Deliverable D6.3:
Revision of the specification for Virtual Polymer as a result of input from WP4

WP6: Development of the open Access TeaM Cables tool and integration of models

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Description: Revision B of the software specification incorporating changes based on WP4 and second version of the software tool.

Table of Contents

Glossary

Abbreviation/ acronym	Description
AO1	Phenolic antioxidant
AO2	Thioether antioxidant
ATH	Tri-hydrated alumina fillers
C=O	Carbonyles species
CO2	Oxygen concentration
COMSY	Condition Oriented Monitoring and Plant Management System (Software)
EDF	Électricité de France
ENSAM	École Nationale Supérieure d’Arts et Métiers
FRA-G	Framatome GmbH
GUI	Graphical User Interface
HW	Hardware
I	Dose rate
MS	Microsoft
O2	oxygen
OS	Operating System
PE	Polyethylene
PH	Polymer substrate
PO_2	Oxygen partial pressure
POOH	Hydroperoxides species
S	Scissions
SO2	Coefficient of oxygen solubility into the polymer
SW	Software
T	Temperature
t	Time
Tbd	To be defined

Abbreviation/ acronym	**Description**
TID	Total Integrated Dose
TMC	TeaM Cables
VM	Virtual Machine
VP	Virtual Polymer (Software)
WP	Work Package
XLPE	Cross-linked polyethylene

1 Executive Summary

In this deliverable the progress achieved in WP6 for the implementation of the TeaM Cables (TMC) Tool is presented to document the project evolution and decisions taken in the course of the software (SW) implementation works in order to achieve the TMC objectives.

The TeaM Cables Tool intends to combine COMSY (Condition Oriented Monitoring and Plant Management System), developed by Framatome GmbH, and VP (Virtual Polymer), developed by EDF.

A first specification of the TeaM Cables Tool was drafted in Deliverable D6.1, which was submitted in September 2019. The Deliverable D6.2 presents the activities made and progress achieved in WP6 for the implementation of the TeaM Cables Tool in order to document the project evolution and decisions made in the course of the SW implementation works in order to achieve the TMC objectives. This deliverable was submitted in May 2019. Both reports can be found at https://www.team-cables.eu/media-centre/.

2 Introduction

COMSY is the front-end software running on Windows OS platform at the customer; all data is stored in an MS Access or MS SQL Server database. For the TeaM Cables Tool, the electrical module of COMSY will be used. In the TeaM Cables Tool, the currently implemented ageing/degradation algorithms for assessment/management of the lifetime for XLPE insulated cables (as part of passive electrical systems) will be replaced/extended with the evaluation of calculation results from VP, using algorithms to be developed and validated within the framework of the TeaM Cables project.

VP is the back-end software running on Linux OS: it is a one-dimension modelling platform composed of a model data base and different calculation components. The chaining of the different parts makes it possible to develop a multi scale and multi physical modelling of the polymer ageing process. The further development and validation of the multi scale and multi physical modelling of the ageing process of XLPE in dependence of specific material properties and environmental conditions is the main objective of the TeaM Cables project.

The features required in the TeaM Cables Tool were identified in Deliverable D6.1 as the following:

- the graphical user interface (GUI) needed for cable data entry and display,
- generates the data needed for degradation calculations in VP,
- receives the calculation results (abacus/solver matrix) from VP,
- allocation/mapping of VP results to the individual cables,
- display of results, calculation of residual life time.

3 VP Data

3.1 Definition of input data provided by COMSY to VP

Key inputs data provided by COMSY to Virtual Polymer are the following:

- **Temperature, T**
  ➔ Range of temperature [T_{min}, T_{max}, step]. The temperature range should be provided in the international system of units, in Kelvins.

  FRA-G suggests to use parameters from the EPR design in the ageing calculation runs. *E.g.* Ambient temperature in the range of 15 to 60°C (60°C is considered as an hotspot).
- **Dose rate, I**
  ➔ Range of dose rate [I_{min}, I_{max}, step]. The dose range should be provided in the international system of units, in Gy/s.

  FRA-G proposes to use parameters from the EPR design in the ageing calculation runs. *E.g.* dose rate in the range of 10E-3 to 100.E-3 Gy/h, which means 2.7E-7 to 2.7E-5 Gy/s.

  From the TMC project point of view it may be interesting to make a VP run using parameters from the accelerated ageing of samples (temperature, dose rate). This would be a first possibility for the researchers to compare data from VP simulation to experimentally obtained data. The environmental parameters used in the TMC project can be taken from Deliverable D2.2.
- **Time, t**
  ➔ Range of duration life [t_{min}, t_{max}, dt]. The time range should be provided in the international system of units, in Seconds.
- **Polymer substrate, [PH]**

  ➔ Polymer substrate corresponds to the content of C-H bonds, corresponding to a potential oxidation site. The polymer substrate concentration should be provided in the international system of units, in mol/L.

  This parameter is not specified in the material datasheet. Thus, there are two options left to the user:
  - Enter a value (in mol/L);
  - Select default value. In polyethylene material, polymer substrate is considered equivalent to [PH] = 60 mol/L (*cf.* Deliverable D4.2).
- **Type of antioxidant, [AO1;AO2,AO1+AO2]**
  ➔ Two types of antioxidants are considered in this project (*cf.* Deliverable D2.1):
  - AO1: Irganox 1076, also called octadecyl-[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate, is a phenolic antioxidant belonging to the family of radical scavengers, stabilization by capture of peroxyl radical (primary AO).
  - AO2: Irganox PS802, also called DiStearyl ThioDiPropionate (DSTDP), is a thioether antioxidant belonging to the family of hydroperoxide decomposers, (secondary antioxidants). Hydroperoxide decomposers are organic molecules capable of transforming hydroperoxides into non-radical and thermally stable species (that is, non-reactive).

  Thus, there are three options left to the user:
  - AO1 corresponding to phenolic antioxidant;
  - AO2 corresponding to thioether antioxidant;
  - AO1+AO2 corresponding to the combination of the two antioxidants.

- **Antioxidant content, [AO]**

  ➔ The antioxidant content should be provided in the international system of units, in mol/L.

  The antioxidants content is not necessarily specified in the material datasheet. De-formulation or also called "reverse engineering" could be necessary to determine this information related to the formulation identity card. Thus, there are two options left to the user:
  - Enter a value provided either by material datasheet or determined by de-formulation procedure (in mol/L);
  - Select default value (realistic ranges must be defined by Nexans):
    - AO1: [0, AO_{min}, AO_{max}];
    - AO2: [0, AO_{min}, AO_{max}];
    - AO1+AO2: [0, AO_{min}, AO_{max}].

- **Oxygen concentration, [CO_2]**

  ➔ Oxygen concentration CO_2 is related to the oxygen partial pressure P_{O2} in the exposure environment by the classical Henry's law:

$$CO_2 = SO_2 \,.\, \mathrm{P}_{O2}$$

  The time range should be provided in the international system of units, in mol/L.

  SO_2 is the coefficient of oxygen solubility into the polymer. Typical values of SO_2 reported for low density polyethylene (LDPE) in the literature are about 1.8×10^{-8} mol.L^{-1}.Pa^{-1} regardless the temperature (Van Krevelen and Nijenhuis, 2009).

  Knowing that: $\mathrm{P}_{O2} = 0.21 \times 10^5$ Pa, it comes finally: $CO_2 = 3.8 \times 10^{-4} \mathrm{mol.L^{-1}}$.

  Thus, there are two options left to the user:
  - Enter a measured value (in mol/L);
  - Select default value (normal oxygen partial pressure).

<u>Optional inputs data provided by COMSY to Virtual Polymer are the following:</u>

- **Thickness, [p]**

  ➔ Simulations carried out by the TeaM Cables tool will be representative of skin properties changes of nuclear power cables. The tickness is provided for informational purpose only. For the sake of consistency, the thickness should be provided in the international system of units, in mm.

- **Fillers content, [ATH]**

  ➔ Only the impact of incorporation of ATH fillers is studied in this project (*cf.* Deliverable D2.1). The studies carried out so far do not make it possible to precisely determine the influence of the fillers. The presence or the absence of fillers is provided for informational purpose only. The fillers content would be provided in %wt.

- **Boundary conditions, [film]**

  ➔ Analytical kinetic models for radio-thermal oxidation suggested in the WP4 deliverables (*cf.* Deliverables D4.3 & D4.6) do not allow to use all the functionalities available in Virtual Polymer. Following oxidation markers in the thickness integrating boundary conditions close to NPP operating conditions will not be possible in the TeaM Cables tool. TeaM Cables simulations consider only thin films (thickness about less than 500µm) and symmetric boundary conditions (oxygen on both surfaces). Simulation of thin films with oxygen on both surfaces is only provided for informational purpose.

3.2 Virtual Polymer simulations

The following files for Virtual Polymer simulations are necessary:

- **teams_cables_2021_create.input**: is an input file to define the couple of parameters for VP run;
- **team_cables_2021.py**: is a Python scrypt to create and execute experimental design for Team Cables;
- **post_test_create_2021_T_$T_I_$I.input**, is an input file for the different couple of parameters to obtain intermediary analytical results of the VP calculation run, *e.g.* constants calculated for the couple of parameters. These files contain:
  - study name;
  - input directory;
  - *.csv output file directory name;
  - analytical equations names;
  - analytical equations;
  - constant names;
  - constant values;
  - result units;
  - universal constant used.
- **c_post_polymer_kinetics_xlpe_T_$T_I_$I_point.csv**: these files contain the results of the intermediary analytical calculations, *e.g.* constants calculated for the couple of parameters;
- **explicit_integration.py**: is a Python scrypt to run the analytical kinetic models for radio-thermal oxidation suggested in the WP4 deliverables (*cf*. Deliverables D4.3 & D4.6) for the different couple of parameters;
- **team_cables_2021_integration_T_$T_I_$I.csv**: these files contain the temporal evolutions of chemical species obtained by VP calculation run for the different couple of parameters:
  - time: time in hour;
  - POOH: concentration of the hydroperoxides species [mol/L];
  - C=O: concentration of the carbonyls species [mol/L];
  - S: concentration of scissions [mol/L].
- **test_create_2021_abaqus.csv:** the abacus associates the following results with each input file:
  - Input file name;
  - Temperature [K];
  - Dose rate [Gy/s];
  - Success_1 is related to criterion 1 [Boolean]. Criterion 1 is equivalent here to [carbonyles] ≈ 0.1 mol/L. “False” means “Criterion not reached”. “True” means “Criterion reached”;
  - End_of_life_1 [sec]. Time to reach criterion 1;
  - Carbonyles content [mol/L]. Carbonyl content when criterion 1 is reached.

3.3 VP clarifications still valid

Clarification results:

1. Model used in the VP run is still a material sheet with free surfaces;
2. Interaction between XLPE and conductor material is not investigated in the TeaM Cables project (there might be some hints from the experimental investigations).

3.4 Next steps

The following steps are:

1. Second VP run with antioxidant content (phenolic antioxidant);
2. Additional calculation outputs other than the parameters already included in the **test_create_2021_abaqus.csv** might be selected for degradation over time evaluations of the XLPE material (aim is the correlation of chemical, mechanical and electrical parameters over time). It is expected that further parameters will be added to and delivered in the abacus of VP to COMSY;
3. Ensure communications between COMSY / VP.

4 References

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