Computers and Structures 182 (2017) 87–103

Contents lists available at ScienceDirect

Computers and Structures

journal homepage: www.elsevier.com/locate/compstruc

# Implicit numerical integration and consistent linearization of inelastic constitutive models of rock salt

Thomas Nagel [a,b,*], Wolfgang Minkley [c], Norbert Böttcher [a,d], Dmitri Naumov [e,a], Uwe-Jens Görke [a], Olaf Kolditz [a,f]

[a] Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany
[b] Trinity College Dublin, Dublin, Ireland
[c] Institut für Gebirgsmechanik GmbH, Leipzig, Germany
[d] Federal Institute for Geosciences and Natural Resources, Hannover, Germany
[e] Leipzig University of Applied Sciences, Leipzig, Germany
[f] Technische Universität Dresden, Dresden, Germany

ARTICLE INFO

*Article history:*
Received 25 July 2016
Accepted 17 November 2016

*Keywords:*
Host rock material
Viscoplastic material
Finite elements
Thermomechanics
Implicit scheme
OpenGeoSys

ABSTRACT

The mechanical behavior of rock salt formations is not only of interest due to mining of salt but also because of its increasing relevance for geotechnical applications, e.g., for the storage of strategic oil and gas reserves, for hosting nuclear waste repositories, for compressed air energy storage (CAES) or the cavern storage of hydrogen. The safety assessment of geotechnical installations as well as long-term convergence predictions of salt caverns require models capturing the inelastic behavior of rock salt under thermomechanical loading. Many models have been derived for uniaxial or triaxial experimental setups and some are inadequately presented to fully describe three-dimensional scenarios. Here, a tensorial representation is chosen to avoid such inconsistencies and their possible consequences on commonly used material parameters are discussed. Two very commonly used material models, the LUBBY2 and Minkley formulations, have been primarily implemented into software relying on explicit time integration schemes. Here, their implicit implementation with analytical Jacobians into a scientific open-source finite element framework is described in detail. The implementations are verified by comparison to suitable analytical solutions for coupled thermomechanical loadings and their convergence behavior is analyzed.



## 1. Introduction

The mechanical behavior of rock salt formations is not only of interest due to mining of salt but also because of the increasing use for geotechnical applications [1]. The tight morphology of rock salt makes it an ideal material for the storage of matter [2,3]. Solution-mined caverns in underground salt domes have been used for the storage of strategic oil and gas reserves for decades. Salt formations are also discussed as candidate formations for hosting nuclear and other waste repositories [4–8]. In the context of the transition to volatile renewable energies, compressed air energy storage (CAES) in salt caverns is discussed to mitigate fluctuations in wind energy for continuous electricity production [9–14]. Finally, the cavern storage of hydrogen as a chemical energy carrier produced electrolytically from renewable energy sources has gained scientific interest [2].

The safety of salt mines as well as the long-term convergence behavior of salt caverns have been assessed based on thermomechanical models of the inelastic behavior of rock salt [5,14–19]. Rock salt is a material exhibiting several modes of creep and plasticity [20,21]. Different, usually viscoplastic, salt models have been developed in the past by various groups of specialists in order to represent the mechanical characteristics of rock salt under laboratory and field conditions [22–29]. Lately, in the context of the novel applications outlined above, an increased and broader interest into the mechanical behavior of rock salt due to a more intense use of the subsurface for energy storage and conversion has developed. These novel applications also shift the focus of the analyses somewhat from the long-term behavior to short-term phenomena induced on the time scale relevant for renewable energy applications [3,7]. For example, while the time scales of pressure changes in caverns used for strategic oil and gas reserves or seasonal energy

* Corresponding author at: Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany.

*E-mail address:* thomas.nagel@ufz.de (T. Nagel).

http://dx.doi.org/10.1016/j.compstruc.2016.11.010
0045-7949/

**Nomenclature**[1]

*Greek symbols*

| | |
|---|---|
| $\alpha_T$ | linear thermal expansion coefficient |
| $\boldsymbol{\epsilon}$, $\boldsymbol{\epsilon}$ | small strain tensor/its Kelvin mapping |
| $\eta$ | shear viscosity |
| $\eta_{\mathrm{vol}}$ | bulk viscosity |
| $\mathrm{d}\Gamma$ | area element |
| $\mathrm{d}\Omega$ | volume element |
| $\Psi^i$ | residual in iteration $i$ |
| $\varrho$ | mass density |
| $\boldsymbol{\sigma}$, $\boldsymbol{\sigma}$ | cauchy stress tensor/its Kelvin mapping |
| $\theta$ | lode angle |

*Operators*

| | |
|---|---|
| $\langle \bullet \rangle$ | McCauley brackets |
| $\boldsymbol{a} \cdot \boldsymbol{b}$ | dot product of $\boldsymbol{a}$ and $\boldsymbol{b}$ |
| $\boldsymbol{A} : \boldsymbol{B}$ | double contraction of $\boldsymbol{A}$ and $\boldsymbol{B}$ |
| $\boldsymbol{a} \otimes \boldsymbol{b}$ | dyadic product of $\boldsymbol{a}$ and $\boldsymbol{b}$ |
| $\boldsymbol{A} \odot \boldsymbol{B}$ | $\frac{1}{2}\left[(\boldsymbol{A} \otimes \boldsymbol{B}^{\mathrm{T}})^{\overset{23}{\mathrm{T}}} + (\boldsymbol{A} \otimes \boldsymbol{B})^{\overset{24}{\mathrm{T}}}\right]$ |
| $\boldsymbol{A} \underline{\odot} \boldsymbol{B}$ | $\frac{1}{2}\left[(\boldsymbol{A} \otimes \boldsymbol{B})^{\overset{23}{\mathrm{T}}} + (\boldsymbol{A} \otimes \boldsymbol{B}^{\mathrm{T}})^{\overset{24}{\mathrm{T}}}\right]$ |
| $(\bullet)^{\mathrm{D}}$ | deviatoric part of a tensor |
| div | divergence operator |
| grad | gradient operator |
| $(\bullet)^{\mathrm{S}}$ | spherical part of a tensor |
| $(\bullet)^{\mathrm{T}}$, $(\bullet)^{\overset{ab}{\mathrm{T}}}$ | transpose operator; transposition of $a$th and $b$th basis vector |

*Roman symbols*

| | |
|---|---|
| $\mathbf{b}$ | external body force |
| $\mathcal{C}$, $\boldsymbol{C}$ | tangent moduli (fourth order tensor/its Kelvin mapping) |
| $\boldsymbol{e}_i$ | Cartesian basis vectors with $\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij}$ |
| $e$ | volume strain |
| $F$ | yield function |
| $G$ | shear modulus |
| $G_{\mathrm{F}}$ | plastic potential |
| $\boldsymbol{I}$ | Kelvin representation of an identity tensor |
| $I_1$ | first principal invariant |
| $J_2$ | second deviatoric invariant |
| $J_3$ | third deviatoric invariant |
| $K$ | bulk modulus |
| $\boldsymbol{n}$ | outward unit normal vector |
| $N_a$, $\boldsymbol{N}$ | nodal shape function, element matrix of nodal shape functions |
| $\boldsymbol{0}$ | Kelvin representation of a zero tensor |
| $\mathcal{P}^{\mathrm{S}}, \mathcal{P}^{\mathrm{D}}$ | spherical and deviatoric projection tensors |
| $\boldsymbol{P}^{\mathrm{S}}, \boldsymbol{P}^{\mathrm{D}}$ | spherical and deviatoric projection matrices |
| $p$ | hydrostatic pressure |
| $\mathbf{t}$ | surface traction |
| $\mathbf{u}$ | displacement vector |
| $\mathcal{V}$ | viscosity tensor |

storage concepts are on the order of months and years, caverns of CAES power plants have to withstand significant pressure fluctuations several times a day or week. The increasing use of the subsurface and the evaluation of partially competing usage concepts are the motivation to revisit the existing formulations for the constitutive behavior of rock salt and to incorporate them into continuum mechanical and numerical frameworks of current standard for large-scale simulations.

Among the models listed above, typical constitutive formulations for rock salt include the LUBBY2 model and the model series by Minkley et al., both of which have been used extensively in practical geotechnical settings. The LUBBY2 model [22,30] is a nonlinear viscoelastic model based on a Burgers-type rheological analogue. Minkley [26] extended this setup by an additional friction element of a modified Mohr-Coulomb type to capture plasticity with strain hardening and softening as well as dilatancy. These effects allow a characterization of, e.g., excavation damaged zones (EDZ) around geotechnical installations. The plastic submodel includes the dependence of the yield surface and the plastic potential on the stress state and on the deformation history, e.g. [28]. Wang et al. [31] used a similar model but employed a Drucker-Prager yield surface with tension cut-off as well as a WIPP creep model, see also [21]. Large displacements and rotations have been taken into account in Ref. [32]. Some studies have investigated hydro-mechanical couplings that become important in the near- and far-field of geotechnical installations when dilatancy or damage open up flow paths in the rock salt that is otherwise considered tight [1–3,33,34]; see also [35,36] for recent works on hydromechanical coupling in a geotechnical context.

Many rock salt models have been derived for uniaxial or triaxial experimental setups and have only later on been generalized to three dimensions in a post hoc manner which is not always appropriate to fully describe three-dimensional scenarios [15,16,22]. Here, a tensorial representation is chosen, overcoming these inconsistencies. We further highlight the different treatment of material parameters existing in the literature due to the mix of uniaxial and three-dimensional formulations.

Specifically for large-scale geotechnical studies, the numerical implementation of the existing rock salt models has hardly been discussed in detail. Most of the known formulations have been implemented into software relying on explicit time integration schemes which are not unconditionally stable [24,28,29,31,32]. An implicit time integration based on a generalized mid-point rule has been employed by Pudewills and Krauss [37] whereas a Crank-Nicholson time integration scheme has been used in [23]. However, none of these studies provide details on the constitutive tangent matrices nor illustrate the convergence behavior of the implemented algorithms. Here, a state-of-the-art implicit implementation of the LUBBY2 and Minkley models into the scientific open-source parallelized finite element framework OpenGeoSys [38] is described in detail, compare for example the Refs. [39–52] regarding implicit finite element implementations. This will form the basis for large scale simulations in the context of competing usage concepts of the subsurface [53].

The outline of the article is as follows: in Section 2, the general numerical framework of the finite element code used in this study is presented. Section 3 clarifies some general aspects of the Burgers model that forms the basis of several constitutive models of rock salt. These considerations are specified for the LUBBY2 model in Section 4. A general tensorial formulation of this model is introduced and compared to the classical version prevalent in literature. In Section 5, the Burgers model is extended by a friction element without considering any specific yield surface or plastic potential to provide the implementation of a generalized viscoplastic model. Plastic flow regularization in the case of softening materials is pro-

[1] Throughout the article bold face symbols denote tensors and vectors. Normal face letters represent scalar quantities.