

**Delivery date: June 30, 2014**

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**MODENA**

## Deliverable 2.1

**Infrastructure of meso-computations: Layout of meso-tools, their interfaces to other tools and an initial set of computational recipes**

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## 1 Description of deliverable

This deliverable introduces the layout of mathematical models of meso-scale level phenomena occurring during the foaming process of polyurethane. The models will describe: (i) the growth of the limited number of bubbles in the polymerizing matrix, (ii) the interaction between individual bubbles by diffusion and coalescence, (iii) the drainage of polymer solution from a wall between two bubbles, (iv) the solidification of the initially liquid matrix, and (v) the wall rupture in flexible polyurethane foams.

In the following sections, we explain requirements placed on each model as well as its basic assumptions and expected results. Each individual model is placed into one of the four meso-scale software tools, which will be developed during this project. The connections to other tools both within and outside of this WP are identified and the form, in which data will be transferred, is discussed. The software environment, in which the models will be developed and formally maintained, is also addressed.

In summary, this deliverable is primarily concerned with Task 2.1: Layout of meso-scale tools of DOW. The following section is copy-pasted from DOW:

### **Task 2.1: Layout of meso-scale tools (VSCHT, M1-M6)**

VSCHT will define the layout of meso-scale tools that will be the blueprint of activities in this WP. This layout contains the following information:

- Review of the existing software that will be used for the meso-scale computations and are suitable for the protocols to be developed.
- 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). Equivalent virtual recipe is going to be constructed as the algorithmic flowsheet describing the flow of information within this WP and interfaces to other WPs.
- Description of the interfaces and communication protocols required for the design of the software adaptors.
- Inputs from WP1 including physical properties, property methods, reaction kinetics and equations of state.
- Inputs from WP3 describing the pressure, temperature and shear-rate profiles along the foaming line.
- Output to WP3 describing the initial bubble distribution, solidification of polymer walls, cell coalescence and rupture of polymer walls in a form suitable for kernels of population balance modelling.
- Description of concepts developed/adopted in meso-scale tools for: (i) initial dispersion of reactants, (ii) bubble initiation and coalescence, (iii) solidification of cell walls, (iv) cell wall drainage and rupture.
- Description of validation procedures for meso-scale modelling tools for WP6.

The layout will not contain information about multiscale communication protocols and their implementation (these will be defined in WP4 and WP5).

## 2 Summary of contribution of involved partners to deliverable

TUE, VSCHT and BASF will develop 4 meso-scopic modelling tools. They contain models for initial dispersion of reactants (TUE), bubble growth (VSCHT, TUE, BASF), polymer solidification (VSCHT) and wall drainage and rupture (VSCHT)

TUE, VSCHT and BASF have provided a review of existing software, (information) protocols and interface which contains information about inputs from WP1 and WP3 and outputs to WP3, concepts developed/adopted and validation procedures for WP6. 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).

After discussions with partners involved in WP2, this deliverable was compiled by VSCHT.

### 3 Meso-scopic tools in flowchart of all tools

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

The meso-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 Recipes for polyurethane foams

In this section, we define characteristic recipes for both types of polyurethane foams, i.e., closed-cell rigid foams and open-cell flexible foams.

Recipes for polyurethane foams used by companies in industrial-scale processes are usually confidential. Thus, open literature often works with the approximate substitutions of real recipes. In this project, one basic recipe for each type of foam is considered. These recipes provide also test-cases of this project.

To avoid potential conflicts with confidentiality, the presented recipes are selected somewhat artificially and are not identical to real industrial recipes.

**Table 1: Recipe for rigid foam**

Monomers	Polyol, polymeric MDI
Blowing agents	Water, n-pentane
Other components	Catalyst, surfactant, fire retardant
Length of foaming process	Typically around 200 s
Temperature rise	Typically around 150 K
Important processing properties	Viscosity, flowability, curing/demould time, panel/board surface quality
Important properties of final foam	Thermal conductivity, closed cell fraction, compressive strength, adhesion to substrates, dimensional stability, non-flammability
Cell size	Typically 100 – 500 $\mu\text{m}$
Fraction of polymer in the struts	Typically 0.7 – 0.9
Typical problems	Extensive wall drainage leading to decreased compressive strength, premature cell opening leading to the loss of the blowing agent

BASF would like to improve the following properties of this foam:

- thermal insulation properties of the final foam: This could be achieved if the foam with smaller cell size is created.
- mechanical properties of the final foam: This could be achieved if most of the polymer is located in the walls instead in the struts.

**Table 2: Recipe for flexible foam**

Monomers	Polyol, TDI
Blowing agents	Water, n-pentane
Other components	Catalyst, surfactant, fire retardant
Length of foaming process	Typically around 200 s
Temperature rise	Typically around 150 K
Important processing properties	Viscosity, flowability, curing/demould time, panel/board surface quality
Important properties of final foam	Open cell fraction, compressive strength, adhesion to substrates, dimensional stability, non-flammability
Cell size	Typically 100 – 500 $\mu\text{m}$
Typical problems	Premature cell opening leading to the collapse of the foam, late cell opening leading to open cell fraction below 1 (i.e., leaving some closed-cells)

BASF would like to improve the following properties of this foam:

- Gain better control over opening of the windows.
- Improve the acoustic insulation properties. This could be achieved if the foam with smaller permeability, i.e., smaller cell size is created.

### **TPU (thermoplastic polyurethane)**

There is no specific task relating to TPU in WP2. The most important morphological aspects of TPU are the hard-soft domains and the dispersion of nano-fillers, which are the objectives of WP1 and WP3, respectively. Thus, no recipe for TPU is given here.

## **5 Tool for initial dispersion of reactants**

### **5.1 Goals**

The main goal of this tool is to determine the initial size distribution of dispersed liquid phase by simulation of micro-mixing. The second output of this tool will be the location of air bubbles with respect to interfaces of both initial liquid phases.

### **5.2 Description**

Prior to the foaming process, liquid solutions of polyols and isocyanates must be mixed together. However, these two solutions are often not entirely miscible. In that case, dispersions with characteristic size of phases about 1-10  $\mu\text{m}$  are created. The formation of such dispersions can strongly influence the rate of polymerization in the initial mixture

### **5.3 Review of existing software and existing knowledge**

No tools are available yet.

### **5.4 Development**

The movement of the droplets and bubbles inside a box depends on the type of the deformation, viscosities of the constituents and surface tension. To retain accuracy and avoid instabilities when the bubbles are approaching close to each other we need to refine our mesh between the bubbles, but also unrefine where needed to reduce computational time. For that reason a method of multilevel adaptive local mesh refinement is used. Our tool is created using TFEM, a toolkit for the finite element method written in Modern Fortran and uses Gmsh for meshing purposes. The interfaces are moving in both normal direction and tangential direction, and stabilized with streamline-upwind/Petrov–Galerkin (SUPG) formulation. Remeshing is invoked if the deformation of

the mesh exceeds a certain threshold. For properly resolving the lubrication layer in between the droplets and bubbles, multilevel adaptive local mesh refinement of the interface is used. The first version of the tool includes Newtonian fluids. The effect of viscoelasticity will be added later

## 5.5 Interface and Protocols

If a tool is needed in the future then the list of input variables for the initial dispersion of reactants are:

- Interfacial tension.
- Diffusion coefficients
- Solubilities (i.e., phase-equilibrium parameters).
- Energy of mixing.
- Fraction and size of air bubbles.
- Type of deformation

The results of the initial dispersion of reactants which BASF currently is able to specify are the outputs then:

- Composition of all phases.
- Descriptors for the size distribution of all phases and their mutual arrangement.

## 6 Tool for bubble growth

### 6.1 Goals

The primary goal of the tool is to predict the rate of the bubble growth and to express it in a form, which could be easily adopted by other meso- and macro-scale tools. The second output of this tool will be the coalescence kernel.

It will consist of several components:

- **Chemistry.** Simplified reaction kinetics will describe polymerization of polyurethane using overall gelling and blowing reactions. Conversion of water and of polyol and isocyanate functional groups as well as the generated carbon dioxide will be implemented.
- **Rheology.** Viscosity of the matrix depending on conversion and temperature.
- **Thermodynamics.** Solubilities and diffusion coefficients of blowing agents. Interfacial tension between liquid and gas phase. Also the dependence of these parameters on temperature and conversion.
- **Mass transfer.** Diffusion of blowing agent in liquid and evaporation at the interface leading to the bubble growth.
- **Coalescence.** Description of both the forces leading to the thinning of a wall between two bubbles and the forces opposing the thinning. Conditions leading to the coalescence

### 6.2 Description

Gas bubbles in polyurethane foam are created during the mixing of reactants. The initial number density and size distribution of bubbles after the mixing will be the input parameter for this simulation. During the foaming process, the blowing agents diffuse to the gas-liquid interface where they evaporate, which leads to the bubble growth. Blowing agents can be dissolved in the reactants prior to foaming (physical blowing agents) or created by chemical reaction during foaming (chemical blowing agents). When two bubbles are in a close proximity, they can influence each other's growth rate by several possible ways:

- **Diffusion coarsening.** Due to the evaporation, the concentration of the blowing agent is locally decreased around the bubble interface. Moreover, the effect of interfacial tension causes that larger bubble can grow at smaller concentration of blowing agent in the liquid phase. When bubbles of distinctly different sizes are at a close proximity, the larger bubble

can consume most of the blowing agent, which leads to shrinking and extinction of the smaller bubble. This mechanism, also known as Ostwald ripening, has the biggest effect at the very start of the foaming.

- **Shear-induced coalescence.** When the velocity between two bubbles is high enough, the inertial forces can cause the bubbles to merge. This mechanism is most pronounced at the places of high shear rate.
- **Coalescence caused by wall drainage.** Once the porosity of the foam exceeds approximately 0.6, flat (or slightly curved) walls are formed between the bubbles. This wall can rupture if it becomes too thin or if it cannot withstand the stress created by stretching of the wall. This mechanism is completely undesirable in the case of rigid polyurethane foams. On the other hand, it is responsible for the opening of the cells at the end of the foaming process in the case of flexible foam.

The tool for bubble growth description should ideally incorporate all of the above mentioned mechanisms of bubble interaction. However, during the development of the tool, specialized models for each mechanism will be created. Moreover, the coalescence by wall drainage will be studied in a separate tool, whose results can be exploited. After the testing of functionality, the models will be combined to form a tool for the prediction of the bubble growth rate and coalescence kernel.

### 6.3 Review of existing software

The phenomenon of bubble growth has been studied in the scientific literature. However, to the best of our knowledge, this was always done through the internal software. Therefore, no software is readily available for the simulation of the bubble growth. Thus, it will be co-developed by VSCHT and TUE. As the programming language, C++ and Fortran will be used and open source general mathematical libraries and differential equation solvers (particularly OpenFOAM) will be utilized.

### 6.4 Development

The bubble growth during the foaming of PU was traditionally modeled as the growth of a single bubble in a shell of polymerizing liquid (Harikrishnan and Khakhar, 2009; Kim and Youn, 2000). This approach was very popular also for other types of foams and was extended to liquids with non-Newtonian viscosity (Feng and Bertelo, 2004) and variable diffusivity and interfacial tension (Chen et al., 2006). The disadvantage of this approach is that it completely neglects both the diffusion coarsening and the coalescence. Nevertheless, the first provisional version of this tool will be based on the combination of the above mentioned models. This version of the tool will provide only the bubble growth rate and will be used to test interfaces to other WPs.

The effect of diffusion coarsening can be evaluated from the simulation of a box containing dissolved blowing agent and multiple growing bubbles. The diffusion process can be modeled using Cahn-Hilliard equation (Naber et al., 2008), Fick law (Sun and Beckermann, 2010) or Lattice-Boltzmann approach (Huber et al., 2014). In these simulations, bubbles extinct simultaneously by diffusion coarsening and coalescence. However, when the effect of disjoining pressure is neglected, the coalescence is seriously overestimated (Bikard et al., 2005). The improved version of the tool will be based on this type of simulation. It will provide the bubble growth rate corrected to diffusion coarsening and to coalescence.

The coalescence kernel can be also evaluated from the simulation of a box with multiple growing bubbles. However, if this proves inefficient, the coalescence kernel will be evaluated from separate simulation. The rate of coalescence can be calculated from the simulation of the direct contact between two bubbles (Mohammadi et al., 2012) while preserving all important forces (Alke and Bothe, 2009) or by statistical approach as described in (Fortelný et al., 2012).

### 6.5 Model assumptions

Here we present the basic assumptions of the bubble growth models. Concentration of the following species is tracked:

- hydroxyl functional groups
- isocyanate functional groups
- water
- carbon dioxide
- physical blowing agent

Skeleton of the models then consists of the following equations:

- mass balances of individual species in liquid and gas phases
- phase equilibria for blowing agents and water
- interface tracking
- continuity equation and momentum balance

## 6.6 Interface, protocols and validation

Here we list input variables for the tool describing the bubble growth and their connection to other work packages:

- Initial concentration of reactants (user)
- Number density and size distribution of initial bubbles (WP6 or user)
- Parameters of kinetic model (WP1)
- Viscosity as a function of temperature and conversion (WP2)
- Diffusion coefficients of blowing agents as functions of temperature and conversion (WP1)
- Solubilities of blowing agents as functions of temperature and conversion (WP1)
- Interfacial tension as a function of temperature and conversion (WP1)
- Temperature (WP3)
- Pressure (WP3)
- Conversion (WP3)
- Shear rate (WP3)
- Parameters of the disjoining pressure model (WP6 or user or literature)
- Stoichiometric coefficients
- Pre-exponential factor
- Activation energy

Alternatively, local concentrations of species can be employed instead of conversion in some of the above mentioned dependencies, especially during the model development.

The results/outputs of the tool for the bubble growth modeling are following:

- Bubble growth rate – dependence on bubble radius, temperature, pressure, conversion (WP2 and WP3)
- Coalescence kernel – dependence on temperature, conversion, shear rate (WP3)

Results of this tool will be validated together with the results of CFD code from WP3. Cell size and number concentration of cells in the final foam can be determined from SEM image or X-ray tomography scanning in WP6. These will be compared with foam density and average cell size predicted by the CFD code.

## 7 Tool for polymer solidification

### 7.1 Goals

The main objective of this tool is to study the gradual solidification of polymer walls. The main output of this tool will be the dependence of viscous and visco-elastic properties of polymer walls on the temperature and on the conversion of reactants' functional groups.

Tool for the polymer solidification will consist of several components:

- **Chemistry.** Evolution of molecular weight with conversion, including branching and/or cross-linking.
- **Thermodynamics.** Solubilities and diffusion coefficients of blowing agents. Plasticizing effect of blowing agent. Temperature of glass transition.
- **Gelation.** Number density of both chemical cross-links created by reactions and physical cross-links created by the separation to hard and soft domains.
- **Rheology.** Prediction of viscous and visco-elastic properties

## 7.2 Description

The transition from low-viscosity to highly viscous mixture, then visco-elastic and finally glassy polymer is caused by several phenomena: (i) growth of polymer chains and polymer concentration, (ii) gelation by branching and cross-linking reactions during polymerization, (iii) gelation by phase separation into hard and soft-domains acting as physical cross-links, (iv) possible strain hardening, (v) diffusion of CO<sub>2</sub> plasticizer out of polymer, and (vi) glass transition.

## 7.3 Review of existing software

Although polymer solidification was extensively studied in scientific literature, no software is currently available that is able to predict evolution of viscosity during polymerization. Therefore, VSCHT will develop this software based on published models. The first version of the tool will be coded in Fortran. The DPD model is going to be implemented in the [LAMMPS](#) software.

## 7.4 Development

The first provisional version of the tool will include only the polymer dilution effect and the plasticizer effect on the glass transition temperature. It will utilize van Krevelen–Hoflyzer ([Van Krevelen and Te Nijenhuis, 2009](#)) Castro-Macosko ([Castro and Macosko, 1980](#)) models. The parameters of this model will be obtained by model fitting to available literature and experimental data.

Later, the model will be extended to include the effects of both the chemical and physical cross-links. The number concentration of the chemical cross-links will be obtained from the detailed simulation of reaction kinetics and the number density of physical cross-links will be the result of the hard-soft domain separation tool in WP1.

Finally, an attempt to predict visco-elastic properties using more rigorous approach will be made. The model will use the state-of-the-art dissipative particle dynamics (DPD) approach with repulsive potential to prevent chain crossing ([Chantawansri et al., 2013](#); [Langeloth et al., 2013](#)).

## 7.5 Interface, protocols and validation

The input variables for the polymer solidification tool are going to be:

- Temperature (WP3)
- Conversion (WP3)
- Average molecular weight as a function of conversion (WP1)
- Number concentration of the chemical cross-links as a function of conversion (WP1)
- Number concentration of the physical cross-links as a function of conversion (WP1)
- Dependence of  $T_g$  on the concentration of blowing agent
- Solubility and diffusivity of blowing agent in cross-linked polymer (WP1)

Here we list results of the tool for bubble growth

- Viscosity as a function of temperature and conversion (WP2 and WP3)
- Visco-elastic properties as a function of temperature and conversion (WP2)

Results of this tool will be validated by rheological measurements of real systems in WP6. However, polymer viscosity can be directly measured only in the absence of foaming, i.e., for the TPU system.

## 8 Tool for wall drainage and rupture

### 8.1 Goals

The tool will simulate the time evolution of the polymer wall thickness between two bubbles until the end of the foaming process or until the wall ruptures. The results of this tool are the thickness of the wall and the characteristic time of drainage (time needed for the drainage and the rupture of a wall).

The tool for wall drainage description will formally consist of several components:

- **Rheology.** Viscous and visco-elastic properties of the polymer matrix depending on time.
- **Thermodynamics.** Diffusion coefficients of surfactants. Interfacial tension between liquid and gas phase depending on surfactant concentration.
- **Morphology evolution.** Description of the stretching and thinning of the wall due to the bubble growth and the flow of polymer between the wall and the Plateau border.

### 8.2 Description

Walls between neighboring bubbles are created when porosity increases above approximately 0.6. As the bubbles continue to grow, the wall is being stretched leading to the thinning of the wall and flow of the liquid phase between Plateau borders and the wall. The flow towards the Plateau borders is mainly driven by the capillary forces and is opposed by the disjoining pressure (when the wall becomes too thin) and by the Marangoni forces when the flow induces gradient in the interfacial tension. Past the gel point, only the low molecular species can flow. However, the flow of individual species is opposed by the osmotic forces.

The wall drainage was most extensively studied for soap films ([Bhakta and Ruckenstein, 1997](#); [Breward and Howell, 2002](#)). The stability of the film is greatly influenced by the disjoining pressure and the interfacial tension. The concept of disjoining pressure was thoroughly discussed by ([Bergeron, 1999](#)) and methods how to measure disjoining pressure isotherm were described by ([Claesson et al., 1996](#)). The type of surfactant influences the surface rheology of the film. Two extreme cases are recognized: mobile surfactants and rigid surfactants ([Hilgenfeldt et al., 2008](#); [Vitasari et al., 2013](#)). In contrast to soap films, the polyurethane films are much more influenced by the film viscosity ([Schwartz and Roy, 2003](#)). The models developed for soap films are usually based on the lubrication approximation and can be utilized only before the gel point.

After the gel point, the viscosity of the walls goes to infinity and the walls behave like a visco-elastic solid. However, even at the gel point, the wall still contains relatively large amount of unreacted monomers. The reaction of these compounds will produce additional blowing agent, which will increase the pressure inside the bubbles that will cause the stress in the walls.

### 8.3 Review of existing software

The phenomenon of wall drainage and rupture in foams was studied in scientific literature mainly in soap froths. Studies investigating wall drainage in polymer foams are much scarcer and were performed using internal software. Therefore, no software is currently available that is able to predict wall drainage and rupture in polyurethane foams. Thus, VSCHT will develop this software based on combination of existing models. The first stage of the tool will be coded in Fortran using only general mathematical libraries. The second stage is going to be implemented in the [LAMMPS](#) software.

## 8.4 Development

The tool will simulate wall drainage in two consecutive stages. Prior the gel point, a model based on the lubrication approximation described in (Schwartz and Roy, 2003) will be used. The model will provide the time evolution of the wall thickness profile. In this stage, the wall will rupture if the wall thickness gets below the critical value at any point. This rather crude model could be potentially refined to more realistic geometries following the procedure described in (Saye and Sethian, 2013).

The DEM (Discrete Element Method) model for the second stage will be used if the gel point is reached before the wall ruptures. This model will provide the stress analysis on a single wall until the end time of the process or until the wall ruptures.

## 8.5 Model assumptions

First we present the basic assumptions of the model for the **first stage of the wall drainage** (before the gel point).

- Flow of polymer solution is caused by the capillary forces, the surface tension gradient and the expansion of the bubble
- No gravitational drainage through struts
- Simplified geometry derived from the uniform bubble size distribution
- No diffusion coarsening

The model primarily consists of the following equations:

- Equation for wall thickness
- Equation for surface speed (slip velocity)
- Surfactant balance

Next, we present the basic assumptions of the model for the **second stage of wall drainage** (past gel point).

- Simplified geometry – analysis of a single wall
- Coarse-grained representation – discrete elements
- No diffusion coarsening

This model consists of the following equations:

- Force balance on discrete elements
- Inter-element potentials as the driving force of transport

## 8.6 Interface, protocols and validation

Here we list input variables for the tool simulating the wall drainage and rupture.

- Temperature as a function of time (WP3)
- Conversion as a function of time (WP3)
- Bubble size as a function of time. (First stage) (WP3)
- Surface tension as a function of surfactant concentration. (First stage) (WP1)
- Viscosity as a function of temperature and conversion (First stage) (WP2)
- Parameters of the disjoining pressure model (First stage) (WP6 or user or literature)
- Viscoelastic properties as a function of temperature and conversion (Second stage) (WP2)

Here we list results for the tool simulating the wall drainage and rupture.

- Mean wall thickness as a function of time
- Fraction of polymer inside the Plateau borders as a function of time
- Time when the wall ruptures

The results of this tool will be validated from the measurement of wall thickness and strut content in the final foam. These will be determined from SEM images or X-ray micro-tomography (struts) in WP6 for various samples of the final foams.

## 9 Conclusions

The layout of the software tools for the modeling of the meso-scale phenomena occurring during the foaming of polyurethane was presented. The developed tools will consider both the rigid and the flexible foams. For both types of foam we provide the recipe describing typical reaction conditions, constraints, important material properties and problems, which are sometimes encountered during the real process. The objectives for possible improvement of these products are also discussed.

All mathematical models related to the meso-scale evolution of morphology in polyurethane foams are formally divided into four software tools: (a) "Initial dispersion of reactants", (b) "Bubble growth", (c) "Polymer solidification" and (d) "Wall drainage and rupture". These tools will help to describe the whole foaming process from mixing of reactants, through growth of interacting gas bubbles, their possible coarsening or coalescence, flow of polymer solution between the walls and the Plateau borders, until the complete solidification of the polymer matrix.

For each software tool we specify its goal, which should clarify the reason, why the tool will be developed. Then we briefly describe the physical phenomena that will be covered by the tool and provide information on the utilized mathematical models. For each model we specify its basic assumptions and list its input and output variables.

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**Delivery date: 21-07-2014**

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**MODENA**

# Appendix A

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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 transferred. 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 sideways (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	$m, \epsilon, \sigma^*$		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	$\rho$	$\text{Kg/m}^3$	real	scalar	WP1 (US)

\* $\epsilon$  (depth of pair potential),  $m$  (segment number per chain),  $\sigma$  (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, $\epsilon$ , $\sigma$ , T, $\rho$ ) Note: vapor pressure, solubilities and general PvT	Algebraic

	<p>behavior are obtained.</p> <p>Bulk density of coexisting phases (<math>\rho_{\text{bulk}}</math>) 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.</p>	
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### c) Output

Variable name	Symbol	Operating range	Data type	Dimension	Dependent on	Passed to (WPs)
Vapor pressures		Pa	real	scalar	Temperature	WP1(improved dispersive force field parameters,(US))
Solubilities		Mol/l	real	scalar		WP2 (initial dispersion, bubble growth, (VSCHT,TUE) )
Bulk densities		kg/m <sup>3</sup>	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, $\epsilon$ , $\sigma^*$		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	$\rho$	Kg/m <sup>3</sup>	real	scalar	WP1 (US)

\* $\epsilon$  (depth of pair potential), m (segment number per chain), $\sigma$  (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 $\rho_{\text{local}}(\mathbf{r}) = f(m, \epsilon, \sigma, T, \rho_{\text{bulk}})$  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 <sup>2</sup>	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	$\nu$	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 <sup>-1</sup> or l·mol <sup>-1</sup> ·s <sup>-1</sup> (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	$\sigma$	10-80 mN/m	real	scalar	WP1 (Thermodynamics (US))
2	Diffusion coefficients (in polymer solution)		$10^{-15}$ - $10^{-9}$ m <sup>2</sup> /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/tens or	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 <sub>2</sub> , physical blowing agent)		0-1000 Kg/m <sup>3</sup>	real	scalar	WP2 (initial dispersion (TUE)), literature
3	Number density of initial bubbles		$10^{15}$ - $10^{24}$ m <sup>-3</sup>	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)	$\eta$	$10^{-3}$ - $10^8$ 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 <sup>2</sup> /s	real	scalar	literature
8	Solubilities of blowing agents, f(T,conversion)			real	scalar	WP1 (Thermodynamics (US)), WP6
9	Interfacial tension, f(T, conversion)	$\sigma$	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 <sup>-1</sup>	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	$\beta$		real		T, conversion, shear-rate	WP3 (CFD (POLITO))

### 2.3. Tool for wall drainage and rupture (1<sup>st</sup> stage and 2<sup>nd</sup> 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 <sup>5</sup> -10 <sup>6</sup> 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 <sup>-6</sup> -10 <sup>-3</sup> m	real	scalar	WP3 (CFD (POLITO))
5	Surface tension, as a f(surfactant conc.)- 1st stage	$\sigma$	10-80 mN/m	real	scalar	WP1 (Thermodynamics (US))
6	Viscosity, as a f(T, conversion)- 1st stage	$\eta$	10 <sup>-3</sup> -10 <sup>8</sup> Pa.s	real	scalar	WP2 (polymer solidification (VSCHT))
7	Viscoelastic property one, as a f(T, conv)- Young modulus-2nd stage		10 <sup>6</sup> -10 <sup>9</sup> Pa	real	scalar	WP2 (polymer solidification (VSCHT))
8	Viscoelastic property two, as a f(T, conv)- relaxation time-2nd stage		10 <sup>-3</sup> -10 <sup>3</sup> 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 (BASE, 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 <sup>3</sup> (may be more)	real	scalar	WP2 (Kinetics (BASE, VSCHT))
6	Dependence of T <sub>g</sub> (glass transition temp.) on the conc. of blowing agent	T <sub>g</sub>	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	$\eta$	$10^{-3}$ - $10^8$ 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	$\nu$	0-2 (typically)	integer	scalar	WP1 (Quantum chemistry (BASF))
2	Pre-exponential factor	A	$10^4 - 10^{13} \text{ s}^{-1}$ or	real	scalar	WP1 (Quantum chemistry)

			$\text{l}\cdot\text{mol}^{-1}\cdot\text{s}^{-1}$ (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	$m_{\text{foam}}$	*Experiments/modeling. Varying in nature by large orders of magnitude (e.g. at shear rate = $0.01 \text{ s}^{-1}$ 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 ( $\text{m s}^{-1}$ )	real	tuple	WP2 (Bubble growth (VSCHT, TUE))
4	Coalescence Kernel	$b$	Experiment/Theoretical or numerical modeling ( $\text{m}^3 \text{ s}^{-1}$ )	real	tuple	WP2 (Bubble growth (VSCHT, TUE))
5	Apparent foam thermal	$l_{\text{foam}}$	Experiment( $\text{Wm}^{-1} \text{ K}^{-1}$ )	real	tuple	WP3 (HT (VSCHT))

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

	<p>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:</p> $C_R = \beta(\gamma, T, v, v') n(v) n(v') \quad ,$ <p>where <math>\beta(\gamma, T, v, v') = \beta_o(\gamma, T) \times (v + v')</math> is the coalescence kernel (function in turn of the shear-rate in the foam and the volume of the coalescing bubbles) and <math>n(v)</math> and <math>n(v')</math> are the number densities of bubbles with volume <math>v</math> and <math>v'</math> .  <math>\beta_o(\gamma, T)</math> has the unit of inverse time (frequency) and could be taken equal to the inverse of a characteristic coalescence (or drainage?) time.</p>	
	<p>4. Apparent viscosity</p> <p>The model for the foam apparent viscosity could have the following form:</p> $\mu_{app} = \mu_1(X, \tau, T) + [\mu_2(X, \tau, T) - \mu_1(X, \tau, T)] [1 + (\gamma \lambda)^2]^{(n-1)/n}$ <p>,</p> <p>where <math>X</math> is the conversion of the gelling reaction, <math>\tau</math> is the residence time, <math>\mu_1</math> and <math>\mu_2</math> are the viscosities at zero and infinite shear-rate <math>\gamma</math> and <math>T</math> is the foam temperature; <math>\lambda</math> and <math>n</math> are model parameters</p>	Algebraic
	<p>5. Apparent foam thermal conductivity</p> <p>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):</p> $\lambda_F = f(\rho_F, T)$	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 (BASEF, 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 <sup>-6</sup>	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 $\text{mWm}^{-1}\text{K}^{-1}$ (gas), 200-700 $\text{mWm}^{-1}\text{K}^{-1}$ (polymer)	real	scalar	user or literature
2	Absorption coefficient of gas and solid phase		$10^{-3}$ - $10^3 \text{ m}^{-1}$ (gas), $10^3$ - $10^7 \text{ m}^{-1}$ (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), $10^{-6}$ - $10^{-3} \text{ m}$ (cell size)	real	scalar	WP3 (CFD (POLITO))
5	Average wall thickness and strut content		$10^{-7}$ - $10^{-5} \text{ m}$ (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 $\text{mWm}^{-1}\text{K}^{-1}$	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 <sup>-1</sup> K <sup>-1</sup>	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	$\sigma$ - $\epsilon$			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	$\sigma_Y$	0-100		scalar	Elastic Moduli and Topology of foam	WP6

