MODA

Modelling data documenting one simulation

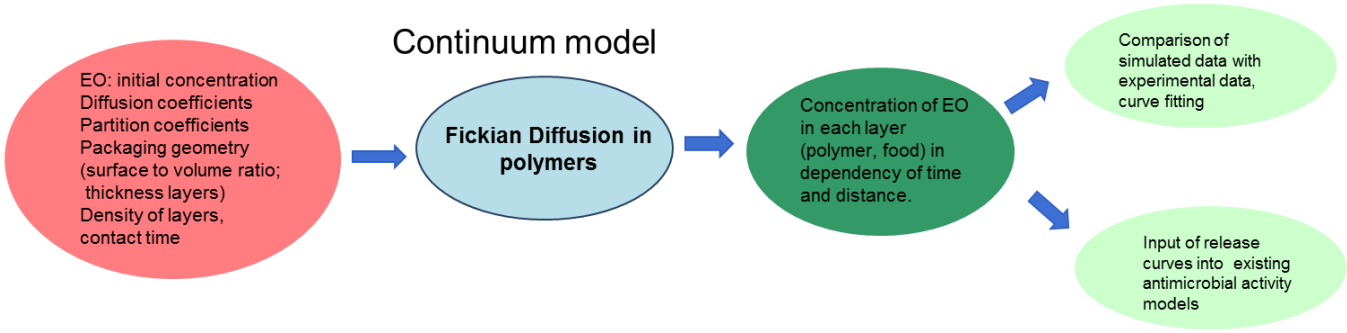
Name <NanoPack, Release of essential oils to food, diffusion model>

Metadata for these elements are to be elaborated over time

Purpose of this document:
Definition of a data organisation that is applicable to ALL materials modelling simulations. The fiche should contain all elements that are needed to describe a simulation. This information spans from the end-user (manufacturer) information to the computational modelling details.

OVERVIEW of the simulation			
1	USER CASE	*General description of the User Case. Please give the properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour to be simulated.* Application of existing physics models to new materials and manufacturing processes: Antimicrobial agents (essential oils) are incorporated in a polymer nanocomposite (nanotubes in polyolefin). Initially, before extrusion, the essential oils are located in the nanotubes and will be released into the polymer and diffuse to the food contact surface. The release of the antimicrobial agents to food or the surface of the food shall be described the diffusion and antimicrobial agents in the polymer along a concentration gradient shall be described and predicted (1) during manufacturing and storage and (2) after contact with food, the transfer into food. predict diffusion of the nanoparticles in the polymer.	
2	CHAIN OF MODELS	MODEL 1	*Please identify the first model* Diffusion model to predict migration of organic molecules into food (and/or polymer layers): Mass transport continuum model, conservation of mass, Fick's 2nd law (use of existing multilayer diffusion models and related software)
		MODEL 2	*Please identify the second model*
		…	…
3	PUBLICATION ON THIS ONE SIMULATION	*Please give the publication which documents **this ONE simulation*** Roduit, B., C. H. Borgeat, S. Cavin, C. Fragniere and V. Dudler (2005). "Application of Finite Element Analysis (FEA) for the simulation of release of additives from multilayer polymeric packaging structures." Food Additives & Contaminants 22(10): 945-955.	
4	ACCESS CONDITIONS	*Please list whether the model and/or data are free, commercial or open source. Please list the owner and the name of the software or database (including web link if available)* The modelling tool (model 1) is available as commercial software (AKTS-SML, AKTS AG, 3960 Siders, Switzerland or alternatively MigratestExp, FABES GmbH, München, Germany) and as freeware (Safe Food Packaging Portal http://sfpp3.agroparistech.fr/). The input parameters (diffusion coefficients, partition coefficients) shall be published.	
5	WORKFLOW AND ITS RATIONALE	*Please give a textual rationale of the choice of models and the workflow. This should include the choice of which aspect of the user case is to be simulated with which model.* Existing diffusion/migration modelling (or better simulation) software is used in which PE/MR and the numerical algorithm are already implemented. For known diffusion and partition coefficients for a given polymer-food system for a defined substance (e.g. from literature), migration can directly be calculated for any time span. All necessary information to solve the Fickian 2nd law by the numerical	

		algorithm is already included with the initial and boundary conditions in the software. For a new material or migrating substance the software can be used to fit the output curve to experimental data by variation of the diffusion and partition coefficients. From the best fit, both parameters for a specific substance in the investigated polymer at a given temperature are obtained. The curve fit procedure is one of several options to experimentally derive diffusion and partition coefficients. Independently how they are derived, they can be used as input parameters for the simulation.



Workflow

Each model used in this simulation can be documented in four chapters:

1. Aspect of the User Case or System simulated with this model
2. Model
3. Computational aspects
4. Post processing

< *Diffusion model to predict migration into food*>

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*Describe the aspects of the user case textually.* Polymer (case: polyolefin films or articles) in which a nanomaterial containing a low-molecular weight organic substance (antimicrobial agent = essential oil) is dispersed. The essential oil is initially encapsulated within the nanomaterial and will be released to the polymer during extrusion and storage. After filling with food or food simulant, the essential oil diffuses to the food contact surface along the concentration gradient and migrates into food. The model assumes in the first instance homogeneous distribution of the essential oil in the polymer. The case described is the release of essential oil into food/food simulant during filling and storage of the food.
1.2	MATERIAL	*Describe the chemical composition:* Polyolefin with Halloysite nanotubes (HNT)
1.3	GEOMETRY	*Size, form, picture of the system (if applicable)* any 3D geometry (flat film, pouch, container, etc. will be transposed to a (less complex) 1-dimensional system with the flux of substances only in one direction along the concentration gradient to the food
1.4	TIME LAPSE	*Duration of the case to be simulated.* Actual case: storage of food package (days – months) Generally depending on the step of manufacture or storage: manufacturing nanocomposite in extruder (seconds to minutes), storage of films (hours-months),
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*If relevant, please list the conditions to be simulated (if applicable).* transfer processes at filling and storage of the polymer with food: filling and storage at room temperature

1.6	PUBLICATION ON THIS ONE SIMULATION	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Model type and name **chosen from RoMM content list** (the PE).* Diffusion in solid polymers: continuum in finite volumes (polymer or food) and migrating substances on mesoscopic scale	
2.1	MODEL ENTITY	*The entity in this materials model is <finite volumes, grains, atoms, or electrons>:* finite volumes	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	*Name, description and mathematical form of the PE* Fick 2nd law: $\frac{\partial c_k}{\partial t} = D_k \left(\frac{\partial^2 c_k}{\partial x^2} + \frac{\partial^2 c_k}{\partial y^2} + \frac{\partial^2 c_k}{\partial z^2} \right)$ The three dimensional relation is simplified to the flux along the concentration gradient (1 dimensional relation) $$\frac{\partial c_k}{\partial t} = D_k \frac{\partial^2 c_k}{\partial x^2}$$
		Physical quantities	*Please name the physics quantities in PE* • t time of migration (diffusion), • 2 ≤ k ≤ n index of the medium (layer: polymer, food), • c_k local concentration (in mg/l oder µg/l) D_k local diffusion coefficient of the substance in the medium k • x, y, z 3D-coordinates The (numerical) solution of the differential equation furthermore needs the quantities: • Initial concentrations in the layers (in mg/l oder µg/l) • partition coefficients K between the layers, • density of layers, • thickness of layers (distance)
2.3	MATERIALS RELATIONS	**Relation**	1. *<Name of the material relation and which PE it completes >* user case input, cooefficients are deduced from experimental data. 2.
		Physical quantities/ descriptors for each MR	1. *Name of the physics quantities, parameters (constants, matrices) and variables that appear in MR* Partition coefficients between each layers describing the equilibrium concentrations 2. *Diffusion coefficients describing the flux of the substance of interest in each layer*
2.4	SIMULATED INPUT	*please document the simulated input and with which model it is calculated.*	

This chapter is similar to the description on input files to simulation software and requires understanding of the underlying architecture of the data in certain class of solvers for the models.

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS	
3.1	NUMERICAL SOLVER	Finite difference method see V. Tosa and P. Mercea (2008) and Tosa et al. (2008) for Migratest Exp software and finite element analysis see Roduit et al. (2005) for AKTS-SML software
3.2	SOFTWARE TOOL	*Please give the name and if this is your own code, please specify if it can be shared, link to website/publication.* Existing commercial simulation software is used: AKTS-SML, AKTS AG, 3960 Siders, Switzerland (http://www.akts.com/sml-diffusion-migration-multilayer-packaging/download-diffusion-prediction-software.html) and/or MigratestExp, FABES

		GmbH, München, Germany (https://www.fabes-online.de/de/software/migratest-exp/)	
3.3	**TIME STEP**	5 s (10 days simulation)	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	*Computational representation of the physics equation, materials relation and material (e.g. "written up for the entity in the model" or in the case of statistical approached "written up for finite volumes")* use of existing software input parameter: Concentration of organic substance (e.g. antimicrobial essential oil (EO) or other substance) in the polymer at a given moment, including initial content; diffusion coefficient of organic substance in each layer (polymer layers, food); partition coefficients between the layers, thickness of layers; time lapsed
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**	*If applicable* • The system packaging/food is isolated: no mass transfer to the environment. • Total mass of the migrant in the system packaging food remains constant (no losses, no chemical reactions) • Initial homogeneous distribution of substance in the polymer layer • No boundary resistance at the interface polymer/food • The diffusion coefficient in each layer remains constant at constant temperature • Partition coefficients remain constant at constant temperature	
3.6	**ADDITIONAL SOLVER PARAMETERS**	*Pure internal numerical solver details, If applicable, like* • *Specific tolerances* • *Cut-offs, convergence criteria* • *Integrator options*	

Post processing

The "raw output" calculated by the model is per definition the physics variable in the PE(s).
This is already specified in the entry 2.2 and will appear in your dark green circle in the workflow picture.

This output is often processed by a post processor in order to calculate values for physics variables for different entities that can be input to the next model. Or the output is homogenised for larger volumes in the form of a MR or Descriptor Rule that are the final output of the total simulation.
This will appear in your light green circle in the workflow picture and also in 2.4 of the next model.

The methodology (often including new physics) used to do this calculation is to be documented.

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT**	*Please specify the post processed output* *If applicable then specify the entity in the next model in the chain fro which this is calculated: electrons, atoms, grains, larger/smaller finite volumes.* *In case of homogenisation, please specify the averaging volumes.* The output of the simulation are time dependent release curves for the migrating substance into the food. Post processing 1: Comparison of the experimental values (migration kinetics) with the simulated curve. Curve fitting by variation of input parameters (diffusion and partition coefficients) using the software above. → experimentally obtained diffusion and partition coefficients Post processing 2: Simulated release of essential oils will be fed into existing models for antimicrobial activity
4.2	**METHODOLOGIES**	*Please describe the mathematics and/or physics used in this calculation.*
4.3	**MARGIN OF ERROR**	*Please specify the margin of error (accuracy in percentages) of the property calculated and explain the reasons.to an industrial end-user.*
4.4		