BEACON
Bentonite Mechanical Evolution

Work Package 3:

Model development

Antonio Gens

Universitat Politècnica de Catalunya (UPC), Barcelona Tech

Workshop on Mechanical Properties of Bentonite Barriers

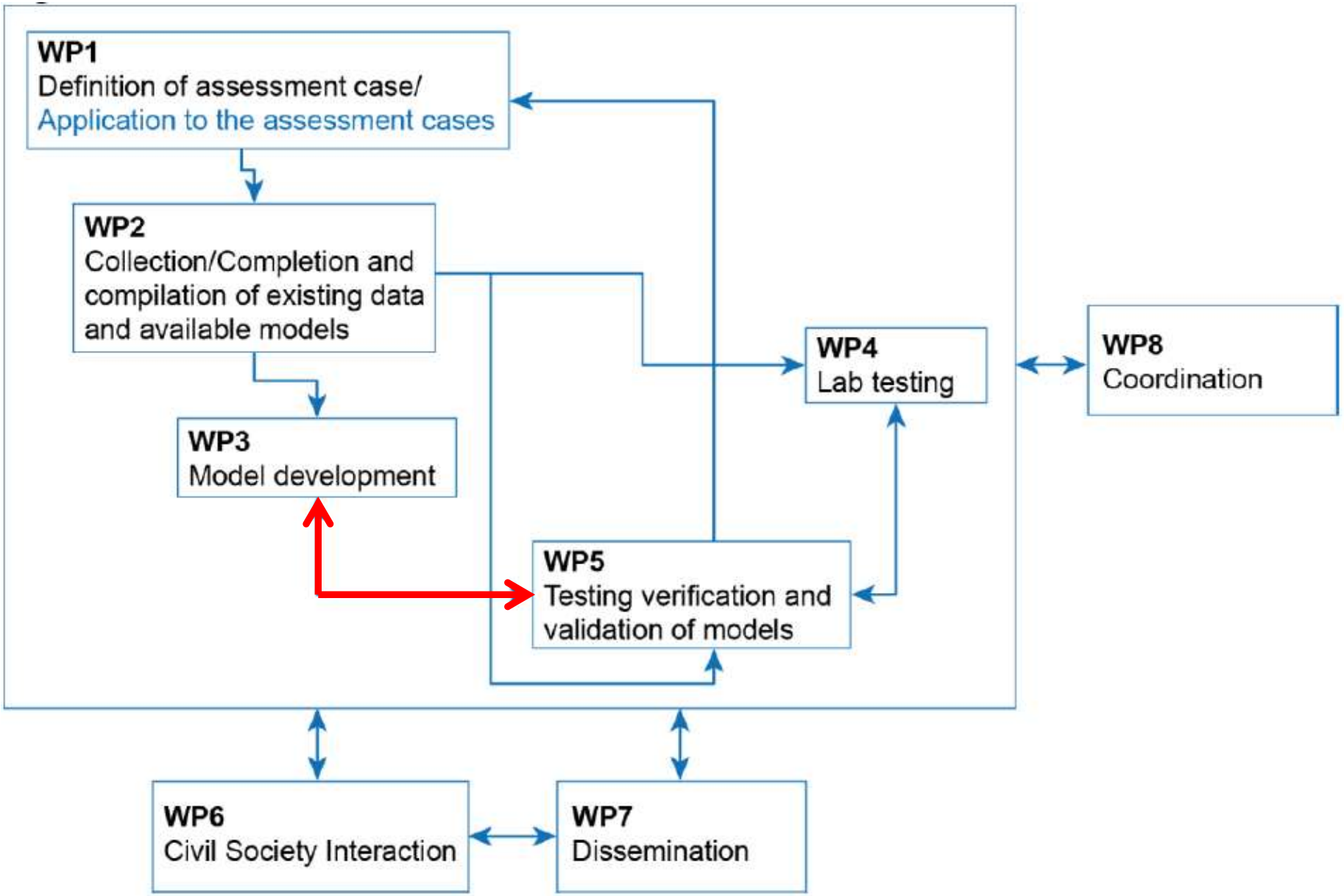
Lithuanian Energy Institute

Kaunas 19-20 June 2017

Objectives of WP3

- The final goal is to develop enhanced, robust and practical numerical tools, firmly grounded on a good understanding of the phenomena involved.
- The numerical tools should have the required predictive capabilities concerning the behaviour of engineered barriers and seals especially in relation to their final state.
- A key component of the numerical tool that requires especial attention is the mechanical (stress-strain) constitutive model because the prediction of the final state of the barrier (including its heterogeneity) is directly dependent on its features and capabilities.

Location of WP3 in BEACON structure



Participants

Work package number	**3**		**Lead beneficiary**			**UPC**
Work package title	**Model development**					
Participant number	3	9	10	11	12	15	16
Short name of participant	Posiva	UPC	GRS	CTU	CU	ULg	BGR
Person months per participant:	1	13	6.6	3	8.55	9	5
Participant number	17	18	19	20	21	22	23
Short name of participant	KIT	LEI	CIEMAT	Clay Tech	EPFL	ICL	Quin-tessa
Person months per participant:	2.2	8	3.5	6	20	8	3.2
Start month	1			**End month**	48		

Features of WP3

- Focus on the mechanical constitutive model because the state of the barrier at the end of the transient period is dependent on the mechanical evolution of the bentonite
  - Issues of irreversibility stress path dependency and long term deformation are critical
  - This focus on mechanical behavior is in contrast with previous projects where thermal and hydraulic behavior were the primary focus
- The following cases should be considered:
  - Saturated and unsaturated material (wide range of densities)
  - Compacted (blocks) bentonite and pellet-based materials
  - Isothermal and non-isothermal conditions
- Implementation into computer codes capable of performing coupled HM and THM analyses.
  - Additional developments (gaps, large displacements) may be required

WP3: Task organization

- Task 3.1 Development of mechanical constitutive models capable of simulating the behaviour and final state of barriers and seals with special focus on features concerning long term behaviour, irreversibility and stress path dependency.
- Task 3.2 Development/Modification of numerical tools capable of performing coupled HM and THM analyses
  - Task 3.2.1 Implementation of the developed mechanical constitutive models
  - Task 3.2.2 Implementation of additional numerical features
- Task 3.3 Verification of the basic features of the models against simple benchmarks

- The full verification, validation and application are performed within WP5

WP3: Tasks of individual participants

- Constitutive model development and numerical implementation

- BGR:
  - Development of mechanical capabilities of OpenGeoSys
  - Development of improved hydro-mechanical coupling
- Clay Tech:
  - Modification of mechanical models in Abaqus to enable plastic hardening for isotropic selling
  - Implementation of a HM mechanical model based on swelling pressure/suction relationship in Comsol Multiphysics
- CTU:
  - Development of an open source FE package (SIFEL)
  - Use of the hypoplastic model developed by CU
- CU:
  - Evaluation and further development of a hypoplastic constitutive model for bentonite
  - Implementation in a single-element driver

WP3: Tasks of individual participants

- Constitutive model development and numerical implementation

- ICL:
  - Constitutive model for swelling clays: double porosity structure
  - Model development based on comparisons with experimental results
  - Implementation in ICFEP
- LEI:
  - Development of a conceptual and numerical model for evaluation of bentonite behaviour
  - Implementation in Comsol Multiphysics
- Quintessa:
  - Improve the conceptual and numerical representation of swelling processes in the ILM
  - Test the coupling of hydraulic processes to mechanical processes that is currently implemented in the ILM
  - Implementation in QPAC

WP3: Tasks of individual participants

- Constitutive model development and numerical implementation

- ULg:
  - Develop a practical model representing the material behaviour with limited parameters
  - Heterogeneity via a model of spatial variability
  - Development and application of an interface model
  - Implementation in LAGAMINE

- UPC:
  - Development of an enhanced and more robust elasto-plastic double porosity model
  - Depending on progress, extension to non-isothermal conditions
  - Implementation in CODE_BRIGHT

WP3: Tasks of individual participants

Model extensions

- GRS and KIT INE:
  - Develop a conceptual model to derive suitable hydraulic parameters
  - Interpretation of density distributions and variation range in terms of porosity/permeability distributions and relate them to large scale hydraulic behaviour
- EPFL:
  - Extension of an existing THM framework to include chemo-osmotic effects
  - Modification of effective stress definition
  - Development of hydraulic and mechanical models
  - Implementation in computer code

WP3: Tasks of individual participants

Auxiliary contributions

- CIEMAT:
  - Experimental mechanical and hydromechanical behaviour of bentonite under hydration
- MKG:
  - Follow the work and coordinate interaction with WP6
- POSIVA:
  - Follow the work and learn form their experiences

WP3: Deliverables and meetings

Deliverables

- Deliverable 3.1
  - Description of the constitutive models available at the start of the project. Conceptual bases, mathematical description and model capabilities and shortcomings.
  - Month of delivery: 9
- Deliverable 3.2
  - Description of improved constitutive models and their implementation and verification.
  - Month of delivery: 27
- Deliverable 3.3
  - Description of the constitutive models developed in the project. Conceptual bases, mathematical description and model capabilities. Assessment of predictive power.
  - Month of delivery: 46.

WP3: Deliverables and meetings

Meetings

- WP3 meetings will be held jointly with WP5 meetings
- Main objectives
  - Presentation and critical discussion of the new model features.
  - Performance of the numerical implementation of the models
  - Validation and verification of the models using the laboratory and in situ tests of WP5
- Most meetings held in conjunction with the project's annual meeting

Meeting schedule			
1	First meeting WP3 (end of WP2)	M6	
2	Intermediate meeting Task 3.1	M13	1 A.M.
3	Final Meeting task 3.1 /Intermediate meeting Tasks 3.2.1 and 3.2.2	M24	2 A.M.
4	Final Meeting task 3.2.1 /Intermediate meeting Task 3.2.2. and 3.3	M35	3 A.M.
5	Final Meeting task 3.2.2/Intermediate meeting Task 3.3	M41	
6	Final Meeting WP3	M46	4 A.M.

WP3: Summary

- A variety of modelling approaches
  - Double porosity models (UPC, CU, ULg, ICL)
  - Hypoplasticity approaches (CTU, CU)
  - Inclusion of hysteresis (ClayTech),
  - Consideration of non-isothermal conditions (UPC, Quintessa)
  - Incorporation of chemical effects (EPFL)
  - Advanced coupling features (BGR)
  - Explicit consideration of spatial heterogeneity (GRS, ULg).:

WP3: Summary

- A variety of computer codes
  - Abaqus (ClayTech)
  - CODE_BRIGHT (UPC),
  - Comsol Multiphysics (Clay Tech, LEI)
  - ICFEP (ICL)
  - Lagamine (ULg, EPFL)
  - OpenGeoSys (BGR)
  - QPAC (Quintessa)
  - SIFEL (CTU)
- Good communication and cooperation among the modelling teams essential
- Constant interaction with WP5 (iterative approach)

Acknowledgment

This project receives funding from the Euratom research and training programme 2014-2018 under grant agreement No 745942