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Safety of Nuclear Waste Disposal
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Supplement of

Methodology of structured development and validation of multiphysical constitutive models using the example of crushed salt compaction under 3D THM load conditions

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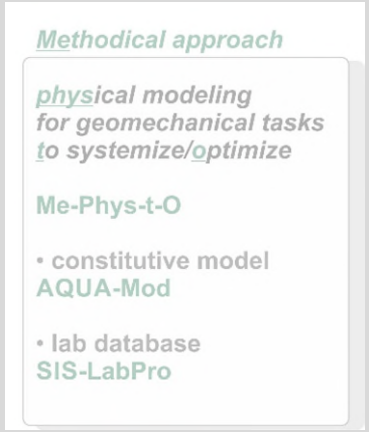
TU Clausthal

safeND Interdisciplinary research symposium on the safety of nuclear disposal practices

Methodology of structured development and validation of multiphysical constitutive models using the example of crushed salt compaction under 3D-THM load conditions



apl. Prof. Dr.-Ing. habil. U. Düsterloh

Dr.-Ing. Svetlana Lerche

Berlin, 10-12.11.2021

1. Methodology for development and validation

   in the framework of physical modeling

2. Demo for the application of the methodology:

   crushed salt behavior

   2.1. Design, creation & analysis of the database:

   TUC-V2

   2.2. Development of the new constitutive model:

   EXPO-COM

3. Summary und Outlook

Methodology for development and validation

What?

Typical task/need:
(Further)-develomment of a numerical equipment

Why?

New areas of application
- **Range of validity**
- **Functionality/influencing factors**
- **Higher quality/realism**

safeND
Interdisciplinary research symposium on the safety of nuclear disposal practices

Methodology for development and validation

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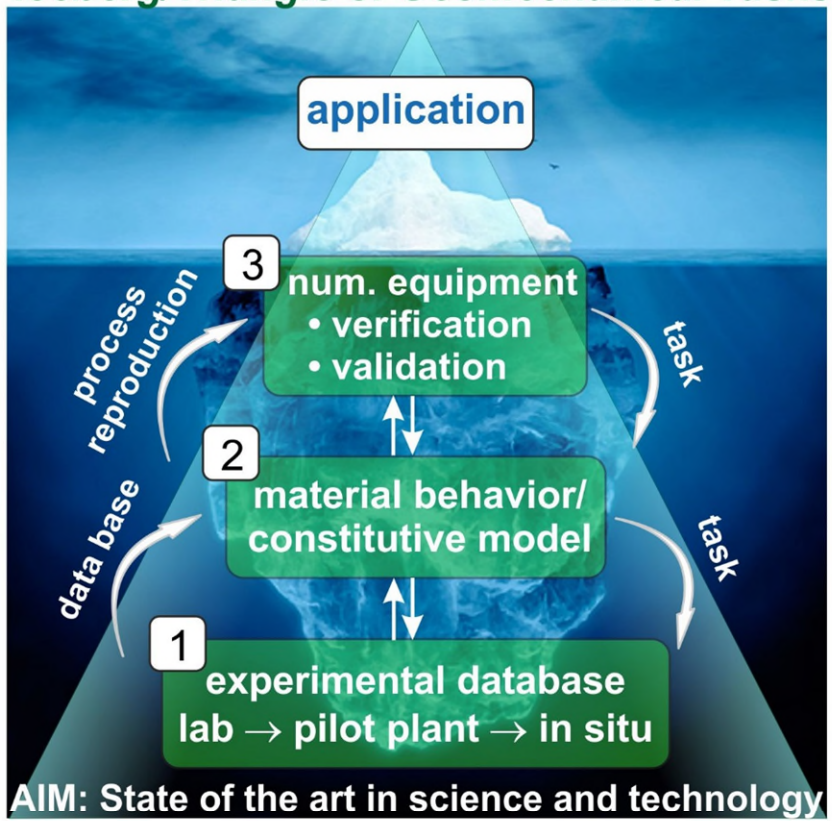
How?

Iceberg/Triangle of Geomechanical Tasks



Methodology for development and validation

safeND Interdisciplinary research symposium on the safety of nuclear disposal practices

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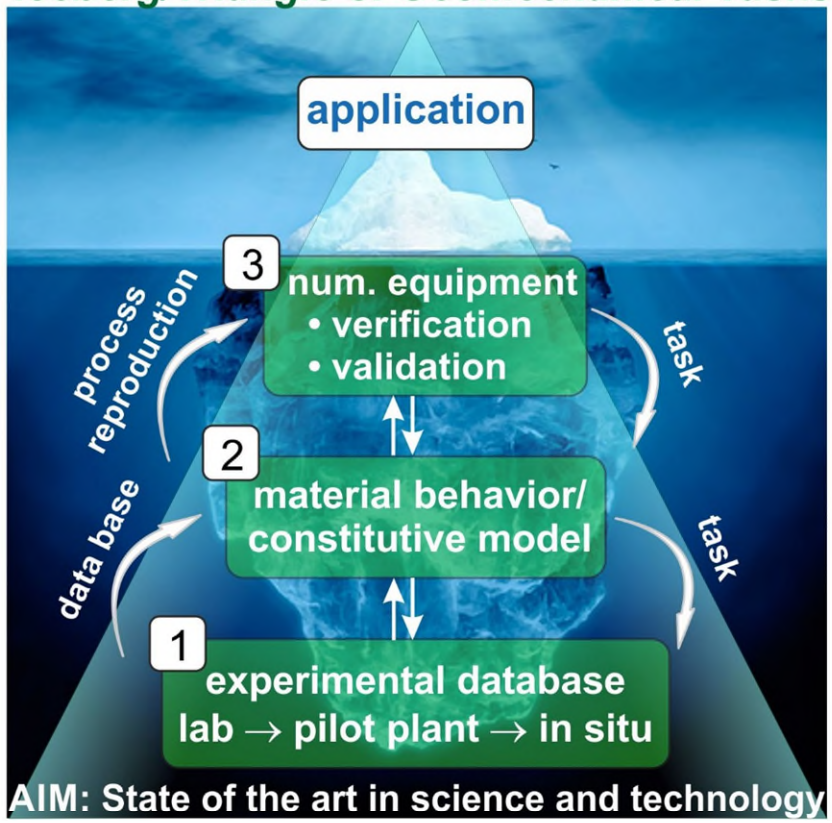


How?

Methodical approach

in the framework of physical modeling for geomechanical tasks/issues to systemize/optimize of the development process
Me-Phys-t-O (TUC)

- Evaluative & comparative analysis
→Structural uniform decomposition

AQUA-Mod

- Design & creation of the database

SIS-LabPro

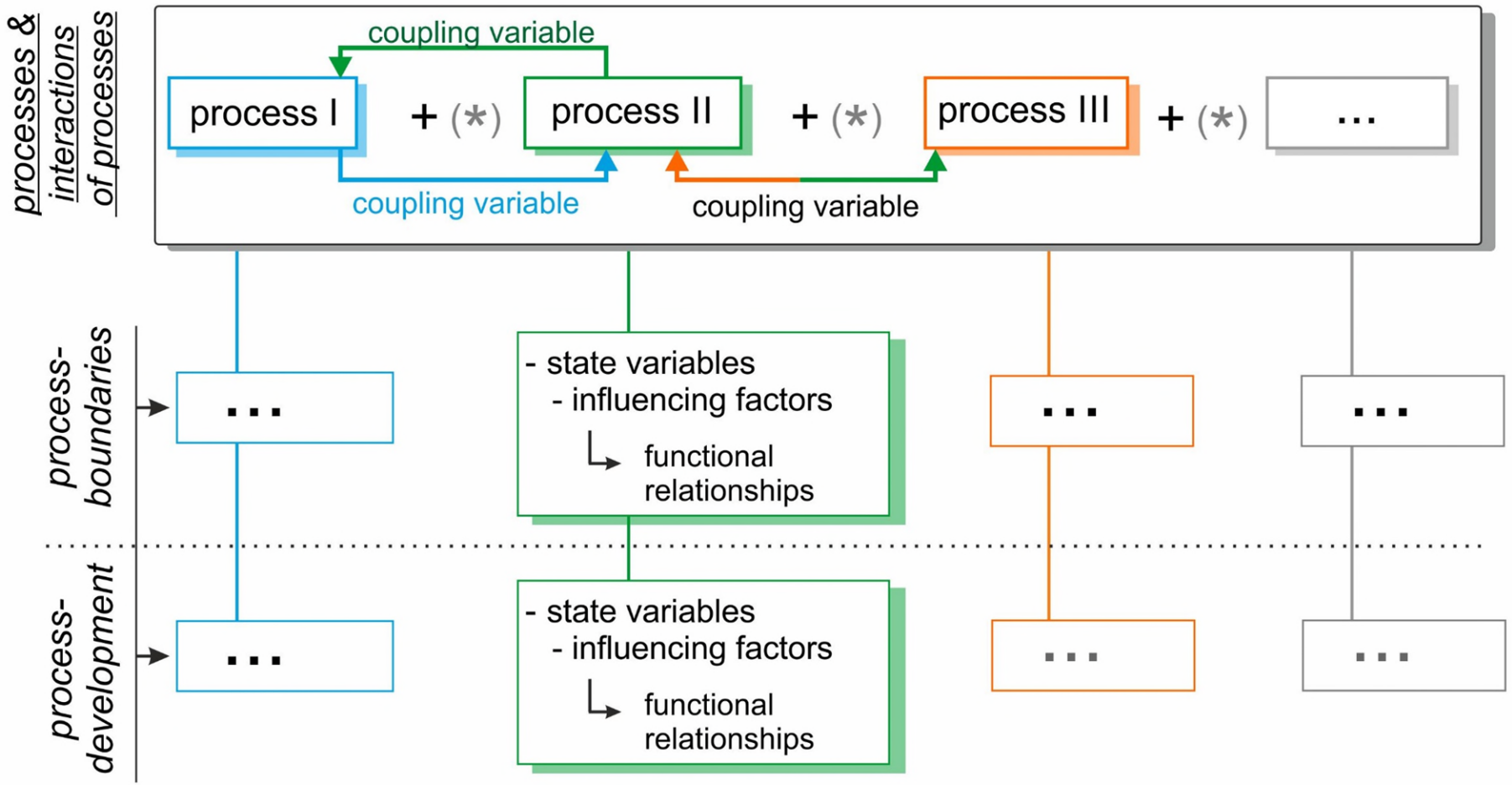
- Analysis of the database
→ Development/validation of the constitutive model

AQUA-Mod

‚AQuA -Mod' → Shema for the Methodology of Unified Comparative and Evaluative Analysis & of (Further) Development for Constitutive Models

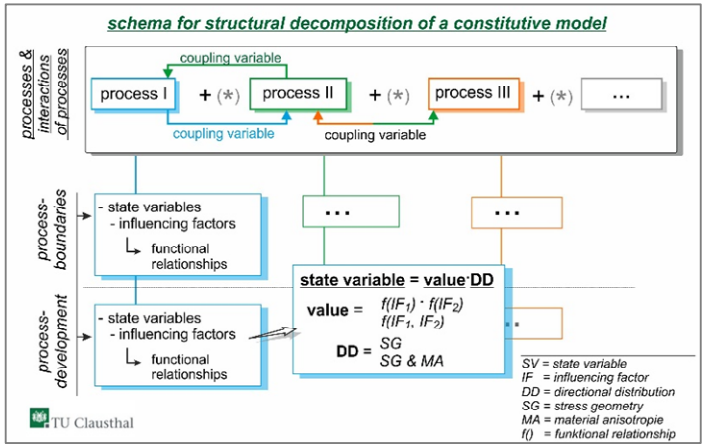
Art of model structure	+	**Quality of model**	⇨	**Areas of application**
▪ statement of grounds/ justification ▪ structure		▪ practicability ▪ plausibility ▪ functionality ▪ realism		areas of validity for ▪ processes ▪ influence factors ▪ outcome variables

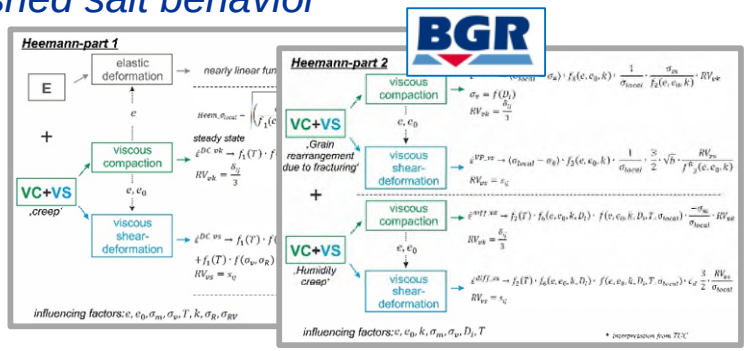
shema for structural decomposition of a constitutive model

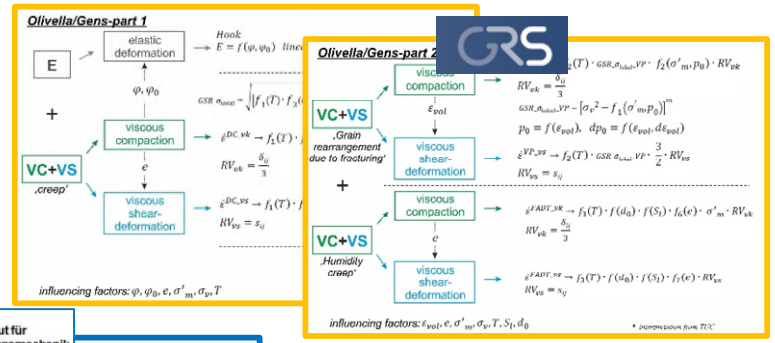


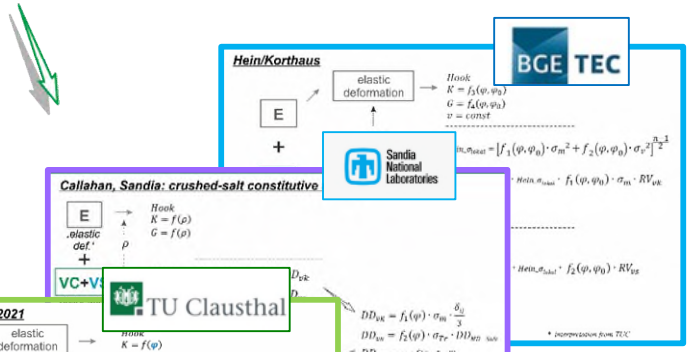
Methodology: example of analysis for constitutive models

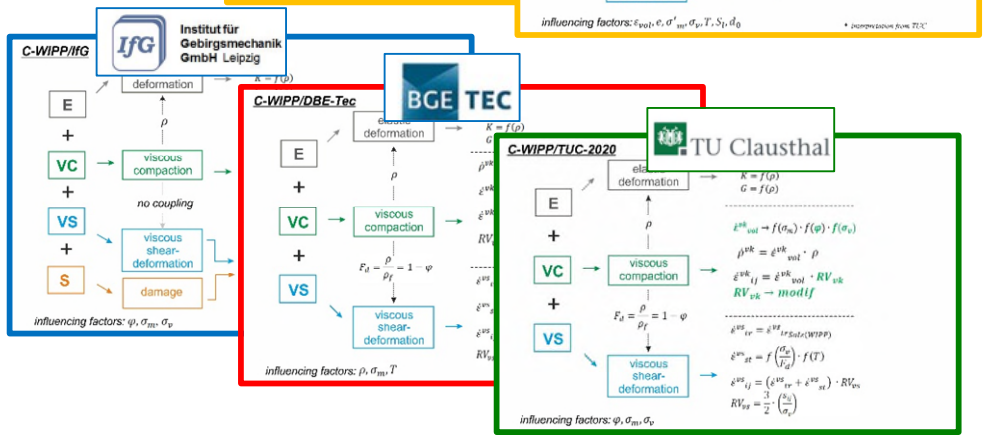
structural decomposition of constitutive models for crushed salt behavior







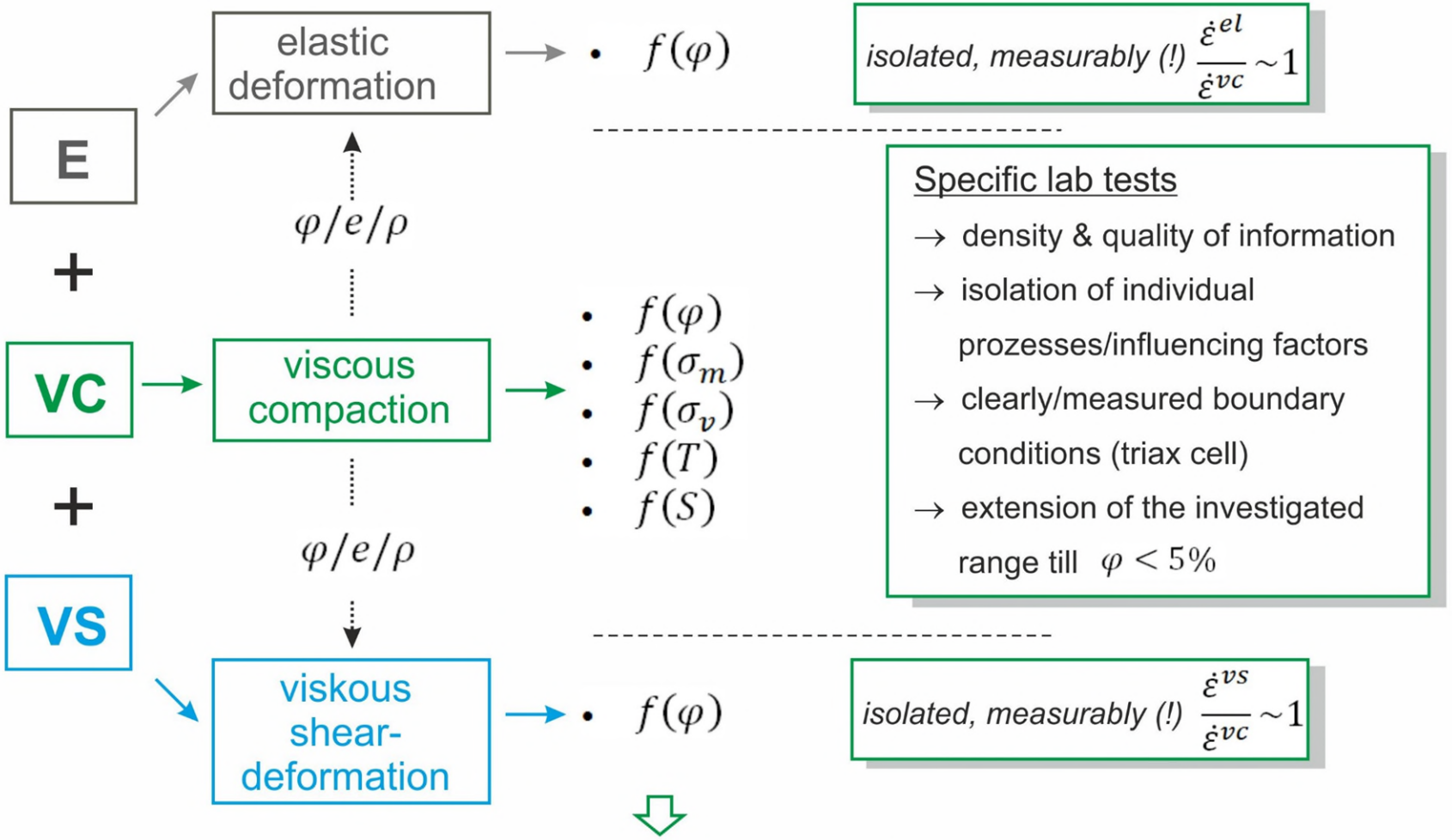




sourses:

- *11th US/German Workshop on Salt Repository Research, Design and Operation, Part 2, 06.2021*
- *KOMPASS I, final report, GRS 608, 09.2020*

crushed salt constitutive models – common investigation need



background for the planning of an extended systematic laboratory program

Methodology: design of lab test program

‚SIS-LabPro‘

shema/guidelines

for optimized design

of the Laboratory Program

→ **Systematics**

- Comparability of tests
- Completeness

→ **Isolability: processes/factors**

- Uniqueness/interpretability
- Exclusion/reduction of scatter

→ **Information density**

- Effort optimization

→ **Structure**

- Prioritization
- Optimized organization/analysis

Methodology: examples for design of lab test program

‚SIS-LabPro‘

shema/guidelines for optimized design of the Laboratory Program

→ **Systematics**
- Comparability of tests
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→ **Isolability: processes/factors**
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→ **Structure**
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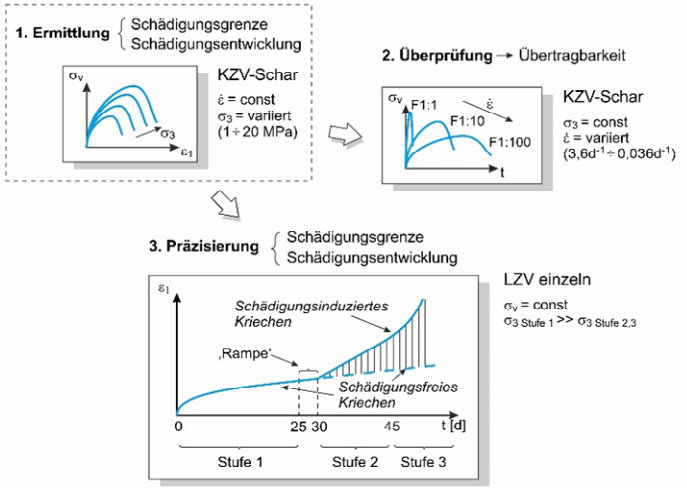
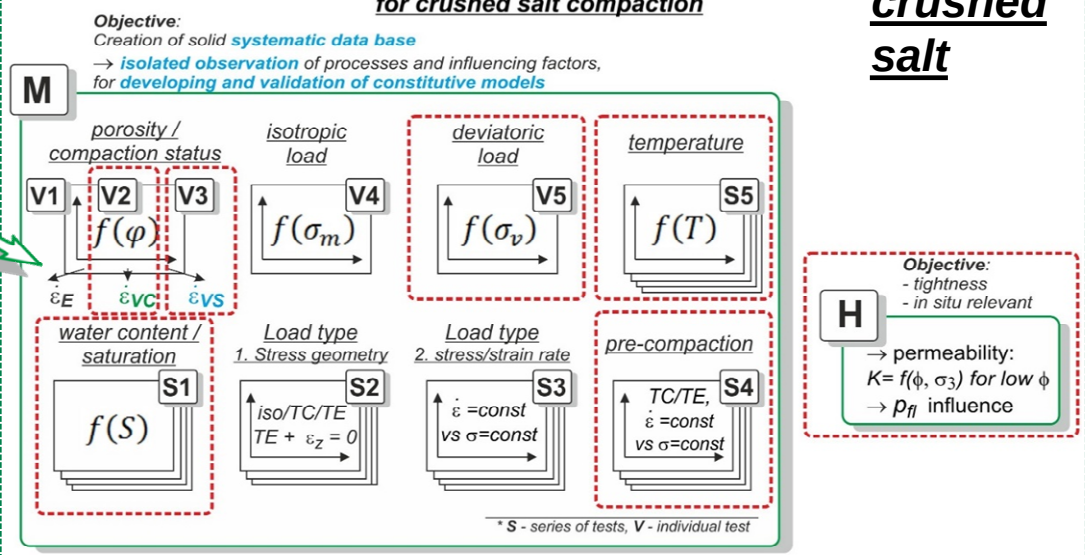
rock salt: damage behavior



source: SALTMECH IX, TUC, Hannover, 09.2018

crushed salt



sources:
- 11th US/German workshop, online, Part 2, 06.2021
- KOMPASS I, final report, GRS 608, 08.2020

Methodology: development of constitutive models

shema/guidelines for optimized design/development of a constitutive model

→ Specifying the model structure

→ Formulation of functional relationships
general considerations

→ Identification of functional relationships
specific detection - lab data related

Methodology: development of constitutive models

shema/guidelines for optimized design/development of a constitutive model

→ **Specifying the model structure**

- Processes
- Influencing factors
- Capability for implementation
- Capability for validation
- Justification (association with microstructural processes/ phenomenological/ reological)

→ **Formulation of functional relationships**
general considerations

- ‚Occam's razor'/principle of minimalism
- Dimensional Analysis → unitless characteristic variables

→ **Identification of functional relationships**
specific detection - lab data related

- Isolation for analysis in individual tests
  of separate processes, influencing factors
  → detection instead of assumptions, instead of curve fitting
- Standardization/scaling for systematic analysis of several tests

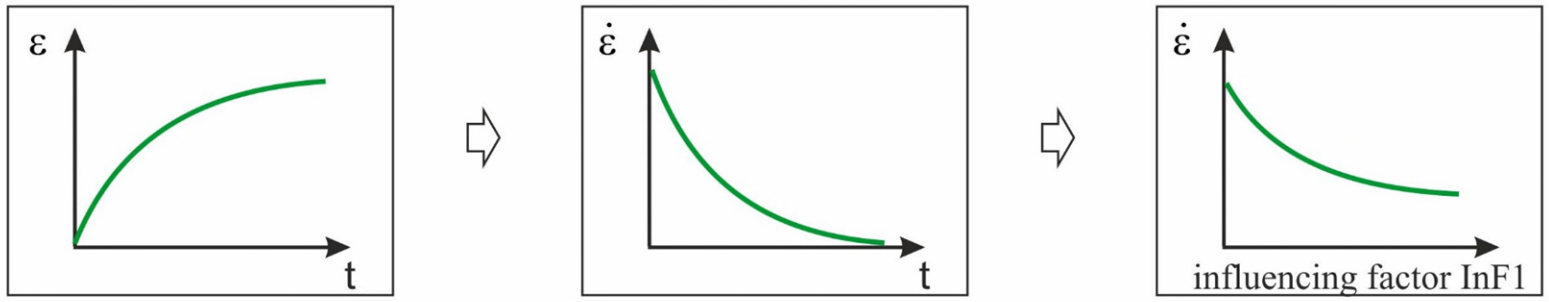
Lab data preparation

independently of the individual constitutive model assumptions

reason: lab $\varepsilon = f(t)$ vs modeling $\dot{\varepsilon} = f(\sigma, \dot{\sigma},...) = f(InF1, InF2, InF3,...)$

isolation

$\varepsilon \rightarrow \dot{\varepsilon}(t) \rightarrow \dot{\varepsilon}(InF)$



ideal for isolation:

→ *InF1 Variation*

→ *Keeping all other factors constant:*
InF2=const, InF3=const, ...
$\dot{\varepsilon} = f(InF1, InF2, InF3,...) = f(InF1)$

→ *low density of information*

- *Lab tests with special BC to avoide/reduce the process overlap*
- *Normalisation of measurement data*
- *Step-by-step procedure for determining of relationships*

* *InF= influencing factor*

Lab data preparation

independently of the individual constitutive model assumptions

reason: possibility of clear cut analysis for indivdual test

→ identification instead of assumtions/curve fitting

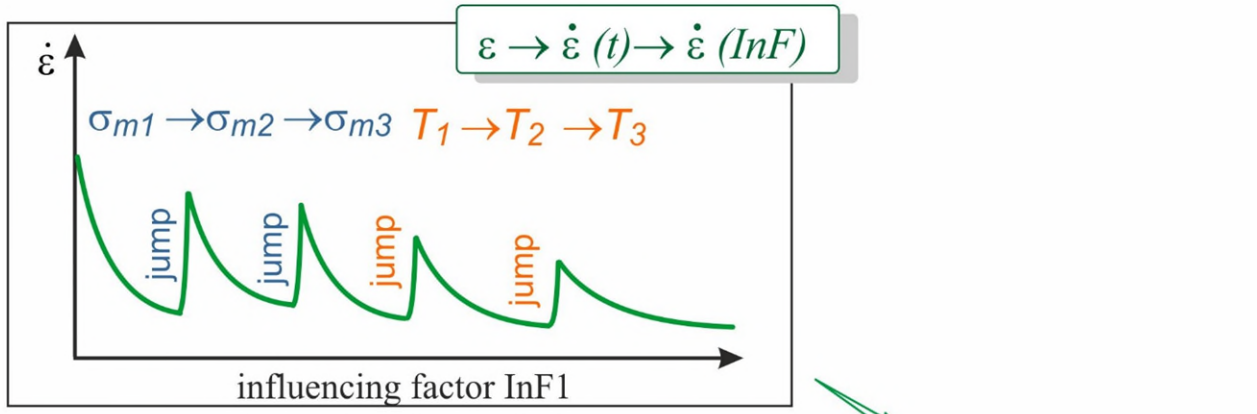
normalisation to isolate

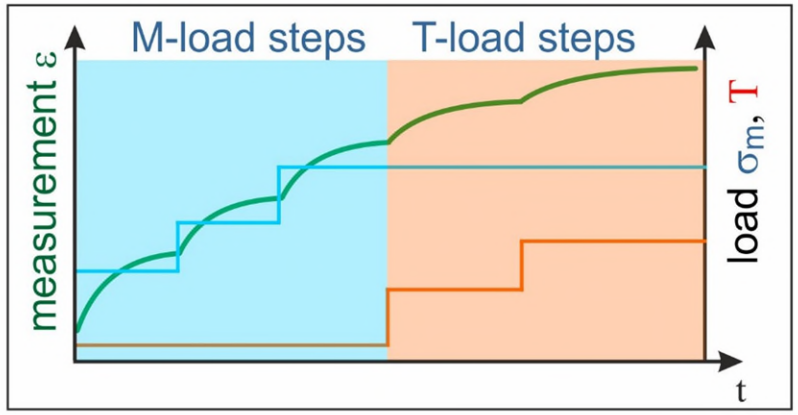
exmaple: isotropic load with σ_m -steps and T-steps

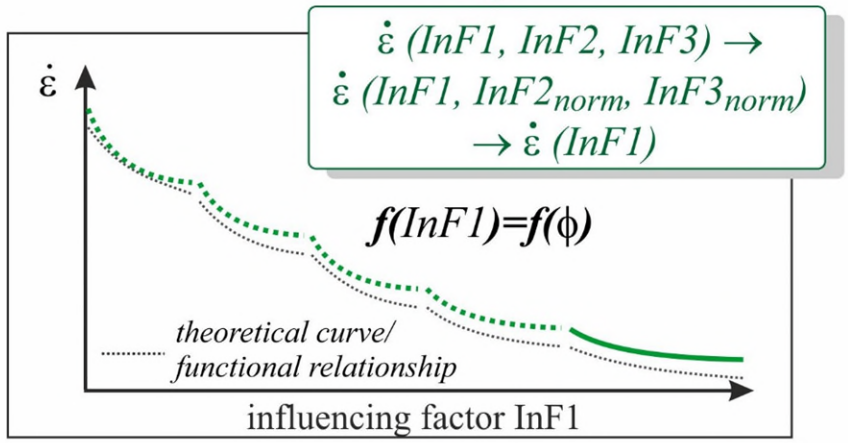
InF1=ϕ

InF2=σ_m

InF3=*T*







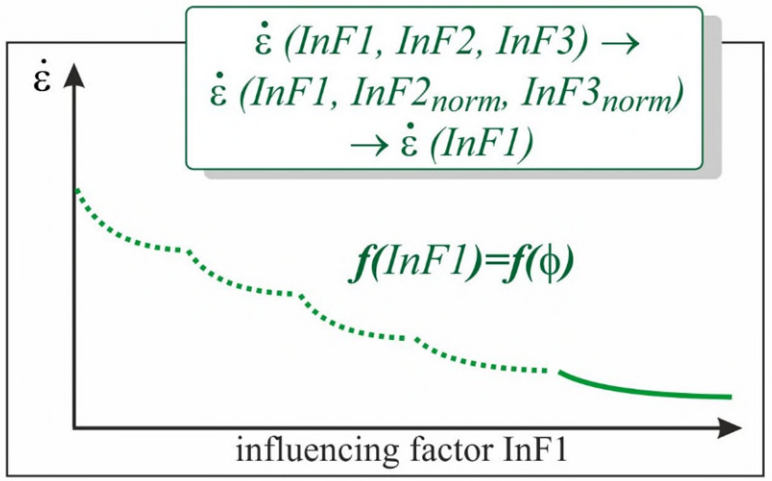
Lab data preparation

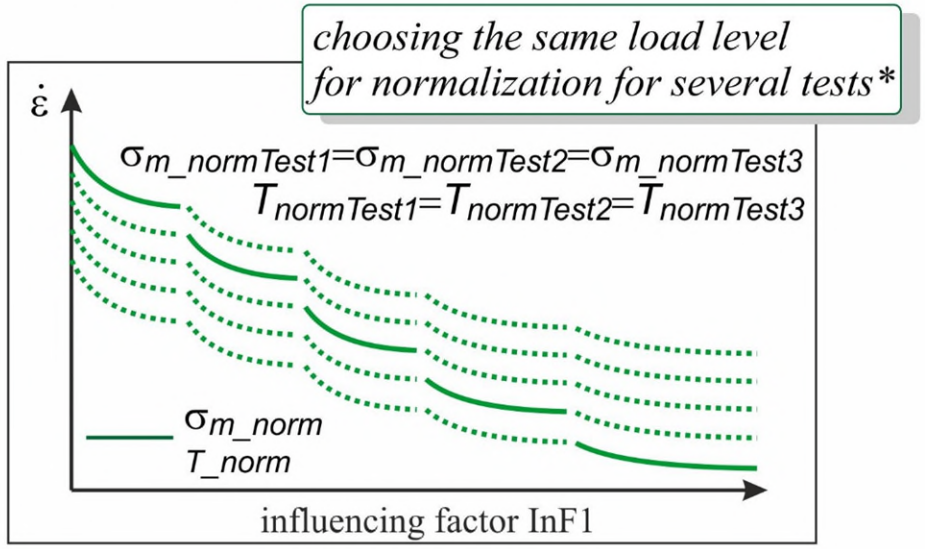
independently of the individual constitutive model assumptions

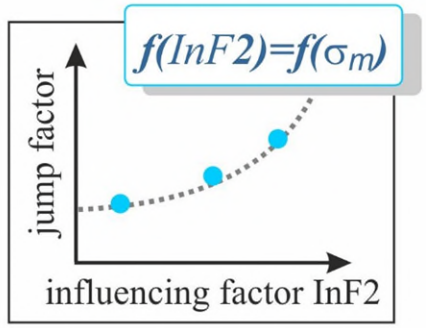
reason: possibility of systematic analysis of several test

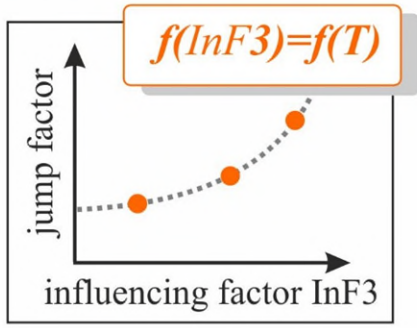
normalisation to isolate
and to compare with another tests
exmaple: isotropic load
with σ_m -steps and T-steps

InF1=ϕ
InF2=σ_m
InF3=*T*









* *if possible/available*

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Lab program designed in the framework of KOMPASS I

TU Clausthal | BGR | IfG Institut für Gebirgsmechanik GmbH Leipzig | GRS

Proposal for extended systematic laboratory program for crush salt compaction

Objective:
Creation of solid systematic data base

Part 1 → isolated observation of processes and influencing factors, for developing and validation of constitutive models (separated functional relationships)

M

porosity / compaction status: V1, V2, V3 — $f(\varphi)$

isotropic load: V4 — $f(\sigma_m)$

deviatoric load: V5 — $f(\sigma_v)$

temperature: S5 — $f(T)$

water content / saturation: S1 — $f(S)$

Load type 1. Stress geometry: S2 — iso/TC/TE, TE + $\varepsilon_z = 0$

Load type 2. stress/strain rate: S3 — $\dot{\varepsilon}$ =const vs σ=const

pre-compaction: S4 — TC/TE, $\dot{\varepsilon}$ =const vs σ=const

* **S** - series of tests, **V** - individual test

P1

Objective: $\phi \leq 1\%$
- in situ relevant
- long term behavior
- not investigated yet: achievable in lab (?!), robust measurably (?!)
- lab benchmark

Part 2

M — V1 — $f(\varphi)$ → BGR, → GRS, → TUC, → IfG

duration t = 1-2years, till $\phi \leq 1\%$

Objective:
- tightness
- in situ relevant

H

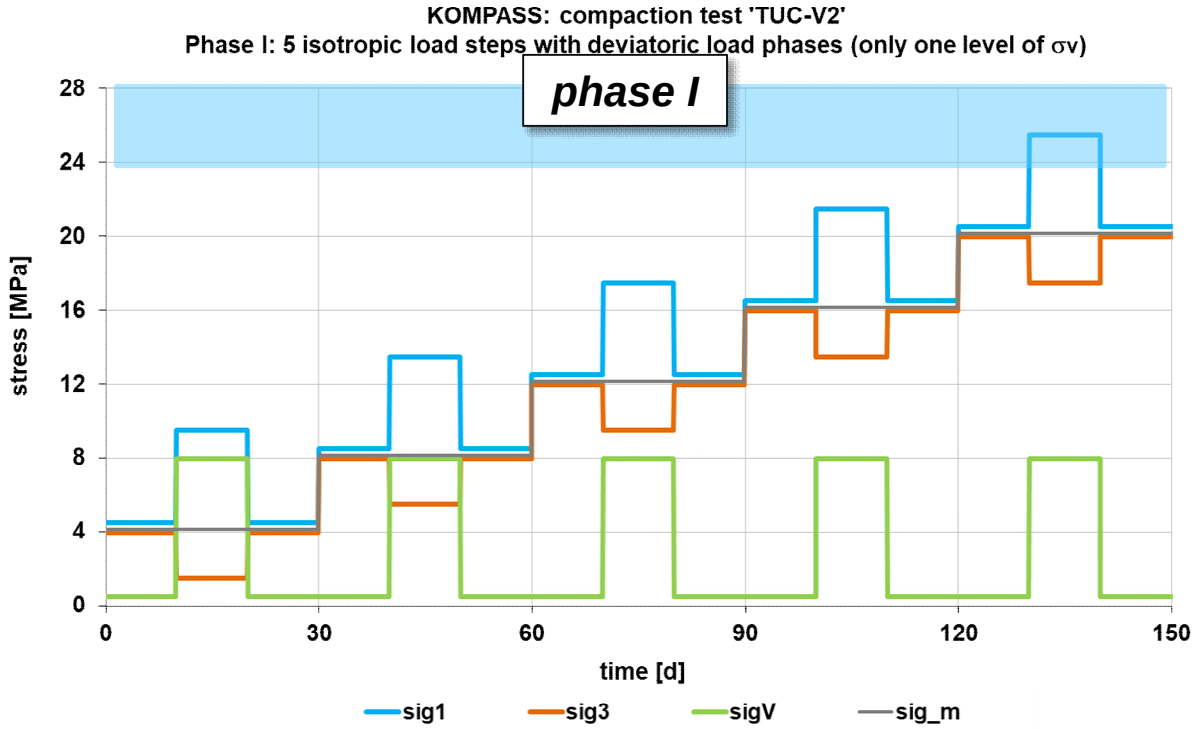
→ permeability: $K = f(\phi, \sigma_3)$ for low ϕ
→ p_{fl} influence

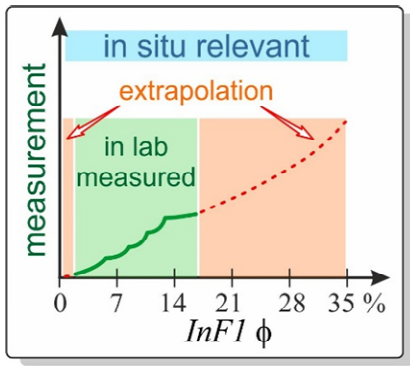
,TUC-V2'

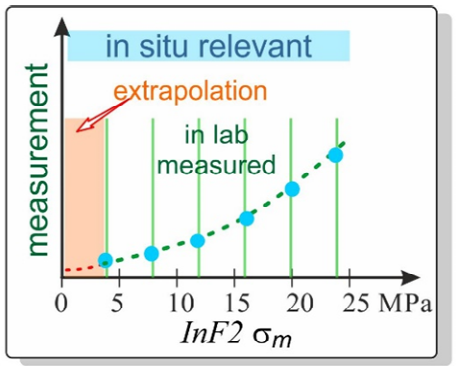
*
P1 = priority 1 – [illegible] significant influence expected, insufficient investigated yet

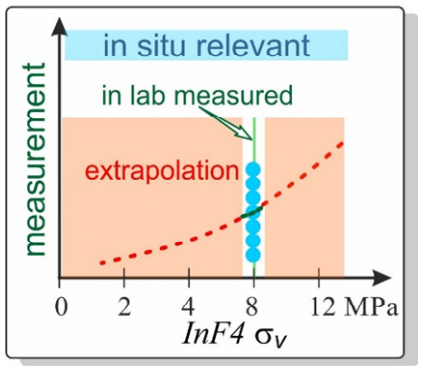
Example for analysis of the database: TUC-V2

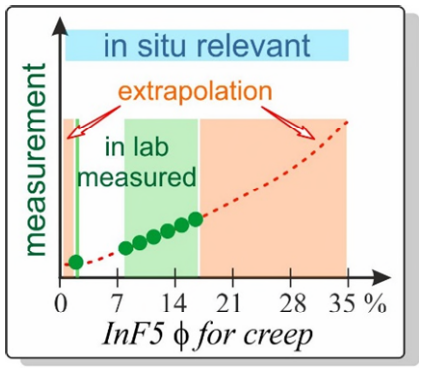
TUC-V2 Phase I: KOMPASS I











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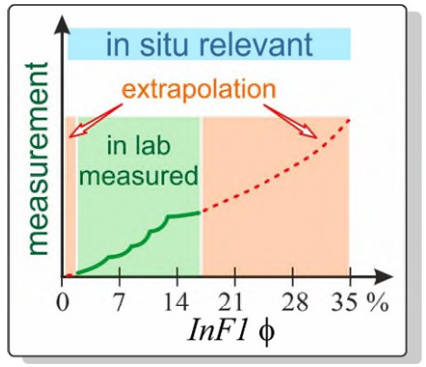
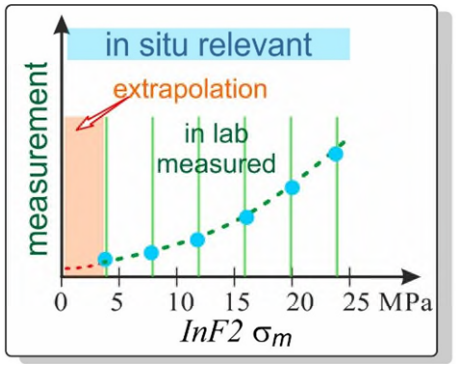
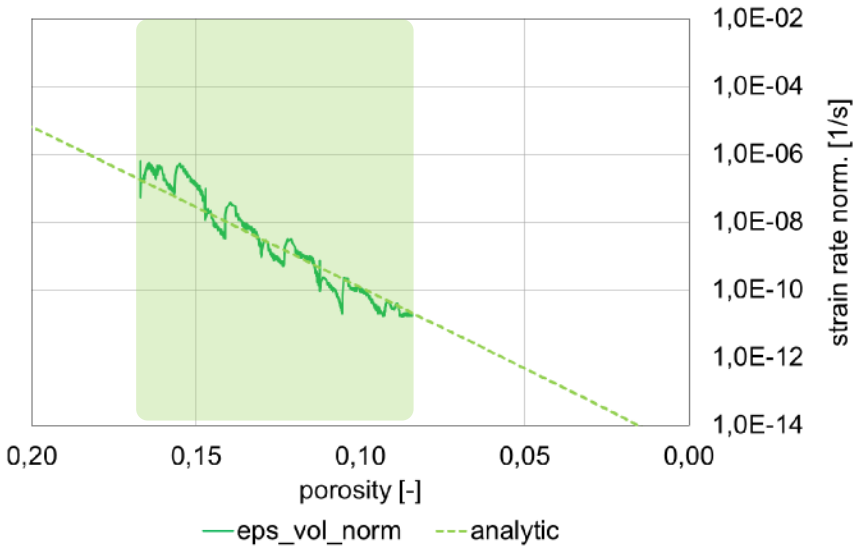
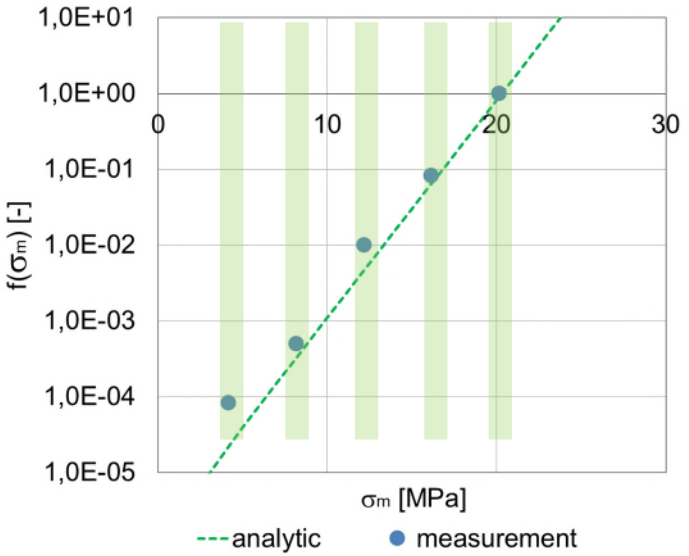


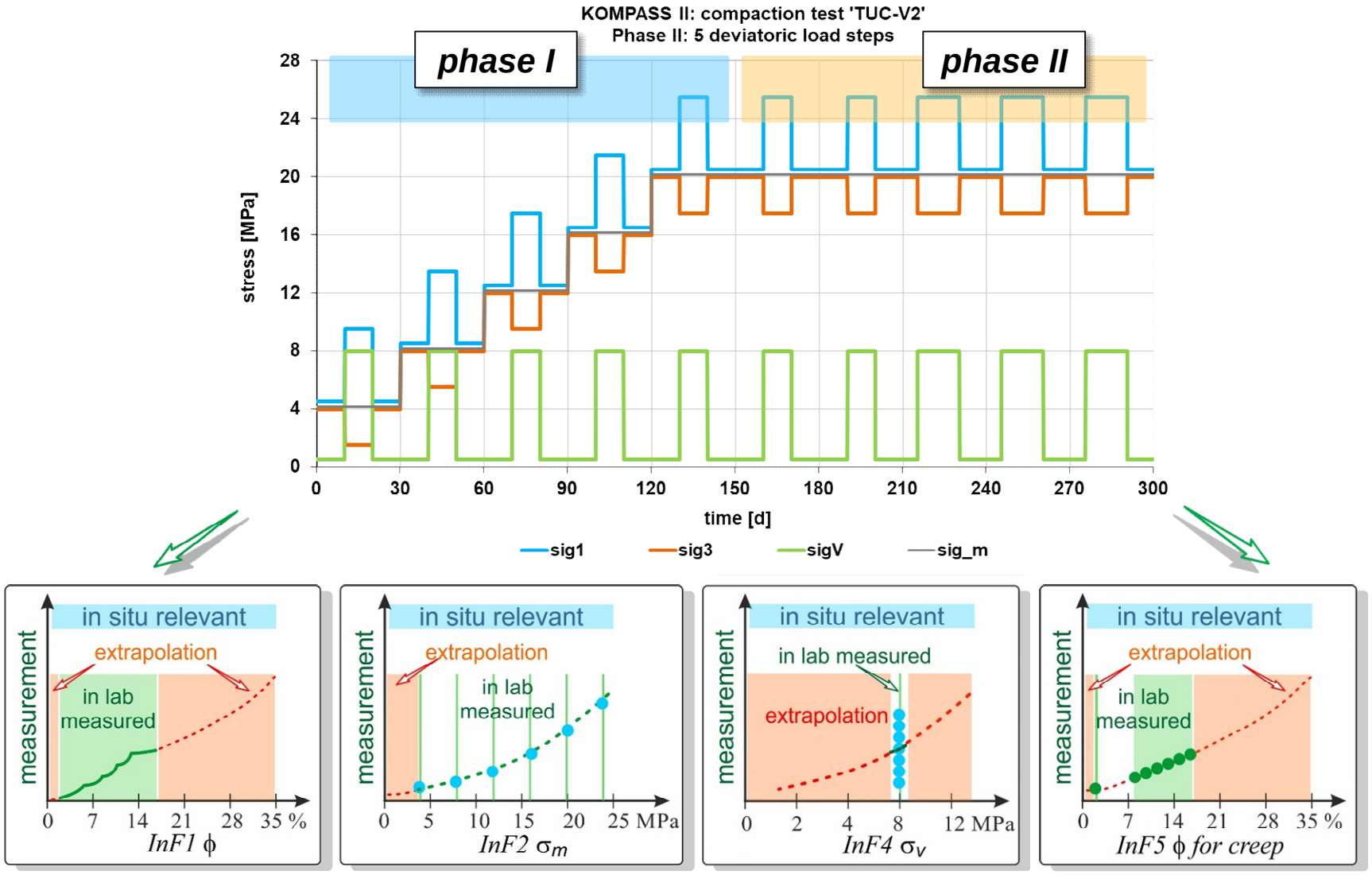






Example for analysis of the database: TUC-V2

TUC-V2 Phase II: KOMPASS II



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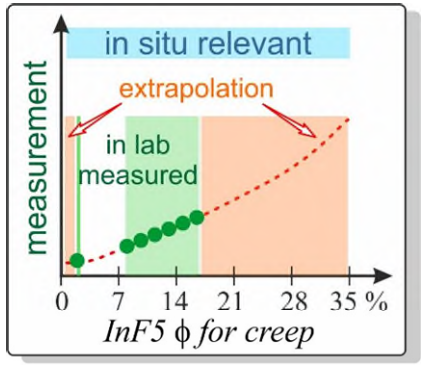
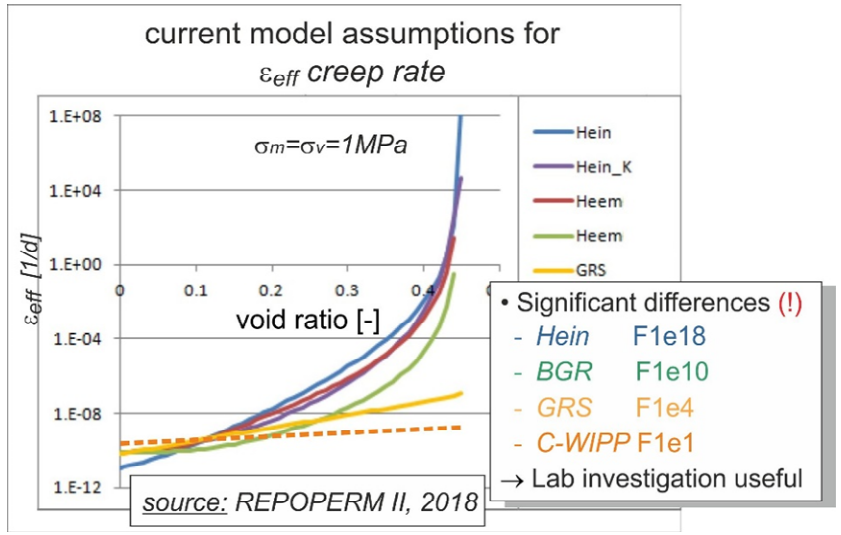
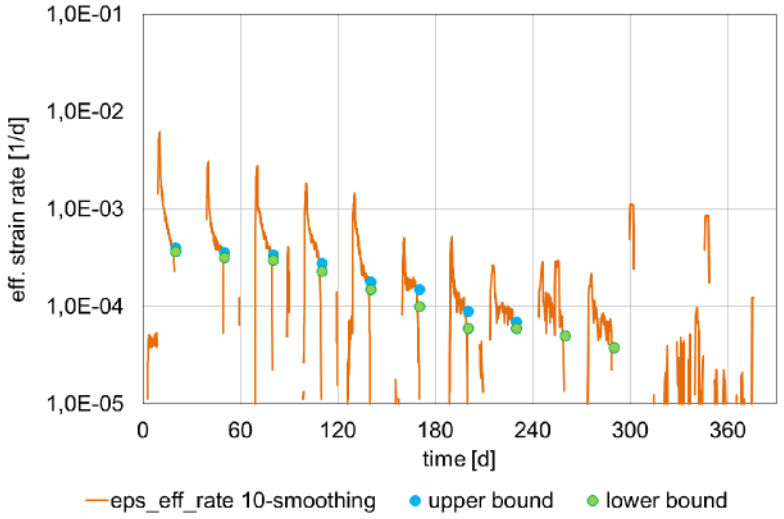
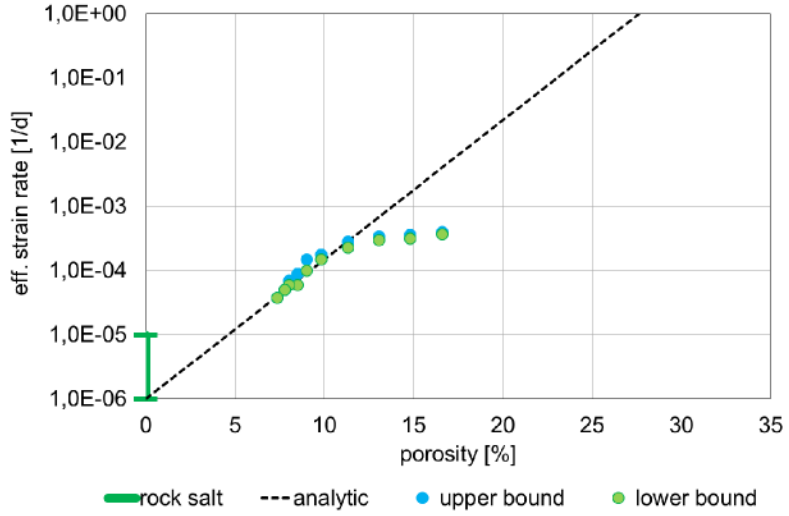
TUC-V2 Phase II: KOMPASS II



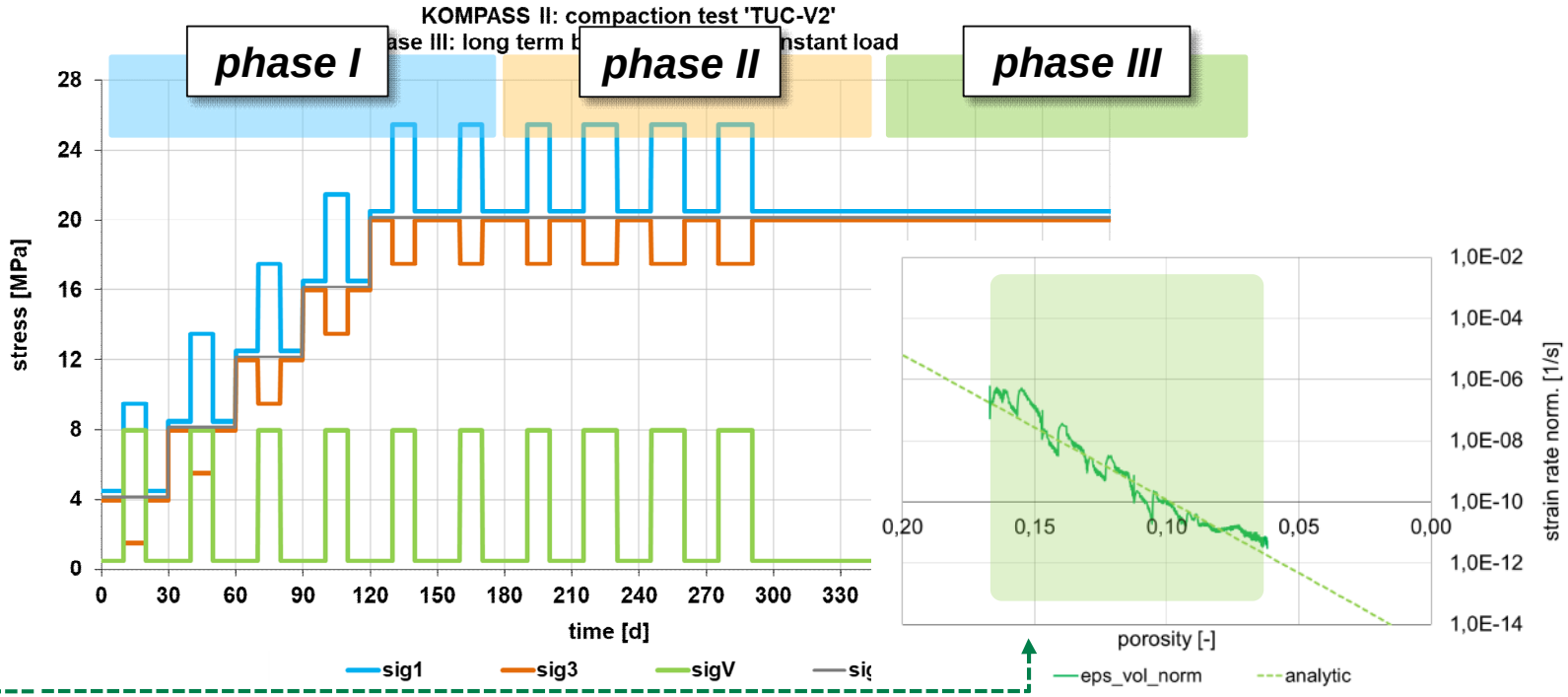


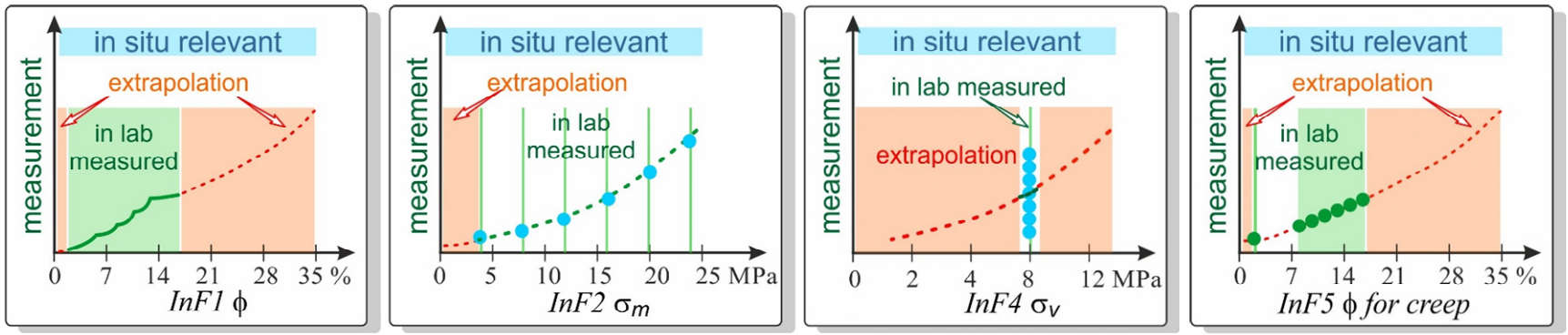




Example for analysis of the database: TUC-V2

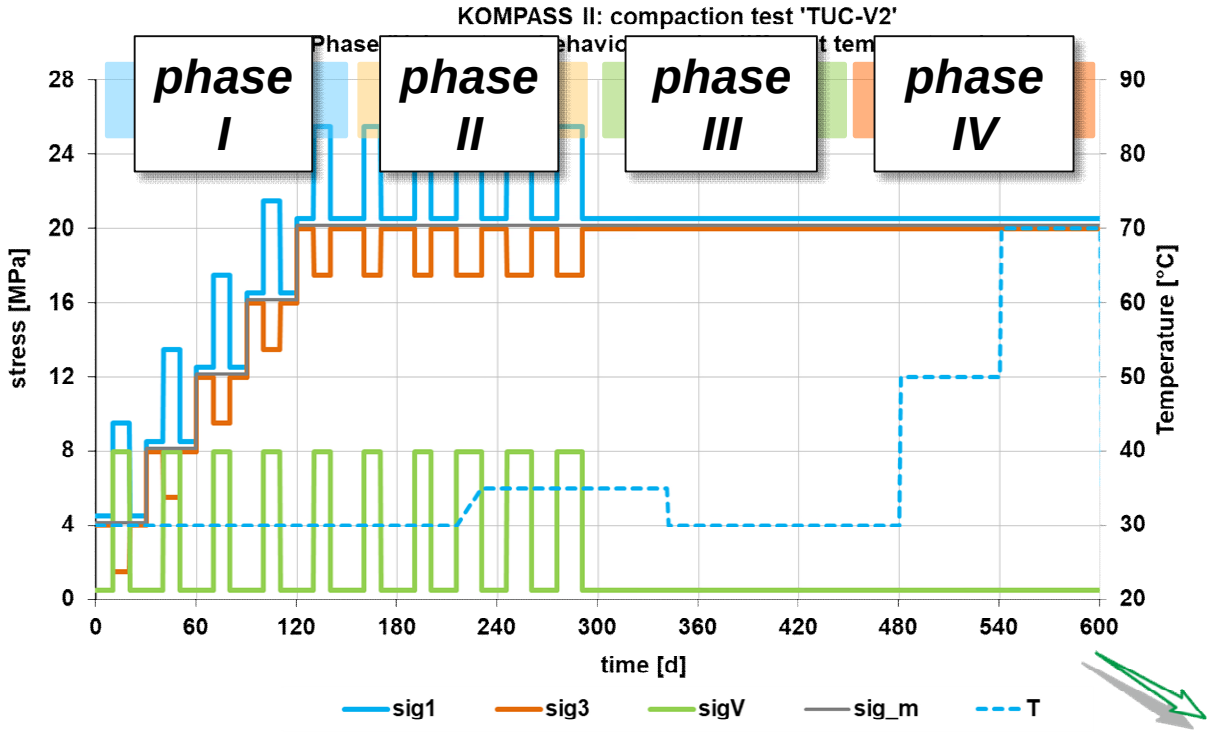
TUC-V2 Phase III: KOMPASS II

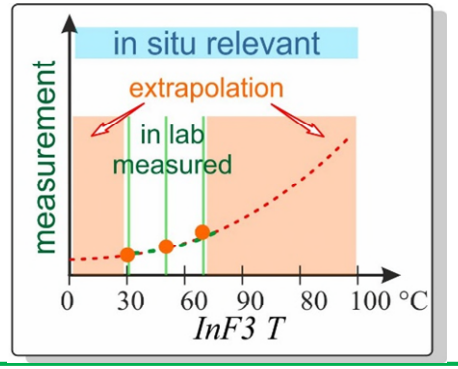




Example for analysis of the database: TUC-V2

TUC-V2 Phase IV & Phase V: KOMPASS II → in ongoing work

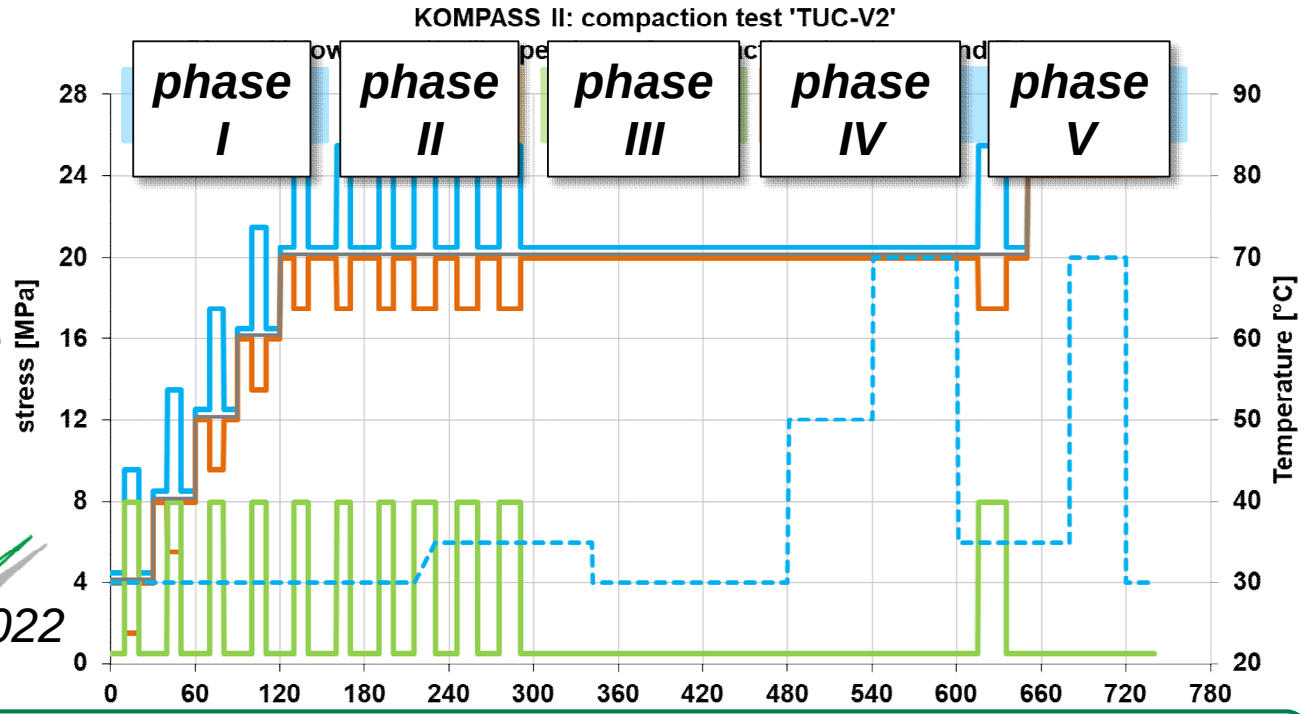


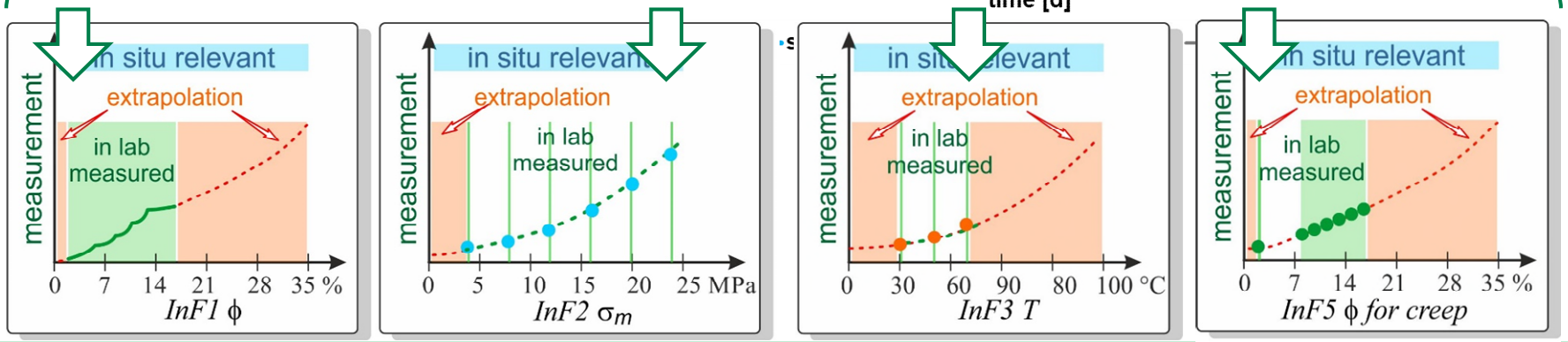


TUC-V2 Phase IV & Phase V: KOMPASS II → in ongoing work

AIM:
Extension of the investigated range
for several influencing factors

More about:
in SALTMECH X, 2022





Interdisciplinary research symposium on the safety of nuclear disposal practices

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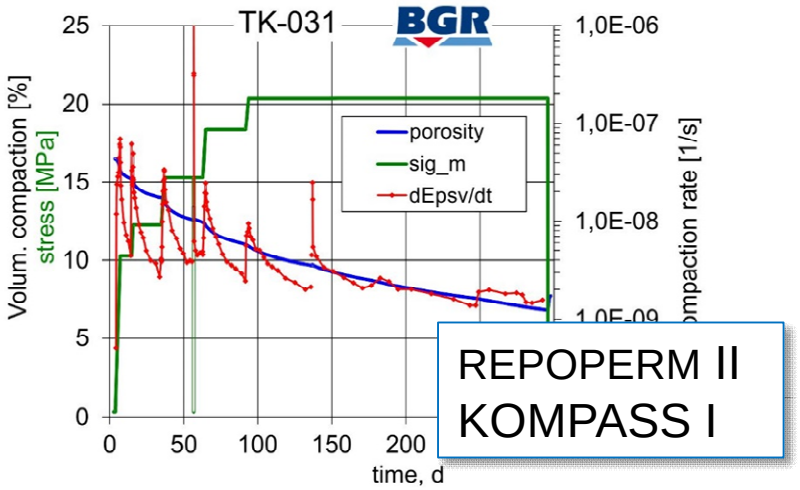
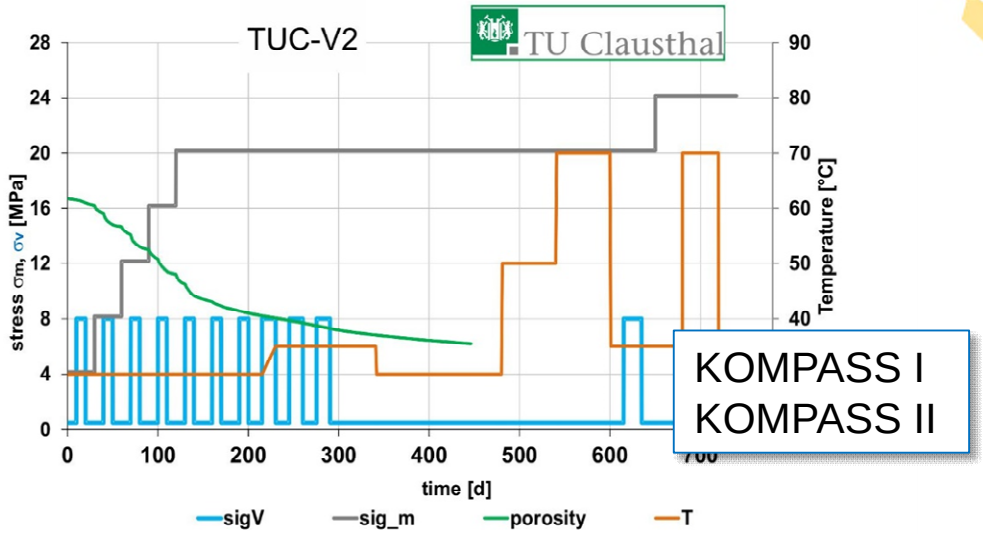
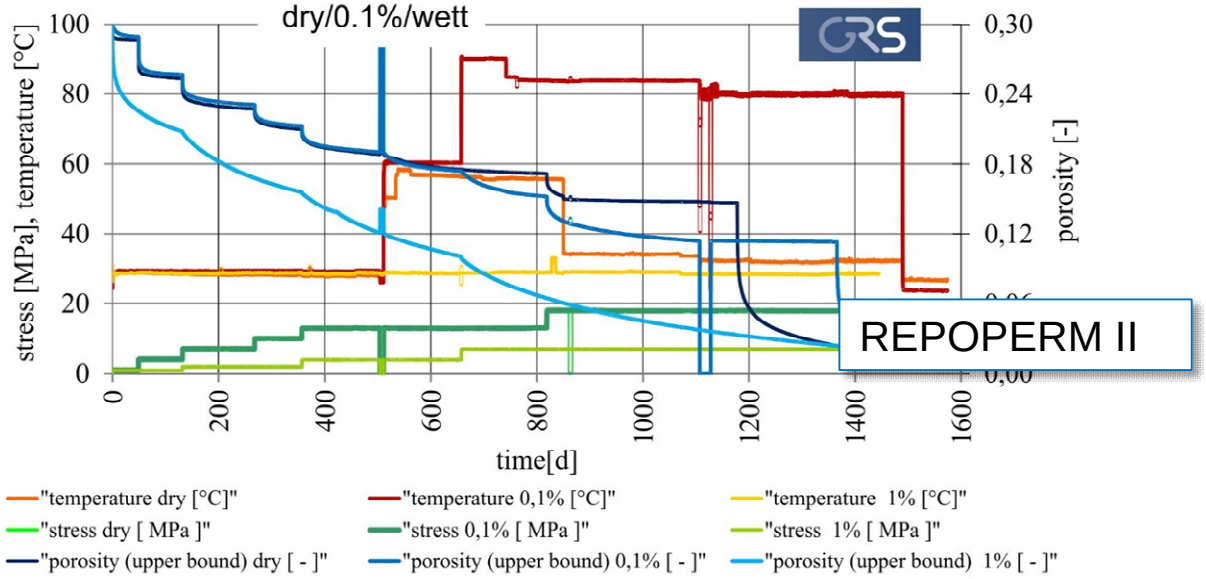
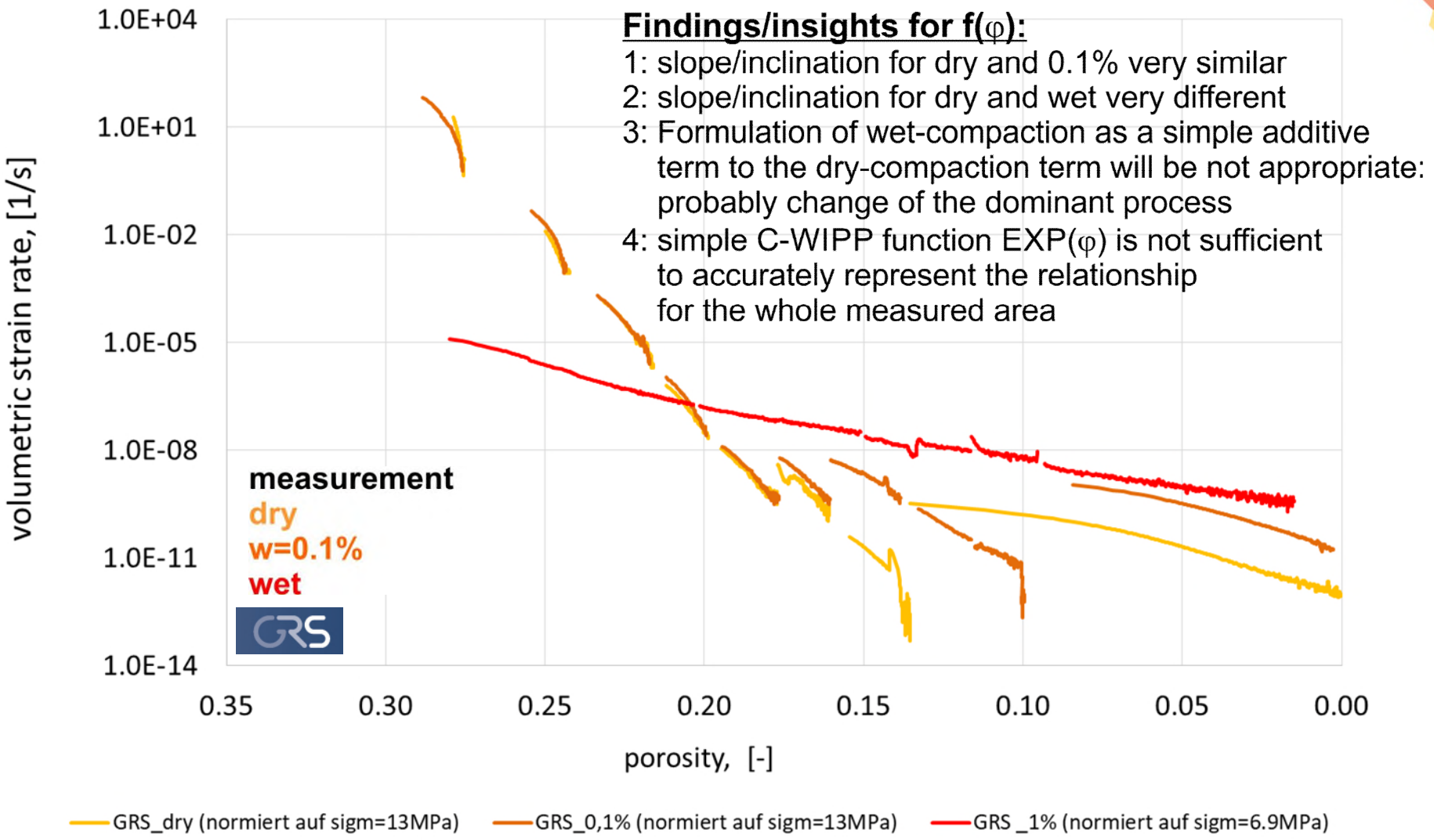
Current database for development of constitutive model





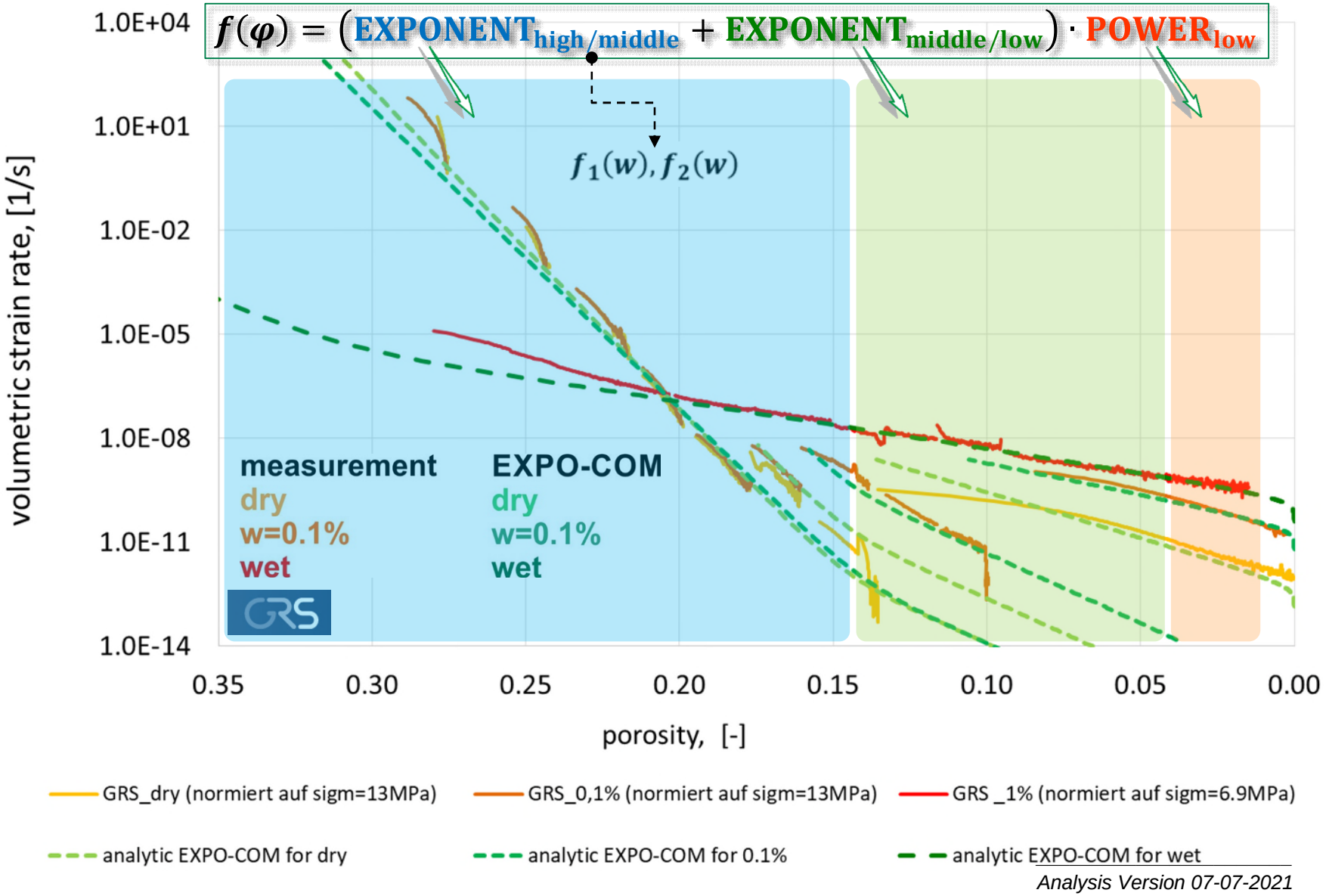


Example for identification of functional relationships: f(porosity)



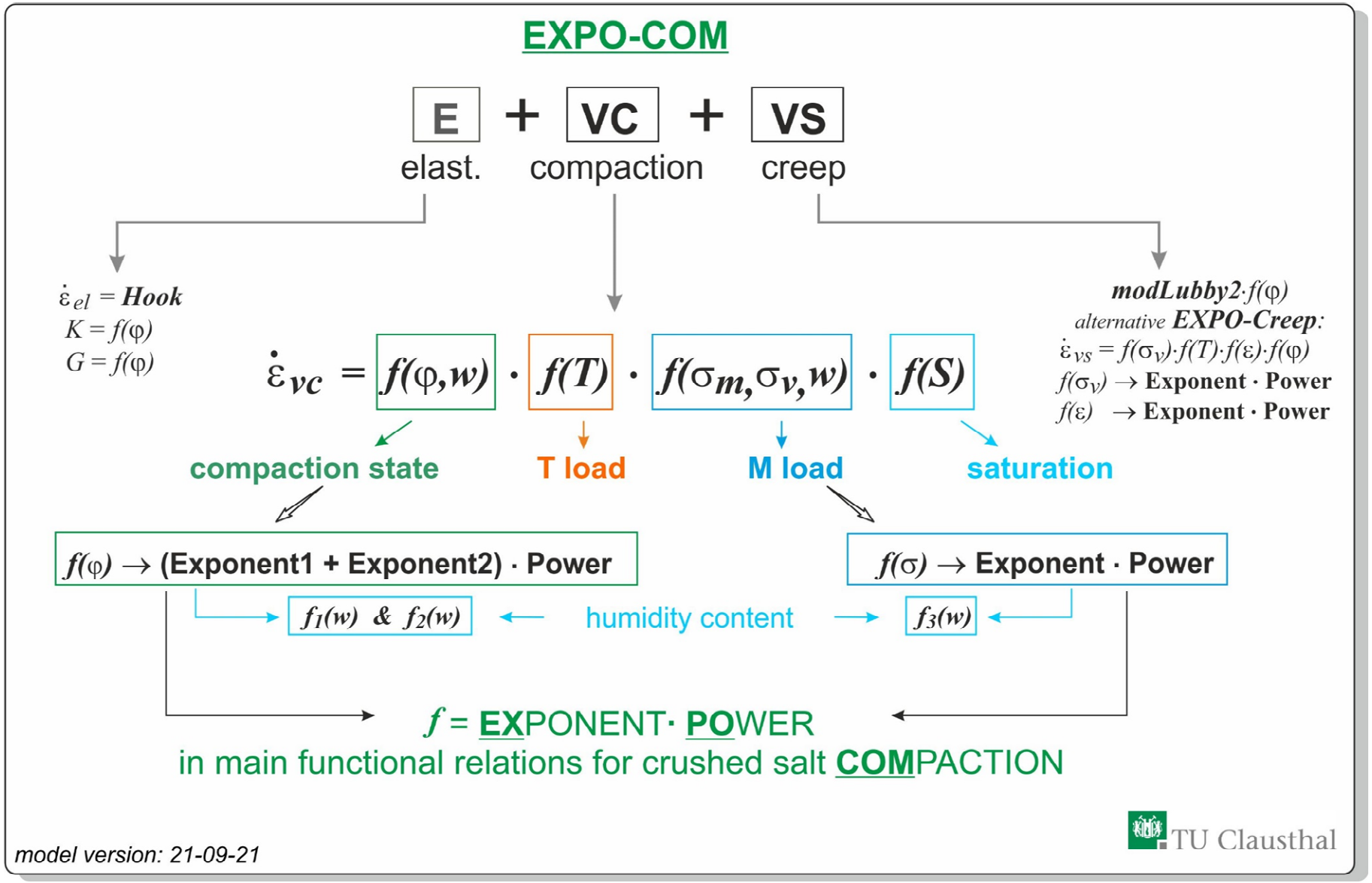
Analysis Version 07-07-2021

Example for identification of functional relationships: f(porosity)



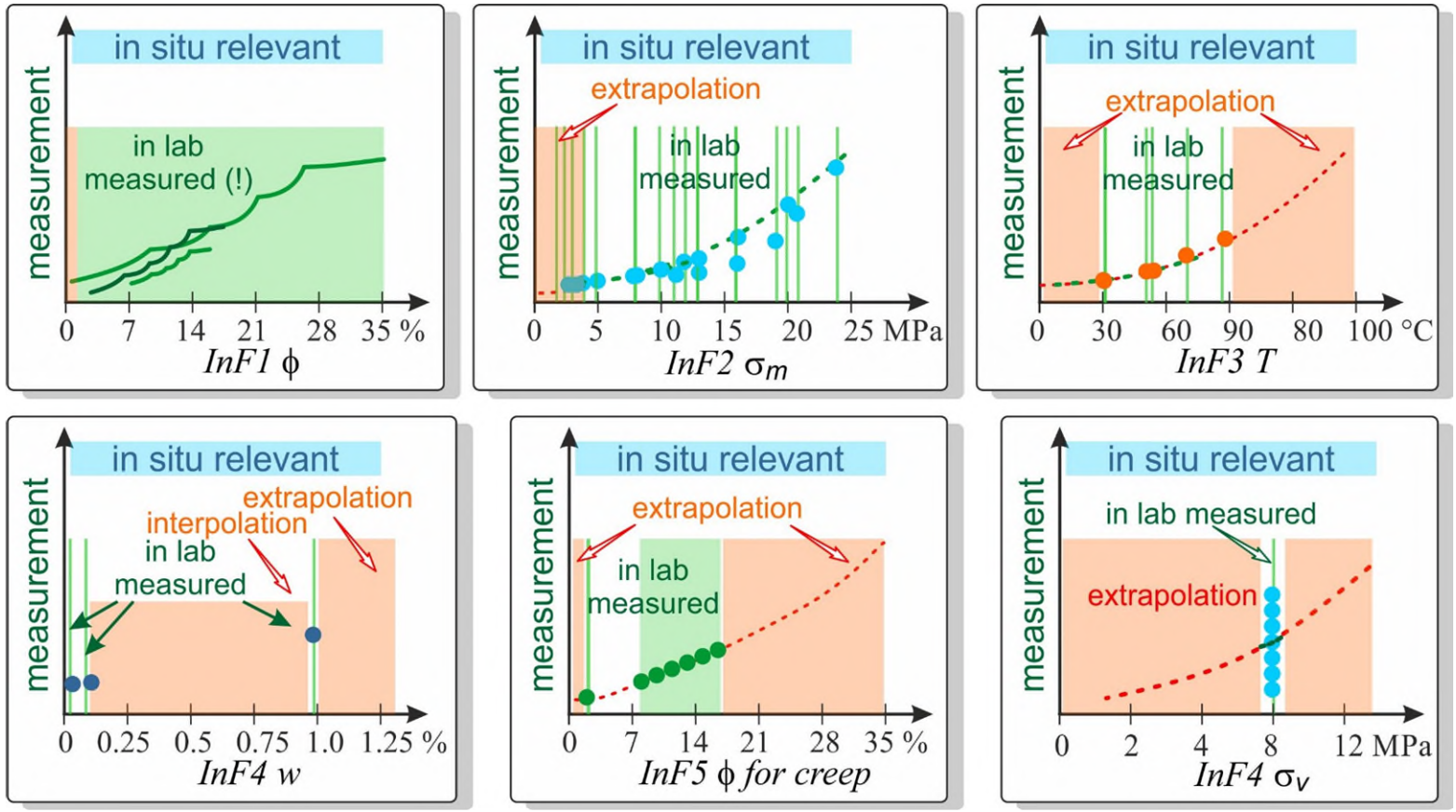
Analysis Version 07-07-2021

New constitutive model EXPO-COM



<u>Validation state</u> → reliability/robustness/realism of statements

- All relevant influencing factors were included
- For each of the factors included, at least one test is available and has been successfully used for development and validation
- Investigated areas for some influencing factors are not yet sufficient
- Number of tests/amount of data base for some influencing factors are not yet sufficient



1. Methodology for development and validation

   in the framework of physical modeling

2. Demo for the application of the methodology:

   crushed salt behavior

   2.1. Design, creation & analysis of the database:

   TUC-V2

   2.2. Development of the new constitutive model:

   EXPO-COM

3. Summary und Outlook

Summary and Outlook

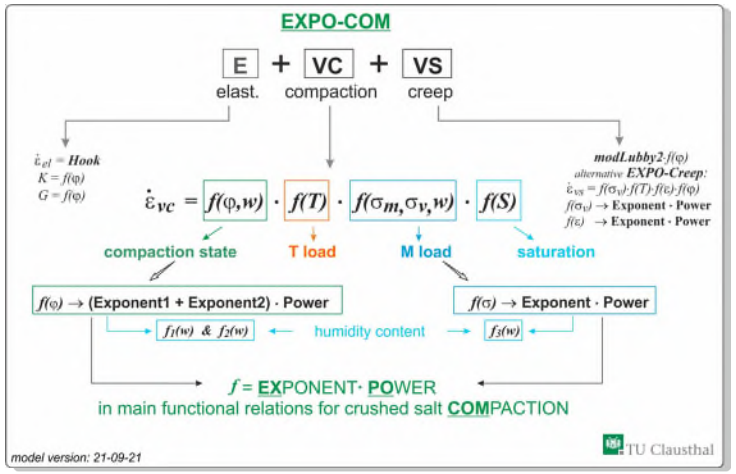
Methodology

Methodical approach in the framework of physical modeling for geomechanical tasks to systemize/optimize

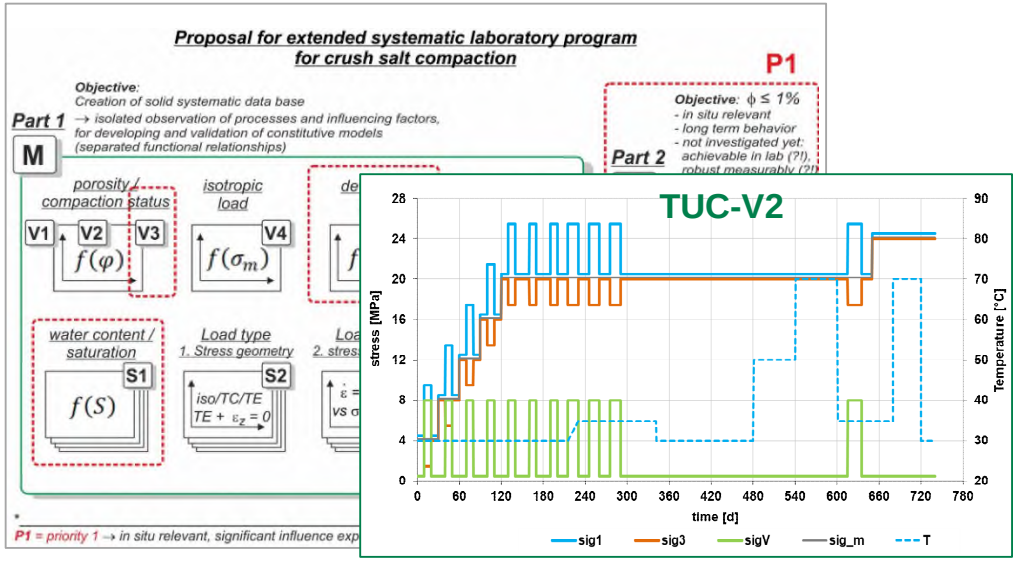
Me-Phys-t-O

- constitutive model **AQUA-Mod**
- lab database **SIS-LabPro**

Model



Lab



Methodology

→ **Experience** of over 10 years systemized

→ **Field of applications**:

- geogenic materials
- backfill materials in mining and repository research

→ **Further development**: correlation to microstructural processes

Lab

- Program is designed
- Realization:
  → **ongoing work**

Model

- Basis/framework is set
- Further development and validation:
  → **ongoing work**

more about in

- KOMPASS II
- Saltmech X, 2022

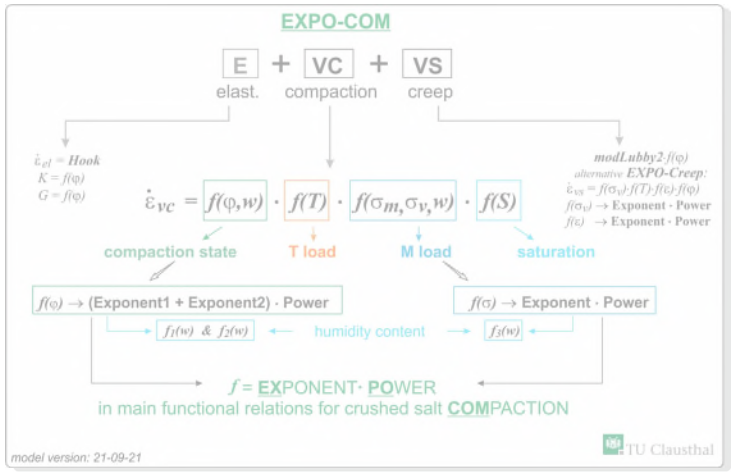
Methodology

Methodical approach in the framework of physical modeling for geomechanical tasks to systemize/optimize

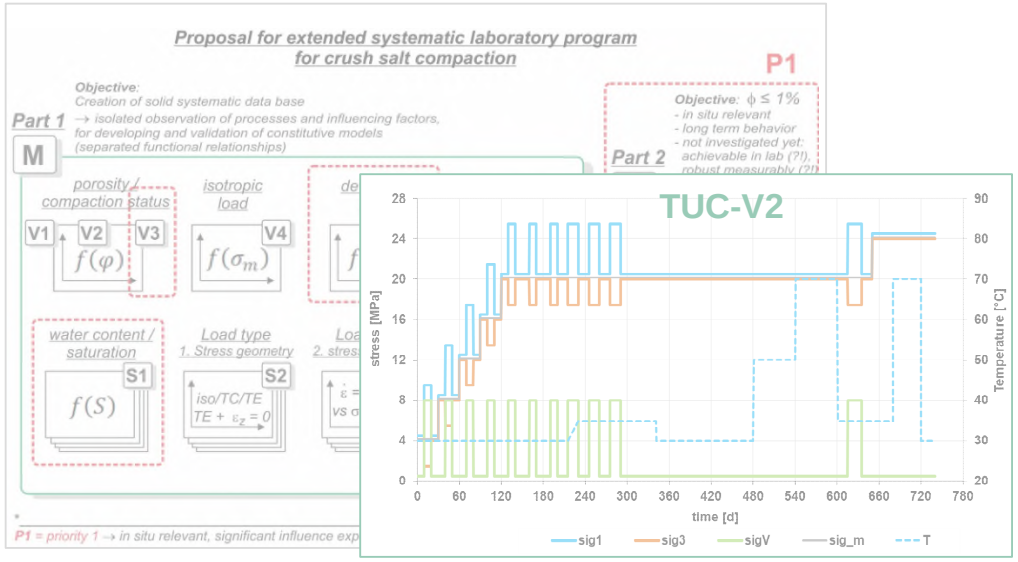
Me-Phys-t-O

- constitutive model AQUA-Mod
- lab database SIS-LabPro

Model



Lab



Thank you for your attention