

1 HYDRATION

1.1 Introduction

Hydration is defined as the chemical absorption of water into a substance, a process by which heat is generated (hydration heat). The setting of concrete — which can be considered as a transition from liquid to solid phase — is the most relevant example for the hydration process in the engineering world.

The effects of the hydration process can be separated into a thermal part and a mechanical part. The implementation of hydration models in *FLAC^{3D}* follows this separation, as the hydration heat generation and heat transfer are dealt with in separate thermal models, material hardening and strength development are implemented as constitutive models.

The coupling parameter between both modules is the hydration grade a , which is defined as the ratio of the accumulated hydration heat at time t to the ultimate hydration heat generated until completion.

$$\alpha(t) = \frac{Q(t)}{Q_\infty} \quad (1.1)$$

The time-dependent evolution of the hydration grade is mainly governed by the temperature boundary conditions. Lower temperatures lead to a longer process with lower hydration heat generation, whereas higher temperatures lead to a shorter process with higher hydration heat generation.

To have a unique reference value, the concrete age t_e , which is the equivalent concrete age at a reference temperature (of 20°C) and is calculated as a function of thermal time t and concrete temperature T , is introduced.

$$t_e = \int_{t=0}^t e^{\frac{E_A}{R} \cdot \left[\frac{1}{293} - \frac{1}{T} \right]} \cdot dt \quad (1.2)$$

where R is the universal gas constant (8.314 J/K/mol) and E_A is the activation energy [J/mol].

In *FLAC^{3D}*, two different thermal hydration models are implemented: a thermal hydration model for German concrete, **th_hyd_concrete1**; and an empirical, more general hydration model, **th_hyd**.

During the hydration process, the values of elastic material parameters can vary over several orders of magnitude. Accordingly, the gridpoint masses have to be adjusted for numerical stability, in small strain mode as well as in large strain mode. The frequency of the update can be set by the user with the *FLAC^{3D}* command **SET geom_rep value**.

1.2 Thermal Hydration Model for German Concrete (th_hyd_concrete1)

In the hydration model for German concrete, **th_hyd_concrete1** (Onken and Rostásy, 1995), the hydration grade α is a function of the concrete age t_e .

$$\alpha(t_e) = e^{-\left(\ln\left(1+\frac{t_e}{t_1}\right)\right)^b} \quad (1.3)$$

where b and t_1 are constants. The hydration heat rate q depends on the gradient of the hydration grade.

$$q(t) = Q_{Ce}^{max} \cdot C \cdot \frac{\Delta\alpha}{\Delta t} \quad (1.4)$$

where C is the cement concentration in $[\text{kg}/\text{m}^3]$, and Q_{Ce}^{max} (in $[\text{J}/\text{kg}]$) is the maximum amount of heat that can be generated, and is estimated to be

$$Q_{Ce}^{max} = \frac{\Delta T \cdot c_c \cdot \rho}{C} \quad (1.5)$$

where c_c is the specific heat of the material $[\text{J}/\text{kg}/\text{K}]$.

The heat transfer is assumed to be isotropic with constant values of specific heat, thermal conductivity and coefficient of thermal expansion.

1.3 General Hydration Model (th_hyd)

In the more general empirical hydration law **th_hyd**, the activation energy E_A , the heat capacity c_p , and the thermal conductivity λ are functions of temperature or temperature and hydration grade, respectively.

The hydration grade is again a function of the effective concrete age t_e .

$$\alpha(t_e) = e^{-\left(\ln\left(1+\frac{t_e}{t_1}\right)\right)^b} \quad (1.6)$$

The activation energy E_A is a function of temperature T .

$$E_A(T) = E_{A,1} + \frac{E_{A,2} - E_{A,1}}{1 + e^{-\frac{T-T_{0,E_A}}{dT}}} \quad (1.7)$$

The heat capacity c_p and the thermal conductivity λ depend on the temperature T and the hydration grade α .

$$\begin{aligned} c_p(\alpha, T) &= c_{p,1} + dc_{p,a} \cdot \alpha + \left(T - T_{T_1,c_p}\right) \cdot dc_{p,T} \\ \lambda(\alpha, T) &= (\lambda_1 + d\lambda_a \cdot \alpha) \cdot (1 + d\lambda_T \cdot T) \end{aligned} \quad (1.8)$$

The hydration heat source strength is limited to a temperature range.

$$q(T) = \begin{pmatrix} Q_{Ce}^{max} \cdot C \cdot \frac{\Delta\alpha}{\Delta t} & , T \leq T_{max,q} \\ 0 & , T > T_{max,q} \end{pmatrix} \quad (1.9)$$

1.4 A Modified Drucker-Prager Model for Hydration

The implementation of hydration in *FLAC^{3D}* is a Drucker-Prager constitutive model with hydration grade α depending on elastic and strength properties (Hinze 1987). During the hydration process, the actual Young's modulus E is a function of the hydration grade α .

$$E(\alpha) = E_{cte} \cdot \left(\frac{\alpha - \alpha_0}{1 - \alpha_0} \right)^a \quad (1.10)$$

where E_{cte} is the Young's modulus after complete hydration and a is a specific parameter for cement (usually of the order of 0.5 – 0.7).

The actual uniaxial compressive strength σ_c , and uniaxial tensile strength σ_t also depend on the hydration grade.

$$\begin{aligned} \sigma_c &= 0.85 \cdot \left(\frac{f_{cte}}{c} \cdot \frac{\alpha - \alpha_0}{1 - \alpha_0} \right)^{3/2} \\ \sigma_t &= f_{cte} \cdot \frac{\alpha - \alpha_0}{1 - \alpha_0} \end{aligned} \quad (1.11)$$

where f_{cte} is the uniaxial strength [MPa] after completion of the hydration process; α_0 is a specific parameter for cement (0.17 – 0.38); and c is a heat capacity factor (0.6 – 1.0).

The yield criterion in the Drucker-Prager constitutive model (see [Section 2.5.1](#) in **Theory and Background**) is

$$0 = \tau + q \cdot \sigma - k \quad (1.12)$$

where q and k are material parameters, and τ and σ are stress invariants. q and k can be derived from the actual uniaxial compressive and tensile strengths, σ_c and σ_t .

$$\begin{aligned} q &= \frac{\sqrt{3} \cdot (\sigma_D - \sigma_z)}{\sigma_D + \sigma_z} \\ k &= \frac{2 \cdot \sigma_D \cdot \sigma_z}{\left(\sqrt{3} \cdot \sigma_D + \sigma_z \right)} \end{aligned} \quad (1.13)$$

1.5 Properties

Table 1.1 Thermal hydration model for German concrete — MODEL th_hyd_concrete1

(1)	e_activate	activation energy, E_A
(2)	gas_const	universal gas constant, R
(3)	t1_const	material parameter, t_1
(4)	b_const	material parameter, b
(5)	cement	cement concentration, C
(6)	qmax	maximum amount of generated heat, Q_{Ce}^{max}
(7)	spec_heat	specific heat, c_p
(8)	conductivity	conductivity, λ
read only		
(9)	t_concrete	effective concrete age, t_e
(10)	heat	hydration heat rate, q

Table 1.2 General thermal hydration model— MODEL th_hyd

(1)	gas_const	universal gas constant, R
(2)	t1_const	material parameter, t_1
(3)	b_const	material parameter, b
(4)	cement	cement concentration, C
(5)	qmax	maximum amount of generated heat, Q_{Ce}^{max}
(6)	E_a1	material parameter, $E_{A,1}$
(7)	E_a2	material parameter, $E_{A,2}$
(8)	T_0EA	material parameter, T_{0,E_A}
(9)	C_p1	material parameter, $C_{p,1}$
(10)	dC_pa	material parameter, $dC_{p,A}$
(11)	T_1pc	material parameter, T_{1,c_p}
(12)	dC_pT	material parameter, $C_{p,T}$
(13)	lambda_1	material parameter, λ_1
(14)	dLambda_a	material parameter, $d\lambda_1$
(15)	dLambda_T	material parameter, $d\lambda_T$
(16)	T_maxq	material parameter, $T_{max,q}$
read only		
(17)	t_concrete	effective concrete age, t_e
(18)	heat	hydration heat rate, q
(19)	e_activate	activation energy, E_A
(20)	spec_heat	specific heat, c_p
(21)	conductivity	conductivity, λ
(22)	dT	temperature change, ΔT

Table 1.3 Modified Drucker-Prager model for concrete — MODEL hydration

(1)	cte_tension	tensile strength for $\alpha = 1$, f_{cte}
(2)	cte_young	Young's modulus for $\alpha = 1$, E_{cte}
(3)	cte_alpha	material parameter, α_0
(4)	a_const	material parameter, a
(5)	c_const	material parameter, c
(6)	tension	tension limit strength, σ_t
(7)	compression	compression limit, σ_D
(8)	Young	Young's modulus, E
(9)	dAlpha_min	minimum difference of $(\alpha - \alpha_0)_{min}$
(10)	qvol	Drucker-Prager material parameter, q_Φ
(11)	kshear	Drucker-Prager material parameter, k_Φ
(12)	qdil	Drucker-Prager material parameter, q_Ψ

1.6 Example Problems for the Hydration Model

1.6.1 Concrete Inclusion in an Elastic Medium

This example consists of a concrete inclusion inside an elastic and thermal isotropic material. The model has a size of 10 m × 1 m × 10 m and is fixed in the y-direction (Figure 1.1). Roller boundary conditions are applied at the model boundaries. The material properties are listed in Table 1.4 (elastic frame) and Table 1.5 (concrete inclusion). The model was run for a thermal time of approximately 250 days.

Figures 1.2 to 1.6 show the evolution of various parameters during the hydration process (gridpoint temperatures at five points (Figure 1.2), hydration grade (Figure 1.3), tensile and compressive strength (Figure 1.4), elastic parameters (Figure 1.5) and the generated hydration heat (Figure 1.6)).

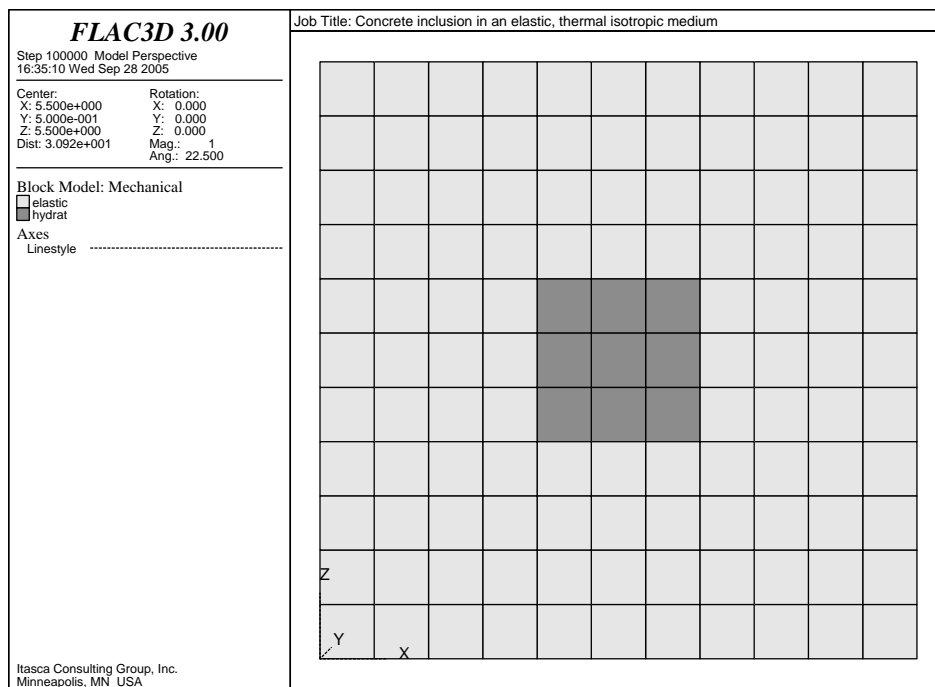


Figure 1.1 FLAC^{3D} model for the concrete inclusion test

Table 1.4 Material properties for the elastic material

Bulk modulus (K)	1000 MPa
Shear modulus (G)	700 MPa
Specific heat (C_P)	0.2 J/kg/K
Thermal conductivity (k)	20.0 W/kg/K
Linear thermal expansion coefficient (α_t)	$10^{-4} \text{ } ^\circ\text{C}^{-1}$

Table 1.5 *Material properties for the concrete material*

Maximum amount of generated heat (Q_{Ce}^{max})	10^5 J/kg
Cement concentration (C)	330 kg/m ³
Material parameter (b)	-1.114
Material parameter (t_1)	7.2×10^4 [s]
Universal gas constant (R)	8.314 J/mol
Activation energy (E_A)	33.5 J/mol
Specific heat (C_P)	0.2 J/kg/K
Thermal conductivity (λ)	2.0 W/m/K
Linear thermal expansion coefficient (α_t)	10^{-5} °C ⁻¹
Specific parameter for cement (α_0)	0.20
Young's modulus after complete hydration (E_{cte})	1000 MPa
Material parameter (c)	0.4
Material parameter (a)	0.6
Minimum value for ($\alpha - \alpha_0$)	10^{-4}

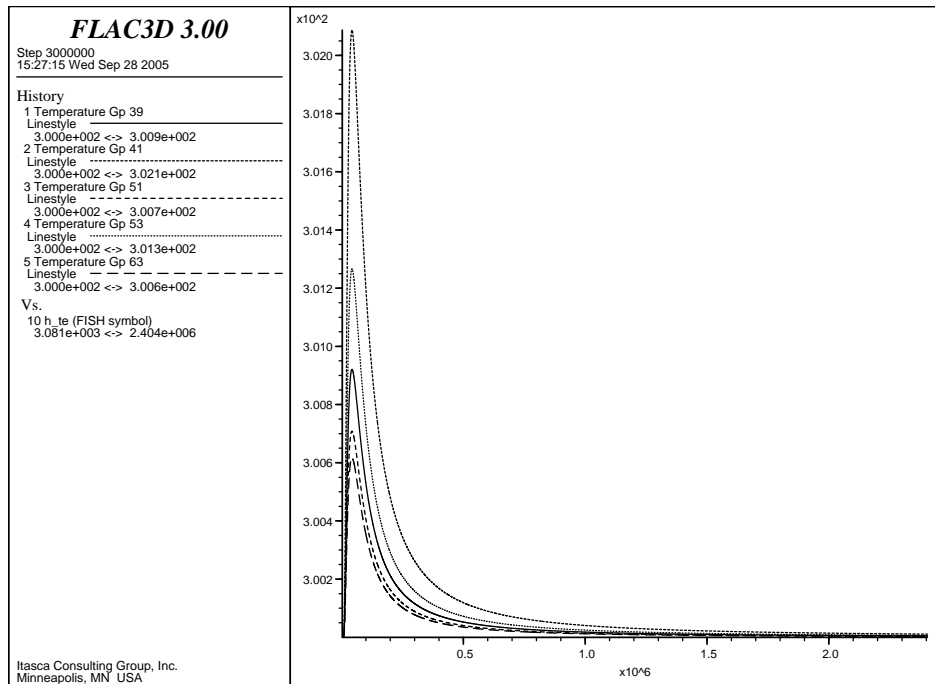


Figure 1.2 *Evolution of gridpoint temperatures for the concrete inclusion test as a function of the concrete age*

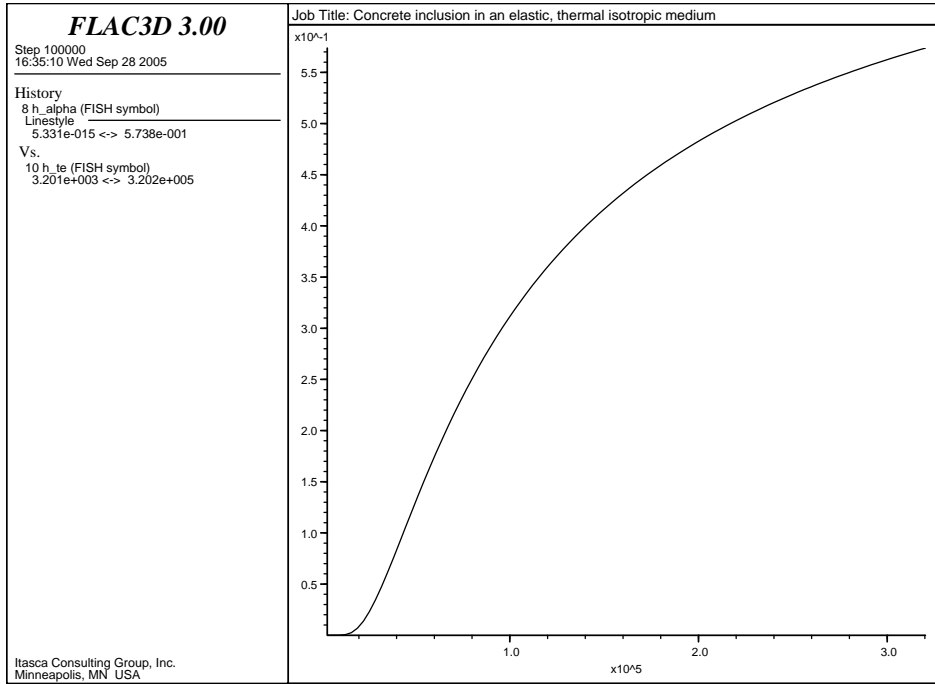


Figure 1.3 Evolution of the hydration grade for the center zone of the concrete inclusion as a function of the concrete age

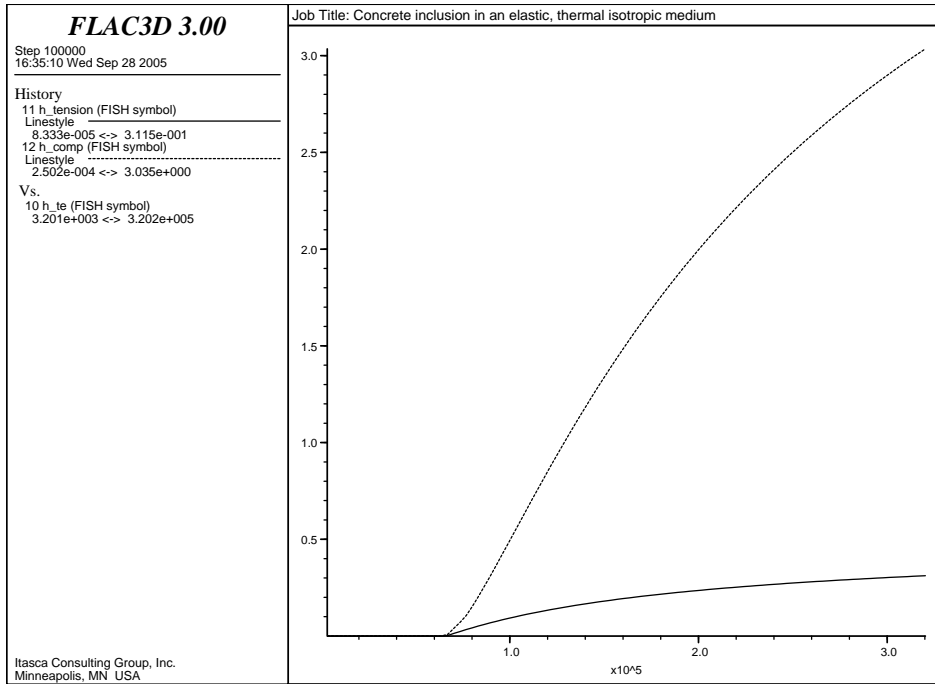


Figure 1.4 Evolution of the tensile and compressive strength for the center zone of the concrete inclusion as a function of the concrete age

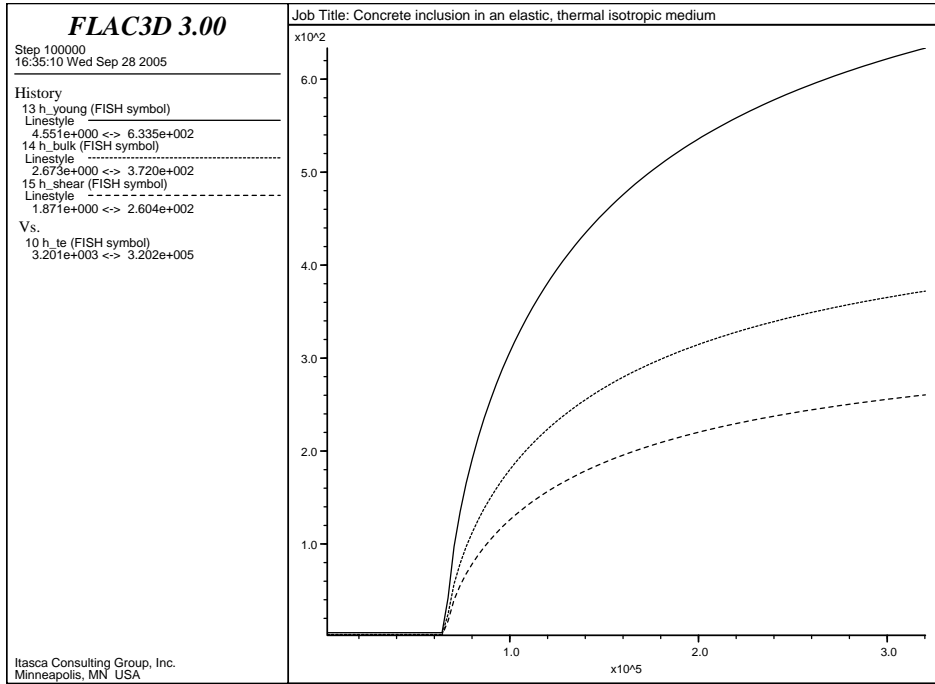


Figure 1.5 Evolution of the elastic parameters for the center zone of the concrete inclusion as a function of the concrete age

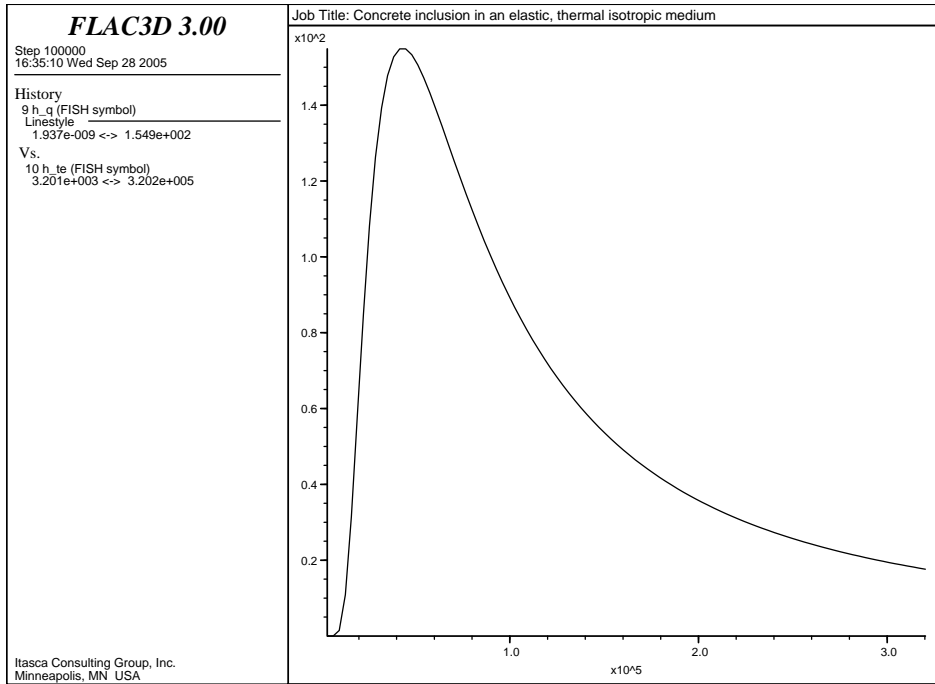


Figure 1.6 Evolution of the hydration heat for the center zone of the concrete inclusion as a function of the concrete age

Example 1.1 HYDRATI.DAT

```

;-----
; Concrete inclusion in an elastic, thermal isotropic medium
;
;-----
new
title
Concrete inclusion in an elastic, thermal isotropic medium

set echo on
config thermal
;
gen zone brick size 11 1 11
macro concrete = 'ra x 4 7 z 4 7'
;willi
model elast th_iso
model hydrat th_hyd_concretel concrete
;
prop dens 2000 bulk 1e3 shear 0.7e3
prop cond 20.0 thex 1e-4 spec_heat 0.2

prop thex 1e-5 cond 2.0 concrete

prop qmax 1e5 cement 330 b_const -1.114 t1_const 7.2e4
concrete
prop gas_const 8.314 e_activate 33.5 cte_alpha 0.20 cte_tension 2.0
concrete
prop cte_bulk 0.98e3 cte_shear 0.50e3 c_const 0.4 a_const 0.6
concrete
prop dalpha_min 1e-4 cte_young 1e3
concrete

ini temp 300
fix temp 300 ra x -0.1 0.1
fix temp 300 ra x 10.9 11.1
fix temp 300 ra z 10.9 11.1
fix temp 300 ra z -0.1 0.1

fix x ra x -0.1 0.1
fix x ra x 10.9 11.1
fix y
fix z ra z -0.1 0.1
fix z ra z 10.9 11.1

```

```

hist gp temp 1 0 5
hist gp temp 2 0 5
hist gp temp 3 0 5
hist gp temp 4 0 5
hist gp temp 5 0 5
hist gp temp 2 0 5

def hist_setup
  hzp = z_nearall(6.5,0.5,6.5)
end
hist_setup

def hyd_hist
  h_alpha = z_prop(hzp,'alpha')
  h_q      = z_prop(hzp,'heat')
  h_te     = z_prop(hzp,'t_concrete')
  h_tension = z_prop(hzp,'tension')
  h_comp   = z_prop(hzp,'compression')
  h_young  = z_prop(hzp,'young')
  h_bulk   = z_prop(hzp,'bulk')
  h_shear  = z_prop(hzp,'shear')
  h_poisson = z_prop(hzp,'poisson')
end

hist hyd_hist
hist h_alpha h_q h_te
hist h_tension h_comp
hist h_young h_bulk h_shear h_poisson

set geom_rep 500
hist nstep 100
cyc 13000
save hyd_inclusion.sav

plot hist 8 vs 10
return

```

1.6.2 Concrete Wall on Elastic Baseplate

The numerical model ([Figure 1.7](#)) used here is based on a model, which was used by Onken & Rostásy (1995) to compare numerical results and temperature measurements. It consists of a new concrete wall ($10 \times 1 \times 40$ elements), footed on a baseplate of old concrete ($10 \times 1 \times 5$ elements). Since the material parameters and the boundary conditions are not available from Onken & Rostásy (1995), the material parameters from [Example 1.1](#) are used together with typical temperature boundary conditions.

For the concrete wall, the thermal hydration model for German concrete (**th_hyd_concrete1**) and the modified Drucker-Prager with hydration (**hydrat**) are used. The baseplate is considered elastic and thermal isotropic.

The model was under summer temperature conditions. The temperatures at the wall boundary are fixed to air temperature, at the baseplate to the initial ground temperature:

Initial wall temperature, 296 K

Wall boundary temperature fixed at 293 K

Initial baseplate temperature, 285 K

Baseplate boundary temperature fixed at 285 K

The numerical results are displayed in [Figures 1.8 to 1.13](#). Shown are the temperature distribution inside the model after 1 and 3 days ([Figures 1.8 and 1.9](#)), evolution of gridpoint temperatures ([Figure 1.10](#)), evolution of the hydration grade ([Figure 1.11](#)), evolution of the strength parameters ([Figure 1.12](#)), evolution of the elastic parameters ([Figure 1.13](#)), and evolution of the generated hydration heat. The results are qualitatively in good agreement with the results given by Onken & Rostásy (1995) (a more detailed comparison is not available due to the limited access to material parameter and boundary conditions).

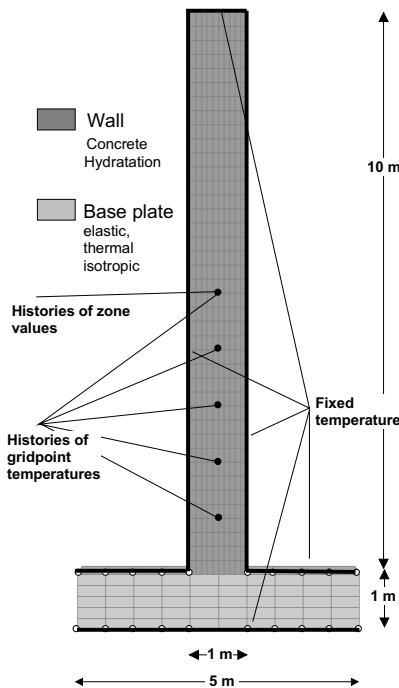


Figure 1.7 *Model of the concrete wall on an elastic baseplate*

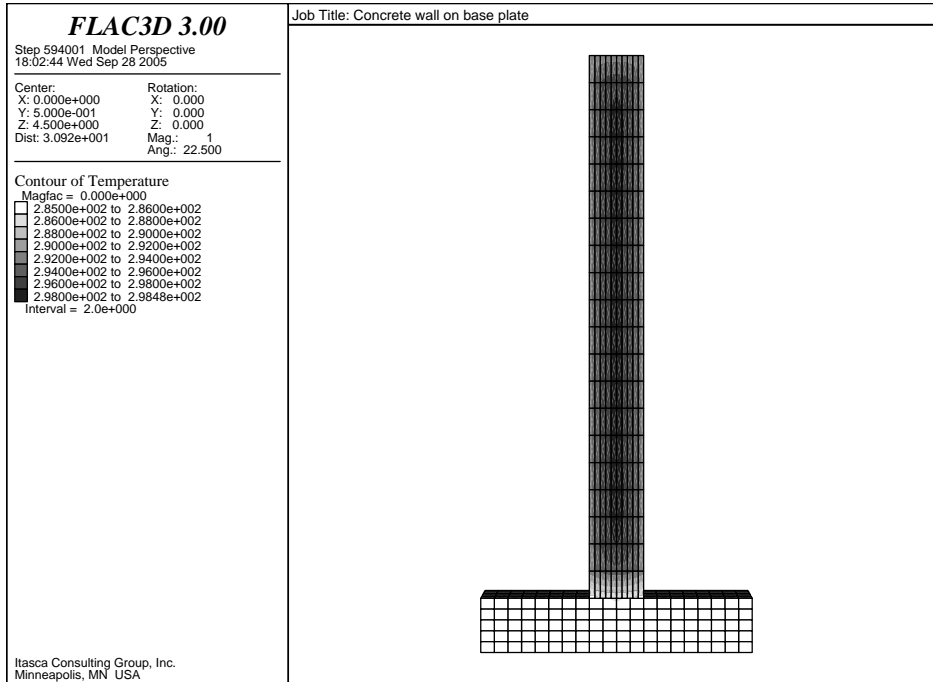


Figure 1.8 *Temperature distribution after 1 day (concrete age)*

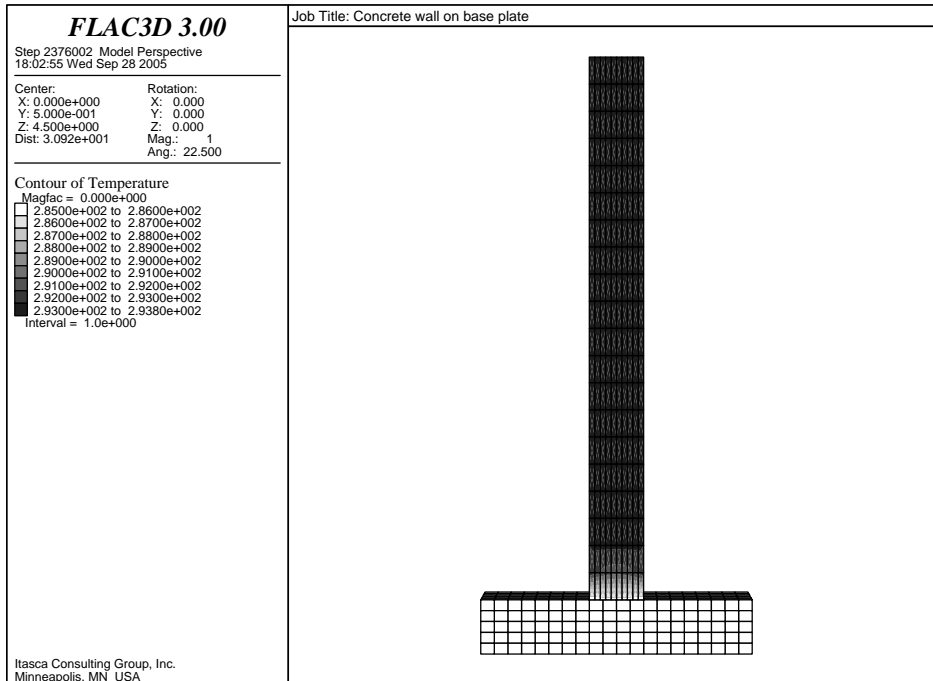


Figure 1.9 *Temperature distribution after 3 days (concrete age)*

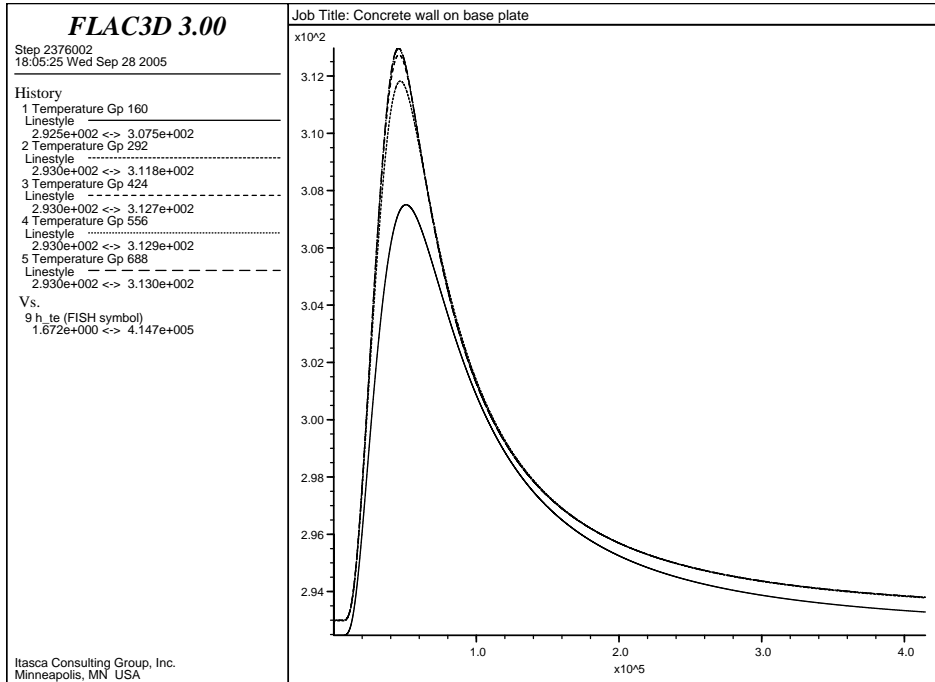


Figure 1.10 Evolution of gridpoint temperatures for the concrete inclusion test as a function of the concrete age

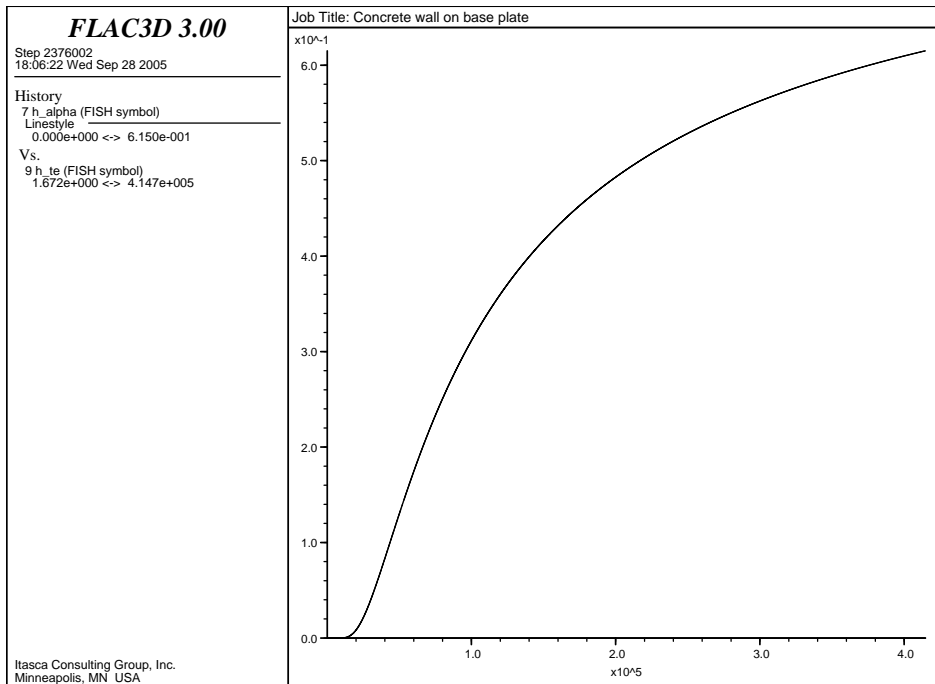


Figure 1.11 Evolution of the hydration grade as a function of the concrete age

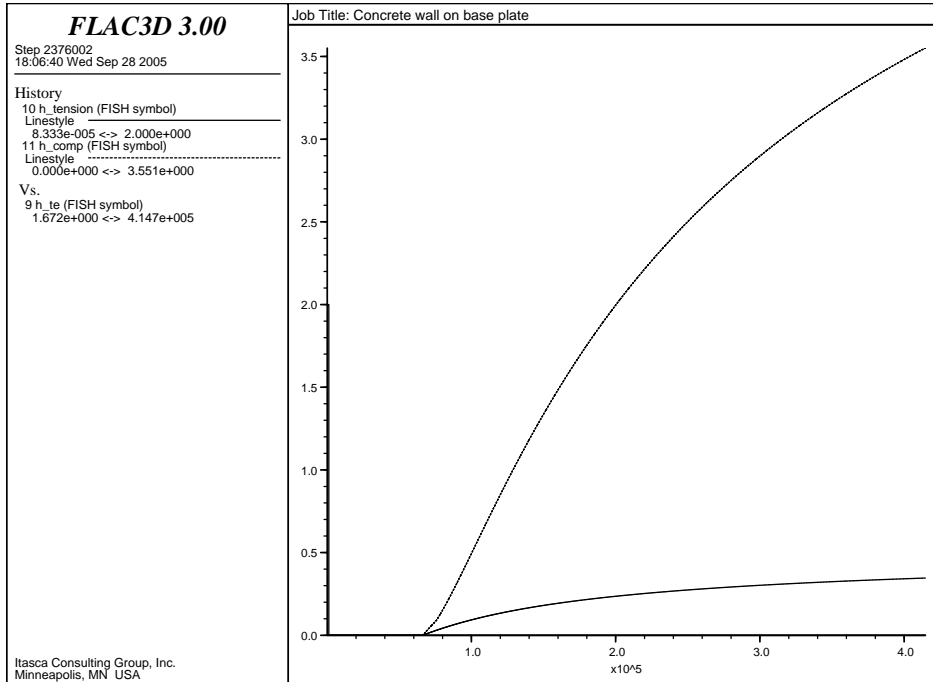


Figure 1.12 Evolution of the tensile and compressive strength as a function of the concrete age

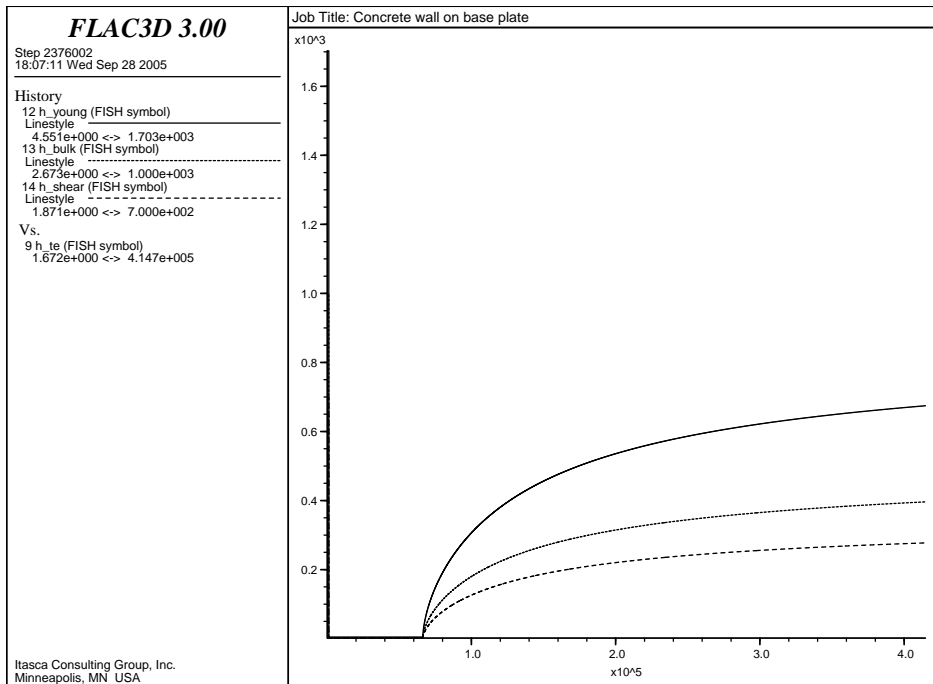


Figure 1.13 Evolution of the elastic parameters as a function of the concrete age

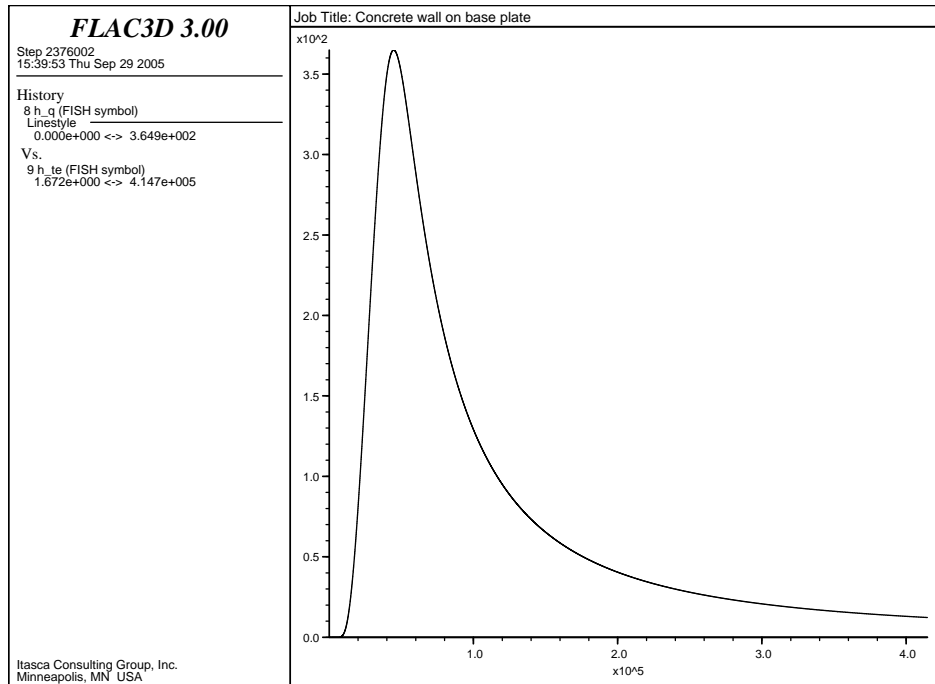


Figure 1.14 Evolution of the generated hydration heat as a function of the concrete age

Example 1.2 HYDRAT2.DAT

```

;-----
; Concrete inclusion in an elastic, thermal isotropic medium
;
;-----
new
title
Hydratation: Concrete wall on elastic base plate - summer temperature
conditions

config thermal
;
gen zone brick p0=(-0.5,0.0,0.0) p1=(0.5,0.0,0.0) p2=(-0.5,1.0,0.0) &
p3=(-0.5,0.0,10.0) size = 10,5,20
gen zone brick p0=(-2.5,0.0,-1.0) p1=(2.5,0.0,-1.0) p2=(-2.5,1.0,-1.0) &
p3=(-2.5,0.0,0.0) size = 20,5,5
attach face ra z -0.01 0.01
;
group concrete range z 0 100
group base_plate range z -100 0

```

```

model elast th_iso          range group base_plate
model hydrat th_hyd_concretel range group concrete

prop dens 2000 bulk 1e3 shear .7e3
prop cond 20. thex 1e-4 spec_heat 0.2
prop cond 2. thex 1e-5      range group concrete

prop qmax 1e5 cement 330 b_const -1.114 t1_const 7.2e4
  range group concrete
prop gas_const 8.314 e_activate 33.5e3 cte_alpha 0.20 cte_tension 2.0
  range group concrete
prop cte_bulk 0.98e3 cte_shear 0.50e3 c_const 0.4 a_const 0.6
  range group concrete
prop dalpha_min 1e-4 cte_young 1e3
  range group concrete

ini temp 296
fix temp 293 ra x -0.51,-0.49 z 0.0 100
fix temp 293 ra x 0.49,0.51 z 0.0 100
fix temp 293 ra z 9.9,10.1

ini temp 285 range group base_plate
fix temp 285 ra z -1.01 -0.99
fix temp 285 ra x -10.0 -0.49 z -0.01 0.01
fix temp 285 ra x 0.49 10.0 z -0.01 0.01

fix x y z ra z -0.9 -1.1
fix x ra x -2.6 -2.4
fix x ra x 2.4 2.6

hist gp temp 0 0.5 1
hist gp temp 0 0.5 2
hist gp temp 0 0.5 3
hist gp temp 0 0.5 4
hist gp temp 0 0.5 5

def hist_setup
  hzp = z_near(0,0,5)
end
hist_setup

def hyd_hist
  h_alpha = z_prop(hzp,'alpha')
  h_q     = z_prop(hzp,'heat')
  h_te    = z_prop(hzp,'t_concrete')
  h_tension = z_prop(hzp,'tension')

```

```
h_comp    = z_prop(hzp,'compression')
h_young   = z_prop(hzp,'young')
h_bulk    = z_prop(hzp,'bulk')
h_shear   = z_prop(hzp,'shear')
h_poiss   = z_prop(hzp,'poisson')
h_time    = thtime
end
```

```
hist hyd_hist
hist h_alpha h_q h_te
hist h_tension h_comp
hist h_young h_bulk h_shear h_poiss
hist h_time
```

```
set geom_rep = 500
solve age 86400
save hyd_exp2_1d.sav
set age 259200
save hyd_exp2_3d.sav
```

1.7 References

Hinze, D. "Dissertation zum Thema: Zur Beurteilung des phsikalischen nicht-linearen Betonverhaltens bei mehrachsigen Spannungszustand mit Hilfe differenzieller Stoffgesetze unter Anwendung der FEM," Hochschule für Architektur und Bauwesen, Weimar (1987).

Onken, P. & Rostásy, F. *Wirksame Betonzugfestigkeit im Bauwerk bei früh einsetzendem Temperaturzwang*. DafStb Heft 449, Berlin: Beuth-Verlag (1995).