Delivery date:

31-08-2015

Authors:

Heinz A Preisig
Henrik Rusche

MoDeNa

Deliverable D5.8

Production Release - Recipes and Adapters

Principal investigators:

BASF: Andreas Daiss, Peter Degelman
IMDEA: Javier Llorca, Mohammad Marvi
POLITO: Daniele Marchisio, Mohsen Karimi
TUE: Patrick Anderson, Christos Mitrias
UNITS: Erik Laurini, Sabrina Pricl
US: Joachim Gross, Jonas Mairhofer
VSCHT: Pavel Ferkl, Juraj Kosek

Collaborators:

Henrik Rusche, Sigve Karolius

Project coordinator:

Heinz A Preisig

heinz.preisig@chemeng.ntnu.no

Abstract:

The MoDeNa framework enables the implementation of dynamic and adaptive simulation work flows that invokes a set of applications modelling the behaviours of detailed models or simpler surrogates. This first production version demonstrates the nature and mechanics of the framework using three cases, the simulation of foam formation, the simulation of foam ageing and the simulation of the foam's mechanical properties. Whilst currently relative simple models are being used, several more complex modules are in place, which one by one will extend the framework for PU foam simulations. The report describes the core concepts of recipes and adaptors, provides respective illustrative examples and summarizes the current status of the modelling module library.

Contents

1 Introduction

This is a brief report on the production release of the MoDeNa software as it relates to the adaptors and recipes as they are currently available on MoDeNa's git repository (MoDeNa consortium, 2015) commit ID 053d5b. There are two simulations available namely foam simulation & foam ageing. A third one is under development, mechanical properties. These simulations utilise the implemented software and define the existing applications, surrogate models, recipes and adaptors. The latter provide the interactions with the applications, surrogate models and software framework.

All software modules are located in the MoDeNa github directory:
https://github.com/MoDeNa-EUProject/MoDeNa/tree/master/applications/PUfoam.
The foam-ageing simulation uses inprocess that is generated off-line applications, each of which may again execute its own work-flow. These are the prerequisites for the above work-flow.

With this release the MoDeNa software will go public with the two simulations, which MoDeNa internally will be expanded to the final industrial simulations. The individual components that can be made public will be updated as they become available.

2 Terminology

Within the MoDeNa framework, we define:

Definition - Application : An implementation of a complex, detailed model

Definition - Simulation : A series of application invocations to solve a defined technical problem (includes specification of all boundary and initial conditions).

Definition - Surrogate model : An implementation of a simple substitute for an application.

Definition - Recipe : An application specific code fragment that executes an application in order to parametrise a surrogate model. It thereby connects the application into the simulation.

Definition - Adaptor : An application specific code fragment that embeds a surrogate model into an application using the interface library. An adaptor consists of three parts:

- construction of surrogate model
- execution surrogate model
- destruction surrogate model

Definition - Connection : An application, surrogate model, adaptor and in the case of backward mapping a recipe, which establish a link between applications. An operational connector implies that sufficient data to parameterise the surrogate model has been obtained from the application.

Standard notation: The notation reflects the current use of terms in MoDeNa. The effort to standardise the notation is ongoing in parallel and reflects into the MODA scheme. At this point in time, the MoDeNa project has not yet adopted the MODA terminology. Once settled this can be adjusted once the standard has been adopted. Work towards the adoption of the MODA documentation is ongoing and the deliverable D4.1 on *Specs of software, models, data and solver methods* will consist of the MODA forms for the various implemented model modules. The components of the notation associated with the platform have not yet converged and are under discussion. This includes particularly the terms *application, adaptor and connection*. The platforms employed in the different projects in the cluster have different uses for those terms and discussions are evolving but have not converged to the level on what has been achieved within the MODA form. The schema approach presented by Thomas Hagelien does though gain increasing acceptance and MoDeNa has a very similar approach using Jinga2 templates (see Deliverable 5.6 Production Release – Orchestrator and Interface Libary).

3 Foaming process simulation

3.1 Description of case

The "foam process simulation" simulates the foaming process for a polyurethane foam chemically and physically blown. The corresponding chemical recipe contains a mixture of polyols and isocynates, water, cyclopenthane, surfactants and catalysts. The simulation describes the evolution of the macroscopic properties of the foam, namely density, viscosity and cell size distribution, by using information coming from quantum chemistry calculations (i.e. chemical reaction rates), molecular dynamics calculations (i.e. diffusion coefficients and polymer density) and mesoscale calculations (for determining for example the individual bubble growth rate belonging to the foam).

3.2 Work-flow diagram

Figure 1 shows a graphical representation of the implemented work-flow for the foam process simulation.

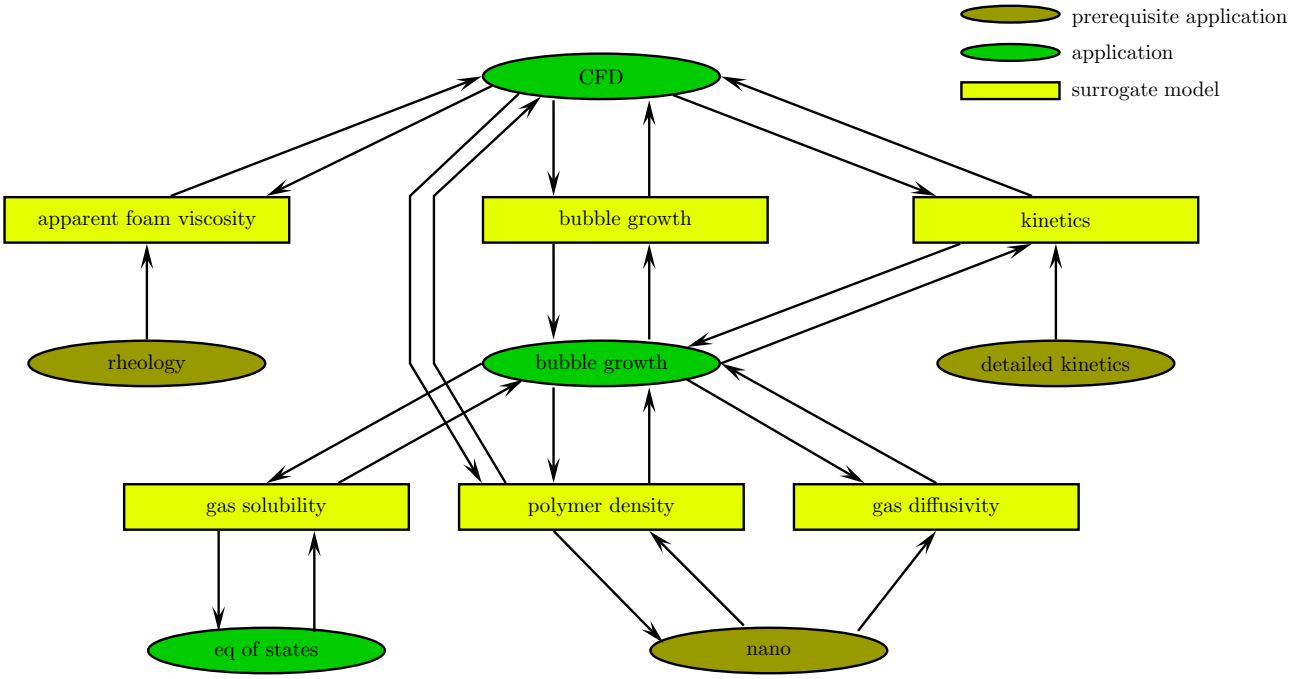

Figure 1: Workflow diagram for foam process simulation

Note: The term *nano* is here used to reflect computations that use *abo inio* models (see Deliverable D4.1 (Preisig et al., 2015))

3.3 Surrogate models, applications, recipes & adaptors

The tables 1 to 3 list the surrogate models, applications and connections being utilised in the computation of the foaming process simulation.

surrogate model	**inputs**	**outputs**	**code reference**
gas diffusivity (UNITS)	temperature	diffusivity of blowing agent and CO_2	`MoDeNaModels/diffusivity/diffusivity.py`
solubility (US)	temperature	Henry coefficients (CO_2, Blowing agent)	`MoDeNaModels/Solubility/Solubility.py`
kinetics (BASF)	temperature, composition (OH, NCO, W)	reaction rate	`MoDeNaModels/Kinetics/Kinetics.py`
polymer density (UNITS)	temperature	Liquid polymer density	`MoDeNaModels/PolymerDensity/PolymerDensity_units.py`
polymer density (US)	temperature	Liquid polymer density	`MoDeNaModels/PolymerDensity/PolymerDensity.py`
bubble growth (VSCHT)	temperature, concentration blowing agent and CO_2, bubble size	growth rates due to blowing agent and CO_2	`MoDeNaModels/bubbleGrowth/bubbleGrowth.py`
app. foam viscosity (TUE)	temperature, shear rage, extent of reaction gelling	apparent foam viscosity	`MoDeNaModels/Rheology/Rheology.py`

Table 1: The list of available surrogate models for foaming process simulation

application	**code reference to application**	**status**
CFD (POLITO)	`MoDeNaModels/CFD_tool_0D/src`	currently only 0D, the 3D code has been tested already and will be included in future releases
bubble growth (VSCHT)	`MoDeNaModels/bubbleGrowth/src`	operational
eq of state (US)	`MoDeNaModels/Solubility/src`, `MoDeNaModels/PolymerDensity/src`	all applications operational, but solubility currently lacks stability and precision
foam rheology (TUE)	`MoDeNaModels/Rheology/src`	application is in principle operational, reducing the computational burden is still the main activity
nano (UNITS)	not submitted to public repository since Material Studio® is closed-source	application operational (external tool), sub-recipes not submitted to public repository
kinetics (BASF)	not submitted to public repository since Predici® is closed-source	application operational (external tool), sub-recipes not submitted to public repository

Table 2: The applications used in foaming process simulations

connection	**status**
CFD – foam rheology	operational, but currently not needed since CFD is only 0D
CFD – bubble growth	operational
CFD – kinetics	operational
CFD – polymer density	operational
bubble growth – kinetics	implemented, but currently replaced by hard-coded model
bubble growth – solubility	implemented, but currently replaced by hard-coded model (see solubility application)
bubble growth – gas diffusivity	operational
bubble growth – polymer density	implemented, but currently replaced by hard-coded model since UNITS's model is currently not submitted into public repository

Table 3: Status of connections in foaming process simulation

4 Foam ageing simulation

4.1 Description of case

The polyurethane foams are usually expanded using chemical and physical blowing agents. These blowing agents typically have lower thermal conductivity than air. Unfortunately, they spontaneously diffuse out of the foam and they are replaced by air. That causes undesirable increase in the thermal conductivity of the foam, and thus the degradation of its insulating properties. This process is called foam ageing.

The application ”foam ageing” predicts the evolution of gas phase composition in foam in time. For the needed diffusivity and solubility of gases in polyurethane it can utilize the ”nano” and ”equation of states” applications, respectively. Once the gas composition is known, the foam insulation properties are calculated by the ”foam conductivity” application. This application utilizes ”nano” and ”reconstruction” applications to predict conductive properties and ”quantum chemistry” to predict radiative properties.

4.2 Work-flow diagram

Figure 2 shows a graphical representation of the implemented work-flow for the foam ageing simulation.

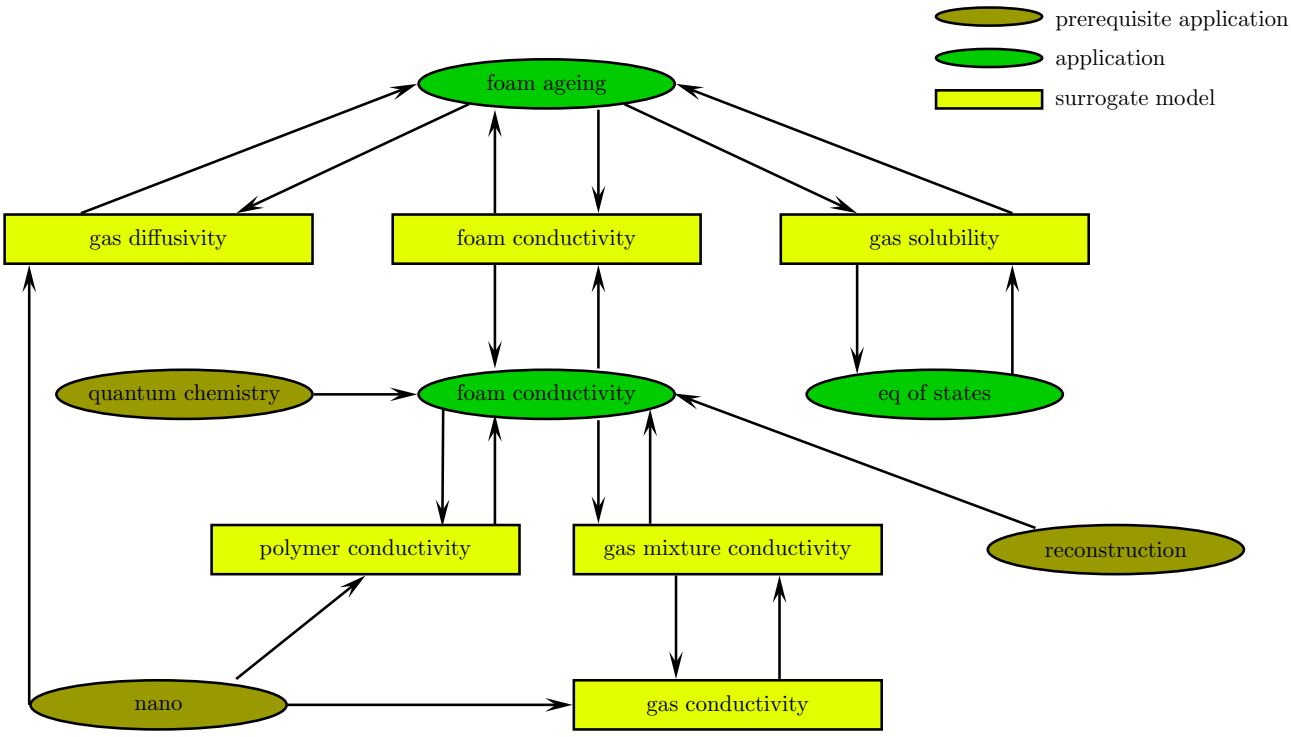

Figure 2: Workflow diagram for foam ageing simulation

4.3 Surrogate models, application, recipes & adaptors

The tables 4 to 6 list the surrogate models, applications and connections being utilised in the computation of foam ageing.

surrogate model	**inputs**	**outputs**	**code reference**
foam conductivity (VSCHT)	porosity, mean cell size, strut content, temperature, mole fractions, gas mixture conductivity, polymer conductivity	foam conductivity	`MoDeNaModels/foamConductivity/foamConductivity.py`
gas mixture conductivity (VSCHT)	temperature, mole fractions, gas conductivity	gas mixture conductivity	`MoDeNaModels/gasMixtureConductivity/gasMixtureConductivity.py`
gas conductivity (UNITS)	temperature	gas conductivity	`MoDeNaModels/gasConductivity/gasConductivity.py`
polymer conductivity (UNITS)	temperature	polymer conductivity	`MoDeNaModels/polymerConductivity/polymerConductivity.py`
gas diffusivity (UNITS)	temperature	gas diffusivity	`MoDeNaModels/diffusivity/diffusivity.py`
gas solubility (US)	temperature, mole fractions	gas solubility	`MoDeNaModels/Solubility/Solubility.py`

Table 4: The list of available surrogate models for foam ageing simulations

application	**reference to application**	**status**
foam ageing (VSCHT)	`MoDeNaModels/CFD_tool_0D/src`	operational
eq of state (US)	`MoDeNaModels/Solubility/src`, `MoDeNaModels/PolymerDensity/src`	all applications operational, but solubility currently lacks stability and precision
foam reconstruction (VSCHT)	`MoDeNaModels/FoamConstruction/foamreconstr/src`	operational
nano (UNITS)	not submitted to public repository since Material Studio® is closed-source	application operational (external tool), sub-recipes not submitted to public repository
quantum chemistry (BASF)	not submitted to public repository, closed-source application	application operational (external tool), sub-recipes not submitted to public repository

Table 5: The applications used in foam ageing simulation

connection	**status**
foam ageing – gas diffusivity	operational
foam ageing – foam conductivity	operational
foam ageing – solubility	implemented, but currently replaced by hard-coded model (see solubility application)
foam conductivity – polymer conductivity	operational
foam conductivity – gas mixture conductivity	operational
foam conductivity – foam reconstruction	operational
gas mixture conductivity – gas conductivity	operational

Table 6: Status of connections in foam ageing simulation

5 Mechanical properties simulation

5.1 Work-flow diagram

Figure 3 shows a graphical representation of the implemented work-flow for the mechanical properties simulation.

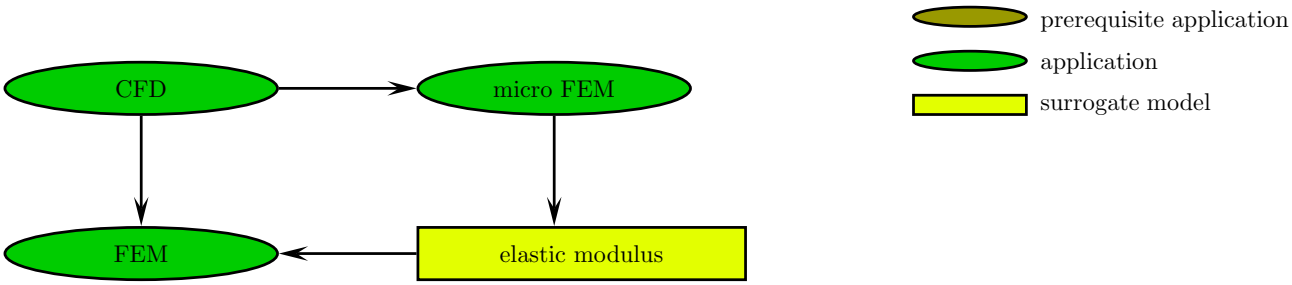

Figure 3: Workflow diagram for mechanical properties simulation

5.2 Surrogate models, application, recipes & adaptors

The tables 7 to 9 list the surrogate models, applications and adaptors being utilised in the computation of the foam mechanical properties.

surrogate model	**inputs**	**outputs**	**code reference**
elastic modulus (IMDEA)	cell size distribution (mean and standard deviation)	elastic modulus	under development

Table 7: The surrogtate models used in mechanical properties simulation

application	**reference to application**	**status**
CFD (POLITO)	`MoDeNaModels/CFD_tool_0D/src`	currently only 0D, 3D code experiences stability problems
micro FEM (IMDEA)	not submitted to public repository, closed-source application	application operational (external tool), sub-recipes not submitted to public repository
FEM (IMDEA)	not submitted to public repository, closed-source application	application operational (external tool), sub-recipes under development

Table 8: The applications used in mechanical properties simulation

connection	**status**
CFD – micro FEM	under development
CFD – FEM	under development
FEM – micro FEM	under development

Table 9: Status of connections in mechanical properties simulation

6 Documentation

MoDeNa has the policy to integrate the software documentation primarily into the software itself and use an automatic documentation tool to generate the on-line documentation. In addition, where appropriate, inprocess is added to describe the implemented model, and on how to build application. A current snapshot of the documentation is available from http://henrus.github.io/MoDeNa/index.html.

References

MoDeNa consortium (2015). Modena github repository. https://github.com/MoDeNa-EUProject/MoDeNa. 1

Preisig, H. A., IMDEA, POLITO, TUE, UNITS, US, and VSCHT (2015). Modena - deliverable D4.1: Specs of software, models, data and solver methods. Technical report, FP7 MoDeNa. 3.2