Computational Materials Science and Engineering of Concrete: Computational rheology and pumping of concrete

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November 10, 2022, Astana
Warm-up Questions

What is the most consumed substance in the world?

What is the second most consumed substance in the world?

What is the most consumed man-made material in the world?
Warm-up Questions

Hoover Dam (Since 1936)  Three Gorges Dam (Since 2003)

https://www.britannica.com/topic/Hoover-Dam#/media/1/271416/213566
https://www.britannica.com/topic/Three-Gorges-Dam#/media/1/593760/113950 (Access Date: November 10, 2022)
Warm-up Questions

What is the most consumed substance in the world?  
**Water**

What is the second most consumed substance in the world?  
**Concrete**

What is the most consumed man-made material in the world?  
**Concrete**

Worldwide, over ten billion tons of concrete are being produced each year.
How cement is made

CO₂ → Rotating kiln → Clinker → Hot air
Ground limestone + clay


https://www.giatecscientific.com/education/concrete-mix-design-just-got-easier/
Burj Khalifa set new standards for reinforced-concrete construction, but there is no room for complacency in future projects.

Materials Science and Engineering of Concrete

The traditional materials science tetrahedron

The emerging systems materials engineering triangle

“System-level planning of theoretical and experimental efforts is increasingly important for the development of modern materials science.”

Materials Science and Engineering of Concrete

Admixtures
• Mineral admixtures
• Chemical admixtures

Admixtures in concrete are like spices in food.
Computational Materials Science and Engineering of Concrete

The traditional materials science tetrahedron

Selected Topics for Computational Studies

- Design of chemical admixtures
- Mix design
- Composition $\rightarrow$ Processing $\rightarrow$ Structure $\rightarrow$ Properties $\rightarrow$ Performance (PSPP) relationships
- Influences of temperature, humidity, and other environmental factors
- Improvement of concrete processability (workability)
- Improvement of concrete durability
- Life Cycle Assessments (LCA)
- Service life prediction
The emerging systems materials engineering triangle

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Computational Materials Science and Engineering of Concrete

The four paradigms of science: empirical, theoretical, computational, and data-driven


https://doi.org/10.1063/1.4946894
Multi-scale & Multi-physics-based Modelling

Shi et al. (2015). Multi-scale computation methods: Their applications in lithium-ion battery research and development. Chinese Physics B, 25(1), 018212.

https://doi.org/10.1088/1674-1056/25/1/018212
Computational Rheology of Concrete

Rheology
rheo: ‘flow’; -logy: 'study of'

Wikipedia:
- Rheology is the study of the flow of matter
- Rheology deals with the deformation and flow of materials

Given composition, can we **compute** the rheological properties of concrete?
Rheology of Concrete

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- Rheology deals with the deformation and flow of materials

Given composition, can we measure the rheological properties of concrete?
Rheology of Fresh Cement and Concrete, Edited By P.F.G. Banfill, 1990

Understanding the Rheology of Concrete, Edited by Nicolas Roussel, 2016

Rheology and Processing of Construction Materials, RheoCon2 & SCC9, Edited by Viktor Mechtherine, Kamal Khayat, Egor Secrieru, 2020

Rheology of Fresh Cement-Based Materials Fundamentals, Measurements, and Applications. By Qiang Yuan, Caijun Shi, Dengwu Jiao. 2023
Rheology as a tool in concrete science: The use of rheographs and workability boxes

Olafur Haraldsson Wallevik\textsuperscript{a}, Jon Elvar Wallevik\textsuperscript{b,*}

\textsuperscript{a} IC Rheocenter, Reykjavik University, Innovation Center Iceland, Keldnaholt, IS-112 Reykjavik, Iceland
\textsuperscript{b} IC Rheocenter, Innovation Center Iceland, Keldnaholt, IS-112 Reykjavik, Iceland

\textbf{A B S T R A C T}

Rheology can supply valuable and practical information regarding the properties of fresh concrete, how to reach an optimization of the product and how to attain it by the use of rheograph. Otherwise, the optimization is largely based on feeling. The rheograph reveals in a systematic way the effects of diverse changes on the rheological behavior of the cement based suspension and thus is a convenient and essential tool to compare different concrete types and examine the behavior relative to changed quantities of constituents. Effects of many admixtures as well as the basic constituents of fresh concrete have been revealed in rheographs. In principle the effect of two or more constituents can be added in a rheograph to estimate the combined effect, which constitutes a so-called vectorized-rheograph approach.

Different applications and types of concrete like slipform, underwater, and high strength, are described by workability boxes. New rheograph with boxes for various types of self compacting concrete is proposed.

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\begin{align*}
\text{Bingham Model} \\
&\quad \text{Yield stress: } \tau_0 \\
&\quad \text{Plastic viscosity: } \mu
\end{align*}
Rheology of Concrete: Rheograph

Bingham Model
- Yield stress: $\tau_0$
- Plastic viscosity: $\mu$

$\tau = \eta \dot{\gamma} = \mu \dot{\gamma} + \tau_0$
CVC = Conventional vibrated concrete; SCC = Self-Compacting Concrete (Self-consolidating concrete);
Easy-CC = East compacting concrete; HY-SCC = High yield SCC; LV-SCC = Low-viscous SCC
LV-HY-SCC = Low-viscous high-yield SCC
**Rheology of Concrete**

Why is fresh self-compacting concrete shear thickening?

*J. F. Faye, R. Verhoeven, G. De Schutter - Cement and Concrete Research, 2009 - Elsevier*

Results on cement pastes prove that the grain inertia theory is not the main... of shear thickening in self-compacting concrete. The influence of several parameters on the shear thickening... ★ Save  Cite  Cited by 222  Related articles  All 7 versions  Web of Science: 144

Fresh self compacting concrete, a shear thickening material

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**Bingham Model (1917)**

\[
\begin{align*}
\tau &= \tau_0 + \mu \dot{\gamma} & \text{for } \tau > \tau_0 \\
\dot{\gamma} &= 0 & \text{for } \tau \leq \tau_0
\end{align*}
\]

**Herschel–Bulkley Model (1926)**

\[
\begin{align*}
\tau &= \tau_0 + K \dot{\gamma}^n & \text{for } \tau > \tau_0 \\
\dot{\gamma} &= 0 & \text{for } \tau \leq \tau_0
\end{align*}
\]
Rheology of Concrete

Modified Bingham Model (Yahia2001, Feys2007)
\[
\begin{align*}
\tau &= \tau_0 + \mu_p \dot{\gamma} + A_2 \dot{\gamma}^2 & \text{for } \tau > \tau_0 \\
\dot{\gamma} &= 0 & \text{for } \tau \leq \tau_0
\end{align*}
\]

“Generalized Bingham” Model: A four-parameter model
(Our work; Under review)
\[
\begin{align*}
\tau &= \tau_0 + \mu_p \dot{\gamma} + K \dot{\gamma}^n & \text{for } \tau > \tau_0 \\
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\]

Zhaidarbek, Balnur and Tleubek, Aruzhan and Berdibek, Galymbek and Wang, Yanwei, Analytical Predictions of Concrete Pumping: Extending the Khatib-Khayat Model to Herschel-Bulkley and Modified Bingham Fluids. Available at SSRN: https://ssrn.com/abstract=4188701 or http://dx.doi.org/10.2139/ssrn.4188701
Table 1. Some special cases of the generalized Bingham model proposed by Zhaidarbek et al. [32]. The constitutive equation corresponds to $\tau \geq \tau_0$.

<table>
<thead>
<tr>
<th>Fluid type</th>
<th>Constitutive model</th>
<th>Rheological parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$\tau_0$</td>
</tr>
<tr>
<td>Newtonian</td>
<td>$\tau = \mu \dot{\gamma}$</td>
<td>0</td>
</tr>
<tr>
<td>Power-law [36,37]</td>
<td>$\tau = K \dot{\gamma}^n$</td>
<td>0</td>
</tr>
<tr>
<td>Sisko [38]</td>
<td>$\tau = \mu_p \dot{\gamma} + K \dot{\gamma}^n$</td>
<td>0</td>
</tr>
<tr>
<td>Bingham</td>
<td>$\tau = \tau_0 + \mu_p \dot{\gamma}$</td>
<td>$\tau_0$</td>
</tr>
<tr>
<td>Casson</td>
<td>$\sqrt{\tau} = \sqrt{\tau_0 + \mu_p \dot{\gamma}}$</td>
<td>$\tau_0$</td>
</tr>
<tr>
<td>Herschel–Bulkley</td>
<td>$\tau = \tau_0 + K \dot{\gamma}^n$</td>
<td>$\tau_0$</td>
</tr>
<tr>
<td>modified Bingham</td>
<td>$\tau_0 + \mu_p \dot{\gamma} + A_2 \dot{\gamma}^2$</td>
<td>$\tau_0$</td>
</tr>
<tr>
<td>Caggioni et al. [33]</td>
<td>$\tau = \tau_0 + \mu_p \dot{\gamma} + K \dot{\gamma}^{1/2}$</td>
<td>$\tau_0$</td>
</tr>
</tbody>
</table>
Figure 1. Schematic representation of the relations between the different rheological models investigated in this work.
Rheology of Concrete

Wang et al. In Preparation (2022)

Five-parameter (5P) model

\[ \tau^m = \tau_0^m + (\mu_p \dot{\gamma})^m + K \dot{\gamma}^n \]

(Parameters: \( \tau_0, \mu_p, K, m, n \))

**Question 1:** Can those model parameters be measured in experiments?

**Question 2:** Can those models be used for anything?

**Figure 1.** Schematic representation of the relations between the different rheological models investigated in this work.
Pumping of Concrete

Pumping of Concrete

Pumping of Concrete

Challenges

(1) Formation of *lubrication layer* in high-performance concrete
(2) Test methods for evaluation of pumpability of fresh concrete
(3) Bends and reducers
(4) Changes in concrete properties due to pumping
(5) Active control

Figure 1. Pumping pressure is well predicted based on Kaplan’s model [14], based on tribology and rheology measurements on different types of concrete. Figure modified from [24].
Pumping of concrete: Understanding a common placement method with lots of challenges

Dimitri Feys\textsuperscript{a,}\textsuperscript{,}a, Geert De Schutter\textsuperscript{b}, Shirin Fataei\textsuperscript{c}, Nicos S. Martys\textsuperscript{d}, Viktor Mechtcherine\textsuperscript{c}

\textsuperscript{a} Department of Civil, Architectural, and Environmental Engineering, Missouri University of Science and Technology, 1401 N. Pine Street, Rolla, MO 65409, United States
\textsuperscript{b} Magel-Vandeputte Laboratory, Department of Structural Engineering and Building Materials, Ghent University, Ghent, Belgium
\textsuperscript{c} Institute of Construction Materials, Technische Universität Dresden, Georg-Schumann-Straße 67, 01067 Dresden, Germany
\textsuperscript{d} Materials and Structural Systems Division, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899, United States

\textbf{ARTICLE INFO}

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Concrete
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 Rheology
Numerical simulation

\textbf{ABSTRACT}

Several million cubic meters of concrete are pumped daily, as this technique permits fast construction. Fundamental research has been performed and practical guidelines have been developed to aid concrete behavior in pipes. However, the pumping process and concrete properties are understood. This paper gives an overview of the current knowledge of concrete pumpability and the flow of concrete in pipes are introduced. A series of experimental studies on concrete flow behavior near a smooth wall to predict pressure-flow rate relationships is discussed. Recent developments in the use of numerical simulations of concrete behavior in pipes are highlighted. The influence of the pumping process on concrete rheology and air-void system is reviewed, and the first developments in active rheology control for concrete pumping are introduced. The last section of this paper gives an overview of open research questions and challenges.
Formation of Lubrication Layer

Fig. 1. Schematic pattern of concrete flow in the pipe.

Solving the Hagen–Poiseuille flow (laminar flow in a pipe) using rheological parameters ($\eta$) of bulk concrete will **over-estimate** the needed pressure for a given flow rate.

Kaplan *et al.* [ACI Materials Journal 2005] considered the formation of a **lubrication layer (LL)** and introduced a **slip-velocity** between bulk concrete and the pipe wall. The Bingham model is used for bulk concrete. The slip-velocity approach corresponds to an infinitely thin LL ($\ell/R \to 0$).
Rami Khatib and Kamal H. Khayat [ACI Materials Journal 2021] relaxed the assumption of an infinitely thin LL ($\ell/R \to 0$) and developed a **two-fluid model**, where both the LL fluid and the bulk concrete are described by the Bingham model.

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**Fig. 6.** Validation of Kaplan’s equations predicting pumping pressure [26,36], based on interface and bulk concrete rheology, pipe radius and flow rate. Measurements are performed on pumpable concrete mixtures with varying consistencies (CVC = conventional vibrated concrete, SCC = self-consolidating concrete, HWC = highly workable concrete with consistency between CVC and SCC). Figure adapted from [52].
Analytical Predictions of Concrete Pumping

Khatib-Khayat Model for Pumping Flowable Concrete

Rheology of Concrete

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Herschel–Bulkley Model (1926)
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Rheology of Concrete

Five-parameter (5P) model
\[ \tau^m = \tau_0^m + (\mu_p \dot{\gamma})^m + K \dot{\gamma}^n \] (Parameters: \( \tau_0, \mu_p, K, m, n \))

4P Models
- Generalized Casson Model
  \[ \tau^m = \tau_0^m + K \dot{\gamma}^n \]
- Generalized Bingham Model
  \[ \tau = \tau_0 + \mu_p \dot{\gamma} + K \dot{\gamma}^n \]
- Carreau-Yasuda model with \( \eta_\infty = 0 \)

3P Models
- Heinz-Casson model
  \[ \tau^n = \tau_0^n + (\mu_p \dot{\gamma})^n \]
- Herschel–Bulkley Model
  \[ \tau = \tau_0 + K \dot{\gamma}^n \]
- Modified Bingham Model
  \[ \tau = \tau_0 + \mu_p \dot{\gamma} + A_2 \dot{\gamma}^2 \]
- Caggioni et al. (2020)
  \[ \tau = \tau_0 + \mu_p \dot{\gamma} + K \dot{\gamma}^{1/2} \]

**Figure 1.** Schematic representation of the relations between the different rheological models investigated in this work.
Analytical Predictions of Concrete Pumping

(a) Pressure drop, $\Delta P = P_0 - P_L > 0$

Fluid rheology, $\dot{\eta}$
Volumetric flow rate, $Q$

Pressure drop per unit length of the pipe, $G = \Delta P / L$

$Q = Q(\dot{\eta}, R, G) = ?$

(b) Rheological properties of the bulk central fluid, $\dot{\eta}_C$
Rheological properties of the Lubrication layer fluid, $\dot{\eta}_{LL}$

Total volumetric flow rate, $Q_{tot} = Q_{tot}(\dot{\eta}_C, \dot{\eta}_{LL}, R, \ell, G) = ?$

Inputs
- Pressure drop per unit length: $G = \Delta P / L$
- Pipe radius (or diameter, $D$): $R = D / 2$
- Fluid rheology: $\dot{\eta} = \{\tau_0, \mu_p, K, m, n\}$

Nondimensionalization
- Base units
  - Pipe radius: $R$
  - Wall shear stress: $\tau_{wall}$
  - Wall shear rate: $\dot{\gamma}_{wall}$

Outputs
- Flow rate as a function of the inputs
  - $\bar{u}_{avg} = \frac{1}{3}[1 - A_3(\tau_0, \mu_p, R, m, n)]$
  - $Q = \pi R^3 \dot{\gamma}_{wall} \bar{u}_{avg}$

Contributions to the flow rate
- $Q_1 = Q_{HP}(\dot{\eta}_{LL}, R, G)$
- $Q_2 = Q_{HP}(\dot{\eta}_{LL}, R - \ell, G)$
- $Q_3 = Q_{HP}(\dot{\eta}_C, R - \ell, G)$

CVC

If $r_{plug} < R - \ell$
- False
  - $Q = Q_1 - Q_2$

If $r_{plug} \geq R - \ell$
- True
  - $Q = Q_1 - Q_2 + Q_3$

Wang et al. In Preparation (2022)
Analytical Predictions of Concrete Pumping

Given a complex generalized Newtonian model, how do we obtain the flow rate – pressure drop relation in Hagen–Poiseuille flow?

Inputs
- Pressure drop per unit length: $G = \Delta P / L$
- Pipe radius (or diameter, $D$): $R = D / 2$
- Fluid rheology: $\eta = \{\tau_0, \mu_p, K, m, n\}$

Nondimensionalization
- Base units
  - Pipe radius: $R$
  - Wall shear stress: $\tau_{\text{wall}}$
  - Wall shear rate: $\dot{\gamma}_{\text{wall}}$

Outputs
- Flow rate as a function of the inputs
  - $\bar{u}_{\text{avg}} = \frac{1}{3} \left[ 1 - A_3(\bar{\tau}_0, \bar{\mu}_p, \bar{K}, m, n) \right]$
  - $Q = \pi R^3 \dot{\gamma}_{\text{wall}} \bar{u}_{\text{avg}}$

Inputs in dimensionless form
- Pressure drop per unit length: $\tilde{G} = 2$
- Pipe radius: $R = 1$
- Fluid rheology: $\tilde{\eta} = \{\tilde{\tau}_0, \tilde{\mu}_p, \tilde{K}, m, n\}$

Analytical Predictions of Concrete Pumping

How to prove our approach for obtaining the flow rate – pressure drop relation in Hagen–Poiseuille flow of two-fluids?

(a) Pressure drop, $\Delta P = P_0 - P_L > 0$

Fluid rheology, $\bar{\eta}$

Volumetric flow rate, $Q$

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Total volumetric flow rate, $Q_{tot} = Q_{tot}(\bar{\eta}_C, \bar{\eta}_{LL}, R, \ell, G) = ?$

CVC

$$Q = Q_{HP}(\bar{\eta}_{LL}, R, G) - Q_{HP}(\bar{\eta}_{LL}, R - \ell, G)$$

SCC

$$Q = Q_{HP}(\bar{\eta}_{LL}, R, G) - Q_{HP}(\bar{\eta}_{LL}, R - \ell, G) + Q_{HP}(\bar{\eta}_C, R - \ell, G)$$

Analytical Predictions of Concrete Pumping: Extending the Khatib-Khayat Model to Herschel-Bulkley and Modified Bingham Fluids

Balnur Zhaidarbek, Aruzhan Tleubek, Galymbek Berdibek, Yanwei Wang

Analytical Predictions of Concrete Pumping

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- Nazarbayev University for Generous research funding
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Comments and suggestions are very welcome.

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