}-10^8 Pa.s	real	scalar	WP2 (polymer solidification (VSCHT))
7	Viscoelastic property one, as a f(T, conv)- Young modulus-2nd stage		10^6-10^9 Pa	real	scalar	WP2 (polymer solidification (VSCHT))
8	Viscoelastic property two, as a f(T, conv)- relaxation time-2nd stage		10^{-3}-10^3 s	real	scalar	WP2 (polymer solidification (VSCHT))

b) Softwares and models

Software	Model type (s)	Type of equations
Software for the first stage will be internal, written in Fortran or python.	First stage-based on article by Schwarz (2003).	System of three PDE.
Software for the second stage might be internal software or LAMMPS (Not decided yet).	Second stage- DEM model	Large system of ODE.

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Mean wall thickness		10^{-7}-10^{-5} m	real	scalar	f(time)	WP3 (HT (VSCHT), mechanical properties (IMDEA))
2	Fraction of polymer inside the plateau borders		0-1	real	scalar	f(time)	WP3 (HT (VSCHT), mechanical properties (IMDEA))
3	Time when the wall ruptures		1-1000s	real	scalar		WP6

2.4. Tool for polymer solidification (VSCHT)

a) Inputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	Temperature	T	300-500 K	real	scalar	WP3 (CFD (POLITO))
2	Conversion	X	0-1	real	scalar	WP3 (CFD (POLITO))
3	Average molecular weight, as a f(conversion)	MW	0-10^6 kg/mol	real	scalar	WP2 (Kinetics (BASF, VSCHT))
4	Number conc. of the physical cross-links (morphology data)			real	scalar	WP1(UNITS)
5	Number conc. of the chemical cross-links, as a f(conversion)		0-10^{12} #/m^3 (may be more)	real	scalar	WP2 (Kinetics (BASF, VSCHT))
6	Dependence of T_g (glass transition temp.) on the conc. of blowing agent	T_g	200-400 K	real	scalar	literature

b) Softwares and models

Software	Model type (s)	Type of equation
	Simplified model based most likely on algebraic equations. DPD model is large system of ODE.	

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Polymer viscosity	η	10^{-3}-10^{8} Pa.s	real	scalar	f(T, conversion)	WP2 (bubble growth (VSCHT, TUE), wall drainage (VSCHT))
2	Visco-elastic property 1-Young modulus		10^{6}-10^{9} Pa	real	scalar	f(T, conversion)	WP2 (wall drainage (VSCHT))
3	Visco-elastic property 2-relaxation time		10^{-3}-10^{3} s	real	scalar	f(T, conversion)	WP2 (wall drainage (VSCHT))

2.5. **Tool for kinetics (co-developed by BASF and VSCHT)**

a) Inputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	Stoichiometric coefficients	ν	0-2 (typically)	integer	scalar	WP1 (Quantum chemistry (BASF))
2	Pre-exponential factor	A	10^{4} – 10^{13} s^{-1} or	real	scalar	WP1 (Quantum chemistry

			$l \cdot mol^{-1} \cdot s^{-1}$ (typically)			(BASF))
3	Activation energy	E	0 – 150 kJ/mol	real	scalar	WP1 (Quantum chemistry (BASF))

b) Softwares and models

Software	Model type (s)	Type of equation
Predici	Kinetic model describing concentrations and molecular weight distributions as a function of time	PDE (molecular weight distributions), ODE (statistical moments of molecular weight distributions, concentrations of low molecular components)

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	C-code for the source terms of the concentration of the low molecular components and the statistical moments of the molecular weight distributions			C code ASCII	vector	Pressure, Temperature, concentrations, statistical moments	WP2 (calculation of local conversion and MWD in meso-scale simulation) WP3 (CFD (POLITO)) (calculation of local conversion and MWD in macro-scale simulation)

3. WP3 input/output data

3.1. CFD tool (POLITO)

a) Inputs

No.	Variable Name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	C-source code (including the source terms for RHS of the kinetic equations)		*Experiment [e.g., values for polyol-isocyanate reaction or gelling include pre-factor = 1, activation energy = 35142.0 J/mol, and enthalpy of reaction = 68500.0 J/mol]	C- code ASCII	vector	WP2 (Kinetic (VSCHT, BASF))
2	Viscosity and solidification model parameters	m_{foam}	*Experiments/modeling. Varying in nature by large orders of magnitude (e.g. at shear rate = 0.01 s^{-1} after 18s of foaming the apparent viscosity is 175 Pa s while after 45s it increases to 988 Pa s)	real	tuple	WP2 (TUE)
3	Bubble growth rate parameters-G_0 and alpha	G_0	Experiment (m s^{-1})	real	tuple	WP2 (Bubble growth (VSCHT, TUE))
4	Coalescence Kernel	b	Experiment/Theoretical or numerical modeling ($m^3 s^{-1}$)	real	tuple	WP2 (Bubble growth (VSCHT, TUE))
5	Apparent foam thermal	l_{foam}	Experiment($Wm^{-1} K^{-1}$)	real	tuple	WP3 (HT (VSCHT))

	conductivity					

***** The example values for the gelling reaction and the foam apparent viscosity have been extracted from the literature and will be updated by the progress on the related WPs.

b) Softwares and models

Software	Model type (s)	Type of equation
OpenFOAM	1. Kinetics Two irreversible reactions will be considered in CFD: gelling and blowing. Only three chemical components will be tracked via the isocyanate, polyol and water concentrations (e.g. c_I, c_P, c_W). The general structure of the kinetic model is as follows: $dc_I/dt = R_G + R_B$, $dc_P/dt = R_G$, $dc_W/dt = R_B$, $R_G = -k_G \exp(E_G/RT) c_I^A c_P^B$, $R_B = -k_B \exp(E_B/RT) c_I^D c_W^E$. The source terms of the kinetics equations will be obtained from WP2 (bubble growth model) which include the activation energies and pre-exponential factors.	Differential
	2. *Bubble growth rate* Bubbles grow because of the blowing reaction (between water and isocyanare that produces carbon dioxide) and the evaporation of the blowing agent. The bubble growth rate can be written as: $G = dv/dt = G_o(T, p, X, \tau) v^{\alpha}$, where $G_o(T, p, X, \tau)$ is a constant that depends on temperature, pressure, conversion, and residence time.	Differential
	3. Coalescence rate	Algebraic

	Bubbles coalesce because of the collapse of the wall between them and because of their relative motion. The bubble coalescence rate is usually written as follows: $C_R=\beta(\gamma,T,v,v')n(v)n(v')$, where $\beta(\gamma,T,v,v')=\beta_o(\gamma,T)\times(v+v')$ is the coalescence kernel (function in turn of the shear-rate in the foam and the volume of the coalescing bubbles) and $n(v)$ and $n(v')$ are the number densities of bubbles with volume v and v' . $\beta_o(\gamma,T)$ has the unit of inverse time (frequency) and could be taken equal to the inverse of a characteristic coalescence (or drainage?) time.	
	4. Apparent viscosity The model for the foam apparent viscosity could have the following form: $\mu_{app}=\mu_1(X,\tau,T)+[\mu_2(X,\tau,T)-\mu_1(X,\tau,T)][1+(\gamma\lambda)^2]^{(n-1)/n}$, where X is the conversion of the gelling reaction, τ is the residence time, μ_1 and μ_2 are the viscosities at zero and infinite shear-rate γ and T is the foam temperature; λ and n are model parameters	Algebraic
	5. Apparent foam thermal conductivity Generally the foam thermal conductivity is written in terms of the temperature and the bubble size distribution in the foam (all the other properties are directly related to these two): $\lambda_F=f(\rho_F,T)$	Algebraic

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Temperature	T	> 273 K	real	tuple	Independent	WP1 (nano-scale (UNITS)) WP2 (kinetics (BASF, VSCHT)) WP2 (bubble growth, wall drainage, polymer solidification (VSCHT, TUE)) WP3 (HT (VSCHT))
2	Pressure	P	Atmospheric (Pa)	real	tuple	Independent	WP1 (nano-scale (UNITS)) WP2 (Bubble growth (VSCHT, TUE))
3	Polyol/isocyanate conversion	X	0-1.0	real	tuple	Kinetics parameters	WP2 (bubble growth, wall drainage, polymer solidification (VSCHT, TUE))
4	Bubble size distribution	n(v)	> 0 m^{-6}	real	tuple	Kinetics parameters, foam apparent viscosity, bubble growth rate, coalesce kernel, foam conductivity	WP2 (initial dispersion (TUE)) WP3 (HT, foam reconstruction (VSCHT))

3.2. Tool for foam thermal insulating properties (VSCHT)-HT

a) Inputs

No.	Variable Name	Symbol	Operating range	Data type	Dimension	Obtained from (WP)
1	Thermal conductivity of gas and solid phase		10-30 $mWm^{-1}K^{-1}$(gas), 200-700 $mWm^{-1}K^{-1}$(polymer)	real	scalar	user or literature
2	Absorption coefficient of gas and solid phase		10^{-3}-10^{3} m^{-1} (gas), 10^{3}-10^{7} m^{-1} (polymer)	real	scalar	user or literature
3	Voxel-based foam morphology			real	scalar	WP3 (foam reconstruction (VSCHT))
4	Foam porosity and average cell size		0-1 (porosity), 10^{-6}-10^{-3} m (cell size)	real	scalar	WP3 (CFD (POLITO))
5	Average wall thickness and strut content		10^{-7}-10^{-5} m (wall thickness), 0-1 (strut content)			WP2 (wall drainage (VSCHT)), WP6

b) Softwares and models

Software	Model type (s)	Type of equations
Fortran code	Coupled conduction and radiation (Fourier law and P_1-approximation)	PDE

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Equivalent foam conductivity		20-700 $mWm^{-1}K^{-1}$	real	scalar	Weakly T, gas-phase composition, morphology	WP3 (CFD (POLITO))

3.3. Tool for foam acoustic insulating properties (VSCHT)

a) Inputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	Voxel-based foam morphology			real	scalar	WP3 (foam reconstruction (VSCHT))
2	Air thermal conductivity		10-30 $mWm^{-1}K^{-1}$	real	scalar	literature

b) Softwares and models

Software	Model type (s)	Type of equation
Internal	Permeability obtained from simulation of Stokes flow inside the porous foam First version-based on laws of Delany and Bazley Extended version- Johnson-Champoux-Allard model	PDE, Algebraic

1.2. Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Characteristic impedance			complex	scalar		WP6
2	Wavenumber			complex	scalar		WP6
3	Acoustic absorption coefficient		0-1	real	scalar	as a f(wavelength)	WP6

3.4. Tool for foam reconstruction (VSCHT)

a) Inputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	Porosity		0-1	real	scalar	WP3 (CFD), WP6
2	Average cell size		10^{-6}-10^{-3} m	real	scalar	WP3 (CFD), WP6
3	Strut content		0-1	real	scalar	WP2 (wall drainage (VSCHT)), WP6
4	Wall thickness		10^{-7}-10^{-5} m	real	scalar	WP2 (wall drainage (VSCHT)), WP6

b) Softwares and models

Software	Model type (s)	Type of equation
	The foam image will be based on Voronoi tessellation. The struts will be created as tetrahedrons and triangular prisms located in the cell corners and along cell edges, respectively.	

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Voxel-based foam morphology						WP3 (HT, acoustics (VSCHT))

3.5. Mechanical properties (IMDEA)

a) Inputs

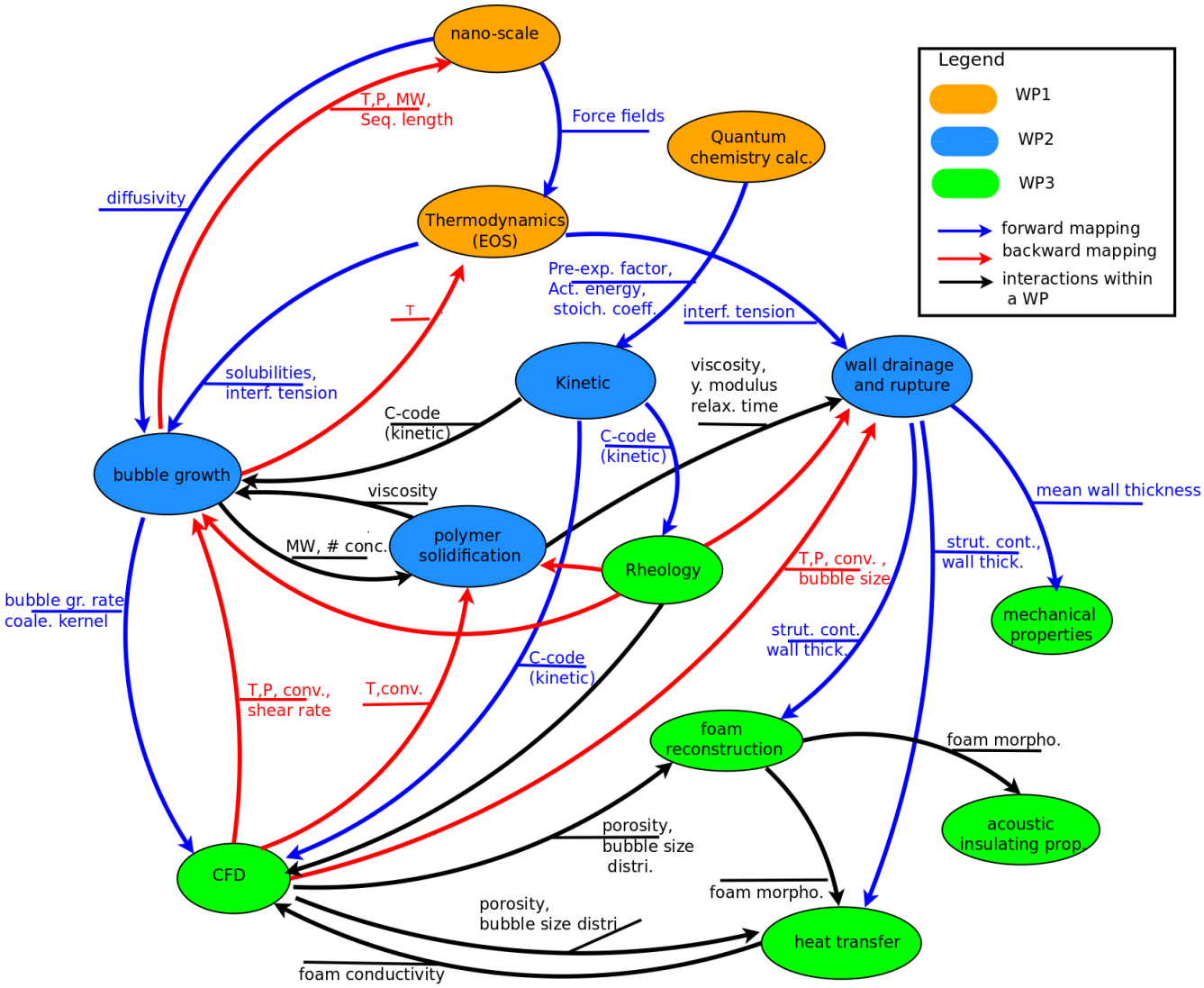
No.	Variable name	Symbol	Operating range	Data type	Dimension	Obtained from (WPs)
1	Elastic Moduli	E	1-100 GPa			WP1
2	Topology of foams					WP3, WP6

b) Softwares and models

Software	Model type (s)	Type of equation
Image J, VG Studio, Hyper Mesh, ABAQUS software package	Representative Volume Element (RVE) including statistical data based on X-ray tomography results will be subjected to deformation through simulation.	Different constitutive equations e.g. Arruda–Boyce model as a dominant mechanical regime

c) Outputs

No.	Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
1	Stress-Strain curves	σ-ε			scalar	Elastic Moduli and Topology of foam	WP6
2	Stress and Strain distributions and failure mechanisms				scalar	Elastic Moduli and Topology of foam	WP6
3	Elastic Moduli in Tensile Rising and Transverse directions	E_T	1-100		scalar	Elastic Moduli and Topology of foam	WP6
4	Elastic Moduli in Compression in Rising and Transverse directions	E_C	1-100		scalar	Elastic Moduli and Topology of foam	WP6
5	Ultimate Tensile Stress in Tension in Rising and Transverse directions	UTS_T	0-100		scalar	Elastic Moduli and Topology of foam	WP6
6	Initial Yield Stress in Compression in Rising and Transverse directions	σ_Y	0-100		scalar	Elastic Moduli and Topology of foam	WP6


nano-scale
T,P, MW,
Seq. length
Force fields
Quantum
chemistry calc.
diffusivity
Thermodynamics
(EOS)
Pre-exp. factor,
Act. energy,
stoich. coeff.
interf. tension
T
solubilities,
interf. tension
Kinetic
viscosity,
y. modulus
relax. time
wall drainage
and rupture
C-code
(kinetic)
C-code
(kinetic)
bubble growth
viscosity
mean wall thickness
MW, # conc.
polymer
solidification
Rheology
T,P, conv. ,
bubble size
strut. cont.,
wall thick.
bubble gr. rate
coale. kernel
mechanical
properties
strut. cont.
wall thick.
C-code
(kinetic)
T,P, conv.,
shear rate
T,conv.
foam
reconstruction
foam morpho.
acoustic
insulating prop.
porosity,
bubble size
distri.
CFD
foam morpho.
porosity,
bubble size distri.
heat transfer
foam conductivity
Legend
WP1
WP2
WP3
forward mapping
backward mapping
interactions within
a WP