Computers & Geosciences 37 (2011) 751–762

Contents lists available at ScienceDirect

Computers & Geosciences

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

Implementation of the Barcelona Basic Model into TOUGH–FLAC for simulations of the geomechanical behavior of unsaturated soils

Jonny Rutqvist [a,*], Yuji Ijiri [b], Hajime Yamamoto [b]

[a] Earth Sciences Division, Lawrence Berkeley National Laboratory, MS 90-1116, Berkeley, CA 947 20, USA
[b] Taisei Corporation, Nuclear Facility Division, 1-25-1 Nishi Shinjuku, Shinjuku, Tokyo 163-0606, Japan

ARTICLE INFO

Article history:
Received 22 June 2010
Received in revised form
1 September 2010
Accepted 3 October 2010
Available online 10 November 2010

Keywords:
TOUGH
FLAC3D
BBM
Coupled modeling
Unsaturated soil

ABSTRACT

This paper presents the implementation of the Barcelona Basic Model (BBM) into the TOUGH–FLAC simulator analyzing the geomechanical behavior of unsaturated soils. We implemented the BBM into TOUGH–FLAC by (1) extending an existing FLAC^{3D} module for the Modified Cam-Clay (MCC) model in FLAC^{3D} and (2) adding computational routines for suction-dependent strain and net stress (i.e., total stress minus gas pressure) for unsaturated soils. We implemented a thermo-elasto-plastic version of the BBM, wherein the soil strength depends on both suction and temperature. The implementation of the BBM into TOUGH–FLAC was verified and tested against several published numerical model simulations and laboratory experiments involving the coupled thermal–hydrological–mechanical (THM) behavior of unsaturated soils. The simulation tests included modeling the mechanical behavior of bentonite-sand mixtures, which are being considered as back-fill and buffer materials for geological disposal of spent nuclear fuel. We also tested and demonstrated the use of the BBM and TOUGH–FLAC for a problem involving the coupled THM processes within a bentonite-backfilled nuclear waste emplacement tunnel. The simulation results indicated complex geomechanical behavior of the bentonite backfill, including a nonuniform distribution of buffer porosity and density that could not be captured in an alternative, simplified, linear-elastic swelling model. As a result of the work presented in this paper, TOUGH–FLAC with BBM is now fully operational and ready to be applied to problems associated with nuclear waste disposal in bentonite-backfilled tunnels, as well as other scientific and engineering problems related to the mechanical behavior of unsaturated soils.

1. Introduction

The Barcelona Basic Model (BBM) is a geomechanical constitutive model for capturing the elasto-plastic behavior of unsaturated soils. The model was first developed and presented in the early 1990s as an extension of the Modified Cam-Clay (MCC) model to unsaturated soil conditions (Alonso et al., 1990). The model can describe many typical features of unsaturated-soil mechanical behavior, including wetting-induced swelling or collapse strains, depending on the magnitude of applied stress, as well as the increase in shear strength and apparent preconsolidation stress with suction (Gens et al., 2006).

In this paper, we present the implementation of the BBM into a coupled multiphase fluid flow and geomechanical simulator called TOUGH–FLAC (Rutqvist et al., 2002; Rutqvist, 2010). The TOUGH–FLAC simulator is based on the sequential coupling of a finite-difference geomechanical code, FLAC^{3D} (Itasca, 2009) and a finite-volume, multiphase fluid flow code, TOUGH2 (Pruess et al., 1999). One great advantage of this approach to coupled-processes modeling is that both TOUGH2 and FLAC^{3D} are being continuously developed and widely used, and therefore contain many constitutive and equation-of-state modules that can be readily applied to a wide range of scientific and engineering problems. In this case, we start with the existing MCC module in FLAC^{3D}, which we then extend and modify to model the geomechanical behavior of unsaturated soil conditions within the framework of the BBM.

We implemented a thermo-elasto-plastic version of the BBM, in which the soil strength depends on both suction and temperature, and includes features for expansive (swelling) clay (Gens, 1995). Fig. 1 presents the three-dimensional yield surface in $p'-q-s$ space and $p'-q-T$ space, where p' is the net mean stress (i.e., total stress minus gas-phase pressure), q is the deviatoric stress (or shear stress), s is suction and T is temperature (Gens, 1995). Under water-saturated conditions ($s=0$), the yield surface corresponds to the MCC ellipse (Roscoe and Burgland, 1968) and the size of the elastic domain increases as suction increases. The rate of increase, represented by the loading–collapse (LC) curve, is one of the fundamental characteristics of the BBM (Gens et al., 2006). Moreover in the thermo-elasto-plastic version of the BBM, the size of the yield surface decreases with temperature (Fig. 1). We implemented

---

[*] Corresponding author. Tel.: +1 510 486 5432; fax: +1 510 486 5686.
E-mail address: jrutqvist@lbl.gov (J. Rutqvist).

0098-3004/$ - see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.cageo.2010.10.011

Nomenclature

c_a, c_b	constants used in the calculation of the plastic multiplier [Pa]
e	void ratio [–]
$\mathbf{e}$	deviatoric-strain tensor [–]
D_v	effective molecular diffusion coefficient of vapor [m^2/s]
f_{LC}	yield surface for loading–collapse in the BBM [Pa]
g_{LC}	plastic potential for loading–collapse in the BBM [Pa]
g_y	parameter describing the shape of the yield surface in the BBM [–]
G	shear modulus [Pa]
$\mathbf{I}$	identity tensor (all components 0, except diagonals which are 1) [–]
k	permeability [m^2]
k_r	relative permeability [–]
k_s	parameter describing the increase of cohesion with suction in the BBM [–]
K	bulk modulus [Pa]
K^s	bulk modulus for suction-induced volumetric strain in the BBM [Pa]
LC	loading–collapse yield surface in the BBM [–]
LC_i	loading–collapse yield surface at initial conditions in the BBM [–]
M	slope of the critical state line in the BBM [–]
p	total mean stress (Eq. (2)), compression positive [Pa]
p'	net mean stress (Eq. (3)), compression positive [Pa]
p^c	a reference stress state for $v-P'$ relation in virgin states in the BBM [Pa]
p_{est}'	estimated mean stress in FLAC^{3D} elastic predictor-plastic corrector algorithm [Pa]
p^g	gas phase, g, pressure [Pa]
p^l	liquid phase, l, pressure [Pa]
p^{φ}	pore pressure [Pa]
p_s	tensile strength in the BBM [Pa]
p_{s0}	tensile strength at saturated conditions in the BBM [Pa]
p_0	net mean yield stress at current suction and temperature in the BBM [Pa]
p_{ref}	reference stress state for relating elastic compressibility to suction in the BBM [Pa]
p_{0T}^*	net mean yield stress for saturated conditions at reference temperature in the BBM [Pa]
r_λ	parameter defining the maximum soil stiffness associated with an LC yield in the BBM [–]
s	suction [Pa]
$\mathbf{s}$	deviatoric-stress tensor [Pa]
S_l	liquid phase saturation [–]
T_0	reference temperature for temperature-dependent cohesion in the BBM [°C]
T	temperature [°C]
q	deviatoric (von Mises) stress [Pa]
q_{est}	estimated deviatoric stress in FLAC^{3D} elastic predictor-plastic corrector algorithm [Pa]
J_2	second invariant of the effective deviatoric-stress tensor [Pa]
J'_2	second invariant of the deviatoric-strain tensor [–]
v	specific volume [–]
v_i, v_{ref}	specific volume at initial and reference stress states [–]
V	volume [m^3]
V^s	volume of solid phase [m^3]
V^ϕ	volume of pores [m^3]
α_a	nonassociativity parameter in flow rule in the BBM [–]
α_B	Biot's effective stress coefficient [–]
α_{ps}	parameter relating elastic compressibility to suction in the BBM [–]
α_{sp}	parameter relating κ_{sp} to net mean stress in the BBM [–]
α_{ss}	parameter relating κ_{sp} to suction in the BBM [–]
α_0, α_2	parameters that relate elastic volumetric strain and temperature changes in the BBM [$^\circ C^{-1}$]
α_T	linear thermal expansion coefficient (equivalent to α_0) [$^\circ C^{-1}$]
β_λ	parameter for the increase of soil stiffness with suction in the BBM [Pa^{-1}]
β_{sw}	moisture swelling coefficient in an LE swelling model [–]
ε_v	volumetric strain ($=\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}$) positive for contraction [–]
$\boldsymbol{\varepsilon}^s$	suction strain tensor [–]
$\boldsymbol{\varepsilon}$	total strain tensor [–]
$\boldsymbol{\varepsilon}^e$	elastic strain tensor [–]
$\boldsymbol{\varepsilon}^p$	plastic strain tensor [–]
$\boldsymbol{\varepsilon}^T$	thermal strain tensor [–]
ε_v^e,ε_q^e	elastic volumetric and deviatoric strains [–]
ε_v^p,ε_q^p	plastic volumetric and deviatoric strains [–]
ε_v^T,ε_v^s	thermal and suction-induced volumetric strains [–]
ϕ	porosity [–]
κ_{ps}	compressibility parameter for elastic $v-p'$ in the BBM [–]
κ_{ps0}	initial (zero suction) slope for elastic $v-p'$ in the BBM [–]
κ_{sp}	compressibility parameter for suction-induced elastic strain in the BBM [–]
κ_{sp0}	κ_{sp} at reference stress P_{ref} and zero suction [–]
λ_{ps}	compressibility parameter in virgin soil states at suction s in the BBM [Pa]
λ_{ps0}	Slope of v–p' relation in virgin soil states at zero suction in the BBM [Pa]
Λ	plastic multiplier [–]
θ	Lode's angle [°]
ρ_d	dry-density, ρ_d [kg/m^3]
ρ_s	parameter that relates cohesion to temperature in the BBM [–]
σ_1, σ_2, σ_3	principal compressive stress components [Pa]
$\boldsymbol{\sigma}$	total stress tensor [Pa]
$\boldsymbol{\sigma}'$	effective stress tensor [Pa]
ν	Poisson's ratio [–]

the BBM into TOUGH–FLAC by (1) extending an existing MCC module within the framework of the FLAC^{3D} User Defined Model (UDM) capability and (2) adding computational routines for suction-dependent strains and net stress in unsaturated soils.

The thermo-elasto-plastic version of the BBM is also part of the CODE_BRIGHT finite element code at the University of Cataluña, Barcelona (CIMNE, 2002; Olivella et al., 1996). It was recently successfully applied to model the coupled thermal–hydrological–mechanical (THM) behavior of an unsaturated bentonite clay associated with the FEBEX in situ heater test at the Grimsel Test Site, Switzerland (Gens et al., 2009). The BBM has also been applied to other types of bentonite-sand mixtures such as MX-80, considered as an option for an isolating buffer in the Swedish KBS-3 repository concept (Kristensson and Åkesson, 2008a, b).