

Awesome Article Title

Atul Agrawal^{1*†}, Erik Tamsen^{2†}, Faidon-Stelios
Koutsourelakis¹ and Jörg F. Unger²

¹*Data-driven Materials Modeling, Technische Universität
München, Boltzmannstraße 15, Garching, 85748, Germany.

²Modeling and Simulation, Bundesanstalt für Materialforschung
und -prüfung, Unter den Eichen 87, Berlin, 12205, Germany.

*Corresponding author(s). E-mail(s): atul.agrawal@tum.de;

Contributing authors: erik.tamsen@bam.de;
p.s.koutsourelakis@tum.de; joerg.unger@bam.de;

[†]These authors contributed equally to this work.

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 ? expands on the background of the work (some overlap with the Abstract is acceptable). The introduction should not include subheadings.

Springer Nature does not impose a strict layout as standard however authors are advised to check the individual requirements for the journal they are planning to submit to as there may be journal-level preferences. When preparing your text please also be aware that some stylistic choices are not supported in full text XML (publication version), including coloured font. These will not be replicated in the typeset article if it is accepted.

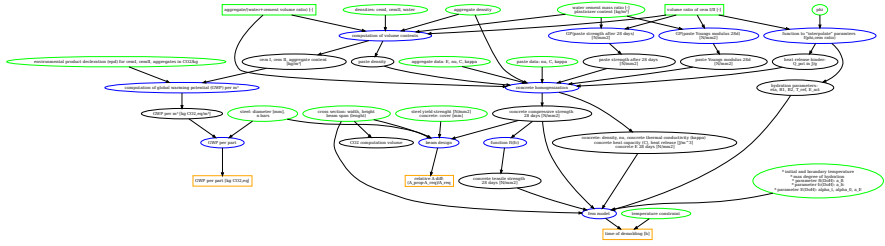


Fig. 1 Testing doit workflow. Figure is created by script. Macro for path is created by other script

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

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

λ is the effective thermal conductivity in $\text{Wm}^{-1}\text{K}^{-1}$. C is the specific heat capacity. ρ is the density. ρC is the volumetric heat capacity in $\text{Jm}^{-3}\text{K}^{-1}$. 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_∞ ,

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

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 ,

$$\frac{\partial Q}{\partial t} = \frac{\partial \alpha}{\partial t} Q_{\infty}. \quad (3)$$

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 $Q_{\infty} = 375\text{--}525$ or Pozzolanic cement $Q_{\infty} = 315\text{--}420$.

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

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

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

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

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

$$a = \exp \left(-\frac{E_a}{R} \left(\frac{1}{T} - \frac{1}{T_{\text{ref}}} \right) \right) \quad (6)$$

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

$$\alpha_{\max} = \frac{1.031w/c}{0.194 + w/c}, \quad (7)$$

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

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

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

2.2.4 Formulation

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

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

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

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

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

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

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 $\Delta \alpha$

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

Now we can solve the nonlinear function

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

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

$$\begin{aligned} \frac{\partial f}{\partial \Delta \alpha} &= 1 - \Delta t a(T) \frac{\partial \tilde{A}}{\partial \Delta \alpha} \quad \text{with} \quad (15) \\ \frac{\partial \tilde{A}}{\partial \Delta \alpha} &= B_1 \exp \left(-\eta \frac{\Delta \alpha + \alpha_n}{\alpha_{\max}} \right) \left[\alpha_{\max} - \frac{B_2}{\alpha_{\max}} - 2\Delta \alpha - 2\alpha_n \right. \\ &\quad \left. + \left(\frac{B_2}{\alpha_{\max}} + \Delta \alpha + \alpha_n \right) (\Delta \alpha + \alpha_n - \alpha_{\max}) \left(\frac{\eta}{\alpha_{\max}} \right) \right] \quad (16) \end{aligned}$$

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 $\frac{\partial \Delta\alpha}{\partial T}$

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

$$\frac{\partial a(T)}{\partial T} = a(T) \frac{E_a}{RT^2} \quad (18)$$

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,

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

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

$$f_c(\alpha) = \alpha(t)^{a_c} f_{c\infty} \quad (20)$$

$$f_t(\alpha) = \alpha(t)^{a_t} f_{t\infty} \quad (21)$$

$$(22)$$

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

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 .

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

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

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 2.4×10^6 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 Example code from template

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

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 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.

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

²Example 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

Project	Element 1 ¹			Element 2 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

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.

¹Example for a first table footnote.

²Example for a second table footnote.

4 Algorithms, Program codes and Listings

Packages `algorithm`, `algorithmicx` and `algpseudocode` are used for setting algorithms in L^AT_EX 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
     $\text{expt}(2, i)$ ;
```

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}	Energy	σ_{expt}
Element 3	990 A	1168	780 A	1239 \pm 100
Element 4	500 A	961	900 A	1092 \pm 40
Element 5	990 A	1168	780 A	1239 \pm 100
Element 6	500 A	961	900 A	1092 \pm 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.

¹This is an example of table footnote.


```

        newline() od           Comments will be set flush to the right margin
where
proc expt( $x, n$ )  $\equiv$ 
   $z := 1$ ;
  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

```

Algorithm 1 Calculate $y = x^n$

Require: $n \geq 0 \vee x \neq 0$

Ensure: $y = x^n$

```

1:  $y \leftarrow 1$ 
2: if  $n < 0$  then
3:    $X \leftarrow 1/x$ 
4:    $N \leftarrow -n$ 
5: else
6:    $X \leftarrow x$ 
7:    $N \leftarrow n$ 
8: end if
9: while  $N \neq 0$  do
10:  if  $N$  is even then
11:     $X \leftarrow X \times X$ 
12:     $N \leftarrow N/2$ 
13:  else [ $N$  is odd]
14:     $y \leftarrow y \times X$ 
15:     $N \leftarrow N - 1$ 
16:  end if
17: end while

```

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

```

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

```

5 Cross referencing

Environments such as `figure`, `table`, `equation` and `align` can have a label declared via the `\label{#label}` command. For figures and table environments use the `\label{}` command inside or just below the `\caption{}` command. You can then use the `\ref{#label}` command to cross-reference them. As an example, consider the label declared for Figure ?? which is `\label{fig1}`. To cross-reference it, use the command `Figure \ref{fig1}`, for which it comes up as “Figure ??”.

To reference line numbers in an algorithm, consider the label declared for the line number 2 of Algorithm 1 is `\label{algln2}`. To cross-reference it, use the command `\ref{algln2}` for which it comes up as line 2 of Algorithm 1.

5.1 Details on reference citations

Standard L^AT_EX permits only numerical citations. To support both numerical and author-year citations this template uses `natbib` L^AT_EX package. For style guidance please refer to the template user manual.

Here is an example for `\cite{...}`: ?. Another example for `\citep{...}`: (?). For author-year citation mode, `\cite{...}` prints Jones et al. (1990) and `\citep{...}` prints (Jones et al., 1990).

All cited bib entries are printed at the end of this article: ?, ?, ?, ?, ?, ?, ?, ?, ? and ?.

6 Examples for theorem like environments

For theorem like environments, we require `amsthm` package. There are three types of predefined theorem styles exists—`thmstyleone`, `thmstyletwo` and `thmstylethree`

<code>thmstyleone</code>	Numbered, theorem head in bold font and theorem text in italic style
<code>thmstyletwo</code>	Numbered, theorem head in roman font and theorem text in italic style
<code>thmstylethree</code>	Numbered, theorem head in bold font and theorem text in roman style

For mathematics journals, theorem styles can be included as shown in the following examples:

Theorem 1 (Theorem subhead) *Example theorem text. Example theorem text. Example theorem text. Example theorem text. Example theorem text. Example theorem text. Example theorem text. Example theorem text. Example theorem text. Example theorem text.*

Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text.

Proposition 2 *Example proposition text. Example proposition text. Example proposition text. Example proposition text. Example proposition text. Example proposition text. Example proposition text. Example proposition text. Example proposition text.*

Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text.

Example 1 Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem.

Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text.

Remark 1 Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem.

Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text.

Definition 1 (Definition sub head) Example definition text. Example definition text. Example definition text. Example definition text. Example definition text. Example definition text. Example definition text.

Additionally a predefined “proof” environment is available: `\begin{proof} ... \end{proof}`. This prints a “Proof” head in italic font style and the “body text” in the roman font style with an open square at the end of each proof environment.

Proof Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. □

Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text. Sample body text.

Proof of Theorem 1 Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. Example for proof text. □

For a quote environment, use `\begin{quote}...\end{quote}`

Quoted text example. Aliquam porttitor quam a lacus. Praesent vel arcu ut tortor cursus volutpat. In vitae pede quis diam bibendum placerat. Fusce elementum convallis neque. Sed dolor orci, scelerisque ac, dapibus nec, ultricies ut, mi. Duis nec dui quis leo sagittis commodo.

Sample body text. Sample body text. Sample body text. Sample body text. Sample body text (refer Figure ??). Sample body text. Sample body text. Sample body text (refer Table 3).

7 Methods

Topical subheadings are allowed. Authors must ensure that their Methods section includes adequate experimental and characterization data necessary for others in the field to reproduce their work. Authors are encouraged to include RIIIDs where appropriate.

Ethical approval declarations (only required where applicable) Any article reporting experiment/s carried out on (i) live vertebrate (or higher invertebrates), (ii) humans or (iii) human samples must include an unambiguous statement within the methods section that meets the following requirements:

1. Approval: a statement which confirms that all experimental protocols were approved by a named institutional and/or licensing committee. Please identify the approving body in the methods section
2. Accordance: a statement explicitly saying that the methods were carried out in accordance with the relevant guidelines and regulations
3. Informed consent (for experiments involving humans or human tissue samples): include a statement confirming that informed consent was obtained from all participants and/or their legal guardian/s

If your manuscript includes potentially identifying patient/participant information, or if it describes human transplantation research, or if it reports results of a clinical trial then additional information will be required. Please visit (<https://www.nature.com/nature-research/editorial-policies>) for Nature Portfolio journals, (<https://www.springer.com/gp/authors-editors/>

[journal-author/journal-author-helpdesk/publishing-ethics/14214](#)) for Springer Nature journals, or (<https://www.biomedcentral.com/getpublished/editorial-policies#ethics+and+consent>) for BMC.

8 Discussion

Discussions should be brief and focused. In some disciplines use of Discussion or ‘Conclusion’ is interchangeable. It is not mandatory to use both. Some journals prefer a section ‘Results and Discussion’ followed by a section ‘Conclusion’. Please refer to Journal-level guidance for any specific requirements.

9 Conclusion

Conclusions may be used to restate your hypothesis or research question, restate your major findings, explain the relevance and the added value of your work, highlight any limitations of your study, describe future directions for research and recommendations.

In some disciplines use of Discussion or ‘Conclusion’ is interchangeable. It is not mandatory to use both. Please refer to Journal-level guidance for any specific requirements.

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

Authors reporting data from electrophoretic gels and blots should supply the full unprocessed scans for key as part of their Supplementary information. This may be requested by the editorial team/s if it is missing.

Please refer to Journal-level guidance for any specific requirements.

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

Please refer to Journal-level guidance for any specific requirements.

Declarations

Some journals require declarations to be submitted in a standardised format. Please check the Instructions for Authors of the journal to which you are submitting to see if you need to complete this section. If yes, your manuscript must contain the following sections under the heading ‘Declarations’:

- Funding
- Conflict of interest/Competing interests (check journal-specific guidelines for which heading to use)
- Ethics approval
- Consent to participate
- Consent for publication
- Availability of data and materials
- Code availability

- Authors' contributions

If any of the sections are not relevant to your manuscript, please include the heading and write 'Not applicable' for that section.

Editorial Policies for:

Springer journals and proceedings:

<https://www.springer.com/gp/editorial-policies>

Nature Portfolio journals:

<https://www.nature.com/nature-research/editorial-policies>

Scientific Reports:

<https://www.nature.com/srep/journal-policies/editorial-policies>

BMC journals:

<https://www.biomedcentral.com/getpublished/editorial-policies>

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.