Awesome Article Title

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Abstract

The abstract serves both as a general introduction to the topic and as a brief, non-technical summary of the main results and their implications. Authors are advised to check the author instructions for the journal they are submitting to for word limits and if structural elements like subheadings, citations, or equations are permitted.

Keywords: keyword1, Keyword2, Keyword3, Keyword4

1 Introduction

The Introduction section, of referenced text Campbell and Gear (1995) expands on the background of the work (some overlap with the Abstract is acceptable). The introduction should not include subheadings.

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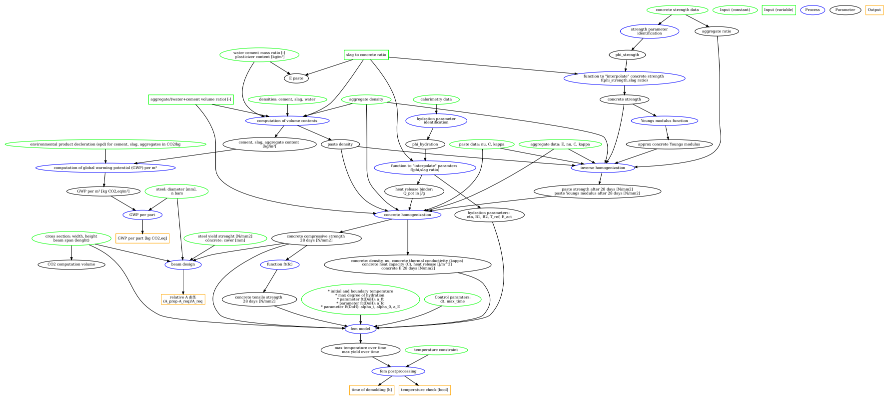

Fig. 1 Testing doit workflow. Figure is created by script. Macro for path is created by other script

2 Models

2.1 Notes on Early Age Concrete Model

Plan is do collect notes, information on the early age concrete model I am implementing. Currently the plan is to include temperature and humidity and couple them the respective mechanical fields. I will start with the temperature field.

2.2 Modeling of the temperature field

Temperature is generally described as

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + \frac{\partial Q}{\partial t} \tag{1}$$

λ is the effective thermal conductivity in $\mathrm{Wm}^{-1}\mathrm{K}^{-1}$. C is the specific heat capacity. ρ is the density. ρC is the volumetric heat capacity in $\mathrm{Jm}^{-3}\mathrm{K}^{-1}$. Q is the volumetric heat, due to hydration, it is also called the latent heat of hydration, or the heat source in Jm^{-3}. For now we assume the density, the thermal conductivity and the volumetric heat capacity as constant, however there are models that make them dependent on the temperature, moisture and/or the hydration.

2.2.1 Degree of hydration α

The degree of hydration α is defined as the ratio between the cumulative heat Q at time t and the total theoretical volumetric heat by complete hydration

Q_∞,

$$\alpha(t) = \frac{Q(t)}{Q_\infty}, \tag{2}$$

by assuming a linear relation between the degree of hydration and the heat development. Therefore the time derivative of the heat source $\dot{Q}$ can be rewritten in terms of α,

$$\frac{\partial Q}{\partial t} = \frac{\partial \alpha}{\partial t} Q_\infty. \tag{3}$$

There are formulas to approximate total potential heat based on composition, approximated values range between 300 and 600 J/g of binder for different cement types, e.g. Ordinary Portland cement $Q_\infty = 375$–525 or Pozzolanic cement $Q_\infty = 315$–420.

2.2.2 Affinity

The heat release can be modeled based on the chemical affinity A of the binder. The hydration kinetics can be defined as a function of affinity at a reference temperature $\tilde{A}$ and a temperature dependent scale factor a

$$\dot{\alpha} = \tilde{A}(\alpha) a(T) \tag{4}$$

The reference affinity, based on the degree of hydration is approximated by

$$\tilde{A}(\alpha) = B_1 \left(\frac{B_2}{\alpha_{\mathrm{max}}} + \alpha \right) (\alpha_{\mathrm{max}} - \alpha) \exp \left(-\eta \frac{\alpha}{\alpha_{\mathrm{max}}} \right) \tag{5}$$

where B_1 and B_2 are coefficients depending on the binder. The scale function is given as

$$a = \exp \left(-\frac{E_{\mathrm{a}}}{R} \left(\frac{1}{T} - \frac{1}{T_{\mathrm{ref}}} \right) \right) \tag{6}$$

An example function to approximate the maximum degree of hydration based on w/c ratio, by Mills (1966)

$$\alpha_{\mathrm{max}} = \frac{1.031 w/c}{0.194 + w/c}, \tag{7}$$

this refers to Portland cement.

2.2.3 Time derivative

For a start I use a simple backward difference, backward Euler, implicit Euler method and approximate

$$\dot{T} = \frac{T^{n+1} - T^n}{\Delta t} \quad \text{and} \tag{8}$$

$$\dot{\alpha} = \frac{\Delta\alpha}{\Delta t} \quad \text{with} \quad \Delta\alpha = \alpha^{n+1} - \alpha^n \tag{9}$$

2.2.4 Formulation

Using (3) in (1) the heat equation is given as

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + Q_\infty \frac{\partial \alpha}{\partial t} \tag{10}$$

Now we apply the time discretizations (8) and (9) and drop the index $n+1$ for readability (8)

$$\rho C T - \Delta t \nabla \cdot (\lambda \nabla T) - Q_\infty \Delta\alpha = \rho C T^n \tag{11}$$

Now, we use (9) and (4) to get a formulation for $\Delta\alpha$

$$\Delta\alpha = \Delta t \tilde{A}(\alpha) a(T) \tag{12}$$

2.2.5 Computing $\Delta\alpha$ at the Gauss-point

As $\Delta\alpha$ is not a global field, rather locally defined information.

2.2.6 Solving for $\Delta\alpha$

To solve for $\Delta\alpha$ we define the affinity in terms of α_n and $\Delta\alpha$

$$\tilde{A} = B_1 \exp\left(-\eta \frac{\Delta\alpha + \alpha_n}{\alpha_{\max}}\right) \left(\tfrac{B_2}{\alpha_{\max}} + \Delta\alpha + \alpha_n\right) (\alpha_{\max} - \Delta\alpha - \alpha_n). \tag{13}$$

Now we can solve the nonlinear function

$$f(\Delta\alpha) = \Delta\alpha - \Delta t \tilde{A}(\Delta\alpha) a(T) = 0 \tag{14}$$

using an iterative Newton-Raphson solver. For an effective algorithm we require the tangent of f with respect to $\Delta\alpha$

$$\frac{\partial f}{\partial \Delta\alpha} = 1 - \Delta t a(T) \frac{\partial \tilde{A}}{\partial \Delta\alpha} \quad \text{with} \tag{15}$$

$$\frac{\partial \tilde{A}}{\partial \Delta\alpha} = B_1 \exp\left(-\eta \frac{\Delta\alpha + \alpha_n}{\alpha_{\max}}\right) \Big[\alpha_{\max} - \tfrac{B_2}{\alpha_{\max}} - 2\Delta\alpha - 2\alpha_n$$

$$+(\frac{B_2}{\alpha_{\max}}+\Delta\alpha+\alpha_n)(\Delta\alpha+\alpha_n-\alpha_{\max})(\frac{\eta}{\alpha_{\max}})\Big] \tag{16}$$

The choice of a good starting value for the iteration seems to be critical. For some reason values close to zero can make to algorithm not converge, or to find negative values, which is non physical. When a starting values of eg. 0.2 is chosen, it seem to be stable. There is room for improvement here.

2.2.7 Macroscopic tangent

To incorporate the heat term in the this in the global temperature field, we need to compute to tangent of the term $Q_\infty \Delta\alpha$. Therefore the sensitivity of $\Delta\alpha$ with respect to the temperature T needs to be computed $\dfrac{\partial\Delta\alpha}{\partial T}$

$$\frac{\partial\Delta\alpha}{\partial T} = \Delta t\tilde{A}(\alpha)\frac{\partial a(T)}{\partial T}, \text{ with} \tag{17}$$

$$\frac{\partial a(T)}{\partial T} = a(T)\frac{E_\mathrm{a}}{RT^2} \tag{18}$$

2.3 Coupling Material Properties to Degree of Hydration

2.3.1 Compressive and tensile strength

Both compressive and tensile strength can be approximated using an generalized exponential function,

$$X(\alpha) = \alpha(t)^{a_x} X_\infty. \tag{19}$$

This model has two parameter, X_∞, the value of the parameter at full hydration, $\alpha = 1$ and a_x the exponent, which is a purely numerical parameter, difficult to estimate directly from a mix design, as the mechanisms are quite complex. The first parameter could theoretically be obtained through experiments. However the total hydration can take years, therefore usually only the value after 28 days is obtained. For now we will assume X_∞ to be a fitting parameter as well. Hopefully a functional relation of the standardized X_28 values and the ultimate value can be approximated. To write (19) in terms of the compressive strength f_c and the tensile strength f_t

$$f_\mathrm{c}(\alpha) = \alpha(t)^{a_\mathrm{c}} f_{\mathrm{c}\infty} \tag{20}$$

$$f_\mathrm{t}(\alpha) = \alpha(t)^{a_\mathrm{t}} f_{\mathrm{t}\infty} \tag{21}$$

$$\tag{22}$$

The publication assumes for their "C1" mix values of $f_{\mathrm{c}\infty} = 62.1$ MPa , $a_{fc} = 1.2$,$f_{\mathrm{t}\infty} = 4.67$ MPa , $a_{fc} = 1.0$.

2.3.2 Young's Modulus

The publication proposes a new model for the evolution of the Young's modulus. Instead of the generalized model (19), the model assumes an initial linear increase of the Young's modulus up to a degree of hydration α_t.

$$E(\alpha < \alpha_t) = E_\infty \frac{\alpha(t)}{\alpha_t} \left(\frac{\alpha_t - \alpha_0}{1 - \alpha_0}\right)^{a_E} \tag{23}$$

$$E(\alpha \geq \alpha_t) = E_\infty \left(\frac{\alpha(t) - \alpha_0}{1 - \alpha_0}\right)^{a_E} \tag{24}$$

Values of α_t are assumed to be between 0.1 and 0.2. For the mix "C1" $\alpha_t = 0.09$, $\alpha_0 = 0.06$, $E_\infty = 54.2$ MPa, $a_E = 0.4$.

2.4 Fitting of model parameters

As an initial example I will use the concrete applied in the "Cost Action TU1404".

2.4.1 Task 1 Adiabatic temperature

Vol therm al capacity 2.4 x 10^6 in J/()m3 K)
therm conductivity 1.75 w/(mK)
Initial temperature 20 degree C
Temperature data given for two initial values (temp and time/hours) Fig 2
results: activation energy 4029-5402 K**-1

2.4.2 Task 2 temperature development in a massive cube

400 mm edge cube
20 degree ambient temp
CEM I (table 4) 52.5R and other stuff...
isothermal calorimetry data 20,30,40,50,60 degree c (fig 5)
Values used by team 2 for massive cube: q pot 500 J/g
Ea/R= 5653 1/K
B1 = 0.0002916 1/s
B2 = 0.0024229
alpha max = 0.875
eta = 5.554

3 Calibration

Here is an empty file as example to start the calibration section. Feel free to create as many sections as necessary :D.

4 Example code from template

4.1 Tables

Tables can be inserted via the normal table and tabular environment.

Table 1 Caption text

Column 1	Column 2	Column 3	Column 4
row 1	data 1	data 2	data 3
row 2	data 4	data 5[1]	data 6
row 3	data 7	data 8	data 9[2]

Source: This is an example of table footnote. This is an example of table footnote.

[1]Example for a first table footnote. This is an example of table footnote.

[2]Example for a second table footnote. This is an example of table footnote.

Table 2 Example of a lengthy table which is set to full textwidth

	Element 1[1]			Element 2[2]		
Project	Energy	σ_{calc}	σ_{expt}	Energy	σ_{calc}	σ_{expt}
Element 3	990 A	1168	1547 ± 12	780 A	1166	1239 ± 100
Element 4	500 A	961	922 ± 10	900 A	1268	1092 ± 40

Note: This is an example of table footnote. This is an example of table footnote this is an example of table footnote this is an example of table footnote this is an example of table footnote.

[1]Example for a first table footnote.

[2]Example for a second table footnote.

In case of double column layout, tables which do not fit in single column width should be set to full text width. For this, you need to use `\begin{table*} ... \end{table*}` instead of `\begin{table} ... \end{table}` environment. Lengthy tables which do not fit in textwidth should be set as rotated table. For this, you need to use `\begin{sidewaystable} ... \end{sidewaystable}` instead of `\begin{table*} ... \end{table*}` environment. This environment puts tables rotated to single column width. For tables rotated to double column width, use `\begin{sidewaystable*} ... \end{sidewaystable*}`.

Table 3 Tables which are too long to fit, should be written using the "sidewaystable" environment as shown here

Projectile	Element 1[1]			Element[2]		
	Energy	σ_{calc}	σ_{expt}	Energy	σ_{calc}	σ_{expt}
Element 3	990 A	1168	1547 ± 12	780 A	1166	1239 ± 100
Element 4	500 A	961	922 ± 10	900 A	1268	1092 ± 40
Element 5	990 A	1168	1547 ± 12	780 A	1166	1239 ± 100
Element 6	500 A	961	922 ± 10	900 A	1268	1092 ± 40

Note: This is an example of table footnote this is an example of table footnote this is an example of table footnote this is an example of table footnote this is an example of table footnote this is an example of table footnote.

[1]This is an example of table footnote.

4.2 Algorithms

Packages `algorithm`, `algorithmicx` and `algpseudocode` are used for setting algorithms in LaTeX using the format:

```
\begin{algorithm}
\caption{<alg-caption>}\label{<alg-label>}
\begin{algorithmic}[1]
. . .
\end{algorithmic}
\end{algorithm}
```

You may refer above listed package documentations for more details before setting `algorithm` environment. For program codes, the "program" package is required and the command to be used is `\begin{program}` ... `\end{program}`. A fast exponentiation procedure:

```
begin
  for i := 1 to 10 step 1 do
      expt(2, i);
      newline() od                Comments will be set flush to the right margin
where
proc expt(x, n) ≡
  z := 1;
  do if n = 0 then exit fi;
      do if odd(n) then exit fi;
          comment: This is a comment statement;
          n := n/2; x := x * x od;
      {n > 0};
      n := n − 1; z := z * x od;
  print(z).
end
```

Similarly, for `listings`, use the `listings` package. `\begin{lstlisting}` ... `\end{lstlisting}` is used to set environments similar to `verbatim` environment. Refer to the `lstlisting` package documentation for more details.

```
for i:=maxint to 0 do
begin
{ do nothing }
end;
Write('Case insensitive ');
Write('Pascal keywords.');
```

Algorithm 1 Calculate $y = x^n$

Require: $n \geq 0 \vee x \neq 0$
Ensure: $y = x^n$
$y \Leftarrow 1$
if $n < 0$ **then**
    $X \Leftarrow 1/x$
    $N \Leftarrow -n$
else
    $X \Leftarrow x$
    $N \Leftarrow n$
end if
while $N \neq 0$ **do**
    if N is even **then**
        $X \Leftarrow X \times X$
        $N \Leftarrow N/2$
    else[N is odd]
        $y \Leftarrow y \times X$
        $N \Leftarrow N - 1$
    end if
end while

Supplementary information. If your article has accompanying supplementary file/s please state so here.

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Acknowledgments. Acknowledgments are not compulsory. Where included they should be brief. Grant or contribution numbers may be acknowledged.

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Appendix A Section title of first appendix

An appendix contains supplementary information that is not an essential part of the text itself but which may be helpful in providing a more comprehensive understanding of the research problem or it is information that is too cumbersome to be included in the body of the paper.

References

Campbell SL, Gear CW (1995) The index of general nonlinear DAES. Numer Math 72(2):173–196