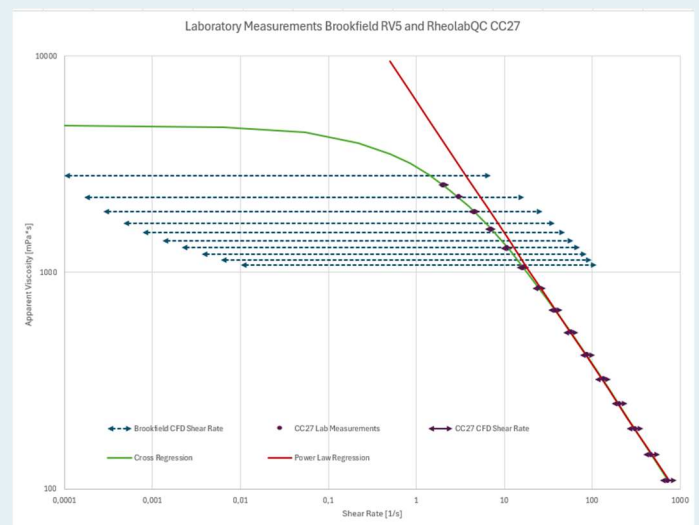
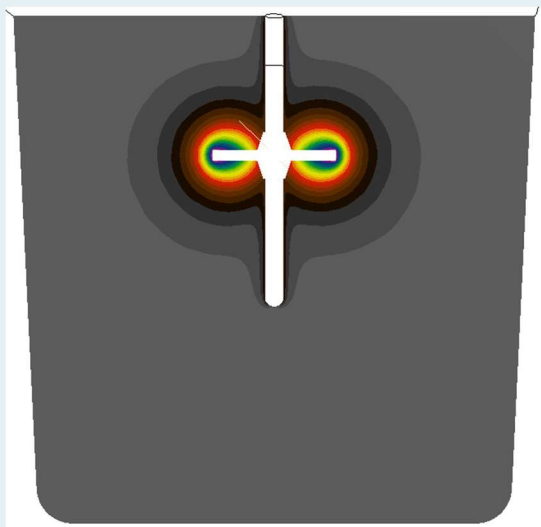




CFD-AI methodology for translating Brookfield measurements into rheometer data

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Thesis for the degree of Master of Science in Engineering
Department of Process and Life Science Engineering
LTH, Faculty of Engineering | Lund University



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June 2026



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Declaration on the Use of AI Tools

AI-based tools were used as supportive aids during the preparation of this thesis. Their use was limited to language refinement, summarization, restructuring of text, and discussion of possible interpretations or formulations. In particular, AI was used as a writing-support tool and as a sounding board during the development of the thesis text.

The scientific content of the thesis, including experimental measurements, CFD simulations, regression procedures, neural network training, data analysis, and interpretation of results, was produced and critically evaluated by the authors. AI tools were not used to create or replace experimental data, simulation data, or final conclusions. All AI-assisted text suggestions were reviewed and edited before being included in the final document.

Acknowledgement

This thesis was carried out in collaboration between the Department of Process and Life Science Engineering at Lund University, and Tetra Pak Processing Systems AB.

We would like to express our sincere gratitude to our industrial supervisors, Dragana Arlov, Hannah Viklund and Sofia Klasen for their continuous support, valuable feedback, and practical insight throughout the project. Their guidance has been highly valuable.

We are also very grateful to our university supervisor, Bernt Nilsson, for his support and guidance throughout this work. We especially appreciate his calm and steady approach during the challenges encountered along the way.

Also, we would like to thank Lecturer Niklas Andersson, the examiner, for reviewing this work.

Finally, we would like to thank our friends and family for their continuous support and encouragement throughout this process

Abstract

Brookfield viscometers are widely used in industrial quality control because they are simple and practical, but the viscosity values obtained are relative to the instrument, spindle, container geometry, and measurement procedure. In contrast, rotational rheometers such as the Anton Paar RheolabQC provide more defined rheological data under controlled shear conditions.

This thesis developed and evaluated a novel workflow combining computational fluid dynamics (CFD) and artificial intelligence (AI) to link Brookfield measurements to rheological model parameters that can be used in CFD simulations. The method combines experimental measurements with the Brookfield DV2T-RV with RV5 spindle and Anton Paar RheolabQC with CC27 geometry, Cross model regression, CFD validation, CFD-generated dataset creation, and artificial neural network prediction into one integrated framework.

An initial Power Law-based approach demonstrated that AI could learn the relationship between CFD-generated torque in the RV5 geometry and rheological parameters, but laboratory comparison showed that the Power Law model was insufficient for transfer between the RV5 and CC27 geometries. Shear rate profile analysis showed that the CC27 geometry mainly samples a higher and narrower shear rate range, while the RV5 includes very low shear rates even at high RPM. The Cross model was therefore selected because it can represent the low-shear plateau, transition region, and shear-thinning behaviour.

CMC30000 solutions at 1.0, 1.4, and 1.5 wt% were used to span a broad torque range measured using the Brookfield viscometer. Due to higher variability in the 1.5 wt% measurements, the main validation and AI evaluation focused on the 1.0 and 1.4 wt% solutions.

CFD validation showed that Cross model parameters regressed from CC27 geometry data reproduced CC27 torque well when end-effect correction was included, reducing the mean torque deviation to approximately 1%. Artificial neural networks were then trained on 5400 CFD-generated RV5 simulations to predict Cross model parameters from Brookfield-type inputs. Both 5-point and 10-point models achieved high accuracy on synthetic test data, but the 10-point model gave lower maximum errors and better torque reconstruction. When AI-predicted parameters were reintroduced into CFD, the 10-point model reproduced measured torque from the Brookfield viscometer with mean deviations of approximately -1.74% to $+0.49\%$ for 1.0 wt% and -1.41% to $+0.16\%$ for 1.4 wt%.

The results show that the developed CFD-AI workflow is a promising proof-of-concept for obtaining CFD-usable Cross parameter estimates from controlled Brookfield measurements. The method is especially valuable because it demonstrates a practical route from simple industrial viscosity measurements to simulation-ready parameter estimates. Although the AI-predicted parameters did not fully match the CC27 geometry-regressed rheological parameters, the torque agreement achieved with the 10-point model indicates strong potential for further development. With improved low-shear measurements, broader CFD datasets, refined uncertainty modelling, and validation on additional fluids and spindle geometries, the workflow could become a useful tool for industrial rheological characterization and process simulation.

Key words: CFD, artificial neural networks, shear-thinning fluids, Cross model, CMC, relative viscometry, absolute rheometry, method development, food engineering.

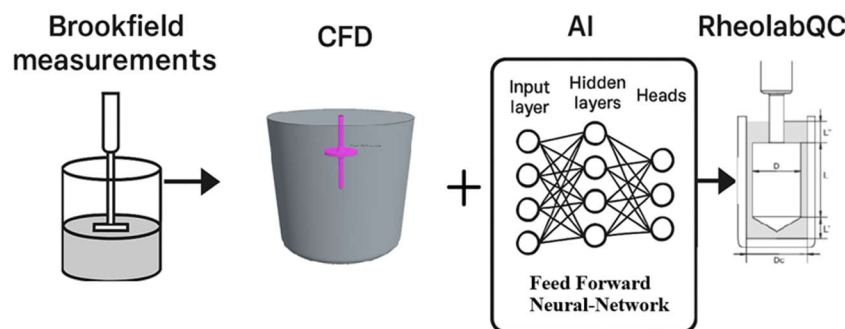
Popular Science Summary - From Simple Viscosity Tests to Useful Design Parameters

What if a simple factory-floor viscosity measurement could help predict how a sauce, cream, or dairy product behaves in a production line? This thesis explores how computer simulations and artificial intelligence can turn simple industrial measurements into more useful process data.

Many food products, such as sauces, creams, dairy products, and other liquid foods, do not flow like water. Some become thinner when they are pumped, stirred, or mixed. This behaviour is important in food production because it affects how products move through pipes, how they are heated, filled into packages, and how stable the final product feels to the consumer.

In industry, viscosity is often measured using simple instruments called Brookfield viscometers. These instruments are practical, robust, and widely used for quality control. However, the values they give depend on the exact measurement setup, such as the rotating measuring tool, container, and procedure. This means that Brookfield measurements are useful for comparing whether a product has changed relative to a previous measurement, but harder to use directly for process design and computer simulations. More advanced laboratory instruments, such as rotational rheometers, can measure flow behaviour under more controlled conditions. These measurements are better suited for describing material properties, but are less common in daily production environments. This creates a gap between practical industrial measurements and the rheological data needed for process calculations.

The aim of this thesis was to investigate whether this gap can be reduced using computer simulations and artificial intelligence. In simple terms, the simulations imitated how the fluid behaves inside the measuring instruments, while the artificial intelligence model was trained to connect simple Brookfield measurements to more useful descriptions of the fluid's flow behaviour.



At first, a simpler mathematical description of the fluid was tested. This showed that artificial intelligence could learn useful patterns from simulated measurement data. However, the two instruments do not “feel” the fluid in exactly the same way. The Brookfield instrument captures more of the slow-moving behaviour of the fluid, while the laboratory rheometer measures under more controlled conditions. Because many food-like fluids behave differently depending on how strongly they are stirred, a more flexible model was needed.

To test the method, controlled model fluids were used. These fluids become thinner when stirred faster, in a similar way to many food products. The results showed that the developed workflow could reproduce Brookfield measurements with good accuracy, especially when more measurement points were used. This suggests that relatively simple viscosity measurements can be transformed into information that is more useful for process calculations and simulations.

The method is not yet a complete replacement for advanced laboratory measurements. The predicted fluid properties did not always match the laboratory-derived values exactly. However, the results show strong potential for creating a practical bridge between everyday production measurements and advanced process design tools. With more testing on different fluids and measurement setups, this type of workflow could help engineers make better use of simple viscosity measurements when designing and optimizing food production processes.

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Nomenclature

Abbreviations

Abbreviation	Meaning
AI	Artificial intelligence
ANN	Artificial neural network
CAD	Computer-aided design
CC27	Anton Paar concentric-cylinder measuring geometry
CFD	Computational fluid dynamics
CMC	Sodium carboxymethyl cellulose
CSR	Controlled shear rate
CSS	Controlled shear stress
FFNN	Feed-forward neural network
GRG	Generalized reduced gradient
MLP	Multilayer perceptron
MRE	Mean relative error
MSE	Mean squared error
ReLU	Rectified linear unit
RPM	Revolutions per minute
RV5	Brookfield RV5 spindle
SSE	Sum of squared errors
WMSE	Weighted mean squared error

Symbols and Variables

Symbol	Meaning	Unit
$\%Tm$	Percentage of maximum torque	%
A	Area over which force acts	m ²
c_L	End-effect correction factor	–
D	Diameter	m
D_c	Cup diameter	m
F	Applied force	N
h	Gap height	m
K	Power Law consistency index	Pa·s ⁿ
L	Effective measuring length	m
L_b	Length or height of bob	m
m	Cross rate constant / Cross exponent	–
n	Power Law flow behaviour index	–

Symbol	Meaning	Unit
N	Selected rotational speed	RPM
R_b	Radius of bob	m
R_c	Inner radius of cup or container	m
R^2	Coefficient of determination	–
s_i	Local slope between neighbouring measurement points	–
T	Torque	N·m
T_{CFD}	CFD-predicted torque	N·m or %Tm
$T_{\text{end-effects}}$	Torque contribution from end-effect surfaces	N·m
T_{Lab}	Experimentally measured torque	N·m or %Tm
T_{total}	Total torque acting on spindle or bob	N·m
T_m	Maximum torque	N·m
V	Velocity of moving surface	m/s
w_i	Loss weight for output i	–
y	True target value	varies
$\hat{y}$	Predicted target value	varies
η	Dynamic viscosity	Pa·s
η_{app}	Apparent viscosity	Pa·s or mPa·s
η_i	Viscosity at measurement point i	Pa·s or mPa·s
η_0	Zero-shear viscosity	Pa·s
η_∞	Infinite-shear viscosity	Pa·s
γ	Shear strain	–
$\dot{\gamma}$	Shear rate	s^{-1}
$\dot{\gamma}_c$	Critical shear rate	s^{-1}
λ	Critical shear rate parameter / Cross transition parameter	s^{-1} or s
μ	Dynamic viscosity	Pa·s
ν	Kinematic viscosity	m ² /s
ρ	Density	kg/m ³
σ	Stress / shear stress	Pa
ω	Angular velocity	rad/s
Ω	Angular velocity	rad/s
ϵ	Small numerical constant used to avoid division by zero	–

1. Introduction

Rheological properties of food products are fundamental to the food industry, where they serve as critical factors in product development, quality control, and process optimization. These properties dictate how the fluid behaves during essential industrial operations such as pumping, heat transfer, and filling. To understand these behaviours, viscosity, a measure of a fluid's internal friction, is used to describe how a substance reacts during stirring and flow.

In a laboratory setting, viscosity is typically measured using advanced rotational rheometers that provide highly accurate data. However, the daily production environment and industrial quality control rely on simpler instruments, primarily Brookfield viscometers. While practical, these viscometers generate relative viscosity values that are challenging to compare directly with laboratory-grade measurements. In this thesis, measurements from a Brookfield DV2T-RV viscometer equipped with an RV5 spindle are compared with measurements from an Anton Paar RheolabQC using the CC27 geometry. These are hereafter referred to as RV5 and CC27, respectively.

This project builds upon the established rheological methods and the specific future work proposed by H. Ekelund (Ekelund, 2025). By utilizing artificial neural networks (ANNs) and Computational Fluid Dynamics (CFD), this research aims to uncover the complex, nonlinear relationships between these different rheological measurement methods. The ultimate goal is to create a "digital bridge" that enables advanced material characterization directly from the simplified instruments used on the production line.

1.1 Problem Statement

A significant communication barrier exists in the food industry because measurement data from Brookfield viscometers and rotational rheometers are not directly comparable. This discrepancy complicates crucial stages of production, such as process scaling, process design and process control. Although some approximations currently exist, they often fail to capture the complex, nonlinear relationships inherent in food products.

This work investigates whether it is possible to accurately correlate measurements from these two distinct rheological techniques. Specifically, it examines the extent to which these correlations can be improved by integrating neural networks with CFD simulations to provide more accurate predictive models than traditional formulas allow.

1.2 Purpose and Goals

The purpose of this work is to bridge the gap between the relative viscosity measurements commonly used in industry and the absolute rheological data required for process line dimensioning. By doing so, the work aims to simplify the estimation of processing parameters from simple measurements obtained with instruments such as a Brookfield viscometer.

The primary goals are:

- **Method Development:** To develop a correlation framework linking Brookfield viscometer measurements with rotational rheometer data using CFD simulations and AI-driven modelling.
- **Predictive Reliability:** To create a model that reliably translates approximate viscometer readings into usable absolute rheological parameters that can recreate the torque measured in physical measurements.

1.3 Expanded Goals and Objectives

To further refine the scope of this project, the following technical objectives have been added to the framework:

- **Shear Rate Range Assessment:** One of the primary technical goals is to determine if the Anton Paar RheolabQC rotational rheometer with CC27 geometry, and the Brookfield rotational viscometer with RV5 spindle operate within overlapping shear rate ranges. Identifying this overlap is critical for establishing whether data from one instrument can be realistically mapped to the other without excessive extrapolation.
- **CFD Feasibility and Validation:** The project seeks to discover if it is possible to accurately simulate the flow behaviour of the Brookfield viscometer using CFD simulations based on absolute measurement data obtained from a rotational rheometer as input.

2. Basic Concepts in Rheology

Rheology is defined as the study of the flow and deformation of materials under applied forces. The term originates from the Greek words *rhein* and *logia*, meaning the study of flow (NETZSCH-Gerätebau GmbH). In practical application, rheology characterizes how a material resists deformation and flows, providing insight into internal structure, intermolecular interactions, and processing behavior, which is critical for product quality and food processing (Zhong & Daubert, 2013). In this thesis, the most relevant rheological quantities are shear stress, shear rate, and viscosity, since both the RV5 and CC27 geometries are based on rotational shear.

2.1 Stress, Shear rate and Viscosity

In rheological measurements a material is subjected to a controlled force or deformation, the resulting response from the examined substance is then measured (Zhong & Daubert, 2013). In rotational rheometry and viscometry the relevant mode of deformation is shear (Zhong & Daubert, 2013), as can be seen in *Figure 1*.

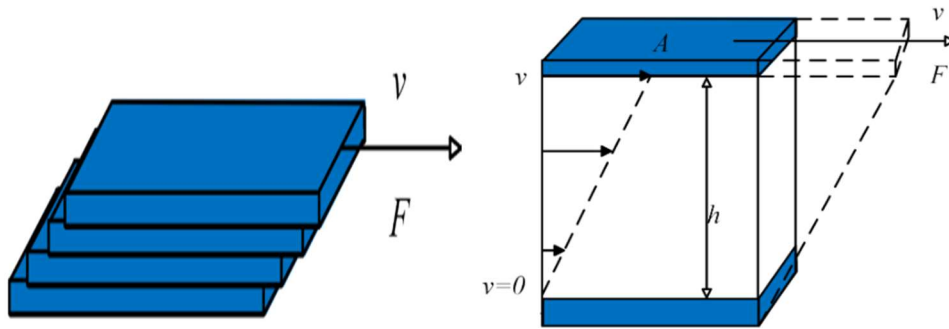


Figure 1: (Left) Parallel fluid layers are displaced relative to each other under tangential force. (Right) Simplified shear flow between a stationary plate and a moving plate, where A is the plate area and h is the gap height. The velocity gradient defines the shear rate, while force over area defines shear stress. (Ekelund, 2025)

Shear Stress is a fundamental concept in rheology, defined as the force per unit area applied to an object (Zhong & Daubert, 2013), as seen in *Figure 1*. It describes the internal resistance of a material to an externally applied load. The unit for stress is Pa (N/m²) and the equation can be written as,

$$\sigma = \frac{F}{A} \quad (1)$$

where σ is stress, F is the applied force, and A is the area over which the force acts (Abbott, 2019). In this work, the relevant stress component is shear stress, which occurs when a force acts parallel to a surface. In rotational measurements, shear stress is related to the torque required to rotate a spindle or measuring geometry through the fluid (Anton Paar GMBH, 2026), this is further detailed in *Section 2.3.1*.

Shear strain is the ratio of the relative displacement of the plates to the distance between them, seen in *Figure 1(right)*.

$$\gamma = \frac{v_{top}}{h} \quad (2)$$

Where h is the vertical height between the plates and v_{top} is the horizontal displacement at the top plate relative to the bottom plate. (Anton Paar GMBH, 2026)

Shear rate then describes how quickly shear deformation occurs (NETZSCH-Gerätebau GmbH). For a simple shear flow, as illustrated in *Figure 1*, where one fluid layer moves relative to another over a gap height, the shear rate can be expressed as:

$$\dot{\gamma} = \frac{d\gamma}{dt} \quad (3)$$

where $\dot{\gamma}$ is the shear rate and γ is the shear strain. The unit of shear rate is s^{-1} . Shear rate is especially important for non-Newtonian fluids, since their apparent viscosity depends on the applied shear conditions (Steffe, 1996).

Viscosity is a measure of a fluid's internal resistance to flow. It describes the frictional resistance that occurs when adjacent fluid layers move relative to each other under shear. For a Newtonian fluid, the shear stress is directly proportional to the shear rate according to Newton's law of viscosity (Barnes, Hutton, & Walters, 1989),

$$\sigma = \eta \dot{\gamma} \quad (4)$$

where σ is the shear stress, η is the dynamic viscosity, and $\dot{\gamma}$ is the shear rate. For Newtonian fluids, the viscosity is constant at a given temperature and pressure. For non-Newtonian fluids, however, the ratio between shear stress and shear rate varies with the applied shear conditions. In such cases, the term apparent viscosity is used (Barnes, Hutton, & Walters, 1989):

$$\eta_{app} = \frac{\sigma}{\dot{\gamma}} \quad (5)$$

The apparent viscosity is only valid for the specific measurement conditions under which it was obtained, such as shear rate, temperature, and measuring geometry.

2.2 Fluid Characterization

A fluid is characterized by its reaction to a change in shear rate. As established in the previous section, the viscosity is determined by its internal resistance to deformation under applied shear rate. However, a fluid's response to shear rate is very different depending on its molecular structures, and all fluids are therefore classified into a range of distinct categories. (Macosko, 1994).

In industrial processing, operating conditions can change a lot, and the fluids can be subjected to a wide range of varying shear rates. For engineers, it is important to map the behavior of viscosity over shear rates in order to not over- or under-estimate operating conditions (Steffe, 1996). The behaviour is most easily visualized using a flow curve, or rheogram, which plots the shear stress of the fluid required to maintain a given shear rate, as shown in *Figure 2*.

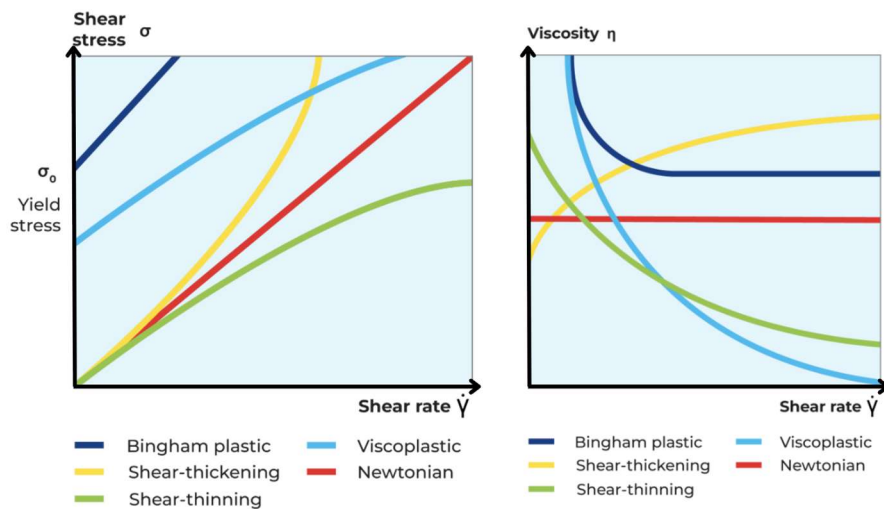


Figure 2: Rheograms illustrating the constitutive behavior of various fluid categories. (Left) Flow curve displaying shear stress versus shear rate. (Right) Viscosity curve displaying apparent viscosity versus shear rate. Adapted from Tetra Pak (2025).

As illustrated in *Figure 2*, plotting common fluid categories behaviors side by side reveals differences in how their internal structures respond to shear rates.

2.2.1 Newtonian Fluids

A fluid is defined as Newtonian if there is a linear relationship between the applied shear stress and the resulting shear rate under laminar flow conditions (Tetra Pak, 2025). In *Section 2.2, Figure 2*, a Newtonian fluid is depicted by the red curves. The linearity is described by the straight line passing through the origin in the left graph, and the horizontal line in the right graph.

The constant of proportionality in this relationship is the dynamic viscosity (η), as defined by Newton's law of viscosity in *Section 2.1, Equation 5*. For a Newtonian fluid, this relationship holds across the entire shear rate range, meaning that the viscosity remains constant regardless of the applied deformation. For a perfectly Newtonian fluid, the dynamic viscosity is therefore a material property at a given temperature and pressure, and it can be described by a single value (Barnes, Hutton, & Walters, 1989).

Common examples of Newtonian fluids include water, mineral oils and vegetable oils (Tetra Pak, 2025). Furthermore, many low concentration liquid foods, such as milk and skim milk, behave with minimal structure resistance and are for simplicity treated as Newtonian fluids for practical engineering and process design purposes.

2.2.2 Non-Newtonian Fluids - Shear Thinning

Most liquid foods, such as yoghurt, cream, salad dressings, and fruit juice concentrates are defined as shear thinning (or pseudoplastic) fluids (Tetra Pak, 2025). As illustrated in the shear stress vs shear rate curve in *Section 2.2, Figure 2 (left)*, a shear thinning fluid shows a nonlinear relationship, where the slope of the curve decrease as shear rate increases. Since the slope of this curve represents the viscosity, this corresponds to a reduction in viscosity at higher shear rates. Further, its apparent viscosity continuously decreases as the applied shear rate increases (*Section 2.2, Figure 2 (right)*).

This behaviour is driven by structural changes in the fluid when in a flowing state. At rest or lower shear rates, suspended particles or polymer chains are randomly oriented and entangled (Tetra Pak, 2025). This creates a high resistance to flow. As shear rate increases, the applied forces cause the internal structures to disentangle and align with the flow. This rearrangement lowers the internal friction and consequently the apparent viscosity of the fluid (Steffe, 1996). The non-linear shear thinning behaviour from a process engineering perspective can massively impact equipment design.

Shear-thinning behavior is often accompanied by additional rheological characteristics depending on the internal structure of the fluid. At low shear rates, some fluids exhibit a Newtonian plateau, where the viscosity increase slows down and at very low shear rates remains approximately constant (Macosko, 1994). In contrast, other fluids exhibit a yield stress, where a minimum stress must be exceeded before flow can occur (Steffe, 1996).

2.2.3 Non-Newtonian Fluids - Plastic Fluids

Certain non-Newtonian fluids require an applied minimum stress before they begin to flow (Tetra Pak, 2025). These fluids are called plastics and they are characterized by the presence of a yield stress, which is defined as the shear stress that must be exceeded for the material to transform from a solid like state to a liquid (Steffe, 1996). Below this yield stress the material behaves as an elastic or viscoelastic solid. Common examples of yield stress fluids are quark, tomato paste and some ketchups (Tetra Pak, 2025).

As illustrated in the shear stress vs shear rate curve (*Section 2.2, Figure 2 (left)*), a yield stress fluid does not begin to flow immediately when a small stress is applied. Instead, a finite shear stress must first be exceeded before flow occurs. This is reflected in the curve, which intersects the shear stress axis at a non zero value corresponding to the yield stress. Once the yield stress has been exceeded, the fluid begins to flow, and the subsequent relationship between shear stress and shear rate depends on the specific material (Steffe, 1996). A fluid that exhibits a linear relationship after yielding is referred to as

a Bingham plastic, while fluids that continue to show shear dependent viscosity after yielding are classified as viscoplastic fluids.

2.2.4 Non-Newtonian Fluids - Thixotropic Fluids

Some fluids exhibit a time dependent behaviour, where the apparent viscosity is not only a function of shear rate, but also the duration of the applied shear (Steffe, 1996). These fluids are defined as thixotropic and the definition is a fluid where apparent viscosity decreases over time when subjected to a constant shear rate, and gradually recovers when the fluid is left in a resting state.

In contrast to pure shear dependent fluids, thixotropic behaviour cannot be described by a single flow curve. Instead, it can experimentally be identified by comparing both increasing and decreasing shear rate sweeps, as shown in *Figure 3*, where a hysteresis loop is formed in the shear stress versus shear rate plot instead.

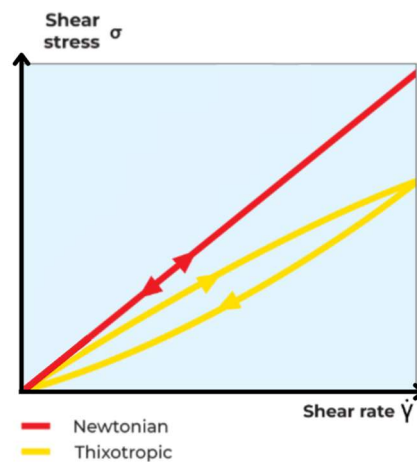


Figure 3: Rheogram illustrating how shear stress is dependent over time for a thixotropic fluid, forming a hysteresis loop when sweeping shear rate up and down. Adapted from Tetra Pak (2025).

This indicates that the internal structures of such a fluid change during shear and does not instantly return to its original state (Steffe, 1996). On the microscopical level this behaviour is governed by the breakdown and rebuilding of the fluids internal structures. In industry, thixotropic behaviour can significantly influence flow stability and make process control more difficult. Since the viscosity is dependent on not only shear rate but also the shear history. The same fluid can exhibit different flow properties depending on the prior handling, mixing or pumping (Steffe, 1996).

2.3 Measurement Instruments

Rheometry is used to determine how materials respond to controlled force or deformation over time. This work combines absolute rheometry and relative rotational viscometry. Absolute methods, such as Couette or Searle rheometry, use well-defined narrow-gap geometries to measure material properties under controlled shear conditions (Barnes, Hutton, & Walters, 1989), (Steffe, 1996). In contrast, Brookfield viscometry is a relative wide-gap method, where the measured apparent viscosity depends on the spindle, container geometry, and measurement procedure. This difference is important because narrow-gap systems provide more defined shear-rate conditions, while wide-gap systems expose the fluid to a broader shear-rate distribution. Rheological instruments may operate in controlled shear rate (CSR) or controlled shear stress (CSS) mode (Anton Paar GMBH, 2026). All the measurements in this thesis are based on CSR mode.

2.3.1 Anton Paar RheolabQC

Absolute measurement systems are designed to determine material properties under well-defined flow conditions. These systems adhere to international standards such as ISO 3219 or DIN 53019 and they use known geometries and controlled gaps, allowing shear rate and shear stress to be calculated from measured torque and rotational speed (Anton Paar GMBH, 2026), (Steffe, 1996). Many rotational

rheometers use concentric-cylinder, or bob-and-cup, geometries based on either the Couette or Searle principle. The Anton Paar RheolabQC, equipped with the CC27, used in this work follows the Searle principle, where the inner bob rotates inside a stationary outer cup (Anton Paar GmbH, 2026). *Figure 4* shows the instrument, while *Figure 5* illustrates the corresponding measuring geometry.



Figure 4: Anton Paar RheolabQC rotational rheometer with heating adapter (Anton Paar GMBH, 2026).

The CC27 is a defined narrow-gap measuring system with a gap of 1.13 mm. Since the bob and cup dimensions are known, the instrument can calculate shear rate and shear stress from the applied rotational speed and measured torque (Anton Paar GMBH, 2026). This makes the CC27 suitable for obtaining flow-curve data and fitting rheological model parameters for later CFD simulations.

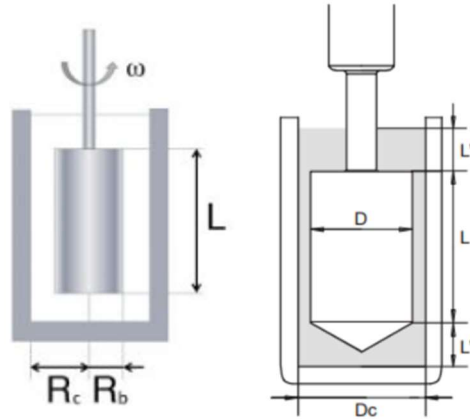


Figure 5: Rotational rheometer geometries. (Left): Simplified concentric-cylinder geometry, showing the bob radius R_b , cup radius R_c , effective bob length L , and angular velocity ω . (Right): Anton Paar CC27 measuring system used in this work, showing the defined cup and bob geometry, including the bob diameter D , cup diameter D_c , effective measuring length L , and end regions L' and L'' .

For the geometry in *Figure 5*, the shear stress can be calculated as,

$$\sigma = \frac{M}{2\pi R_b^2 L} \quad (6)$$

where M is the measured torque, R_b is the bob radius, and L is the effective length. The effective shear rate in the gap is calculated from the angular velocity and geometry dimensions as,

$$\dot{\gamma} = \frac{2\omega R_c^2}{(R_c^2 - R_b^2)} \quad (7)$$

where ω is the angular velocity, R_c is the cup radius, and R_b is the bob radius. This equation is a valid approximation for a shear rate profile in the gap exhibits linearity. The angular velocity is related to rotational speed, N , by,

$$\omega = \frac{2\pi N}{60} \quad (8)$$

The apparent viscosity is then obtained from the same Newtonian viscosity relation as described in *Section 2.1, equation 5*. For Newtonian fluids, this value is constant at fixed temperature and pressure. For non-Newtonian fluids, the calculated viscosity is shear rate dependent and should therefore be reported as apparent viscosity. (Anton Paar GMBH, 2026)

2.3.2 Brookfield DV2T-RV

Relative measurement systems are dependent on the complete measurement geometry, including the spindle, cup or container, sample volume, immersion depth, and measurement procedure. Unlike absolute rheometers, which use well-defined geometries to calculate shear stress and shear rate, relative viscometers produce apparent viscosity values that are specific to the instrument setup (Anton Paar GMBH, 2026), (Steffe, 1996). The AMETEK Brookfield DV2T-RV Viscometer (shown in *Figure 6*) is the global standard in this field, widely used for quality control to ensure that there hasn't been any relative change to the viscosity of a product in a process stream. (AMETEK Brookfield, 2026)



Figure 6: Brookfield DV2T-RV Viscometer. (AMATEK Brookfield, n.d.)

These relative measurement systems work similarly to the absolute measurement tools in that they also use the measured torque of the equipment to calculate viscosity. The difference between a Brookfield viscometer and an Anton Paar rheometer, is that the viscometer uses a calibrated spring to measure the torque. The core mechanism for measurement in one of these viscometers is driving a spindle through a fluid and as the spindle rotates, the spring is wound up in proportion to the torque required to maintain that motion. The available RV spindles are shown in order 2-7 from the left in *Figure 7*. (AMETEK Brookfield, 2026)



Figure 7: RV spindle-set for the Brookfield viscometer, RV2-7 in order left to right. (AMATEK Brookfield, 2026)

The measurement range of the Brookfield DV2T-RV depends on several factors: the rotational speed, spindle size and shape, container geometry, and the full-scale torque of the calibrated spring. Brookfield provides four basic spring torque series: LV, RV, HA, and HB. The DV2TRV model has a spring torque of 7187 dyne·cm, corresponding to 0.7187 mN·m. A higher torque calibration gives a higher measurable viscosity range. (AMETEK Brookfield, 2026)

For a Brookfield DV2T-RV viscometer using standard RV spindles, the maximum measurable viscosity can be estimated from the spindle range coefficient,

$$\eta_{max} = \frac{\text{Range coefficient}}{\text{RPM}} \quad (9)$$

where η_{max} is the full-scale viscosity range in cP and RPM is the rotational speed. For the RV torque range, the spindle range coefficients are shown in *Table 1*.

The range coefficient shows that larger spindle numbers generally correspond to higher measurable viscosity ranges. For example, using the RV5 spindle, the RV range coefficient is 400,000. This means that the full-scale viscosity range is approximately 40,000 cP at 10 rpm and 4,000 cP at 100 rpm. Since $1 \text{ cP} = 1 \text{ mPa} \cdot \text{s}$, these values are numerically equivalent to 40,000 mPa·s and 4,000 mPa·s, respectively.

Table 1: Brookfield RV spindle range coefficients for the RV type viscometer

Spindle	RV Range Coefficient
RV1	10 000
RV2	40 000
RV3	100 000
RV4	200 000
RV5	400 000
RV6	1 000 000
RV7	4 000 000

Brookfield recommends collecting viscosity data only within the 10–100% torque range. Above 100%, the measurement is outside the instrument range, while below 10% the uncertainty becomes large relative to the measured value. The DV2T accuracy is specified as $\pm 1.0\%$ of the full-scale range, corresponding to approximately ± 1 percentage point in torque rather than $\pm 1\%$ of the displayed torque value. The repeatability of a measurement is likewise ± 0.2 percentage points. Low-torque readings therefore have higher relative uncertainty and should be treated carefully when used for model fitting, CFD validation, or AI input data. For the Brookfield DV2T, the full-scale viscosity range can be calculated as,

$$\text{Full-scale viscosity range} = \frac{TK \cdot SMC \cdot 10000}{RPM}$$

where TK is the torque constant for the viscometer model, SMC is the spindle multiplier constant, and RPM is the rotational speed.

For the RV5 spindle on a Brookfield DV2TRV viscometer: $TK = 1$, $SMC = 40$ which gives,

$$\text{Full-scale viscosity range} = \frac{1 \cdot 40 \cdot 10000}{RPM} = \frac{400000}{RPM} \quad (10)$$

This is the same relationship used later when converting torque percentage to Brookfield-equivalent viscosity in the CFD-generated dataset. (AMETEK Brookfield, 2026)

2.3.3 Wall slip and End-effect Phenomena

Accurate rheological measurements rely on the assumption of no-slip boundary conditions, meaning that the fluid in direct contact with a measuring surface has the same velocity as that surface (Anton Paar GMBH, 2026). When this condition is violated, measurement errors occur.

Wall slip arises when the fluid does not adhere to the surface but instead slides along it. This effect is particularly common in high-viscosity or structured fluids, where a thin depleted layer can form near the wall. As a result, the measured shear rate is lower than assumed, leading to an underestimation of viscosity (Macosko, 1994).

In concentric cylinder rheometry, an additional source of systematic error arises from something called end effects (Hamedi, 2018). The theoretical expressions for shear stress and viscosity assume that the

torque acting on the rotating spindle originates exclusively from the cylindrical side surface of length L seen in *Section 2.3.1, Figure 5 (right)*. In practice, however, additional torque contributions arise from fluid shearing at the bottom and top regions (L' and L'' in *Figure 5(right)*) of the spindle, outside the idealised measurement zone. As a result, the total measured torque is higher than the torque predicted by the ideal equation model. These contributions are commonly referred to as end effects.

If these contributions are not accounted for, they lead to an overestimation of shear stress and, consequently, viscosity, since both quantities are directly derived from the measured torque (Hamed, 2018). This makes end-effect corrections essential for obtaining accurate rheological data, especially when using absolute measuring systems such as the CC27 geometry.

To compensate for this, rheometers introduce an effective length, denoted L_{eff} , which replaces the physical cylindrical length in the calculation (Macosko, 1994). The effective length accounts for the additional torque by effectively extending the measurement region. The viscosity expression for the concentric cylinder system is therefore instead written as,

$$\eta = \frac{M}{4\pi L_{eff} \omega} \left(\frac{1}{R_b^2} - \frac{1}{R_c^2} \right) \quad (11)$$

where L_{eff} incorporates the influence of end effects. For the Anton Paar CC27 measuring system, the effective length is typically implemented through a correction factor,

$$L_{eff} = c_L L \quad (12)$$

where c_L is the dimensionless correction factor. A standard value of $c_L = 1.1$ is applied in the RheolabQC software, but can vary. This provides a practical approximation for many fluids, particularly those that are close to Newtonian.

The magnitude of end effects is not constant, but depends on the rheological properties of the fluid (Hamed, 2018). In particular, more shear-thinning fluids tend to exhibit larger end effects than less shear-thinning fluids. As the viscosity decreases in high-shear regions near the boundaries, a more non-uniform shear field is formed applying more torque on the ends where rotational speeds are lower. Consequently, the use of a constant correction factor may introduce additional uncertainty when analysing strongly non-Newtonian materials.

2.4 Curve Fitting and Fluid Models

Analysis of rheological data is performed through the use of mathematical models. These models describe the relationship between shear stress and the applied shear rate with an equation for a specific shear rate region (NETZSCH-Gerätebau GmbH). The benefit is the ability to summarize a fluid's complex flow data, into a number of constants that approximate the rheology over that shear rate region. By identifying the flow behavior and defining it with a mathematical model, process engineers can get a better understanding of how the fluid reacts during pumping and mixing, and use the model to predict flow behavior at a range of shear rates. Although a more complex model may provide a more accurate description of the fluid behaviour, a sufficiently accurate approximation is often adequate for process understanding. In *Figure 8*, the different behaviours of shear-thinning fluids with Newtonian plateau or yield stress is illustrated.

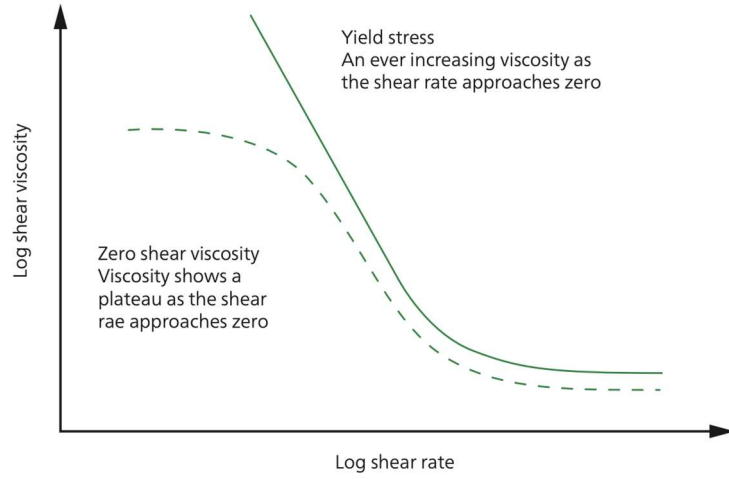


Figure 8: Schematic illustration of zero-shear viscosity and yield-stress behaviour for a shear-thinning fluid. Adapted from (NETZSCH-Gerätebau GmbH).

Two different mathematical models are needed to describe the curves shown in Figure 8. In the middle part of the curve, the fluid is in the shear-thinning region, where viscosity decreases with increasing shear rate and appears approximately linear on a logarithmic scale. At low shear rates, some shear-thinning fluids reach a Newtonian plateau, also called the zero-shear viscosity, where the viscosity approaches a nearly constant value (Barnes, Hutton, & Walters, 1989), (Barnes, Hutton, & Walters, 1989). In contrast, yield-stress fluids behave differently. Their apparent viscosity increases sharply as the shear rate approaches zero. Therefore, different rheological models are required depending on whether the fluid exhibits a low-shear plateau or yield-stress behaviour.

2.4.1 Power Law Model

The Power Law model (also known as the Ostwald-de Waele model) is one of the most widely used equations to characterize non-Newtonian behavior (Barnes, Hutton, & Walters, 1989). It is one of the most simple models to employ due to its two parameter nature, and interpretable expression of fluid behavior. The Power Law equation can be written as,

$$\eta = K\dot{\gamma}^{n-1} \quad (13)$$

or,

$$\sigma = K\dot{\gamma}^n \quad (14)$$

where K is the consistency index, and n is the flow behavior index. These parameters are material Power Law constants for a given fluid at a specific temperature (Macosko, 1994). The parameter n, indicates the degree of Newtonian behavior. If $n < 1$ the fluid exhibits a shear thinning behavior and if $n > 1$, the fluid exhibits a shear thickening behaviour. A fluid with $n = 1$ behaves as a Newtonian fluid.

The Power Law model is versatile for quick understanding of a fluid's behaviour, but comes with limitations for more exact modelling (Abbott, 2019). Power Law approximates that the viscosity is linearly proportional to the shear rate on a double logarithmic axis as shown in Figure 9 for a shear-thinning fluid with Newtonian plateau (NETZSCH-Gerätebau GmbH).

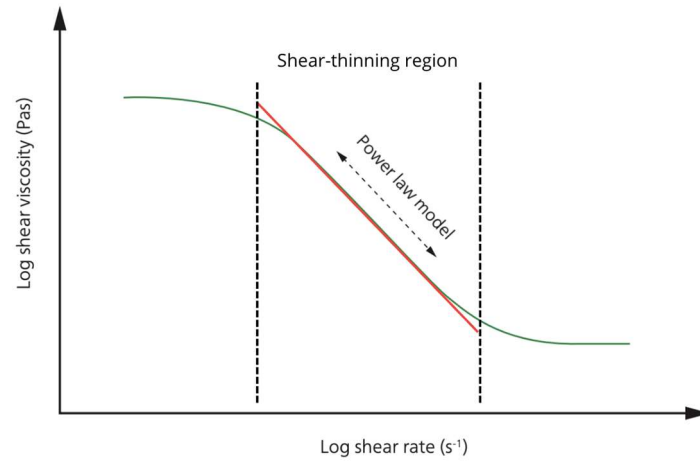


Figure 9: Validity range of the Power Law model regression (red) for example a typical shear-thinning fluid with Newtonian plateau (green).

This is a valid approximation as long as the fluid is within its shear-thinning region and within its fitting data range (Steffe, 1996). The shear thinning region varies with the fluid's nature and is typically within middle shear rate regions, 1 - 1000 reciprocal seconds (Barnes, Hutton, & Walters, 1989). At shear rates outside the linear behaviour, Power Law is only valid over a limited range and should be used as an approximation.

2.4.2 Herschel-Bulkley Model

The Power Law model provides a simple and effective description of rheology, but it does not describe the flow behavior of fluids that exhibit both yield stress and non-Newtonian characteristics (Abbott, 2019). To address this limitation, the Herschel-Bulkley model is an extension of the Power Law by including a yield stress term, making a total of three parameters. The Herschel-Bulkley equation can be written with shear stress or viscosity as,

$$\sigma = \sigma_y + K\dot{\gamma}^n \quad (15)$$

or,

$$\eta = \frac{\sigma_y}{\dot{\gamma}} + K\dot{\gamma}^{n-1} \quad (16)$$

where K is the consistency index, and n is the flow behaviour index, and σ_y is the yield stress for a plastic fluid (NETZSCH-Gerätebau GmbH). When $\sigma_y = 0$ the Herschel-Bulkley reduces to the Power Law model. Similarly to the Power Law the Herschel-Bulkley is valid over a limited shear rate range, and is most accurate within the region of curve fit (Macosko, 1994). To include a yield stress term can improve the fit in lower shear rate regions closer to the yield stress for fluids exhibiting a plastic behavior. The upwards curvature of the red curve in Figure 10, at low shear rates, indicates the presence of a yield stress, where a finite stress is required to initiate flow, in contrast to the Newtonian plateau observed for the green curve.

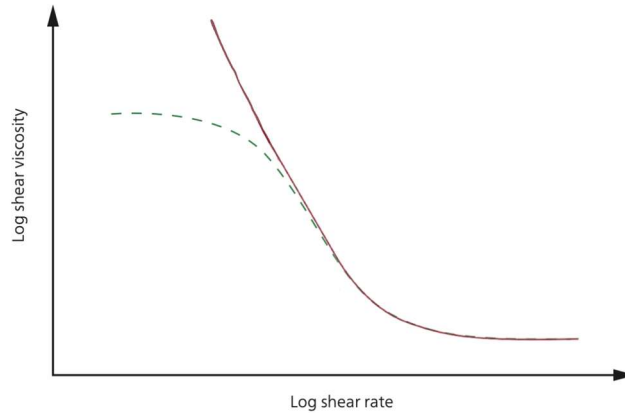


Figure 10: Typical shear thinning yield stress fluid behaviour (red) vs shear thinning plateau behaviour (green).

With the Herschel-Bulkley equation in viscosity form, the model predicts an infinite viscosity as $\dot{\gamma} \rightarrow 0$, which needs to be considered when modelling viscosity at lower shear rates (Abbott, 2019).

2.4.3 Cross Model

For modelling of a typical shear-thinning fluid that exhibits a Newtonian plateau behaviour at lower shear rates, a more extensive mathematical equation is required. The Cross model is a four parameter equation capable of describing viscosity behavior across both low and high shear rate regions including the viscosity plateaus observed in many shear thinning fluids (Macosko, 1994). The Cross model is commonly written as (Siemens Digital Industries Software, n.d.) ,

$$\eta = \frac{\eta_0 - \eta_\infty}{1 + (k\dot{\gamma})^m} + \eta_\infty \quad (17)$$

where η_∞ is the infinite-shear viscosity, η_0 is the zero-shear viscosity, k is called the time constant, and m is the rate index describing flow behaviour (Siemens Digital Industries Software, n.d.). The parameters η_∞ and η_0 represent the limiting viscosity plateaus (*Figure 11*), at infinite shear rate and as shear rate approaches zero. In cross modelling the parameter k is often interpreted through the critical shear rate, $\dot{\gamma}_c = \frac{1}{k}$, which can be visualized as intersection point between the slopes of Newtonian plateau and the shear thinning region in *Figure 11*.

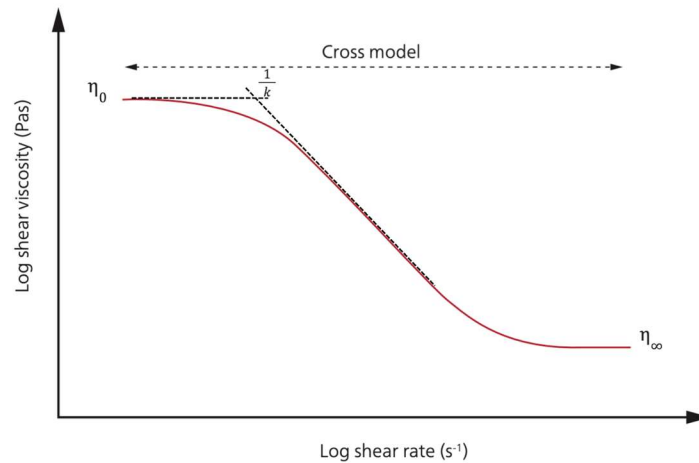


Figure 11: A typical cross model regression (red). Showing zero-shear viscosity η_0 , infinite-shear viscosity η_∞ and how the intersect for critical shear rate $\dot{\gamma}_c = \frac{1}{k}$ is interpreted.

Unlike the Power Law model, the Cross model captures both viscosity plateaus for a shear thinning fluid, while also reducing to shear thinning behaviour in the intermediate shear rate region (Barnes, Hutton, & Walters, 1989). In this shear-thinning region, the Cross model curve appears approximately linear on a logarithmic viscosity as a function of shear rate plot, corresponding to a Power Law

dependence over a limited shear rate interval. Therefore, viscosity values obtained from the Cross model within this interval can be used to determine apparent Power Law parameters, K and n , for the selected shear rate range. This makes the model suitable for describing fluids over a wide shear rate range.

In practical curve fitting, the infinite-shear viscosity is sometimes approximated and fixed to a known value, such as the viscosity of the solvent (Macosko, 1994). This in order to reduce the number of parameters used in the fitting to improve the stability of the regression. This approximation is typically applied when high shear data is limited or when the infinite-shear plateau lies outside the range of interest and the measured range.

2.5 Sodium Carboxymethyl Cellulose CMC

Sodium carboxymethyl cellulose, CMC, is a water-soluble cellulose derivative commonly used as a model shear-thinning fluid in rheological studies. (Wagner, Róžańska, Warmbier, & Mitkowski, 2023), (Nouryon, 2020). In this work, CMC30000 was selected as the primary validation material because it provides more controlled and reproducible non-Newtonian behaviour than more complex food products.

A CMC solution's viscosity depends strongly on concentration and temperature. Increased concentration increases viscosity and generally gives more pronounced shear-thinning behaviour, while increasing temperature lowers the fluid's viscosity (Nouryon, 2020). A key feature of high-viscosity CMC solutions is the presence of a low-shear viscosity plateau followed by a transition into the shear-thinning region (Chalah, Benmounah, Mahdad, & Kheribet, 2022). This makes CMC relevant in the present work because the RV5 geometry is sensitive to low-shear behaviour.

Time-dependent effects, such as thixotropy, may occur in high-molecular-weight CMC solutions at higher concentrations (Chalah, Benmounah, Mahdad, & Kheribet, 2022).

3. Computational Fluid Dynamics (CFD)

Computational Fluid Dynamics (CFD) is a numerical approach used to analyze, simulate and solve fluid flow problems. CFD serves as a powerful tool for the prediction of fluid behavior in complex geometries and operating conditions where experimental measurements are challenging or impossible to obtain (Anderson, 1995). It provides an insight to data as, velocity, pressure, and shear distributions, which enables improved understanding of fluid systems and design. In this work, Siemens Simcenter STAR-CCM+ will be used as CFD tool.

3.1 Governing Equations and Theoretical Basis

The governing equations of fluid motion are based on the fundamental laws for mass, momentum and energy conservation, commonly expressed through the Navier-Stokes equations (Versteeg & Malalasekera, 2007). Due to their non-linear and coupled nature, analytical solutions are only possible for simplified cases, meaning that the numerical methods are in most cases required to solve realistic engineering problems. The continuity equation for incompressible flow is given as,

$$\nabla \cdot \mathbf{u} = 0 \quad (18)$$

and the equation for conservation of momentum can be written as,

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \boldsymbol{\tau} \quad (19)$$

where $\mathbf{u}$ is the velocity vector, ρ is the density, p is the pressure, and $\boldsymbol{\tau}$ is the stress tensor. For modeling of non-newtonian fluids, the stress tensor is dependent on shear rate through the chosen fluid model (Macosko, 1994). In CFD these governing equations are often expressed in a generalized form for transport. This approach describes the rate of change for any flow variable as a balance between convection, diffusion and internal source terms, providing a universal framework for solving fluid dynamics problems and analyzing the transport phenomena in fluid systems (Anderson, 1995).

3.2 The Numerical Methods in CFD

In order to solve the governing equations numerically, the continuous space or spatial domain is discretized into a finite number of individual volumes (cells), forming a mesh. Within each individual volume, the governing partial differential equations are discretized into an algebraic form, transforming the partial differential equations into a system of equations that can be solved for each iteration run (Anderson, 1995).

In this work, the finite volume method (FVM) is applied, which is the standard in Star-CCM+. In FVM, the equations are integrated over each individual cell, and the divergence terms between cells are converted into surface integrals using Gauss' divergence theorem (Versteeg & Malalasekera, 2007). This formulation ensures the conservation of mass and momentum within each cell, as fluxes are evaluated across the cell faces. The values for primary variables are typically stored in the cell centers. This means that profile plots in a system require a good cell resolution to be visibly interpretable.

The numerical solution is obtained by an iterative process where the discretized equations are solved repeatedly until convergence is reached (Ferziger & Perić, 2002). Convergence is assessed by the monitoring of residuals, to ensure change in the solution between iterations is small enough. Due to the non-linearity of certain models, a stable convergence may require careful numerical treatment. As for example, under-relaxation factors to avoid value oscillations, which limits the value update for each cell through each iteration to a set percentage.

3.3 Mesh Quality and Mesh Sensitivity Analysis

The computational mesh affects both the accuracy and stability of a CFD simulation. Since the governing equations are solved over discrete control volumes, insufficient mesh resolution can lead to spatial discretization errors, especially in regions with large velocity, shear-rate, or viscosity gradients. In this work, this is particularly relevant near the spindle and cup walls, where wall shear stress directly

influences the predicted spindle torque. Mesh quality is therefore important for obtaining reliable torque predictions.

A mesh sensitivity analysis is used to ensure a sufficient mesh quality and to make sure that the solution is mesh independent (Beghami, 2020). This is done by repeating the same simulation using different mesh sizes and comparing the main output quantity. In this thesis, spindle torque is used as the monitored quantity, since it is the primary CFD result compared with experimental measurements. A mesh is considered sufficiently refined when further refinement only gives small changes in the predicted torque. Residuals are also monitored to assess iterative convergence, but mesh sensitivity is evaluated primarily through the convergence of torque, residuals and shear rates, rather than residual reduction alone.

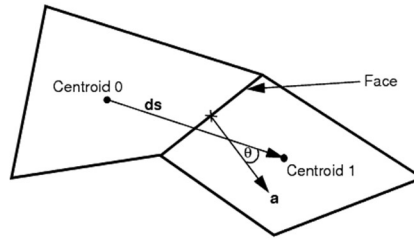


Figure 12: Illustration of the cell skewness angle, θ , defined as the angle between the face area vector, a , and the centroid 0 to 1 vector, ds , across a shared cell face. Adapted from Siemens Digital Industries Software (n.d.).

Mesh quality is also affected by cell shape and distortion (Siemens Digital Industries Software, n.d.). One commonly used mesh quality metric in Siemens Simcenter STAR-CCM+ is the cell skewness angle. The skewness angle is defined as the angle between the face area vector, normal to the cell face, and the vector connecting the centroids of the two neighbouring cells (*Figure 12*). High skewness can reduce numerical accuracy and solver robustness, since the calculation of diffusive fluxes across cell faces becomes less reliable when the face normal and centroid connecting vector are poorly aligned. In STAR-CCM+, cells with skewness angles above approximately 85° are typically considered poor-quality cells, while skewness angles approaching or exceeding 90° may lead to convergence issues.

4. Neural Networks for Rheological Modelling

Neural networks, introduced in the 1940s, are powerful tools for predictive modelling and regression analysis. They can analyse large datasets and identify complex patterns that may be difficult to capture using traditional methods. In fields such as pharmaceutical sciences and food processing, neural networks are used to model complex non-linear relationships, for example between rheological properties such as viscosity and different process or measurement conditions. (Duarte, 2026), (Chen, o.a., 2026) (Lennon, 2023)

4.1 Neural Networks and Regression

Neural network models can be adapted to different data structures and prediction tasks. The choice of model depends on the type of input data, the prediction goal, and the physical relationships represented in the dataset. One common category is black-box models, which learn relationships between input and output parameters without explicitly using physical laws. These models can give accurate predictions, but they usually provide limited insight into the underlying physical relationships between the parameters. (Duarte, 2026), (Chen, o.a., 2026), (Elkhatny, 2019)

Feed-forward neural networks, also called multilayer perceptrons, are models where information moves in one direction from input to output through hidden layers. Each layer applies weights, biases, and a nonlinear activation function, allowing the network to model complex nonlinear relationships (Goodfellow, Bengio, & Courville, 2016), (Lennon, 2023). In this thesis, this makes them suitable for mapping Brookfield-type measurement data to rheological model parameters, where the relationship is difficult to describe using traditional regression methods.

Neural networks can be used for supervised regression, where input variables are mapped to continuous output variables. In rheological modelling, inputs may include RPM, torque, shear stress, or viscosity, while outputs may be model-specific parameters such as those used in the Cross model. During training, the model adjusts its weights and biases to minimize a loss function, such as mean squared error, MSE, or weighted mean squared error, WMSE. Compared with classical linear regression, neural networks can better capture nonlinear relationships, making them useful for rheological correlations where measurement data and model parameters are not linearly related. (Goodfellow, Bengio, & Courville, 2016), (Lennon, 2023)

4.2 Network architecture, feature engineering and training

Neural network design involves selecting an architecture suitable for the prediction task. In a feed-forward neural network, the structure consists of an input layer, hidden layers, and an output layer. The input layer receives the selected features, the hidden layers transform these inputs into internal representations, and the output layer produces the predicted target values. The number of hidden layers defines the model depth, while the number of neurons in each layer defines the model width. (Goodfellow, Bengio, & Courville, 2016)

Activation functions are applied after the linear transformation in each hidden layer. Without activation functions, the network would behave as a linear model, regardless of the number of layers (Goodfellow, Bengio, & Courville, 2016). Nonlinear activation functions allow the network to learn more complex relationships between input and output variables. In this work, ReLU was used as the activation function,

$$g(z) = \max(0, z) \quad (20)$$

Rectified Linear Unit (ReLU) was selected because it is simple and efficient to optimize. Other activation functions, such as sigmoid and tanh, are also common, but were not used in the final model.

Feature engineering transforms raw measurement data into variables that better describe the physical behaviour being modelled. In rheology, logarithmic transformations are useful because viscosity and shear-rate relationships are often easier to describe in log-log space. Local slopes between neighbouring measurement points can also be used to describe how viscosity changes with shear rate:

$$\text{Slope} = \frac{\Delta \log(\eta)}{\Delta \log(\dot{\gamma})} \quad (21)$$

These slope features provide information about the curve shape and can help the model identify transition regions between low-shear behaviour and shear-thinning behaviour. (Lennon, 2023)

Before training, input features are commonly scaled or normalized because neural networks are sensitive to the numerical magnitude of input values. Scaling places features on comparable numerical ranges and improves numerical stability during training. (Lennon, 2023), (Chen, o.a., 2026), (Goodfellow, Bengio, & Courville, 2016)

Experimental rheological measurements contain variation from instrument noise, sample handling, and measurement uncertainty. If a neural network is trained only on idealized data, it may perform less reliably on new measurements. Artificial noise can therefore be added during training to encourage the model to learn the general trend of the flow curve rather than exact individual points. (Lennon, 2023), (Chen, o.a., 2026), (Goodfellow, Bengio, & Courville, 2016)

For multi-output rheological models, a neural network can use a shared trunk with separate output heads. A shared trunk corresponds to the common hidden layers of the neural network, where the input features are processed and general patterns are learned. The output heads are comparable to separate output-layer branches, where each branch takes the shared hidden representation and specializes in predicting one specific target parameter. In other words, instead of one shared output layer predicting everything directly, the model first uses shared hidden layers and then splits into parameter-specific output heads. (Goodfellow, Bengio, & Courville, 2016)

During training, an optimizer updates the network weights to reduce the loss function. Adam and AdamW are commonly used optimizers. A learning-rate scheduler can reduce the learning rate when the validation loss stops improving, allowing larger updates early in training and smaller refinements later (Loshchilov & Hutter, 2019). This is done over several epochs, where one epoch corresponds to one complete pass through the training dataset. Multiple epochs allow the network weights to be updated repeatedly, helping the model improve its prediction accuracy during training. (Goodfellow, Bengio, & Courville, 2016)

For multi-output regression, a weighted mean squared error can be used:

$$\text{Loss} = \sum_i w_i (y_{\text{pred},i} - y_{\text{true},i})^2 \quad (22)$$

where w_i is the weight assigned to each output. Weighting allows certain parameters to be prioritized during training, for example if one parameter is more difficult to predict or more important for describing the flow curve. (Lennon, 2023)

To evaluate generalization, data are divided into training, validation, and test sets. The training set updates the model weights, the validation set monitors training progress, and the test set is used for final evaluation on unseen data. The R^2 score describes the overall agreement between predicted and true values, while relative error is useful for identifying individual prediction deviations. (Goodfellow, Bengio, & Courville, 2016), (Elkatatny, 2019), (Duarte, 2026)

5. Materials and Methods

In this chapter the materials and method behind the finalized workflow is described. A central part of this work regards the suggestion of a workflow that can be followed repeated for other fluid models and geometries. The workflow created is detailed in *Figure 13* and is divided into methods for physical measurements (blue boxes), excel regression (yellow), CFD simulation/modelling (green) and AI training/prediction (purple). Experiments were performed mainly on Nouryon, Cekol CMC30000 solutions 1.0, 1.4 and 1.5wt%, but some initial tests on condensed milk, tomato ketchup and sugar solution was also done with this method.

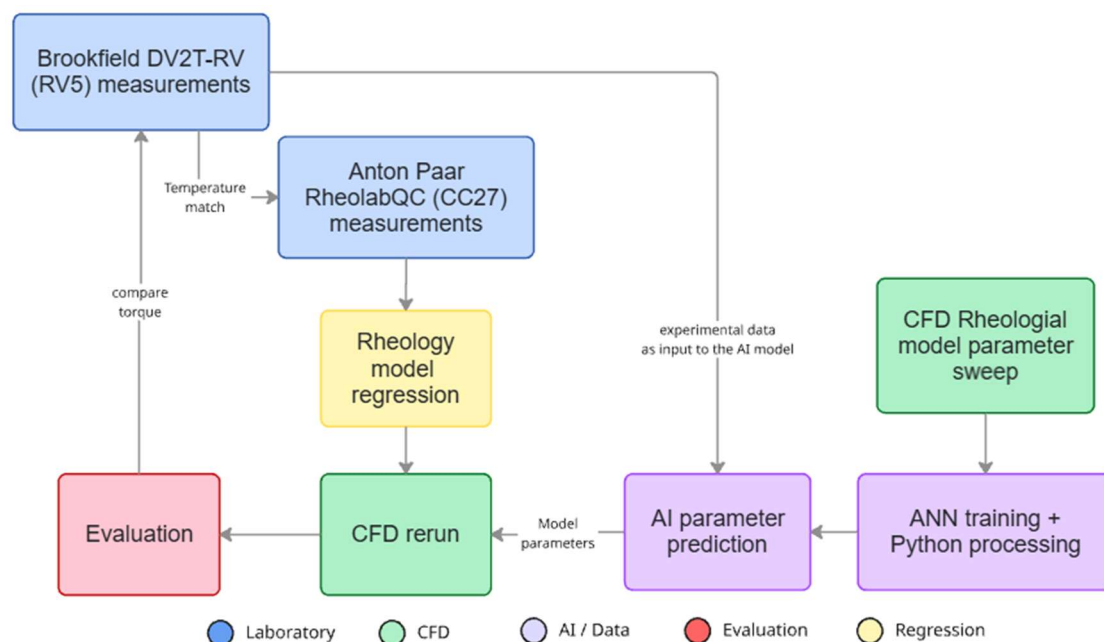


Figure 13: Workflow diagram detailing the different steps taken in this work. Starting with the physical/laboratory measurements (Blue), then Regression (Yellow), CFD simulation/modelling (Green), followed by Data preprocessing and AI training/development (Purple) and finally output evaluation (red)

The developed workflow above (*Figure 13*), shows how CFD simulations (green right box) are used to create a dataset of torque at RPMs 10-100 in the RV5 geometry with their corresponding rheological model parameters. With data restructuring, training of the AI models and AI parameter predictions from Brookfield torque inputs (purple boxes) rheological parameters are estimated for a fluid. Physical measurements are performed at matching temperatures (blue boxes), where excel regression (yellow box) is used to extract laboratory rheological model parameters. The parameters predicted from the AI model are compared against the excel regressed parameters, either directly or as their predicted torque in a CFD rerun (green left box) for both RV5 and CC27 geometries.

5.1 Method for Experimental Brookfield Measurements

The viscosity measurements were performed using a Brookfield DV2T-RV rotational viscometer equipped with an RV5 spindle. According to the manufacturer, the DV2T viscometer has a viscosity accuracy of $\pm 1.0\%$ of the full-scale range.

A standard Brookfield 600 ml beaker was filled with 500 ml of sample (exact measurements can be seen in *Section 5.4.2, Figure 22 (right)*). The RV5 spindle was immersed into the sample at an angle to reduce the risk of air entrapment around the spindle. The spindle was then attached to the Brookfield DV2T-RV and lowered until reaching the marked part of the spindle (visible in *Section 2.3.2, Figure 7*) before the measurement was started.

For each fluid, two samples were measured twice, giving four measurement series per batch. The rotational speed was increased from 10 to 100 RPM in increments of 10 RPM. At each rotational speed, the sample was sheared for 60 s before the measurement was recorded.

The recorded parameters for each measurement point were rotational speed, torque percentage, apparent viscosity, and sample temperature, since viscosity is temperature dependent. The temperature was measured between each rotational-speed step using an external thermometer. The measurements were used to obtain an initial viscosity profile for each fluid and to identify the relevant temperature conditions for the subsequent RheolabQC measurements.

An example of the recorded Brookfield measurement data can be seen in *Table 2*. The full Brookfield measured data are provided in *Appendix A1*.

Table 2: Example Brookfield DV2T RV viscosity measurement data for sample 1.1 using the RV5 spindle and a shearing time of 60 s.

RPM	Temperature (°C)	Torque (%Tm)	Viscosity (cP)
10	21.3	6.9	2760
20	21.3	10.7	2140
30	21.3	13.6	1813
40	21.3	16.0	1600
50	21.3	18.1	1448
60	21.3	19.9	1327
70	21.3	21.6	1234
80	21.3	23.2	1160
90	21.3	24.6	1093
100	21.3	25.9	1036

5.2 Method for Experimental RheolabQC Measurements

The rheological measurements were performed using an Anton Paar RheolabQC equipped with a CC27 measuring system (*Section 5.4.1, Figure 21*). For each measurement, approximately 19 mL of sample was added to the CC27 cup, ensuring that the filling level reached the indicated mark. Each fluid was measured in triplicate using three independently prepared samples in order to assess repeatability and reduce the influence of measurement variability. The detailed measurement settings are presented in *Figures 14-18*. *Figure 14*, shows an overview of the RheolabQC measurement sequence used for the

shear rate sweeps. The method consisted of three main intervals: temperature conditioning, pre-shear at constant shear rate, and the final shear rate sweep.

	1	2	3
Points	10000	10	15
Duration	1 s	15 s	50 s
$\dot{\gamma}$	100 1/s	100 1/s	2...720 1/s
T	23; ΔT : -0,133333 °C	21,3 °C	21,3 °C

Figure 14: Overview of the RheolabQC measurement sequence used for the shear-rate sweeps. The method consisted of three main intervals: temperature conditioning, pre-shear at constant shear rate, and the final shear-rate sweep. The sample was first adjusted from room temperature to the target temperature, followed by pre-shearing at 100 s^{-1}

Since viscosity is temperature dependent, the RheolabQC measurements were performed at the same temperatures as those observed during the Brookfield measurements. Before the shear rate sweep, the sample temperature was adjusted from room temperature to the target temperature using a temperature-conditioning step. Event control was applied during this interval to ensure that the method did not proceed until the desired temperature had been reached (Figures 15 and 16).

Data points		Set value	
Number:	10000	Variable: T	Temperature
Duration:	Constant	Profile:	Rate with initial
Point:	1 s	Initial:	23 °C
Interval:	10000 s	Rate:	-0,133333 °C/s

Figure 15: Temperature-conditioning interval used as a first step (interval 1) The sample temperature was adjusted from room temperature to the same temperature as used during the Brookfield measurements. This ensured that the RheolabQC measurements were performed under comparable thermal conditions.

Reactions and events		Parameters	
Step forward by x interval(s)...	Number of intervals:	1	
...if value < limit	T	Temperature	Default
	21,3		°C

Figure 16: Event-control settings for the temperature-conditioning interval (interval 1). Event control was used to prevent the method from continuing before the sample had reached the target temperature. The next measurement interval (interval 2) was started only after the temperature condition had been fulfilled.

After the temperature-conditioning step, the sample was pre-sheared at the target temperature, as shown in Figure 17. This step was included to standardize the shear history of the sample prior to the viscosity measurement.

Details	
Data points Number: 10 Duration: Constant Point: 15 s Interval: 150 s ☒ Set value Variable: T Temperature Profile: Constant Value: 21,3 °C	

Figure 17: Pre-shear settings used before the shear-rate sweep (interval 2). The sample was pre-sheared at a constant shear rate of 100s^{-1} at the target temperature. This step was included to standardize the shear history of the sample prior to the viscosity measurement.

The final measurement interval (interval 3) consisted of a shear-rate sweep from low to high shear rate (Figure 18). The sweep range was adapted from the standard Tetra Pak method in order to improve the resolution in the low-shear region of the viscosity curve. Before the triplicate measurements for each temperature, an initial low-shear test sweep was performed for each fluid to determine the lowest reliable shear rate measurable by the RheolabQC based on the instrument torque limit (0.2mNm - 75mNm). This was done to better capture the transition region, of the viscosity curve, which was required for the subsequent Cross model parameter fitting.

Details	
Data points Number: 15 Duration: Constant Point: 50 s Interval: 750 s ☒ Set value Variable: T Temperature Profile: Constant Value: 21,3 °C	

Figure 18: Settings for the shear-rate sweep (interval 3) used to obtain the viscosity curve. The final measurement interval consisted of a shear-rate sweep from low to high shear rate. The lower shear-rate limit was adjusted based on initial test sweeps in order to capture the low-shear transition region of the viscosity curve, while the upper limit was set to 720s^{-1}

The lower shear-rate limit was adjusted depending on the fluid concentration. For the 1.4 wt% CMC30000 and 1.0 wt% samples, the sweep was started at approximately 2s^{-1} , whereas for the 1.5 wt% sample, the sweep was started at approximately 0.5s^{-1} . The upper shear-rate limit was set to 720s^{-1} for all measurements. From each sweep, tables containing shear rate, apparent viscosity, temperature and shear stress were exported. These data were subsequently used in Excel for Cross model regression, with the infinite-shear viscosity fixed to the viscosity of water.

An example of the measurements done in the Rheolab QC showing the data which was later used in excel to find the cross regression curve fitting those measurement points is shown in Figure 19.

Test: CMC30000_1pct_S1_21.3°C_CC27									
Program temperatures 1									
Point No. №	Shear Rate $\dot{\gamma}$ [1/s]	Shear Stress τ [Pa]	Viscosity η [mPa·s]	Temperature T [°C]	Torque M [mN·m]	Status Stat	Time t [s]	Rotational Speed n [1/min]	Angular Velocity ϕ [rad/s]
1	2	5,0491	2524,5	21,32	0,26815		234	1,5505	---
2	3,05	6,8445	2247,7	21,31	0,3635		294	2,3607	---
3	4,64	8,8709	1913,2	21,30	0,47112		354	3,5946	---
4	7,06	11,18	1583,6	21,29	0,59377		414	5,4732	---
5	10,7	13,938	1296,6	21,30	0,74025		474	8,3337	---
6	16,4	17,225	1052,4	21,29	0,91481		534	12,689	---
7	24,9	21,072	845,52	21,29	1,1191		594	19,321	---
8	37,9	25,4	669,35	21,29	1,349		654	29,418	---
9	57,8	30,48	527,52	21,30	1,6188		714	44,793	---
10	88	36,61	416,13	21,29	1,9443		774	68,203	---
11	134	43,053	321,4	21,29	2,2865		834	103,85	---
12	204	50,535	247,76	21,29	2,6838		894	158,12	---
13	311	58,919	189,72	21,29	3,1291		954	240,76	---
14	473	68,003	143,81	21,29	3,6115		1014	366,58	---
15	720	78,744	109,37	21,29	4,182		1074	558,17	---

Figure 19: Rheological flow-curve measurement (data obtained in interval 3) of CMC 30000 (1 wt%) obtained using an Anton Paar RheolabQC with CC27 geometry at approximately 21.3 °C. The measurement was performed over a shear-rate range of 2 to 720 s⁻¹. The viscosity decreased from approximately 2525 mPa·s at low shear rate to 109 mPa·s at the highest shear rate, indicating pronounced shear-thinning behaviour

5.3 Excel Regression Tool

The rheological data obtained from the RheolabQC measurements were used to determine the parameters required for the Cross viscosity model implemented in the CFD simulations. The measured shear rate and apparent viscosity values were imported into Microsoft Excel, where the Cross model parameters were fitted using the GRG Nonlinear Solver.

The infinite-shear viscosity, η_{∞} , was set equal to the viscosity of water, while the zero-shear viscosity, η_0 , the time constant, a , and the Cross rate constant, c , were varied during the fitting procedure. Exact settings for the solver can be seen in *Appendix B1*.

The Solver objective was defined as the minimization of the sum of squared errors between the measured and calculated viscosity values. Parameter constraints were applied to keep the fitted values within physically reasonable limits. The resulting Cross model parameters were then used as material input data in the CFD simulations. The optimization objective was defined as the minimization of the sum of squared errors,

$$SSE = \sum_{i=1}^n (\eta_{measured,i} - \eta_{model,i})^2 \quad (22)$$

where $\eta_{measured,i}$ is the measured apparent viscosity at measurement point i , $\eta_{model,i}$ is the corresponding viscosity calculated by the Cross model, and n is the number of measurement points. The Solver objective cell was set to minimize the total squared error by varying η_0 , a , and c . Constraints were applied to the fitted parameters to ensure physically reasonable values.

The fitted viscosity curve was plotted together with the measured RheolabQC CC27 data to visually assess the quality of the regression. Both shear rate and apparent viscosity were plotted on logarithmic axes due to the large range of measured values. The fitted Cross model parameters were subsequently used as material input data in the CFD simulations. Full setup and example can be seen in *Appendix B*.

5.4 CFD Setup

This section describes the CFD geometry creation, parameterization, physics setup, torque reports, mesh settings, and mesh sensitivity analysis used for the simulations. The rheological behaviour of the fluids between the spindle and cup was simulated using Siemens STAR-CCM+ CFD software.

Two CFD geometries were created: one representing the RV5 spindle in a standard 600 mL Brookfield cup, and one representing the CC27 measuring system. Both geometries were constructed in the 3D-

CAD tool in STAR-CCM+ by sketching the geometry outlines in the xy-plane and revolving them around the y-axis.

5.4.1 CC27 Geometry

The CC27 spindle (bob) and cup geometry were obtained from the Anton Paar CC27 manual, confirmed with a calliper and sketched as shown in *Figure 20*. For the CC27 spindle, with radius of the large cylinder 13.33 mm and height 40 mm. The cone with an angle of 30 deg as shown in *Figure 20 (left)*, and the small cone with a radius of 4 mm and a height of 15 mm (this height was decreased later to fit the fluid volume of 19ml for the cup). For the Cup, a wall was sketched 14.46 mm from the y axis to give the gap width 1.13 mm. The cup bottom was sketched 5 mm under the cone tip. Each geometry outline was sketched in the xy-plane in a 3D-CAD model in STAR-CCM+. Each sketch was then revolved around the y axis forming separate Body Groups. A Boolean Subtraction was performed on the CC27 cup part with the CC27 spindle as a stance tool to remove the volume taken by the spindle to form the final geometry shown in *Figure 21*.

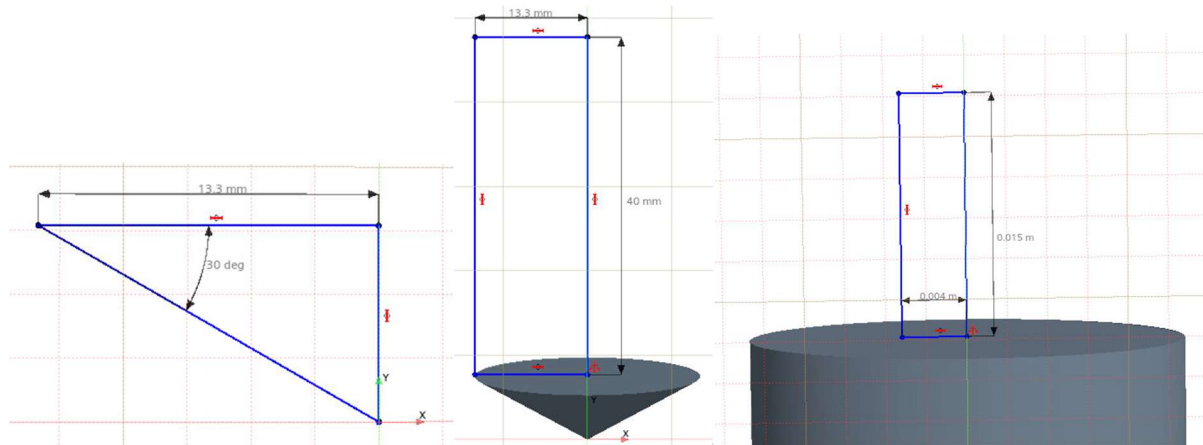


Figure 20: Dimensions of the CC27 spindle split into three parts, cone part (left), large cylinder (middle) and small cylinder (right). Length dimension for radius of the spindle, large cylinder, is 13.33 mm but shows 13.3mm in the figure due to limitations of decimals in the 3D-CAD tool.

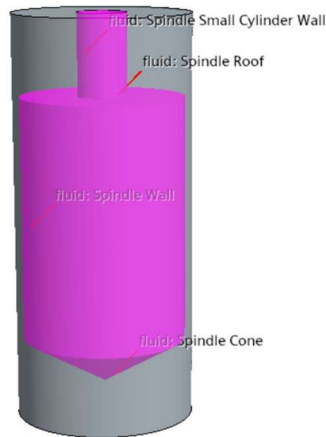


Figure 21: The full geometry of the fluid part (grey) and of the CC27 spindle (pink) with notation of each individual wall name.

The surface of the fluid was split up into six individual boundary groups. The fluid surface, the cup walls and CC27 spindle that consisted of four internal parts, the spindle cone, spindle wall, spindle roof and spindle small cylinder wall. The split up of the CC27 spindle was essential to later isolate the torque contribution of the different parts to examine the end effects caused by the geometry.

5.4.2 RV5 Geometry

The RV5 spindle and the standard Brookfield 600 mL cup, filled to the 500 mL mark, were measured using a calliper and approximated according to the dimensions shown in *Figure 22*. The spindle and cup

outlines were sketched separately in the xy-plane in a 3D-CAD model and revolved around the y-axis to create separate body groups. A Boolean subtraction was then performed, where the RV5 spindle was subtracted from the cup volume to create the fluid domain.

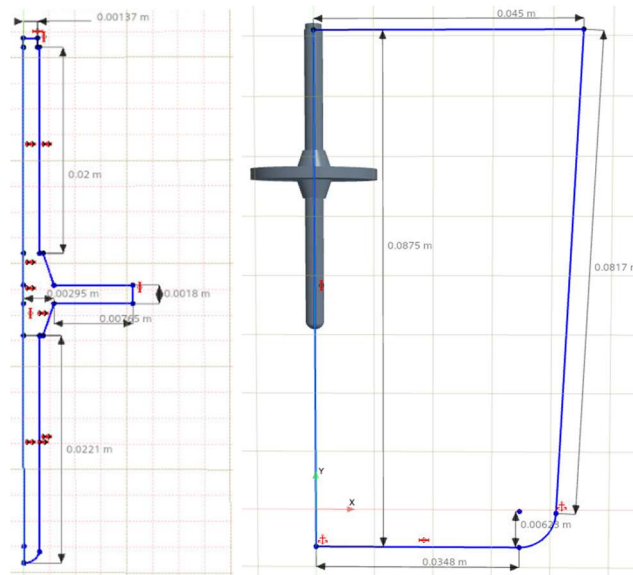


Figure 22: Dimensions of the RV5 spindle (left) and standard 600ml (to 500ml mark) Brookfield cup (right).

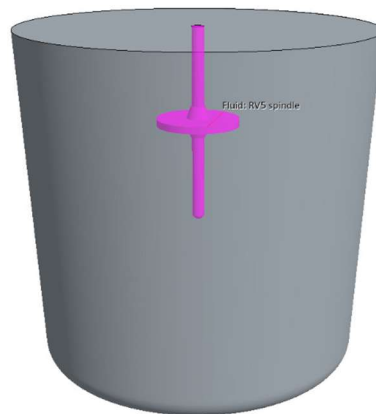


Figure 23: The full RV5 fluid domain geometry (grey) and the RV5 spindle boundary (pink).

The fluid surfaces were divided into three individual boundary groups, fluid surface, cup wall and RV5 spindle wall. The full final RV5 geometry is visualized in Figure 23.

5.4.3 Physics and Parameter setup

A separate physics continuum was created for each rheological model. The selected physics models for the Power Law and Cross model simulations are shown in Figure 24.

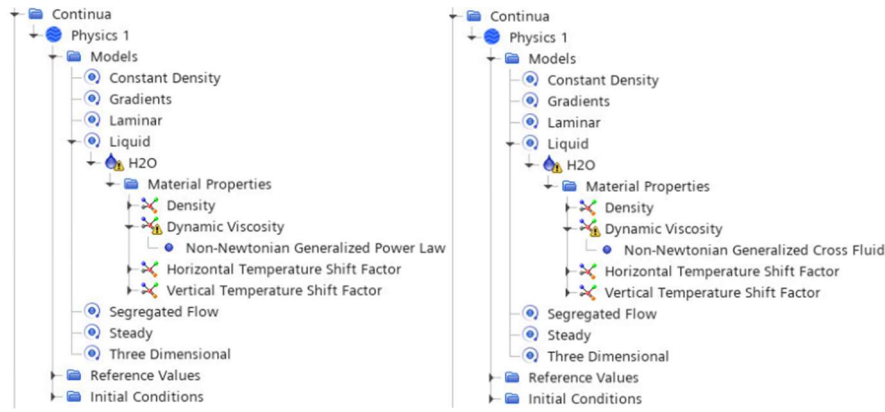


Figure 24: Physics models used for simulation of the Power Law model (left) and the Cross model (right).

In both continua, the fluid density was kept constant, the flow was laminar, and the horizontal and vertical temperature shift factors were set to isothermal. The dynamic viscosity was defined as a function of either the Non-Newtonian Generalized Power Law model or the Non-Newtonian Generalized Cross Fluid model, depending on the simulation case. The corresponding fluid model parameter settings are shown in Figure 25.

Non-Newtonian Generalized Power Law - Properties ×		Non-Newtonian Generalized Cross Fluid - Properties ×	
▼ Properties		▼ Properties	
Yield Stress Threshold	0.0 Pa	Yield Stress Threshold	0.0 Pa
Yielding Viscosity	1.0 Pa·s	Yielding Viscosity	1.0 Pa·s
Consistency Factor	$\{P_consistency_K\}$	Cross Rate Constant	$\{P_CrossRateConstant_m\}$
Power Law Exponent	$\{P_index_n\}$	Zero Shear Viscosity	$\{P_ZeroShearViscosity\}$
▼ Expert		Infinite Shear Viscosity	$\{P_InfShearViscosity\}$
Viscosity Under-Relaxation Factor	0.7	Critical Shear Rate	$\{P_CriticalShearRate\}$
Minimum Viscosity Limit	0.001 Pa·s	▼ Expert	
Maximum Viscosity Limit	10000.0 Pa·s	Viscosity Under-Relaxation Factor	0.9

Figure 25: Fluid model parameter properties for the Power Law (left) and Cross model (right) simulations.

For the Power Law model, three parameters were introduced: $P_consistency_K$, P_index_n , corresponding to the consistency index and flow behavior index, respectively (From Section 2.4.1, Equation 14), and P_RPM , representing the spindle rotational speed in revolutions per minute.

For the Cross model, four additional parameters were defined (From Section 2.4.3, Equation 17): $P_CriticalShearRate$, $P_CrossRateConstant_m$, $P_InfShearViscosity$, and $P_ZeroShearViscosity$. The infinite-shear viscosity was approximated by the viscosity of the solvent, assumed here to be water, with a value of 0.001 Pa·s.

In each simulation the minimum viscosity limit was reduced to 0.001 Pa·s. Additionally, the relative boundary condition of angular speed was set onto the rotating wall.

5.4.4 Reports

The spindle torque was extracted using a Moment report in STAR-CCM+. In this thesis, the moment of the spindle rotation axis is referred to as torque. The report was created using the force option Pressure + Shear and units of Nm. For both geometries, a report named Spindle Torque was created by selecting all spindle boundaries in contact with the fluid. For the CC27 geometry, an additional report named End-Effects was created using the same settings, but selecting all spindle surfaces except the main spindle wall. This allowed the end-effect torque contribution to be separated from the torque generated on the main cylindrical wall.

5.4.5 Mesh Setup

Automated mesh operations were created for the part “Fluid” for both the CC27 geometry and the RV5 spindle geometry. For CC27, the base size was set to 0.3 mm with 12 prism layers, stretching of 1.6 and

prism layer total thickness to 80% of base size. Which resulted in the following mesh across the gap *Figure 26*.

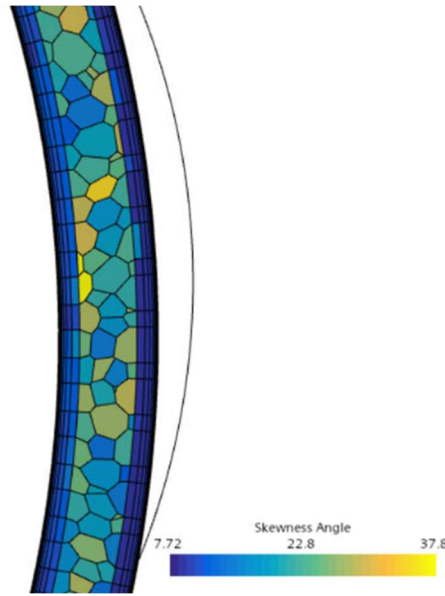


Figure 26: CC27 mesh in 1.13mm gap with skewness angle for each cell. 12 prism layers on each wall are visible as well as three to four cells inbetween. The skewness angle range from 7.72 to 37.8.

For RV5, the base size was increased to 0.4 mm due to the larger radius of the cup with 12 prism layers, stretching of 1.3 and prism layer total thickness to 100% of base size. Resulting in the following mesh below in *Figure 27*. Skewness angle for both geometry meshes was kept below the recommended limit of 85 ° discussed in *Section 3.3*.

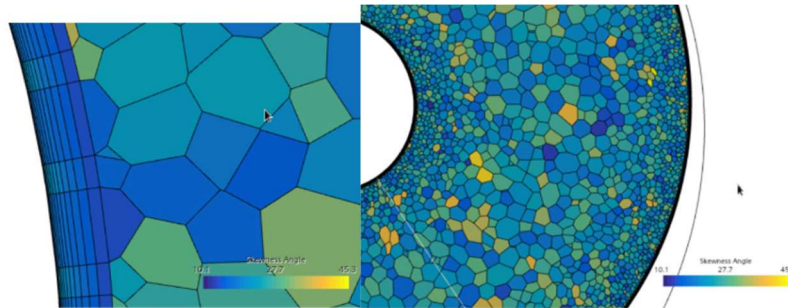


Figure 27: RV5 geometry mesh in gap with skewness angle for each cell.

5.4.6 Mesh sensitivity analysis

The mesh sensitivity analysis was needed to make sure that a mesh independent solution was acquired, according to *Section 3.3*. Since the validation of the simulations was based on predicted torque on the spindle, torque was selected as the primary parameter in the analysis. In addition, the individual cell shear rate was evaluated as a local parameter to determine whether the local shear rate profile across the measurement gap was affected by the mesh resolution. This chapter first presents the initial Power Law mesh sensitivity analysis, followed by a final Cross model mesh sensitivity analysis for both geometries, CC27 and RV5. Finally, the local shear rate profiles are compared for the tested mesh to confirm that the selected mesh resolve both the global torque and the local shear rate accurately.

5.4.6.1 Initial Power Law Mesh Sensitivity

In the beginning of the work, before performing the final validation simulations, an initial mesh sensitivity analysis was carried out using the Power Law model for the CC27 geometry. This was done to make sure the results were mesh independent in the initial results presented in *Section 6.1*. As

described in *Section 3.3*, spindle torque was used as the quantity of interest, since this is the primary CFD output used for validation against experimental measurements.

Only the mesh base size was varied, while the remaining mesh settings, including the prism layer settings, were kept unchanged. The relative deviation was calculated with respect to the finest mesh, according to,

$$\text{Relative deviation} = \frac{|T_{\text{mesh}} - T_{\text{fine}}|}{|T_{\text{fine}}|} \cdot 100 \quad (23)$$

where T_{fine} is the spindle torque obtained using the finest mesh.

Table 3: Initial Power Law mesh sensitivity results for the CC27 geometry. Relative deviation calculated using 0.20 mm as the reference.

Base size [mm]	Spindle torque [Nm]	Relative deviation to 0.20 mm [%]
0.65	$7.631440 \cdot 10^{-3}$	0.200
0.60	$7.622116 \cdot 10^{-3}$	0.322
0.55	$7.614882 \cdot 10^{-3}$	0.416
0.50	$7.624206 \cdot 10^{-3}$	0.294
0.45	$7.629598 \cdot 10^{-3}$	0.224
0.40	$7.633062 \cdot 10^{-3}$	0.179
0.35	$7.636046 \cdot 10^{-3}$	0.140
0.30	$7.641621 \cdot 10^{-3}$	0.067
0.25	$7.644125 \cdot 10^{-3}$	0.034
0.20	$7.646720 \cdot 10^{-3}$	0.000

The initial Power Law mesh sensitivity analysis showed that the predicted spindle torque was only slightly affected by mesh base size variation. *Figure 28* depicts how the torque slightly increase with the decreasing base size. For base size > 0.55 mm, the mesh becomes too coarse and affects the trend.

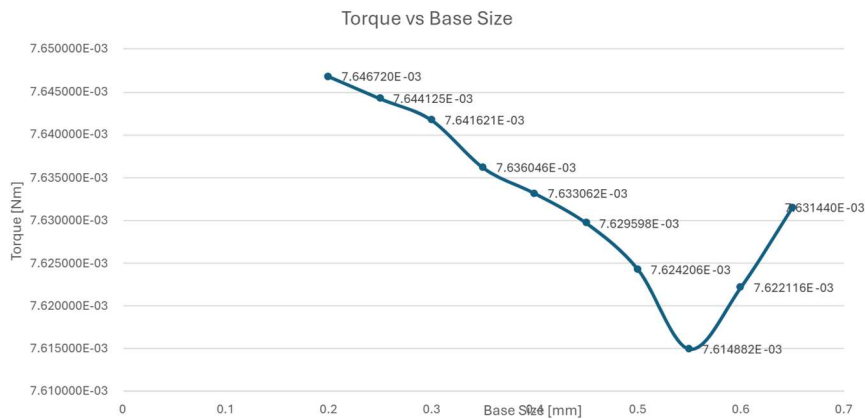


Figure 28: Initial Power Law mesh sensitivity analysis for the CC27 geometry, showing the predicted spindle torque as a function of mesh base size. The torque variation becomes small for the finer mesh. A torque increase for base size > 0.55 mm can be seen.

The initial Power Law mesh sensitivity analysis showed that the predicted spindle torque was only slightly affected by the mesh base size. The maximum deviation from the finest mesh was approximately 0.416% for the 0.55 mm mesh, while the deviation for the 0.30 mm mesh was 0.067%. Based on the

values presented in *Table 3*, a torque deviation below 0.1% was considered sufficiently small for the purpose of this initial mesh evaluation. Although the torque curve in *Figure 28* does not show a clear plateau around 0.30 mm, further mesh refinement is expected to have only a minor influence on the predicted torque. It should also be noted that torque is a global parameter and therefore provides only a first indication of mesh independence. A more detailed evaluation of the local flow field, including the shear rate distribution, is required to assess the mesh-independent behaviour more completely and is presented in the following sections. Furthermore, the cells in the gap region for the 0.30 mm base size showed a systematic increase in size, as discussed in *Section 5.4.5* and shown in *Figure 26*. Based on the low torque deviation and the mesh quality in the gap region, a base size of 0.30 mm was selected for the CC27 geometry.

5.4.6.2 Cross Model Mesh Sensitivity - Global Parameter

The final mesh sensitivity analysis was performed using the Cross model for both geometries, CC27 and RV5, to verify that the predicted spindle torque was independent of the mesh resolution for the final validation and data set creation. The global parameter spindle torque was evaluated, using the same relative deviation definition as in *Section 5.4.6.1*. Only the mesh base size was varied, while all other mesh settings were kept unchanged.

The same representative Cross parameter set was used for both geometries, 1.4 wt% CMC30000 at 20.5 °C which is the most viscous fluid used in the validation. The exact parameters used was zero-shear viscosity at 16510.79 mPas, critical shear rate 1.370724 s^{-1} , cross rate constant 0.704276 and infinite shear viscosity 1 mPas. This to challenge the mesh with the highest viscosity used in simulations. For CC27, the mesh sensitivity analysis was performed at 558.17 RPM, corresponding to a shear rate of 720 s^{-1} .

Table 4: CC27 mesh sensitivity results. Relative deviation calculated using 0.20 mm as reference.

Base size (mm)	Total spindle torque (Nm)	Relative deviation to 0.20 mm (%)
0.50	$8.3289 \cdot 10^{-3}$	0.056
0.40	$8.3279 \cdot 10^{-3}$	0.045
0.30	$8.3379 \cdot 10^{-3}$	0.165
0.20	$8.3242 \cdot 10^{-3}$	0.000

The CC27 torque showed no significant dependence on base size. All tested meshes were within 0.138% of the finest mesh, and the 0.30 mm mesh was therefore considered sufficiently refined for the CC27 simulations. The 0.30 mm base size had already been selected during the initial Power Law mesh sensitivity analysis and was kept for the Cross model simulations to maintain consistency. This resulted in a total cell count of 2,313,608. The outside of the finalized CC27 mesh is showed in *Figure 29*.



Figure 29: The finalized CC27 mesh with a base size of 0.30 mm and cell count of 2,313,608 cells. The outside and upper surface of the cup geometry is visible.

The mesh structure inside of the gap is shown in Section 5.4.5, Figure 26.

For the RV5 geometry, the mesh sensitivity analysis was performed at 100 RPM, corresponding to the highest rotational speed used in the Brookfield validation.

Table 5: RV5 mesh sensitivity results. Relative deviation calculated using 0.30 mm as reference.

Base size (mm)	Spindle torque (Nm)	Relative deviation to 0.30 mm (%)
0.60	$4.445976 \cdot 10^{-4}$	1.179
0.50	$4.428817 \cdot 10^{-4}$	0.789
0.40	$4.398304 \cdot 10^{-4}$	0.094
0.30	$4.394157 \cdot 10^{-4}$	0.000

The RV5 torque in Table 5 showed a smooth convergence trend with decreasing base size. The difference between the 0.40 mm mesh and the finest mesh, 0.30 mm, was only 0.094%, since the torque deviation was less than 0.1% it was sufficient. Therefore, the 0.40 mm mesh was considered sufficiently refined and was selected as the production mesh for the final RV5 simulations. This resulted in a total cell count of 3,783,388. The outside of the finalized RV5 mesh is showed in Figure 30.



Figure 30: The finalized RV5 mesh with a base size of 0.40 mm and cell count of 3,783,388 cells. The outside and upper surface of the cup geometry is visible. Figure is zoomed in to visualize the contour of the cells, another Figure is available in Appendix C1.

The mesh structure inside of the gap is shown in Section 5.4.5, Figure 27.

5.4.6.3 Cross Model Mesh Sensitivity - Local Parameters

In addition to the global torque comparison, the mesh sensitivity was also evaluated at a local parameter. The local parameter selected for this analysis was the shear rate, given from the ShearRateMod field function, evaluated along a line-section through the measurement gap which are visible in Section 6.1.2, Figures 44 and 45 for the two different geometries. This was done to assess whether changes in mesh base size affected the predicted shear rate distribution locally, even when the global torque was mesh independent.

The shear rate profiles are here compared as a function of radial coordinate in the gap, for each tested mesh. For each profile, the minimum and maximum shear rate along the sampled line were also extracted.

The local mesh sensitivity results for the CC27 geometry are presented first. The analysis was performed for the same Cross model case as used in the global torque comparison, at 558.17 RPM, corresponding to a nominal shear rate of 720 s^{-1} .

Table 6: CC27 local shear rate range for different mesh base sizes. Deviations are calculated using the 0.20 mm mesh as reference.

Base size [mm]	Minimum shear rate [s^{-1}]	Deviation in minimum shear rate [%]	Maximum shear rate [s^{-1}]	Deviation in maximum shear rate [%]
0.50	545.40	0.989	927.43	0.141
0.40	556.03	0.940	927.87	0.094
0.30	558.54	1.396	936.36	0.820
0.20	550.85	0.000	928.74	0.000

The minimum and maximum shear rates show small variation between the tested mesh base sizes. The minimum shear rate varied between 545.40 and 558.54 s^{-1} , and the maximum shear rate varied between 927.43 and 936.36 s^{-1} . The largest deviation in minimum shear rate was 1.396%, occurring for the 0.30 mm mesh. The largest deviation in maximum shear rate was 0.820%, also occurring for the 0.30 mm mesh.

The 0.30 mm mesh, which was selected as the production mesh for the CC27 geometry, gave a shear rate range of $558.54 - 936.36 \text{ s}^{-1}$. This was close to the range obtained with the finest 0.20 mm mesh,

which gave $550.85 - 928.74 \text{ s}^{-1}$. Together with the global torque deviation of only 0.165%, this indicated that the 0.30 mm mesh was sufficiently refined both in terms of global torque prediction and local shear rate resolution.

The shear rate profile over the gap for different base size mesh is shown in *Figures 31-34* below.

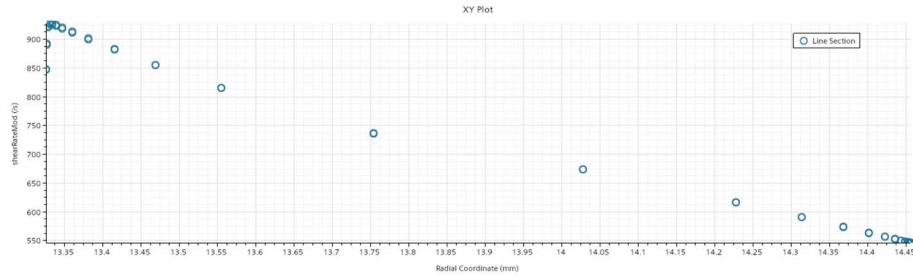


Figure 31: Shear rate profile for mesh base size 0.50 mm for the CC27 geometry plotted as a function of radial coordinate (mm) across the measurement gap. The line-section extends from the spindle surface at $r = 13.33 \text{ mm}$ to the cup wall at $r = 14.46 \text{ mm}$. The profiles are used to compare how the predicted local shear rate distribution changes with mesh base size.

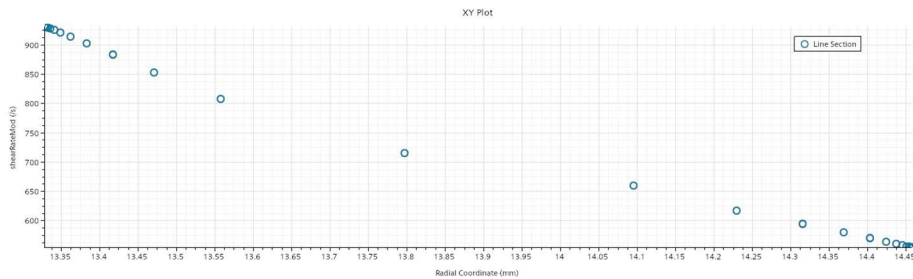


Figure 32: Shear rate profile for mesh base size 0.40 mm for the CC27 geometry plotted as a function of radial coordinate (mm) across the measurement gap.

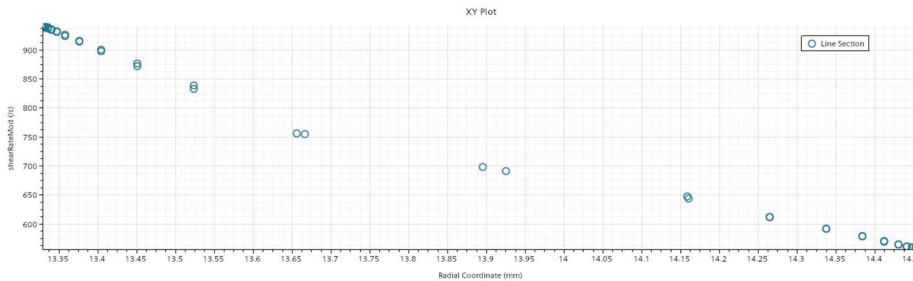


Figure 33: Shear rate profile for mesh base size 0.30 mm for the CC27 geometry plotted as a function of radial coordinate (mm) across the measurement gap.

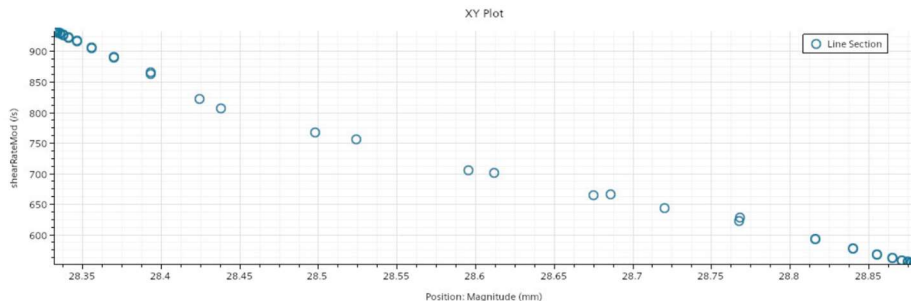


Figure 34: Shear rate profile for mesh base size 0.20 mm for the CC27 geometry plotted as a function of radial coordinate (mm) across the measurement gap.

Minimal visual change in the shear rate profiles were recorded, indicating that the mesh once again was sufficient for mesh independent solutions. The only deviation present is for 0.50 mm (*Figure 31*) where a non-systematic dip in shear rate occurred close to the spindle.

The local mesh sensitivity results for the RV5 geometry are presented in *Table 7*. The analysis was performed for the same Cross model case as used in the global torque comparison, at 100 RPM.

Table 7: RV5 local shear rate range for different mesh base sizes. Deviations are calculated using the 0.30 mm mesh as reference.

Base size [mm]	Minimum shear rate [s^{-1}]	Deviation in minimum shear rate [%]	Maximum shear rate [s^{-1}]	Deviation in maximum shear rate [%]
0.60	0.04711	4.945	141.57	3.517
0.50	0.04720	5.146	136.17	0.431
0.40	0.04623	2.985	133.71	2.230
0.30	0.04489	0.000	136.76	0.000

The extracted minimum and maximum shear rates for the RV5 geometry show some variation between the tested mesh base sizes. The minimum shear rate varied between 0.04489 and 0.04720 s^{-1} , while the maximum shear rate varied between 133.71 and 141.57 s^{-1} . The largest minimum shear rate deviation was 5.146%, for the 0.50 mm mesh. The largest deviation in maximum shear rate was 3.517%, for the 0.60 mm mesh.

The 0.40 mm mesh, which was selected as the final mesh for the RV5 geometry, gave a shear rate range of 0.04623 – 133.71 s^{-1} . This was close to the range obtained with the finest 0.30 mm mesh, which had 0.04489 – 136.76 s^{-1} . The deviation for the 0.40 mm mesh was 2.985% for the minimum shear rate and 2.230% for the maximum shear rate. Together with the global torque deviation of only 0.094%, this indicates that the 0.40 mm mesh was sufficiently refined for the RV5 simulations.

The shear rate profiles across the RV5 gap for the different mesh base sizes are shown in *Figures 35 - 38* below.

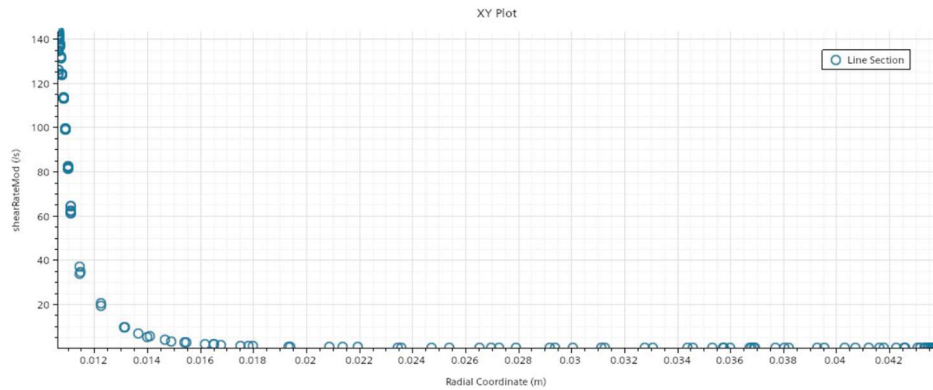


Figure 35: Shear rate profile for mesh base size 0.60 mm for the RV5 geometry plotted as a function of radial coordinate (mm) across the measurement gap. The line-section extends from the spindle surface at $r = 10.5965$ mm to the cup wall at $r = 43.8235$ mm. The profiles are used to compare how the predicted local shear rate distribution changes with mesh base size.

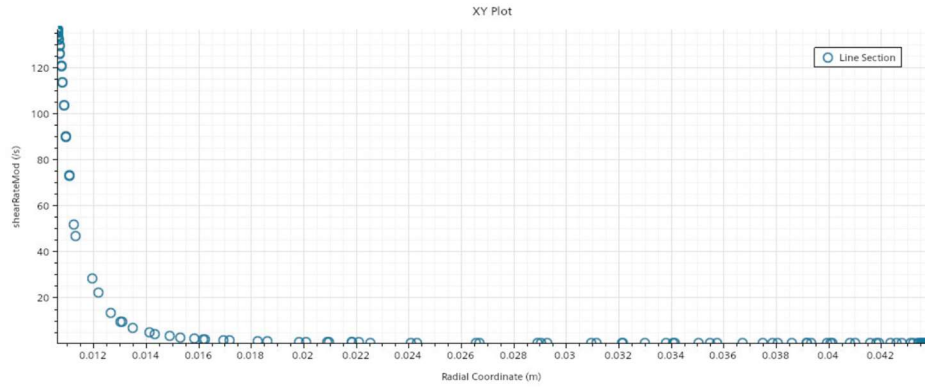


Figure 36. Shear rate profile for mesh base size 0.50 mm for the RV5 geometry plotted as a function of radial coordinate (mm) across the measurement gap.

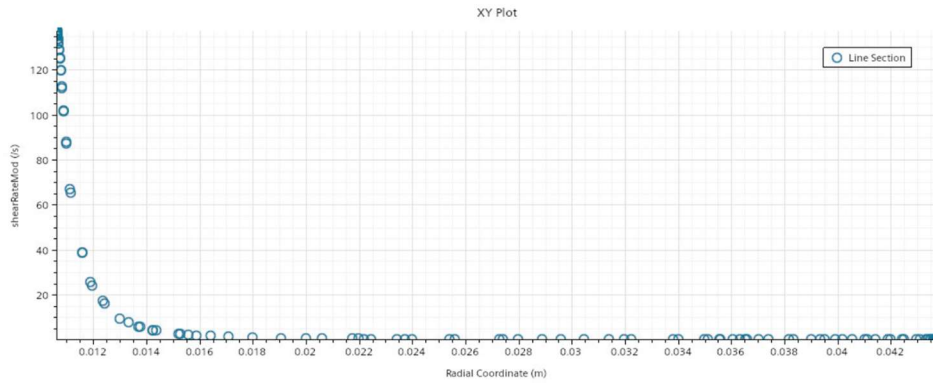


Figure 37: Shear rate profile for mesh base size 0.40 mm for the RV5 geometry plotted as a function of radial coordinate (mm) across the measurement gap.

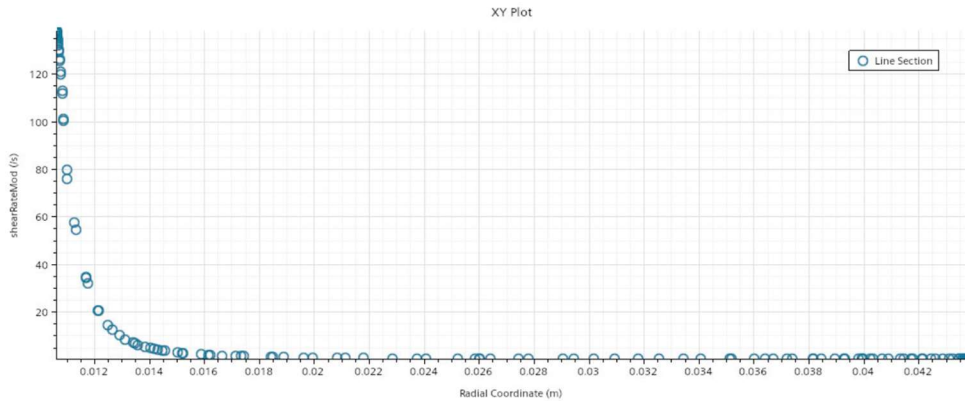


Figure 38: Shear rate profile for mesh base size 0.30 mm for the RV5 geometry plotted as a function of radial coordinate (mm) across the measurement gap.

The RV5 shear rate profiles show similar overall behaviour for all tested mesh base sizes. The shear rate remained low in large parts of the gap and increased closer to the spindle surface as expected, where the highest velocity gradients occurred. This trend was captured by all meshes, indicating that the main local shear rate distribution was not strongly affected by the mesh resolution.

Some differences were observed in the maximum shear rate close to the spindle surface. The coarsest mesh, 0.60 mm, gave the highest maximum shear rate of 141.57 s^{-1} , while the chosen final mesh, 0.40 mm, gave 133.71 s^{-1} . The finest mesh, 0.30 mm, gave 136.76 s^{-1} . This indicates that the local shear rate field was slightly more sensitive to mesh resolution than the global torque. However, the overall profile shape remained consistent, and the global torque deviation for the 0.40 mm mesh was only 0.094%.

Therefore, the 0.40 mm mesh was considered sufficiently refined for the final RV5 simulations. Based on the agreement in both global torque and local shear rate distribution, the selected meshes were considered mesh independent to a sufficient degree for the scope of this work.

5.5 CFD Validation

The purpose of the CFD validation is to assess whether simulations using the Cross model can with accuracy, reproduce experimentally measured torque for both the RV5 and the CC27 geometries.

Validation was conducted by comparing CFD predicted torque with laboratory measured torque. This was done for both geometries and under matching temperature conditions. Since the CFD model relies exclusively on the rheological parameters used as input, these parameters first needed to be regressed from real experimental data. In this work, Cross model parameters were obtained through regression from RheolabQC measurements using the CC27 geometry performed at the same temperature as the corresponding Brookfield measurements.

The overall validation approach follows a structured workflow, designed to capture the full modeling chain from experimental measurement to numerical prediction. This sequence can be seen in the workflow (*Section 5, Figure 13*) excluding the box “AI parameter prediction” and everything right of it. The validation workflow is summarized as follows:

1. Perform experimental torque measurements using RV5 and CC27 geometries (*Sections 5.1 and 5.2*).
2. Obtain Cross model parameters from regression of CC27 data (*Section 5.3*).
3. Use the identified parameters as input to CFD simulations and predict torque on the spindles.
4. Compare CFD-predicted torque with experimentally measured torque.

This procedure ensures that the validation reflects not only the numerical accuracy of the CFD model but also the combined effects of experimental uncertainty, estimations and rheological model parameter regression.

In this approach, Brookfield measurements were performed according to the procedure described in *Section 5.1*. For each prepared CMC batch, two separate samples of 500 mL were extracted. Each sample was swept over the rotational speed range of 10-100 RPM with 10 RPM increments, twice. This resulted in four Brookfield datasets per batch, denoted as samples 1.1, 1.2, 2.1 and 2.2. For the same batches and temperatures, CC27 measurements were carried out according to *Section 5.2*, to ensure consistent fluid properties. Triplicate measurements were performed for each condition, and the temperatures were matched to those of the Brookfield measurements as closely as possible. This alignment in temperature is critical, as the rheological behavior of fluid solutions is highly sensitive to temperature shifts.

Cross model parameters were obtained from the experimental CC27 data using the regression procedure described in *Section 5.3*. Regression was performed on the averaged CC27 triplicate data. For each CC27 dataset, three regression strategies were evaluated:

- i. Inclusion of all measured shear rate data points.
- ii. Exclusion of the lowest shear rate point.
- iii. Exclusion of the lowest shear rate point combined with an end-effect correction.

The exclusion of the lowest shear-rate data point was investigated due to the uncertainty associated with low shear-rate measurements. Variability in the first shear-rate point was observed across CC27 triplicate measurements, indicating reduced measurement consistency in this region. This point further lies at the lower end of the operational shear-rate range of the CC27 geometry, where measurement uncertainty is higher. Based on these observations, the exclusion of the lowest shear-rate point was included as a regression strategy to evaluate its effect on the robustness of the Cross model parameter estimation.

End-effect correction factors, c_L for each individual shear rate were calculated using *Equation 24* to be directly applicable to the Anton Paar methodology for end-effect correction (*Section 2.3.3*). In this work, the end-effect contribution was approximated by extracting torque applied to all spindle parts except the spindle wall with an end-effect report (*Section 5.4.4*) from the CFD results using the Cross parameters obtained from the “all points included” regression case.

$$c_L = \frac{T_{\text{total}}}{T_{\text{total}} - T_{\text{end-effects}}} \quad (24)$$

In *Equation 24* above T_{total} is the total torque (moment) applied to the spindle and $T_{\text{end-effects}}$ is the torque from end effects only. The new calculated correction factors were then applied to corresponding calculation of the viscosity using *Section 2.3.1, Equation 6*. This approach provided a practical estimate of the influence of end effects without introducing a loop where regression parameters and end-effect factors would repeatedly update each other.

To validate that the CFD model can reproduce experimentally measured torque, CFD simulations were conducted. For the RV5 geometry, simulations were performed for each Brookfield sample at its measured temperature. Cross model parameters from the CC27 regressions were used as CFD input for three cases: (i) all shear-rate points included, (ii) lowest shear-rate point excluded, and (iii) lowest shear-rate point excluded with end-effect correction. Each parameter set was simulated over the RV5 sweep range of sweep range of 10 to 100 RPM in 10 RPM increments. The spindle torque was extracted from CFD and converted to percent of maximum torque (%Tm) using the Brookfield maximum torque (*Section 2.3.2*), enabling direct comparison to the experimental %Tm at the same RPM and temperature. For the CC27 geometry, agreement was evaluated using the absolute spindle torque (N·m) at the corresponding operating points. Agreement was quantified by calculating the signed relative deviation between CFD-predicted torque and laboratory measured torque at each operating point using the deviation definition, which is applied consistently for both geometries as long as T_{CFD} and T_{Lab} are expressed in the same form (both as %Tm for Brookfield or both as absolute torque for CC27).

$$\text{Deviation (\%)} = \frac{T_{\text{CFD}} - T_{\text{Lab}}}{T_{\text{CFD}}} \cdot 100 \quad (25)$$

Where T_{CFD} is the CFD simulated torque and T_{Lab} is the experimental measured torque. Mean deviation was calculated as the average of the signed relative torque difference over the investigated operating range for each geometry. For Brookfield, this corresponds to RPMs 10-100. For CC27, the mean deviation was computed over the 15 CC27 operating points included in the measurement procedure. Negative values indicate CFD underprediction of RV5 torque.

In addition to mean deviation, a deviation trend analysis was performed to determine whether deviations changed systematically across the operating range (e.g., increasing mismatch at high RPM or high shear rate). The operating range was divided into low, mid, and high regions, and the mean signed deviation was computed within each region.

Table 8: Shows the low, mid, and high RPM regions for RV5 (left) and shear rate regions for CC27 (right).

RPM	Range(RPM)	Shear Rate	Shear Rate Range(s ⁻¹)
Low	10-30	Low	2-7
Mid	40-60	Mid	10-25
High	70-100	High	≥30

For each dataset and each simulation case, the mean signed deviation was computed within each group. Deviation trends were reported for two transitions, Low→Mid and Mid→High. The direction of the trend was assigned based on whether the magnitude of the mean deviation increased or decreased

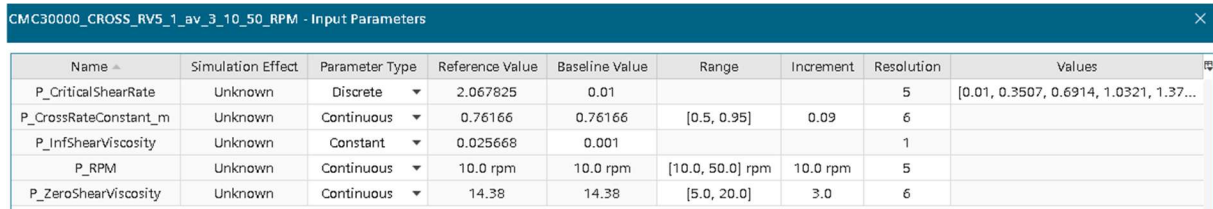
between consecutive groups. To avoid effect of very small changes, differences smaller than approximately 0.5 percentage points were treated as negligible.

- Increasing Magnitude $\rightarrow \uparrow$
- Decreasing Magnitude $\rightarrow \downarrow$
- Change ≤ 0.5 %units across bins $\rightarrow \approx$

This trend classification was used consistently for both Brookfield and CC27 to indicate whether the CFD vs lab mismatch was approximately constant over the operating range or became more pronounced at higher RPM (Brookfield) or higher shear rates (CC27).

5.6 Creation of Datasets

The dataset used for training the artificial neural network was generated CFD simulations and later preprocessed in Python to fit the input structure of the AI. The CFD part consisted of a parameter sweep performed in a STAR-CCM+ Design Manager file. The Design Manager reads a reference simulation and performs multiple simulations with varied parameters. Rheology model parameters and rotational speed were varied in the RV5 geometry. The purpose of the sweep was to generate a synthetic dataset, linking known Cross model parameters to the corresponding RV5 torque response. The interface for input parameter range selection used in the CFD sweep are shown in *Figure 39*.



Name	Simulation Effect	Parameter Type	Reference Value	Baseline Value	Range	Increment	Resolution	Values
P_CriticalShearRate	Unknown	Discrete	2.067825	0.01			5	[0.01, 0.3507, 0.6914, 1.0321, 1.37...
P_CrossRateConstant_m	Unknown	Continuous	0.76166	0.76166	[0.5, 0.95]	0.09	6	
P_InfShearViscosity	Unknown	Constant	0.025668	0.001			1	
P_RPM	Unknown	Continuous	10.0 rpm	10.0 rpm	[10.0, 50.0] rpm	10.0 rpm	5	
P_ZeroShearViscosity	Unknown	Continuous	14.38	14.38	[5.0, 20.0]	3.0	6	

Figure 39: Shows the Design Manager interface used for selecting Cross parameter's range, increment and resolution. Note that this is only 900 simulations and 1/6 of the total dataset used for the AI training.

The critical shear rate was varied between 0.01 and 4.78 s⁻¹ for increased resolution since it is a hard parameter to predict, the Cross rate constant between 0.50 and 0.95, and the zero-shear viscosity between 5 and 20 Pa·s. The infinite-shear viscosity was fixed at 0.001 Pa·s, corresponding approximately to the viscosity of water. The rotational speed was varied between 10 and 100 rpm.

The selected parameter ranges were based on initial regressions performed for CMC30000 at 1.4 wt%, in combination with preliminary simulation trials. These initial tests indicated that the chosen span covered a broad response range, extending from approximately 0% torque to above 100% of the maximum torque of the Brookfield viscometer. The range was therefore selected to include both the predicted parameter values and the full measurable torque interval of the instrument, although the final bounds were to some extent chosen pragmatically rather than through a strict optimization procedure.

In total, 5400 CFD simulations were performed, and since one simulation is for one RPM, this resulted in more than 1000 usable data rows after post-processing and filtering for the 5 point model, and more than 500 rows for the 10 point model. Both models will be explained in more detail in section 5.7.

The raw CFD output was then processed using Python. The processing consisted of filtering, sorting, combining, and formatting the simulation results into a structure suitable for neural network training. The measured torque percentage from the CFD simulations was used to calculate an equivalent Brookfield viscosity according to,

$$\eta = \frac{400000}{RPM} \cdot \frac{T}{7.187 \cdot 10^{-4}} \quad (26)$$

where η is the relative viscosity in mPas, RPM is the rotational speed (revolutions per minute), and T is the torque percentage. This calculation was applied during the Python post-processing stage for each rotational speed and torque value.

Rows containing torque values outside the usable Brookfield measurement range were removed before ANN training. For the five-point dataset, rows were removed if any torque value was above 99% or below 10%, while the ten-point dataset used torque limits of 1-99%. The five-point dataset was filtered to remove both torque saturation regions and low-torque points with reduced reliability, whereas the ten-point dataset retained a broader low-torque range to increase the measurement span and improve prediction performance at lower torque levels. The Brookfield-equivalent viscosity was then calculated from the simulated torque percentage and rotational speed. The final filtering limits resulted in different viscosity ranges for the two datasets. At 100 s^{-1} , the five-point dataset covered approximately 103-3050 mPa·s, while the ten-point dataset covered approximately 24-1852 mPa·s. These ranges define the approximate viscosity space represented by each ANN model.

The final ten-point dataset contained rows of ten rpm values, ten torque percentage values, ten calculated viscosity values, and the three target Cross model parameters. A hard check was included in the script to verify that each output row contained 33 columns, corresponding to 30 input-related columns and 3 output parameters.

An additional augmentation script was used to expand the dataset by generating alternative five-point combinations from available RPM, torque, and viscosity triplets associated with the same fluid parameter set. For each unique set of Cross model parameters, the corresponding measurement points were grouped, and random combinations of five points were sampled. This approach increased the number of training samples while preserving the underlying relationship to the same Cross parameter set.

The final processed datasets were then used as input for the ANN training. The input features consisted of the CFD produced RPM, torque percentage and calculated viscosity. The output targets were the Cross model parameters: zero-shear viscosity, critical shear rate, and Cross rate constant.

5.7 Neural Network Setup

An artificial neural network was developed using a feed-forward architecture to predict three parameters of the Cross model: zero-shear viscosity, critical shear rate, and the Cross rate constant. The model consisted of a shared fully connected trunk followed by three separate output heads, one for each predicted parameter.

The network architecture comprised a common core with four hidden layers, followed by separate prediction branches. For the 5-point model, the shared trunk consisted of four layers with 512, 512, 512, and 256 units. After the shared layers, the network split into three branches, each containing a 64-unit hidden layer followed by a single linear output neuron. This structure allowed the model to learn a shared representation of the rheological input data while still enabling target-specific prediction of each Cross-model parameter.

For the 10-point model, the same overall architecture was retained, but with an increased trunk capacity of (512, 512, 512, 512) units to account for the higher-dimensional input representation. The final selected model architectures are summarized in *Section 5.7.9*.

A feed-forward neural network was chosen because the task involved mapping a fixed set of engineered rheological features to continuous model parameters. The model was developed iteratively, starting from smaller architectures and increasing network capacity where prediction performance was insufficient. Rectified linear unit (ReLU) activation functions were used throughout as a general-purpose non-linear activation function.

5.7.1 Input feature construction

The neural network input for the 5-point model was based on five measurement points from Brookfield-type viscosity measurements. Rather than using raw rotational speed and viscosity values directly, the input representation was engineered to better capture the shape of the viscosity curve.

Viscosity values were transformed using a base-10 logarithm. Rotational speed values were also transformed using a base-10 logarithm and were used to calculate local slopes between consecutive measurement points. The local slope between two neighbouring points was calculated as,

$$s_i = \frac{\log_{10}(\eta_{i+1}) - \log_{10}(\eta_i)}{\log_{10}(\text{rpm}_{i+1}) - \log_{10}(\text{rpm}_i)} \quad (27)$$

where η_i is the viscosity at measurement point i . These slope features provided information on how viscosity changed as a function of rotational speed and helped the model identify curvature and shear-thinning behaviour. Without these slope features, the model exhibited unstable convergence and produced maximum relative errors exceeding 4000% in some training iterations.

The final input vector for the 5-point model consisted of: 5 log-transformed viscosity values, 5 torque values and 4 local slope values, resulting in a total of 14 input features as can be seen in *Figure 40*.

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
rpm_1	pct_t_1	relative_vi rpm_2	pct_t_2	relative_vi rpm_3	pct_t_3	relative_vi rpm_4	pct_t_4	relative_vi rpm_5	pct_t_5	relative_vi	P_ZeroShe	P_CriticalS	P_CrossRa				
20	34,32402	6864,804	30	42,95041	5726,722	40	49,63121	4963,121	50	55,09451	4407,561	70	63,74527	3642,587	14	3,0764	0,77
10	13,24769	5299,074	20	15,27179	3054,358	30	16,17908	2157,211	60	17,42152	1161,435	80	17,86968	893,4839	20	0,6914	0,95
10	21,02695	8410,78	30	33,93638	4524,85	50	38,80789	3104,631	80	42,40313	2120,157	100	43,84849	1753,939	14	2,7357	0,95
20	31,95019	6390,037	30	39,2232	5229,76	40	44,97521	4497,521	50	49,7914	3983,312	80	61,01725	3050,863	20	1,0321	0,68
10	25,35551	10142,2	20	40,26059	8052,118	60	69,2254	4615,027	70	73,41428	4195,102	100	82,97555	3319,022	14	4,78	0,86
60	19,73105	1315,404	70	20,49148	1170,942	80	21,1126	1055,563	90	21,62878	961,2792	100	22,06954	882,7817	5	4,0986	0,95

Figure 40: Snippet of dataset used for the 5 point model

For the 10-point model, the same feature-engineering strategy was applied to ten measurement points, resulting in: 10 log-transformed viscosity values, 10 torque values and 9 local slope values, for a total of 29 input features. This extended representation provided additional resolution of the viscosity curve, particularly in the shear-thinning region and a snippet of the dataset with 10 points can be seen in *Figure 41*.

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG
rpm_1	pct_t_1	relative_vi rpm_2	pct_t_2	relative_vi rpm_3	pct_t_3	relative_vi rpm_4	pct_t_4	relative_vi rpm_5	pct_t_5	relative_vi rpm_6	pct_t_6	relative_vi rpm_7	pct_t_7	relative_vi rpm_8	pct_t_8	relative_vi rpm_9	pct_t_9	relative_vi rpm_10	pct_t_10	relative_vi	P_ZeroShearViscosity_5	P_CriticalShearRate_5	P_CrossRateConstant_m_5									
10	4,2382	9807,3	20	6,935	919	30	8,4793	100	40	10,083	9008,3	50	11,519	521,05	60	12,094	854,25	70	14,016	800,39	80	14,108	758,91	90	16,186	718,91	100	17,189	607,36	5	0,9507	0,5
10	3,7827	9050,1	20	5,5394	1807,3	30	6,0495	913,26	40	7,5286	782,86	50	8,8955	708,44	60	9,6908	645,39	70	10,429	595,32	80	11,198	595,81	90	11,795	522,44	100	12,353	434,13	5	0,9507	0,59
10	3,2011	1021,3	20	4,8196	280,21	30	5,409	721,19	40	6,0862	608,12	50	6,8432	531,41	60	7,1294	475,29	70	7,582	432,12	80	7,9504	397,81	90	8,2121	365,43	100	8,6463	245,71	5	0,9507	0,68
10	2,6842	1037,7	20	3,893	170,61	30	4,1628	505,03	40	4,5434	454,34	50	4,9571	388,08	60	5,116	340,77	70	5,3287	306,07	80	5,5415	277,66	90	5,7947	254,43	100	5,993	235,72	5	0,9507	0,77
10	2,3896	955,85	20	2,8482	589,84	30	3,103	416,57	40	3,2846	329,46	50	3,4339	275,15	60	3,5605	237,37	70	3,6844	203,4	80	3,7952	187,81	90	3,8988	170,62	100	3,9944	155,57	5	0,9507	0,86
10	1,9496	778,24	20	2,1392	407,84	30	2,2391	288,95	40	2,3076	230,76	50	2,3691	188,89	60	2,4058	160,35	70	2,4448	138,7	80	2,4797	123,39	90	2,5117	111,63	100	2,5434	101,65	5	0,9507	0,95

Figure 41: Snippet of dataset used for the 10 point model

All input features were scaled using StandardScaler from the *scikit-learn (sklearn)* python library. This method standardizes each feature by subtracting the mean and dividing by the standard deviation, resulting in features with zero mean and unit variance. This scaling ensures that all input variables contribute equally during training and prevents features with large magnitudes from dominating the learning process.

5.7.2 Target variables and scaling

The model was trained to predict three Cross-model parameters: zero-shear viscosity (η_0), critical shear rate (λ), and Cross rate constant (m).

The zero-shear viscosity and critical shear rate were transformed using a base-10 logarithm prior to scaling, as these parameters can span several orders of magnitude. The Cross rate constant was kept in its original scale. All target variables were then standardized using StandardScaler. During evaluation, predictions were inverse-transformed back to their original physical scale before performance metrics were calculated.

5.7.3 Data splitting

The dataset was divided into training, validation, and test subsets to ensure reliable model evaluation.

For the 5-point model, a fixed random seed of 39 was used for reproducibility. First, 10% of the data was held out as unseen test data. The remaining 90% was then split into training and validation data, with 15% of this subset used for validation. This resulted in an approximate split of 76.5% training data, 13.5% validation data, and 10% test data.

For the 10-point model, a slightly different splitting strategy was used. A fixed random seed of 42 was applied, and the data was divided into 80% training, 10% validation, and 10% test data using two

consecutive splits. First, 10% of the data was separated as the test set. The remaining 90% was then split with 10% allocated to validation, resulting in the final 80/10/10 distribution.

The validation set was used during training for learning-rate scheduling and early stopping, while the test set was reserved exclusively for final model evaluation on unseen data.

5.7.4 Physics-aware noise augmentation

The training data originated from fitted or processed rheological curves and was therefore relatively noise-free compared with real experimental Brookfield measurements. To improve robustness to experimental variation, physics-aware noise was applied to the input features during training.

Torque values were perturbed using a multiplicative noise factor. The corresponding log-viscosity values and slope features were then adjusted consistently using the same perturbation, ensuring that the augmented inputs remained physically plausible. A maximum noise variance of 1% was used. Noise was applied only during training and was not applied to validation or test data.

5.7.5 Loss function

The model was trained using a weighted mean squared error loss function calculated on the standardized target variables:

$$L = \text{mean}(w \cdot (\hat{y} - y)^2) \quad (28)$$

where w is the vector of loss weights, $\hat{y}$ is the predicted target vector, and y is the true target vector.

For the 5-point model, the loss weights were set to $w = [1, 2, 1]$, giving increased emphasis to the critical shear rate, which was found to be the most difficult and sensitive parameter to predict accurately. For the 10-point model, a normal weighting was used, $w = [1, 1, 1]$.

5.7.6 Model evaluation

The model was evaluated using both R^2 scoring and relative error. The R^2 score was used to assess the overall correlation between predicted and true values. However, since high R^2 values can still occur even when individual predictions have large deviations, relative error was also calculated.

The relative error was calculated as:

$$\text{Relative error} = \frac{|\hat{y} - y|}{|y| + \epsilon} \quad (29)$$

where $\epsilon = 10^{-1}$ was added to avoid division by zero.

The maximum relative error was calculated separately for: Zero-shear viscosity, Critical shear rate and Cross rate constant.

The maximum relative error of the critical shear rate was used as the primary model-selection criterion, since this parameter was the most sensitive and difficult to predict. The worst maximum error across all three outputs was also considered to ensure that the selected model did not sacrifice performance on the other outputs.

5.7.7 Training procedure

The neural network was trained for a maximum of 500 epochs (iterations). The AdamW optimizer was used with a learning rate of 1×10^{-3} and a weight decay of 1×10^{-4} . A learning-rate scheduler was used to reduce the learning rate when the validation loss stopped improving. A ReduceLROnPlateau scheduler was applied with a patience of 30 epochs to reduce the learning rate when the validation loss stopped improving.

Early stopping was employed to prevent overfitting. Training was terminated if the validation loss did not improve for 50 consecutive epochs, and the model state with the lowest validation loss was retained.

5.7.8 Hyperparameter optimization

A deterministic hyperparameter grid search was performed, for parameters shown in *Table 9*, to identify suitable model configurations for both the 5-point and 10-point models. The sweep was implemented using the same training pipeline as the final models to ensure full transferability of results.

A total of 144 model configurations were evaluated, covering variations in shared trunk architecture, loss weights, optimizer choice, learning-rate scheduler patience, early-stopping patience, and batch size. The top 10 tested configurations and their resulting maximum relative errors are reported in the final sweep output in *Appendix D1*.

Table 9: Hyperparameter sweep for both AI models

Hyperparameter	Values tested
Hidden trunk architecture	(512, 512, 512, 256), (512, 512, 512, 128), (512, 512, 512, 512)
Loss weights	(1.0, 1.0, 1.0), (1.0, 2.0, 1.0), (1.0, 3.0, 1.0)
Optimizer	AdamW, Adam
Learning-rate scheduler patience	20, 30
Early-stopping patience	40, 50
Batch size	32, 64
Learning rate	0.001
Weight decay	0.0001

5.7.9 Selected final model

For the 5-point model, the best-performing configuration in the hyperparameter sweep can be seen in *Table 10*, which achieved the lowest maximum relative error for the critical shear rate and the lowest worst-case error across all three outputs.

Table 10: 5 point model final hyperparameters

Parameter	Selected value
Hidden trunk	(512, 512, 512, 256)
Loss weights	(1.0, 2.0, 1.0)
Optimizer	AdamW
Learning-rate scheduler patience	30
Early-stopping patience	50
Batch size	64
Learning rate	0.001
Weight decay	0.0001

For the 10-point model, the best-performing configuration in the hyperparameter sweep can be seen in *Table 11*, which achieved the lowest maximum relative error for the critical shear rate and the lowest worst-case error across all three outputs.

Table 11: 10-point model final hyperparameters

Parameter	Selected value
Hidden trunk	(512, 512, 512, 512)
Loss weights	(1.0, 1.0, 1.0)
Optimizer	AdamW
Learning-rate scheduler patience	30
Early-stopping patience	50
Batch size	32
Learning rate	0.001
Weight decay	0.0001

The selected models achieved the following maximum relative errors on the test set, as presented in Table 12-13 below.

Table 12: 5-point model maximum relative errors.

Target	Maximum relative error
Zero-shear viscosity	4.80%
Critical shear rate	9.84%
Cross rate constant	2.78%

Table 13: 10-point model maximum relative errors.

Target	Maximum relative error
Zero-shear viscosity	2.84%
Critical shear rate	2.457%
Cross rate constant	0.441%

5.7.10 Derivation of power-law parameters

After predicting the Cross-model parameters, approximate Power Law parameters K and n were obtained by fitting a Power Law relationship to viscosity values generated from the predicted Cross model over the shear-thinning region. Viscosity values were calculated for the shear rate range:

$$\dot{\gamma} = [24.9, 37.9, 57.8, 88, 134, 204, 311, 473, 720]$$

These values were fitted using the Power Law expression (Section 2.4.1, Equation 13), which was linearized in logarithmic space. A least-squares regression was applied, where the slope corresponds to $n - 1$ and the intercept to $\log_{10}(K)$. The resulting parameters represent apparent Power Law values valid for the selected shear-rate interval rather than the full viscosity curve.

6. Results and Discussion

This chapter presents and discusses the results of the thesis work in relation to the overall objective of developing a methodology for estimating rheological model parameters from Brookfield measurements, using CFD and artificial intelligence.

The interpretation of the results requires consideration not only of prediction performance, but also of rheological model suitability, experimental uncertainty, and the transferability of parameter sets between different measurement geometries. The discussion therefore addresses the work as an integrated framework in which laboratory measurements, numerical simulations, and AI-based predictions are strongly interdependent.

The following work-flow will be used in this Chapter:

- **Section 6.1** first examines the initial results and the limitations of the early Power Law-based approach, which provided useful insight, but proved insufficient for reliable transfer between the RV5 and CC27 geometries.
- **Section 6.2** then discusses the laboratory measurements and variations that occurred in the experiental part of the work.
- **Section 6.3** then follow with an evaluation of the CFD validation using the Cross model. Discusses wether CFD sufficient to reconstruct the fluid behaviour and torque in both geometries from CC27-derived parameters.
- **Section 6.4** discusses the final AI model in terms of parameter prediction accuracy and consistency. Discusses how our AI-models predict Cross parameters compared to CC27 regression. And how well RV5 torque can be reconstructed in CFD with the predicted AI Cross parameters.

6.1 Initial Power Law based CFD-AI results

The initial AI modelling approach was based on the Power Law model, using the consistency index, K , and the flow behaviour index, n . This Power Law model was selected as a first approach due to its simplicity and its common use for describing shear-thinning fluids. The dataset was generated using 500 CFD simulations of the RV5 geometry, where K and n were varied over a defined parameter range shown in *Table 14*. The dataset was then split into test (20%), validation (16%) and training (64%) data. It is important to note that for this initial Power Law approach a CFD validation step was never conducted.

Table 14: Design manager parameters for CFD dataset, 10 different K values, 10 different n values and 5 different RPMs. Totalling 500 unique datapoints

Variable	Range	Increment
K (Pa*s ⁿ)	0.5-10	1.05
n	0.5-1	0.055
RPM	10-50	10

An initial artificial Neural Network was trained on this Power Law dataset with torque at RPMs 10-50 as input and Power Law parameters as output. This model, used 5 RPM measurements, and the corresponding torque and relative viscosity, similarly to the 5 point model described in *Section 5.7*, the difference beeing the outputs are K and n instead of the Cross parameters described in that section. This AI model showed promising guessing performance on the CFD RV5 test split not used in the training, the results of which can be seen in *Table 15*. The Neural Networks predictions based on the test dataset resulted in high R^2 –scores and low relative errors, indicating that the FFNN framework itself was capable of learning the relationship between Brookfield measurement data and Power Law model parameters.

Table 15: Initial AI results, R^2 , mean and max relative error for K and n . Predictions based on CFD dataset of 100 rows, 20 rows were randomly selected as test dataset and used as basis for these prediction results.

Metric	n	K
R^2	0.9992	0.9998
Mean relative error (%)	0.525	0.714
Max relative error (%)	1.397	3.815

Since these results were based on the synthetic RV5 CFD dataset it also needed to be compared to actual measurements and torques. This was done by having the AI model predict the Power Law parameters of condensed milk. This prediction was based on the average of three RV5 measurements series of five measurements ranging from 10-50 RPM with 10 RPM increments, which can be seen in Table 16.

The Power Law parameters predicted by the AI model from the condensed milk Brookfield measurements were evaluated by using them as input parameters in CFD simulations of both the RV5 and CC27 geometries. If the predicted parameters were physically transferable, the simulated torque would be expected to agree with the experimental torque in both systems. The RV5 simulations showed relatively good agreement, with only small deviations from the measured Brookfield torque, as shown in Table 16.

Table 16: Shows Mean measured laboratory % of max torque from the Brookfield with Condensed Milk. The Mean CFD simulation % of max torque in RV5 geometry with Power Law parameters obtained from the initial AI model. The Mean difference between laboratory measurements and CFD simulations.

RPM	Lab Mean %Tmax	CFD Mean %Tmax	Mean % Difference (CFD-Lab)/Lab *100
10	17.53%	17.90%	-2.03%
20	35.17%	34.77%	1.15%
30	51.83%	51.25%	1.13%
40	67.03%	67.50%	-0.69%
50	81.17%	83.55%	-2.85%

Applying the same parameters to the CC27 geometry, however resulted in poor agreement, with torque deviations exceeding 130% as shown in Table 17.

Table 17: Shows the CFD torque obtained from simulation in CC27 geometry with average Power Law parameters obtained from the initial AI model. The corresponding laboratory measured torque at same shear rate. And the difference (CFD-Lab)/Lab *100 between CFD and Lab.

Shear Rate (1/s)	Lab Torque (mN·m)	CFD Torque (mN·m)	% Difference (CFD-Lab)/Lab *100
20.0	2.635	6.386	+142.3%
29.8	3.952	9.365	+136.9%
44.3	5.875	13.703	+133.3%
66.0	8.695	20.093	+131.1%
98.3	12.765	29.452	+130.8%
146.0	18.631	43.057	+131.2%

218.0	27.001	63.266	+134.2%
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The calculated difference in *Table 17* show that the CFD largely overpredicted the torque in the CC27 geometry. This indicated that the Power Law parameters obtained from the RV5 region by the AI model were not transferable to the CC27 measurement region. At the same time, *Table 17* should not be interpreted as proof that Power Law extrapolation was the only cause of the error. The fluid food products used in the initial tests are difficult validation materials because their measured response can depend on temperature, wall slip, and thixotropy behaviour. This was especially clear for condensed milk. *Figure 42* shows an upward and downward shear rate sweep for sweetened condensed milk, where the separation between the curves indicates thixotropic behaviour.

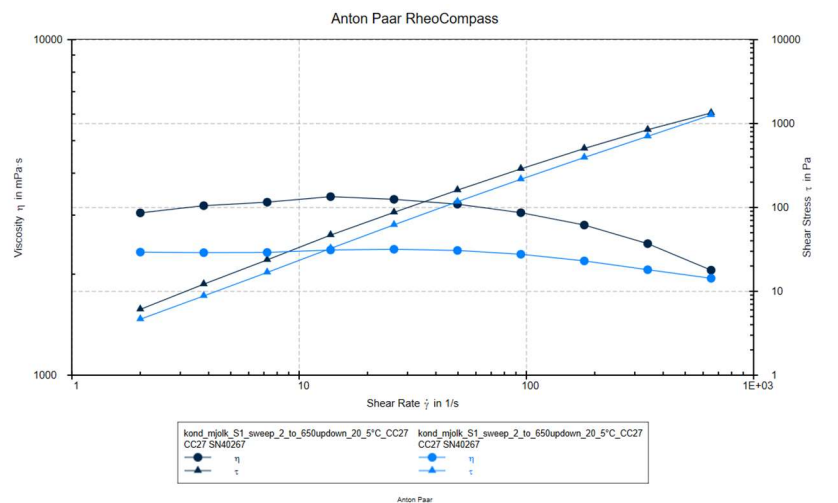


Figure 42: Sweep up (black) and down (blue) for sweetened condensed milk showing clear thixotropy as the two sweeps exhibit difference in viscosity (lines with dots) at the same shear rates.

This proof of thixotropy also shows a reason to why the measurements do not coincide, since Power Law is not a valid model for time dependant fluids. Since the CC27 measurements included a defined measurement protocol and pre-shear, while the CFD simulation represents only a steady state response based only on the fitted rheological parameters, the large overprediction in *Table 16* may have resulted from a combination of rheological model limitations and material behaviour.

Ketchup was also considered as a validation fluid, but was excluded from the main analysis due to poor repeatability and likely wall-slip or yield-stress effects. Overall, the initial results show that suitable food fluids were difficult to identify, since many industrially relevant products exhibit thixotropy, wall slip or yield-stress behaviour. The Power Law model is not suitable for thixotropic fluids. Further, these effects made it difficult to isolate whether the disagreement came from the CFD model, the laboratory measurements or the fluid behaviour itself.

To test whether the disagreement was only caused by complex food rheology, a close to Newtonian sugar solution (Brix 70) from a previous Master's thesis (Ekelund, 2025) was also evaluated. A Power Law regression of the available average CC27 measurements resulted in Power Law parameters, $n = 0.983$ and $K = 0.6224$. Since the reference measurements used an LV1 spindle, the CFD comparison was also performed using the LV1 geometry. No separate mesh sensitivity analysis was performed for the LV1 geometry here. Since this comparison was used only as an initial indication, the mesh settings from the CC27 mesh sensitivity study were adopted. The results should therefore be interpreted as indicative rather than fully validated. The comparison between the laboratory data from Ekelund (2025) and the CFD-simulated torque is shown in *Table 18*.

Table 18: Mean laboratory torque with Brookfield LV1 spindle from Ekelund (2025) vs CFD simulated torque for sugar solution Brix70 with difference, (CFD-Lab)/Lab*100.

RPM	Lab mean %Tm	CFD %Tm	Difference (%)
20	12.93	16.70	+29.1
30	19.73	24.81	+25.7
50	33.43	40.83	+22.1
60	40.83	48.77	+19.4
100	68.97	80.26	+16.4

The systematic overprediction behaviour for lower RPM shown in Table 18 supports the interpretation illustrated in Figure 43. A Power Law fit can describe a limited shear rate region well, but it does not include a low-shear plateau or transition region. It was known that the Brookfield geometry exhibited lower shear rates compared to the CC27 (Section 2.3). If such a fit is extrapolated outside the region where it was determined, it can systematically overpredict or underpredict viscosity and therefore torque. Figure 43 illustrates this problem schematically. The Power Law curve may follow the shear-thinning region but deviate strongly from a fluid with plateau behaviour at lower shear rates.

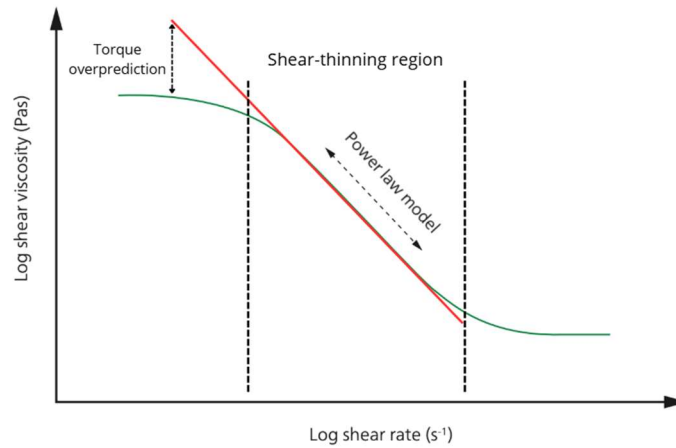


Figure 43: Shows how Power Law (red) parameters regressed in the shear-thinning region can systematically cause overprediction in CFD torque for lower shear rate regions if the fluid is shear-thinning with plateau (green).

The initial trials showed that the main limitation was not the CFD-ANN framework itself, but the rheological model used to describe the fluids along with the material behaviour. The Power Law model performed well when the data followed the same idealized assumptions used to generate the training set, but it was not sufficiently flexible for experimental fluids measured across different shear rate regions, especially the low shear rate region where Brookfield geometries operate. This motivated the transition to the Cross model and the use of controlled CMC solutions for continued validation. The suitable Brookfield spindle for CMC30000 solutions used in this work is the RV5 spindle.

Key takeaway in this section is that The initial Power Law-based CFD-AI approach provided a useful proof-of-concept, showing that AI could learn the relationship between CFD-generated Brookfield torque data and Power Law parameters. Laboratory comparison showed that the Power Law model was limited for transfer between RV5 and CC27, mainly because it cannot capture the low-shear plateau or transition region. The initial trials therefore demonstrated the potential of the CFD-AI workflow, while motivating the shift to the Cross model and controlled CMC solutions for the main validation work.

6.1.2 Shear Rate Profile Analysis

Shear rate profiles were analysed to understand in what regions the RV5 and the CC27 operate for CMC solutions, and why the initial Power Law approach did not transfer well between them. The profiles also

provide insight into how a single shear rate registered in the CC27 actually corresponds to a distribution of local shear rates in the gap. This is important because both the local shear rate range and the rheological model influence the simulated torque response.

Figure 44 show the shear rate profile in the CC27 geometry gap for the 1.4 wt% CMC30000 solution at 20.5 °C. The profile was extracted 25 mm above the cup floor, and the simulation was performed at 558.17 RPM, corresponding to the nominal 720 s^{-1} CC27 data point. The local shear rate range was approximately $550 - 940 \text{ s}^{-1}$. This shows that even though CC27 is treated experimentally as a controlled shear rate measurement, the actual CFD result contains a finite shear rate distribution in the gap for the high-viscosity CMC solution.

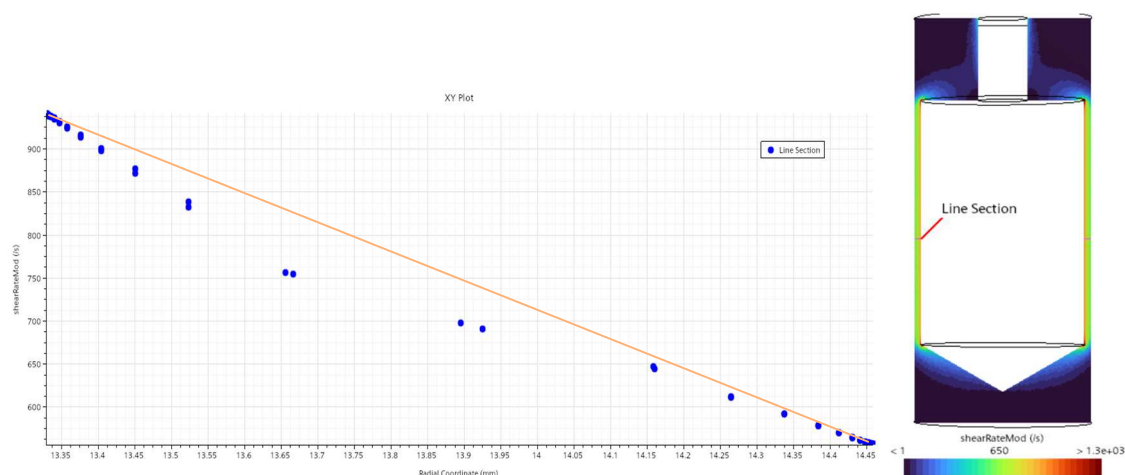


Figure 44. CC27 shear rate profiles in the gap depicted as blue measurement points for each cell (Left), with function *ShearRateMod* against Radial coordinate. An orange linear curve is drawn as the theoretical approximation. Also, full CC27 cup profile (Right) for 1.4 wt% CMC30000 at 20.5 °C using regressed Cross parameters. The profile (Right) was extracted 25 mm above the cup floor (At the marked Line Section) at 558.17 RPM, corresponding to the 720 s^{-1} data point. The local shear rate range in the gap was $556 - 938 \text{ s}^{-1}$.

The shear rate profile exhibit a behaviour similar but not identical to the expected linear (orange curve in Figure 44 above) that is used in the effective shear rate calculation in Section 2.3.1, Equation 7. Since this is the most shear-thinning fluid used in this work, shear rate profiles for 1wt% solutions should also appear somewhat linear. The shear rate profile of 1wt% 21.0°C can be seen in Appendix C2, and does not show much of a difference.

Figure 45 show the corresponding shear rate profile for the RV5 geometry, using the same Cross parameters as in Figure 44 but at 100 RPM. 100 RPM was chosen due to being the highest RPM run in the RV5. The profile was extracted from the spindle edge to the cup wall, 57 mm from the cup bottom. In contrast to CC27, the RV5 geometry produced a much lower shear rate range, $0.046 - 136 \text{ s}^{-1}$. Majority of the gap exhibited low shear rates compared with the maximum shear rate close to the spindle surface. This demonstrates that fluids in the RV5 geometry gap includes very low-shear regions even at the highest rotational speed used in the validation.

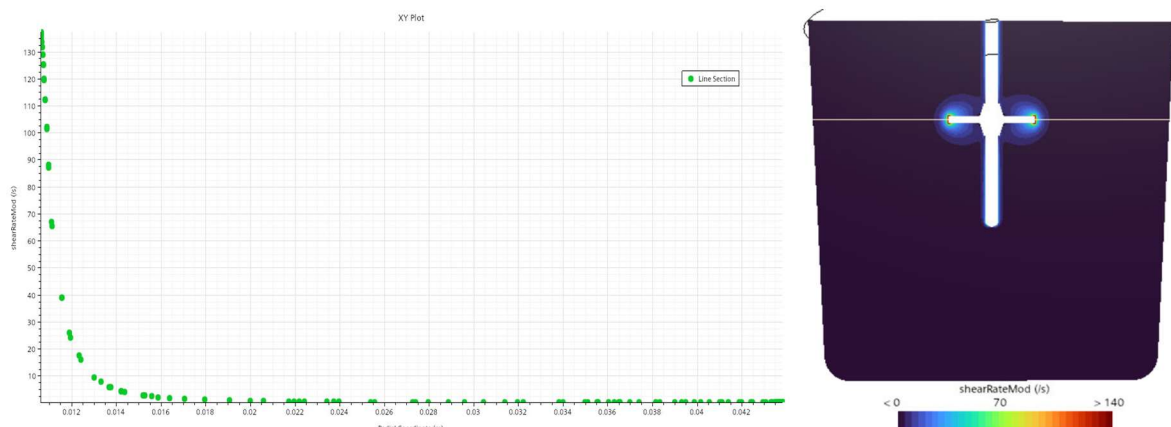


Figure 45: RV5 shear rate profiles in the gap (Left) with function ShearRateMod vs Radial coordinate. Also, full RV5 cup profile (Right) for 1.4 wt% CMC30000 at 20.5 °C using regressed Cross parameters. The profile (Right) was extracted 57 mm above the cup floor (At the marked Line Section) at 100 RPM. Local shear rate range was 0.046 - 136 s^{-1}

The difference between Figures 44-45 is important to understand why the Power Law model did not transfer reliably between the geometries. CC27 mainly samples a shear rate region that is centered around the calculated effective shear rate due to its narrow gap geometry, while RV5 spans a range that reaches shear rates close to zero due to its wide gap. Therefore, the RV5 torque response can be strongly influenced by the viscosity in low-shear plateau and the transition region of the viscosity curve. Since the Power Law model only describes a continuous shear-thinning trend and cannot represent for example a Newtonian plateau, it is not suitable for extrapolation across such a wide shear rate range. The Cross model was therefore selected for continued work, since it can represent the low-shear plateau, transition region, and shear-thinning behaviour within one continuous viscosity function. While also being a simple rheology model compared to other models describing multiple shear rate regions.

To further illustrate the difference in shear rate conditions between the two measurement geometries, an example comparison was made using Cross model parameters obtained from a CC27 measurement and regression. These parameters were then used in CFD simulations of both the RheolabQC CC27 and RV5 geometries. The parameters used for the comparison are shown in Table 19, and the resulting shear rate ranges are visualized in Figure 46.

Table 19: Example of cross parameters and Power Law parameters for CMC30000 1 wt%, based on triplicate CC27 Measurements made at 21.3°C.

Sample	K ($\text{Pa} \cdot \text{s}^n$)	n	Infinite shear viscosity, η_∞ ($\text{mPa} \cdot \text{s}$)	Zero-Shear Viscosity, η_0 ($\text{mPa} \cdot \text{s}$)	Cross rate constant	Critical shear rate, $\dot{\gamma}_c$
CMC 30000 21.3°C 1wt%	6.165789	0.391618	1	4772.942	0.659715	2.440387

Figure 46 illustrates that the Anton Paar RheolabQC with CC27 and Brookfield DV2T-RV with RV5 spindle measurements represent shear conditions in fundamentally different ways. In the CC27 geometry, the shear rate range is relatively close to the laboratory stated effective shear rates. In contrast, each RV5 measurement corresponds to a broad local shear rate distribution, where the lower part of the range approaches 0 s^{-1} even at higher RPM values. This means that successful transfer between the two measurement methods requires a rheological model that accurately describes the low-shear behaviour of the fluid.

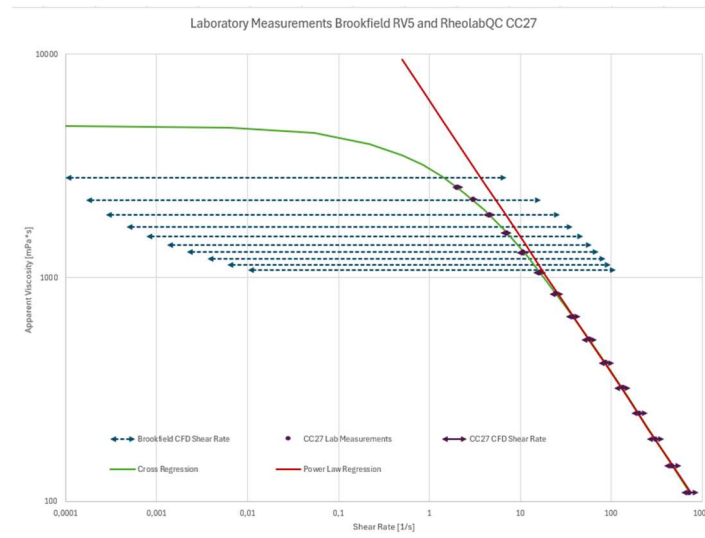


Figure 46: Plot of shear rate ranges in the Brookfield DV2T-RV viscometer with RV5 spindle and RheolabQC with CC27 spindle. Power Law extrapolation and Cross Regression to give perspective to the ranges. The long lines are from the Brookfield DV2T-RV, from 10RPM to 100RPM. The short lines around the measurement points are from the RheolabQC CC27, from 2/s to 720/s

This difference is important when transferring rheological parameters between the two geometries. A simple Power Law model can describe the shear-thinning region over a limited shear rate interval, but it cannot represent low-shear effects such as a zero-shear viscosity plateau, yield-stress behaviour, or transition-region behaviour. As shown in Figure 46, extrapolating the Power Law regression toward the low-shear region would lead to unrealistically high apparent viscosities compared with the Cross model. The figure therefore supports the conclusion that the Power Law model is insufficient for reliable transfer between the RV5 and CC27 geometries, and that the Cross model is more appropriate for the continued work.

Key takeaway here is that the shear-rate analysis shows that the CC27 and RV5 geometries measure different parts of the viscosity curve. CC27 mainly operates in a higher and narrower shear rate range, while RV5 includes very low shear rates even at high RPM. This explains why the Power Law model was not sufficient and supports the use of the Cross model for the main validation work.

6.1.3 CC27 Stabilisation Time

To ensure measurement stability, the measurement time was first evaluated using CMC30000 at 1.5 wt%. During the initial CC27 measurements, shear rate sweeps were performed using 6 s stabilisation time per shear rate point. These measurements showed unexpected behaviour in the low-shear region, as measured points in Figure 47 appear to plateau rapidly.

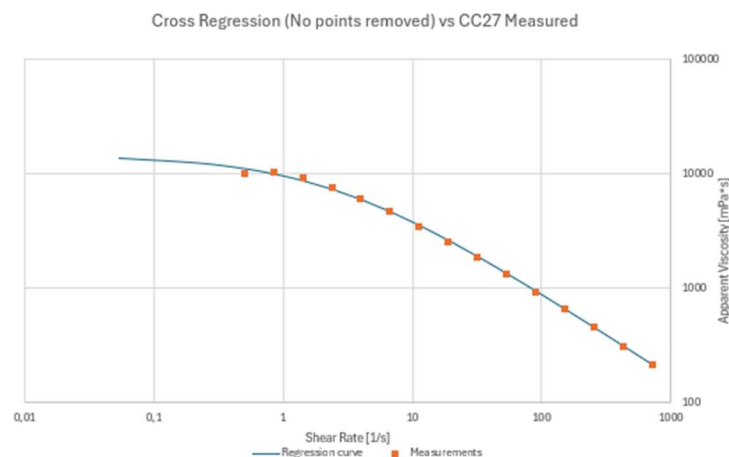


Figure 47: Cross parameter regression for CMC30000 1.5wt% without any points removed.

This caused the Cross model regression to acquire a lower R^2 of 0.9925 and a relatively bad fit. It was investigated if the exclusion of the lowest shear rate point would result in a better fit. The regression with first shear rate point excluded resulted in a regression showed in *Figure 48*, and a R^2 value of 0.9997. The exclusion of two points was also investigated (*Appendix B5*) and showed even better R^2 of 0.9999. Combined with the observed instability at low shear rates, this indicated that the lowest shear rate points were less reliable and should be treated with caution in the subsequent regression.

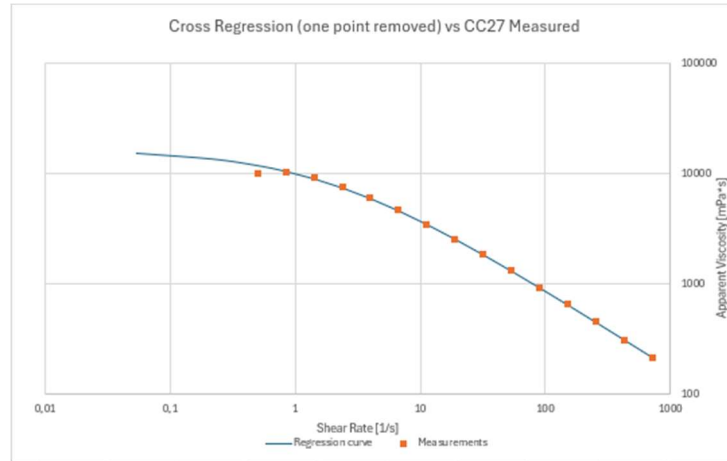


Figure 48: Cross parameter regression for CMC30000 1.5wt% with the first measurement shear rate removed

To investigate if the short stabilisation time caused the unexpected low-shear behaviour, additional CC27 measurements were performed using a longer stabilisation time of 60 s per shear rate point. *Figure 49* compares the 6 s and 60 s measurements for CMC30000 1.0 wt% at 21.3 °C. The main difference is observed at low shear rates, where the 6 s measurements result in lower viscosity values than the 60 s measurements. This indicates that the fluid's viscosity profile was not fully developed in the gap within 6 s, especially at the lowest shear rate points. At higher shear rates, the difference between the two measurement times becomes negligible, suggesting that the influence of stabilisation time is most important in the low-shear region.

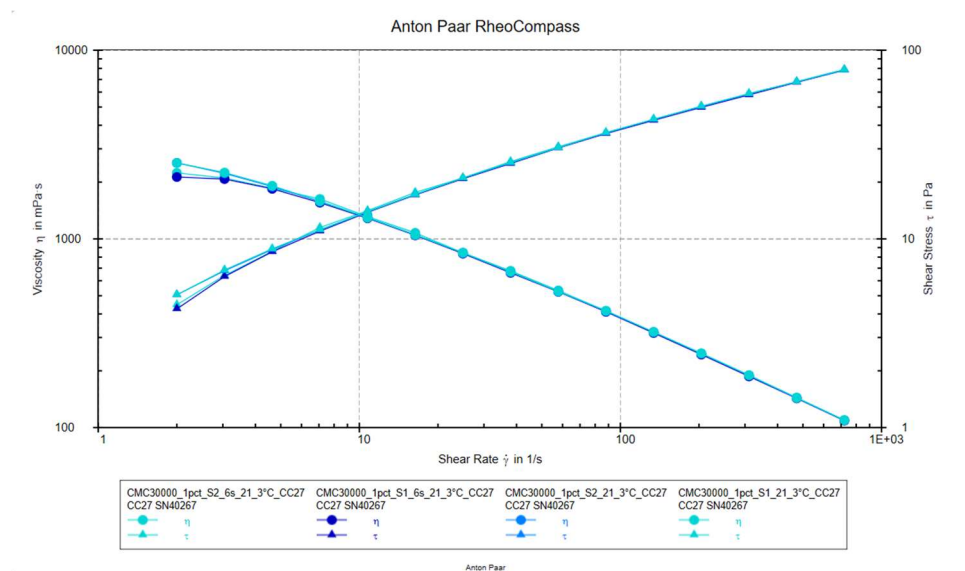


Figure 49: Shows the Anton Paar Rheocompass regressions of measured samples of CMC30000 1wt% at 21.3 °C for two measurements of 6s per shear rate, and two of 60s per shear rate. For lower shear rates a deviation is shown, where 6s datapoints measure lower viscosity.

A comparison between 50 s and 60 s measurement intervals was also performed for the CMC30000 1.4 wt% at 20.5 °C. The resulting curves were nearly identical as can be seen in *Figure 50*, for most of the measurement range. This indicating that the sample response was close to steady state after

approximately 50 s. Based on this comparison, a measurement time of 60 s per point was used for the final CC27 measurements.

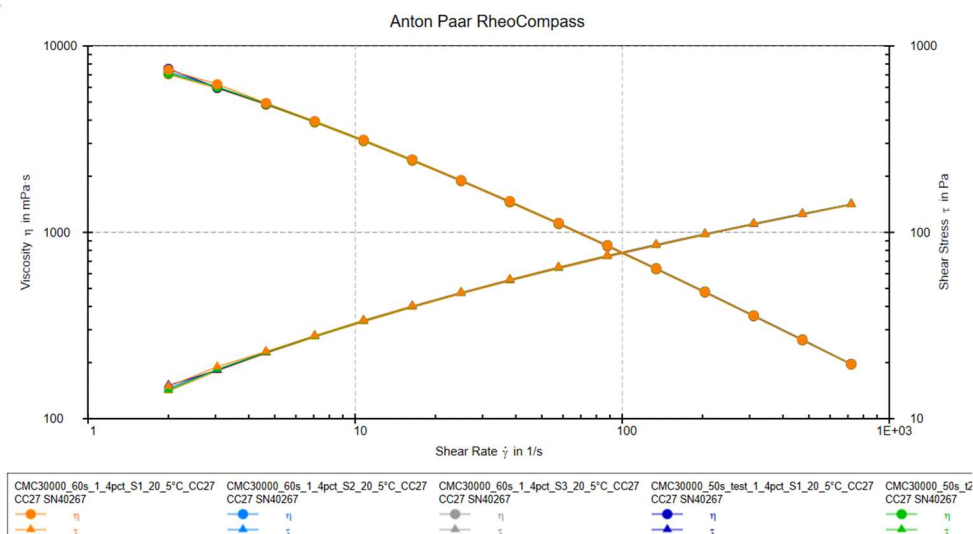


Figure 50: Shows the regressions of CMC30000 1.4wt% at 20.5 °C for three measurements of 60s and two of 50s. An inaccuracy at the lowest shear rate point can be seen but no systematic difference between 50 and 60s datapoints.

Although the comparison in Figure 50 supports that 60 s was sufficient for most of the shear rate range, the lowest shear rate point still showed noticeable scatter. This was especially visible for the higher concentration CMC samples. The deviation at the first point may be related to instrument limitations at very low shear rates, low torque resolution, or incomplete stabilisation after the initial loading of the sample. For this reason, the lowest shear rate point was treated with caution during regression and model evaluation.

The measurement time comparison was important because the Cross model regression is sensitive to the low-shear region. If the low-shear data are not stabilised, the fitted zero-shear viscosity and critical shear rate may be affected. The final procedure therefore used longer measurement times to improve the reliability of the measured viscosity curves before performing the Cross model regression.

Key takeaway It was found that for high viscosity, strong shear-thinning fluids, it is not enough with 6s stabilisation, especially not in the low shear rate region. A point duration of 60 s was selected for the final CC27 measurements, which proved to produce stable results for the highest viscosity fluid used in this work. There still was some instability in the first measurement points however, so those were treated with caution.

6.2 Experimental Results from physical measurements

The experimental laboratory results obtained with the Brookfield DV2T-RV (RV5) and the Anton Paar RheolabQC (CC27) are summarized and presented here. These measurements describe how the CMC30000 solutions responded to increasing rotational speed or shear rate, and how the measured torque and apparent viscosity varied with concentration and temperature. For both instruments, the results showed the expected shear-thinning behaviour as torque increased with increasing RPM or shear rate, while apparent viscosity decreased. The overall variation between measurements is represented by the coefficient of variation (CV), defined as,

$$CV = 100 \cdot \frac{\text{standard deviation}}{\text{mean}}$$

where the standard deviation is calculated for each sample at a given RPM, and the mean represents the average response at that RPM. A low CV indicates good repeatability with small variation between measurements, while a higher CV reflects increased variability.

The RV5 measurement's temperature range, Torque CV range and Viscosity CV range for each batch (concentration of CMC solution) are summarized in *Table 20*. The full tables with individual sample torque and apparent viscosity for each RPM is presented in *Appendix A1*.

Table 20: Summary table of Brookfield Measurements. Temperature range, CV range for the whole measurement series and Max CV for a single measurement in the series.

Concentration CMC30000	Temperature range (°C)	Torque CV range (%)	Viscosity CV range (%)
1.0 wt%	21.0 - 21.4	1.07-0.63	1.07-0.63
1.4 wt%	20.4 - 20.8	2.25-0.84	2.25-0.84
1.5 wt%	21.0 - 21.3	5.74-5.25	5.74-5.25

The data in *Table 20* show that measurement variability increased with CMC concentration. The 1.0 wt% solution exhibited the lowest coefficient of variation and the most stable torque response, whereas the 1.5 wt% solution showed the highest variability, with consistently elevated CV values across the measurement series. This trend is also evident in *Figure 51*, where the spread between repeated measurements increases with concentration.

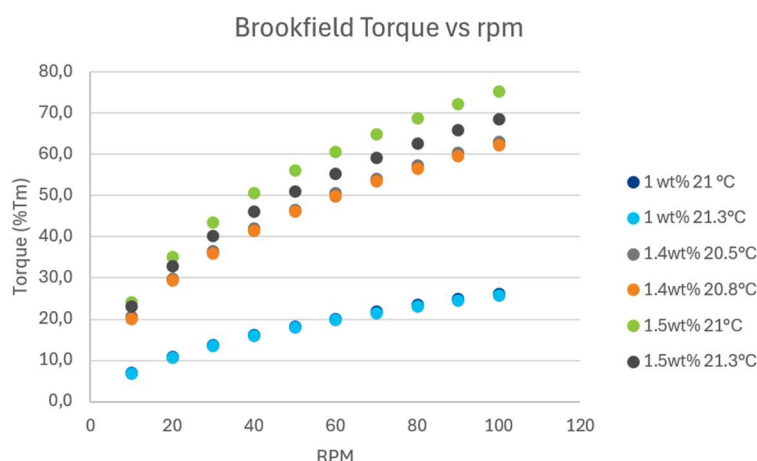


Figure 51: Brookfield RV5 torque response for CMC30000 solutions. Torque increased with RPM for all samples, and higher concentrations produced higher torque. The 1.5 wt% samples showed the largest variation, while the 1.0 wt% samples were the most stable.

As shown in *Figure 51*, torque increased with RPM for all samples, and higher concentration resulted in higher torque levels. However, the 1.5 wt% data show a larger spread between repeated measurements compared to the 1.0 wt% and 1.4 wt% datasets, indicating reduced repeatability at higher viscosities.

The recorded temperature spans were relatively narrow for all measurements, although small variations were present between repeated runs. Possible contributing factors include temperature fluctuations, spindle positioning, sample preparation, and local temperature gradients within the beaker. Based on the available data for CMC30000 at concentrations between 1.0 and 1.5 wt%, it is not possible to determine which of these factors had the greatest influence. A dedicated sensitivity analysis of the Brookfield method would be required to identify and quantify the dominant sources of uncertainty.

The 1.5 wt% RV5 measurements showed substantially larger variation than the 1.0 wt% and 1.4 wt% datasets. In several cases, the scatter was large enough that it exceeded what would be expected from simple repeatability alone, which is ± 0.2 percentage points as detailed in *Section 2.3.2*. This is important because the 1.5 wt% sample also showed less stable behaviour in the low-shear CC27 measurements discussed earlier in *Section 6.1.3*. For this reason, the 1.0 wt% and 1.4 wt% datasets were considered more reliable for the later CFD validation and AI-based parameter evaluation, while the 1.5 wt% results were mainly used to illustrate concentration-dependent trends and measurement limitations.

The CC27 measurements are summarized in *Table 21*, where Torque CV range, Viscosity CV range and temperature span for each batch (concentration of CMC solution) is presented. All individual sample measurement data is presented in *Appendix A2*.

Table 21: Coefficient of variation for RheolabQC CC27 measurements. CV values for torque and apparent viscosity are shown over the shear-rate range 2–720 s⁻¹. The ranges indicate the highest and lowest relative variation observed across the sweep, with the largest deviation occurring at the lowest shear rates.

Sample	Shear-rate range (s ⁻¹)	Temperature span (°C)	Torque CV range (%)	Viscosity CV range (%)
1wt%	2-720	21-21.3	4.32 – 8.3E(-15)	4.32-0.001
1.4wt%	2-720	20.5-20.8	1.67-0.56	1.63-0.56

Compared with the RV5 measurements in *Table 20*, the CC27 measurements showed smaller relative variation between repeated measurements and between the investigated temperatures. The highest number in the CV ranges of both torque and Viscosity in *Table 21*, correspond to the lowest shear rates in the measurement series, this difference can be seen in *Figure 52*. Overall the deviations for the CC27 were generally quite small, and the measured curves were smooth and internally consistent.

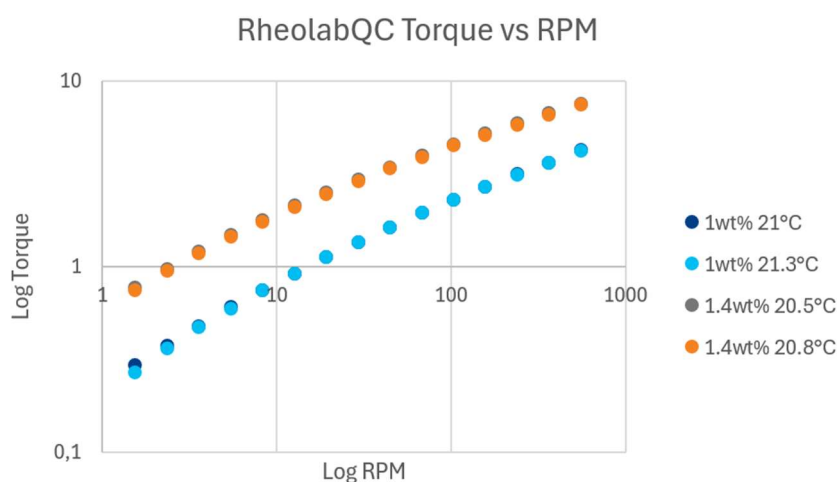


Figure 52: RheolabQC CC27 Torque response for CMC30000 solutions. Torque increased with RPM for all samples, biggest deviation between the samples with the same wt% was at the lowest RPM measurement points. Log scale was used to increase visibility of low shear measurements.

Some studies report thixotropic behaviour in high-molecular-weight CMC systems, including CMC30000. However, no pronounced thixotropy was observed in the present measurements, as illustrated by the measurement-time comparison in Section 6.1.3 (*Figure 49*). Although no dedicated thixotropy tests were performed for the 1.5 wt% sample, the comparison between 6 s and 60 s point durations showed minimal differences in the measured response, except at the lowest shear rate points.

This indicates that thixotropic effects were not significant under the conditions investigated. Instead, the deviations observed at low shear rates are more likely related to measurement instability rather than time-dependent fluid behaviour. Nevertheless, the increased variability observed for the 1.5 wt% sample means that possible time-dependent effects cannot be completely excluded at the highest concentration.

Key takeaway: The RV5 measurements showed larger variability than the CC27, which was expected considering the large acceptable error of the DV2T-RV, especially for the 1.5 wt% sample. Since it was outside the scope of this work, the available data were not sufficient to determine whether this was mainly caused by temperature variation, spindle positioning, sample loading, local temperature gradients, or instrument uncertainty. The RheolabQC CC27 measurements for the lowest shear rate points showed higher variability, which may affect fitted zero-shear viscosity and critical shear rate.

Because the 1.5 wt% sample showed the largest variability in both Brookfield and low-shear CC27 measurements, the 1.0 wt% and 1.4 wt% datasets were considered the most reliable basis for CFD validation and AI-based parameter evaluation.

6.3 Validation of CFD with Cross model

This section assesses how well CFD simulations using the Cross model reproduce experimentally measured torque in both the Anton Paar RheolabQC (CC27) and the Brookfield DV2T-RV (RV5) geometry. CFD predicted torque is compared directly against laboratory torque at matching spindle rotational speeds.

The Cross parameters were obtained for each sample with three different regression strategies from the CC27 laboratory data. The regression method described in *Section 5.3* was used for all regressions here.

Three rheological regression strategies are evaluated for each CC27 dataset (sample):

- (i) all shear rate points included,
- (ii) lowest shear rate point excluded, and
- (iii) lowest shear rate point excluded with end-effect correction.

Since the Cross parameters are identified from CC27 measurements, the validation is first evaluated in the CC27 geometry, i.e., within the same shear rate region used for parameter identification. This establishes whether the Cross implementation in CFD can reproduce the torque in the domain where the parameters are fitted. The same rheological parameter sets are then transferred to the RV5 geometry to test predictive performance across a different instrument and shear rate distribution.

The agreement between simulated and measured torque is evaluated using mean deviation over the sweep range, deviation trends across low/mid/high RPM and shear rate regions, and minimum/maximum deviations to distinguish systematic discrepancies from random variation. The split between Low, Mid and High RPM and shear rate regions for the two geometries are defined in *Section 5.5, Table 8*.

6.3.1 CC27 validation

Table 22 shows the mean torque deviation for both temperature samples in the 1.4 wt% CMC30000 batch. It also shows a deviation trend and maximum and minimum deviations for each rheological regression strategy used ((i), (ii), and (iii)).

Table 22: 1.4 wt% CMC30000 CC27 at 20.5 and 20.8 °C. Deviation trends across low, mid and high operating regions are shown as defined in *Section 5.5, Table 8* in order to highlight systematic deviations.

1.4wt% Temperature	CFD simulation case	Mean deviation (%)	Deviation trend (Low→Mid Mid→High)	Minimum deviation (%) [s ⁻¹]	Maximum deviation (%) [s ⁻¹]
20.5 °C	No points excluded (i)	+5.86	↑ ↑	+0.31 [2]	+10.20 [720]
	First point excluded (ii)	+5.58	↑ ↑	+1.46 [3.05]	+9.97 [720]
	First excl + end effect corr. (iii)	+0.87	↑ ↓	+0.24 [88]	+2.68 [720]
20.8 °C	No points excluded (i)	+5.81	↑ ↑	+0.66 [2]	+10.02 [720]

	First point excluded (ii)	+5.61	↑ ↑	−0.66 [2]	+9.85 [720]
	First excl + end effect corr. (iii)	+0.95	↑ ↓	+0.13 [3.05]	+2.60 [720]

Table 22 shows that without end-effect correction, CFD overpredicted CC27 mean torque by approximately 5 - 6% at both 20.5 °C and 20.8 °C. Excluding the lowest shear rate point alone did not improve agreement much. However, when end-effect correction was included, the mean deviation decreased sharply to approximately 1%. The deviation trend also changed from increasing with shear rate (↑ | ↑) to a flatter or partly reversed trend (↑ | ↓) with lower maximum deviations, showing that end effects were a major source of systematic mismatch in the CC27 geometry.

Table 23 shows the corresponding results for 1.0 wt% CMC30000 batch at 21.0 °C and 21.3 °C.

Table 23: CC27 validation results for 1.0 wt% CMC30000 at 21.0 and 21.3 °C.

1.0wt% Temperature	CFD simulation case	Mean deviation (%)	Deviation trend (Low→Mid Mid→High)	Minimum deviation (%) [s ⁻¹]	Maximum deviation (%) [s ⁻¹]
21.0 °C	No points excluded (i)	+4.89	↑ ↑	−0.63 [2]	+9.29 [720]
	First point excluded (ii)	+4.55	↑ ↑	+0.28 [3.05]	+8.98 [720]
	First excl + end effect corr. (iii)	+0.96	↑ ≈	+0.05 [88]	+3.52 [720]
21.3 °C	No points excluded (i)	+4.68	↑ ↑	+0.39 [3.05]	+9.07 [720]
	First point excluded (ii)	+4.80	↑ ↑	+0.93 [3.05]	+9.17 [720]
	First excl + end effect corr. (iii)	+1.27	≈ ≈	+0.08 [88]	+3.05 [720]

The same pattern is observed, where uncorrected cases overpredicted torque by approximately 4 - 5%, while end-effect correction reduced the mean deviation to approximately 1%. The corrected cases also showed flatter deviation trends (↑ | ≈ or ≈ | ≈), indicating reduced shear rate dependence of the mismatch.

The improvement from end-effect correction should not be interpreted as a correction of the CFD, but rather as an adjustment of the measured torque to viscosity interpretation for the real CC27 measurements. The rheometer viscosity calculation assumes an effective measuring length in *Section 2.3.3, Equations 11-12*, and this assumption may not fully represent the end-effect contribution for shear-thinning fluids as the end effect contribution is not always 10% of the total torque. In this work the end-effect contribution according to CFD was in the range 10-20% depending on the shear rate, meaning end-effect correction generally lowers the total torque in the 20-720 s⁻¹ range.

For both concentrations, including end-effect correction reduced the mean deviation. Without end-effect correction, the mismatch generally increased with shear rate ($\uparrow \mid \uparrow$). With end-effect correction, the trend became flatter or partly reversed at higher shear rates, indicating that end effects contributed significantly to the apparent torque mismatch in the CC27 geometry. The larger effect observed for the 1.4 wt% cases may be related to differences in viscosity level and shear-thinning behaviour, although this would require a dedicated end-effect sensitivity study to confirm.

Overall, best CC27 torque agreement is achieved when taking end-effects into account, and this corrected CC27 fit is therefore used as the baseline before transferring the same parameter sets to the RV5 geometry.

6.3.2 RV5 validation

In *Section 6.3.1* it is showed that Cross parameters obtained from a CC27 geometry measurement and regression can predict CC27 CFD torque with good accuracy. Here it is instead evaluated how well the same Cross parameters transfer to and can predict torque in a different geometry, RV5, with a different shear rate distribution. CFD predicted RV5 spindle torque was compared directly against RV5 laboratory torque at matching RPM and temperature. For Brookfield measurements, torque is reported as percent of maximum torque (%Tm), and mean deviation is calculated over RPMs = 10 -100.

Table 24 summarize the RV5 validation results for the 1.4 wt% solution batch at 20.5 °C and 20.8 °C samples. It describes the mean torque deviation between CFD simulation and real laboratory measurements along with a deviation trend and maximum and minimum deviations for each rheological regression strategy used ((i), (ii), and (iii)).

Table 24: Brookfield RV5 validation results for 1.4 wt% CMC30000. Mean deviation calculated over RPM = 10 - 100.

1.4wt% Temperature	CFD simulation case	Mean deviation (%)	Deviation trend (Low→Mid Mid→High)	Best deviation (%) [RPM]	Worst deviation (%) [RPM]
20.5 °C	No points excluded (i)	-2.44	↓ ↑	-1.51 [30]	-4.67 [10]
	First point excluded (ii)	-2.79	↓ ↑	-0.63 [50]	-6.60 [10]
	First excl + end effect corr. (iii)	-6.69	≈ ↑	-4.80 [20]	-8.50 [100]
20.8 °C	No points excluded (i)	-3.93	↓ ↑	-2.93 [40]	-7.19 [10]
	First point excluded (ii)	-4.30	↓ ≈	-3.27 [40]	-8.65 [10]
	First excl + end effect corr. (iii)	-7.86	↓ ↑	-5.95 [60]	-9.53 [100]

Across all regression strategies and both temperatures, the mean deviation is negative, indicating systematic CFD underprediction of the Brookfield torque for the high-viscosity fluid. The underprediction becomes larger when the lowest shear rate point is excluded from the CC27 regression and increases further when end-effect correction is included.

Two main factors likely contribute to this behaviour. First, proper end-effect correction reduces the amount of torque attributed to end-effect surfaces during regression, which lowers the fitted rheological parameters and therefore reduces the simulated torque in the Brookfield geometry. Second, excluding unstable low-shear points tends to reduce the fitted zero-shear viscosity while simultaneously shifting

the critical shear rate to higher values. Since the RV5 geometry contains large low-shear regions, the simulated torque is highly sensitive to these parameters. Underestimating the zero-shear viscosity and overestimating the critical shear rate therefore both contribute to lower predicted torque.

The end-effect corrected cases show the largest mismatch at higher RPM, although the low-to-mid RPM trend differs slightly between temperatures. The consistently negative deviations at both 20.5 °C and 20.8 °C indicate that this behaviour is systematic rather than random.

A likely contributing factor is the limited resolution of the low-shear measurement region in the CC27 data. Improved measurement resolution and stability at low shear rates would likely make the regression behaviour easier to interpret and help distinguish whether the observed deviations are mainly caused by end-effect correction, low-shear regression uncertainty, or limitations in the rheological model itself.

Table 25 summarizes the RV5 validation results for the 1.0 wt% solution at 21.0 °C and 21.3 °C. In contrast to the 1.4 wt% case, the mean deviation is positive in the baseline cases, indicating systematic CFD overprediction of RV5 torque. Including end-effect correction improves agreement substantially and reduces the mean deviation to approximately 2.3% at both temperatures. The end-effect corrected cases reduce the overall bias and show decreasing or approximately constant to decreasing trends across the RPM range.

Table 25: Brookfield RV5 validation results for 1.0 wt% CMC30000. Mean deviation calculated over RPM = 10 - 100.

1.0wt% Temperature	CFD simulation case	Mean deviation (%)	Deviation trend (Low→Mid Mid→High)	Best deviation (%) [RPM]	Worst deviation (%) [RPM]
21.0 °C	No points excluded (i)	+5.92	≈ ↓	+4.69 [100]	+6.72 [30]
	First point excluded (ii)	+4.65	≈ ↓	+3.64 [100]	+5.43 [40]
	First excl + end effect corr. (iii)	+2.27	↓ ↓	−0.05 [100]	+4.74 [10]
21.3 °C	No points excluded (i)	+4.25	↑ ≈	+1.32 [10]	+4.92 [40]
	First point excluded (ii)	+4.48	↑ ≈	+2.09 [10]	+5.15 [40]
	First excl + end effect corr. (iii)	+2.33	≈ ↓	+0.90 [100]	+3.50 [20]

Overall, the RV5 validation shows systematic deviations when using a Cross model from regression of CC27 rheometer data in a geometry with a different shear rate distribution. CFD torque can deviate from laboratory measurements, even though the CC27 measurements are supposedly correct.

For the 1.4 wt% CMC solution, CFD underpredicted the measured RV5 torque for all regression strategies, with the largest deviation observed when using the end-effect corrected Cross parameters. This suggests that the simulated fluid response in the RV5 geometry was effectively less viscous than the experimental response, even though the same correction improved agreement in the CC27 geometry. For the 1.0 wt% CMC solution, the baseline cases instead overpredicted RV5 torque, indicating an effectively too viscous simulated response, while end-effect correction substantially improved the agreement. These concentration-dependent trends suggest that the remaining RV5 mismatch is mainly

related to limitations in transferring CC27-regressed Cross parameters across geometries and shear rate ranges, rather than an incorrect Cross model implementation in CFD.

The most likely explanation is that RV5 torque is more sensitive to the low-shear plateau and transition region of the viscosity curve. A Cross parameter set, regressed from a higher shear rate region, can give good agreement in the CC27 while still not fully capturing the low-shear behaviour needed for accurate RV5 prediction. Especially, since the wide gap geometry in the RV5, force a majority of the fluid to obtain a low shear rate (*Section 6.1.2*). Excluding the lowest CC27 shear rate point can also remove information about the low-shear plateau, which may shift the fitted Cross curve and increase RV5 underprediction, notably for 1.4 wt%. But this could not be confirmed from the available measurement data. However, the 6 s and 60 s CC27 comparison (*Section 6.1.3, Figure 49*) does not support the interpretation that 60 s CC27 measurements were biased downward by longer pre-shear breakdown, since the shorter 6 s measurements gave lower viscosity values at low shear rates. Dedicated torque versus time measurements would therefore be required to determine whether thixotropy contributes to the RV5 mismatch.

Key takeaways from this section is that the Cross model provided a coherent description of both measurement geometries. In the CC27 geometry, applying end-effect correction reduced the systematic torque mismatch and improved agreement between CFD and experiment to approximately 1%, showing that the CFD implementation and Cross model can reproduce the measured torque well within the fitted shear rate region. When the same CC27-derived parameters were transferred to the RV5 geometry, some systematic concentration-dependent deviations remained, mainly due to the broader and lower shear-rate range of the RV5 geometry. Even so, the results show that the Cross model gives a much stronger basis for cross-geometry prediction than the Power Law model, while also highlighting the importance of accurate low-shear regression, stable measurements, and careful treatment of end effects for further improving transferability.

6.4 AI Results

This section evaluates the final AI models from three perspectives.

- **Section 6.4.1** first evaluates the prediction accuracy on synthetic CFD-generated test data. This determine whether the models can learn the inverse mapping between Brookfield torque and Cross parameters from similar data to which it is trained on.
- **Section 6.4.2** compare the AI-predicted parameters with independently regressed CC27 parameters.
- **Section 6.4.3**, evaluate if the AI-predicted Cross parameters can be reintroduced into the CFD model to reproduce measured RV5 torque.

6.4.1 Final AI model

The finalised AI framework was evaluated using two input configurations, a 5-point model and a 10-point model. The 5-point model was the main focus during most of the project and therefore underwent the most systematic optimisation. While the 10-point model was introduced later as an exploratory extension to investigate whether using all available Brookfield input points, could improve prediction accuracy without relying on artificial dataset enlargement through cross-linking of RPM values.

Although the 10-point model was explored less extensively due to time limitations, the results indicate that it is a promising alternative.

The predictive performance of both models on the test split is summarized in *Table 26* using the coefficient of determination (R^2), mean relative error, and maximum relative error. The reported metrics correspond to the final models trained with noise-augmented input data, as described in *Section 5.7.4*.

Table 26: Test-set predictive performance of the 5 point AI and 10 point AI models for ZeroShearViscosity, CriticalShearRate, and CrossRateConstant, expressed as coefficient of determination (R^2), mean relative error, and maximum relative error.

AI model	Parameter	R^2	Mean relative error (%)	Max relative error (%)
5 point AI	ZeroShearViscosity	0.999703	0.345	4.803
	CriticalShearRate	0.999670	0.721	9.839
	CrossRateConstant	0.999907	0.126	2.784
10 point AI	ZeroShearViscosity	0.999537	0.387	2.84%
	CriticalShearRate	0.999346	0.866	2.457%
	CrossRateConstant	0.999954	0.101	0.441%

As can be seen in *Table 26*, both models achieved very high R^2 values, showing strong agreement between predicted values and unseen CFD-generated test data values. Although, R^2 alone does not fully describe practical prediction performance. This is especially relevant for synthetic CFD-generated data, where the model may risk learning the idealized mapping too closely, causing overfitting. As a result, model performance was evaluated using both R^2 and relative error metrics, where the maximum relative error was particularly important for identifying occasional poor predictions, which should be avoided in our work.

The formulation of the noise augmentation is important. In this work, a 1% relative torque noise was used during training. This is not equivalent to adding an absolute uncertainty of ± 1 percentage point in %Tm, which would better represent the Brookfield full-scale torque accuracy. Absolute noise has a larger relative effect at low torque values, while relative noise affects all values proportionally. This noise formulation was selected due to time limitations and may therefore underestimate the uncertainty in low-torque measurements. Future work should evaluate alternative noise formulations, including absolute %Tm perturbations, to assess their effect on model stability and prediction accuracy.

The relative error metrics in *Table 26* show that the two models perform slightly differently depending on whether mean relative error or max relative error is considered. The 5-point model gives lower mean relative errors for zero-shear viscosity and critical shear rate, while the 10-point model reduces the maximum relative error for all three predicted parameters. The largest improvement is observed for critical shear rate, where the maximum relative error decreases from 9.84% for the 5-point model to 2.46% for the 10-point model. The maximum error for the Cross rate constant also decreases substantially, from 2.78% to 0.44%.

The difference between mean and max error is important for evaluating practical usefulness. A low mean error indicates that the model performs well on average, while a high max error shows that some poor predictions still occur. From this perspective, the 5-point model gives very accurate average predictions, but the 10-point model appears more stable because it reduces the largest errors. This is particularly relevant for critical shear rate, which describes the transition from the zero-shear plateau into the shear-thinning region and was one of the more difficult parameters to predict reliably. The lower maximum error of the 10-point model suggests that the additional RPM inputs provide useful information about this transition region.

The parity plots in *Figures 53-55* below further supports this interpretation. For zero-shear viscosity, both models follow the ideal 1:1 parity line closely, although the 10-point model shows slightly tighter

clustering and lower scatter, particularly at intermediate and high values. A similar trend is visible for critical shear rate, where both models perform well overall, but the 5-point model exhibits somewhat greater scatter at the highest values. This observation is consistent with the larger maximum error reported in *Table 26* and reinforces the conclusion that critical shear rate is more difficult to infer reliably when fewer input points are available. For the Cross rate constant, both models show near perfect agreement with the parity line, but the 10-point model again displays the tightest clustering, which aligns with its very low maximum relative error of 0.44%.

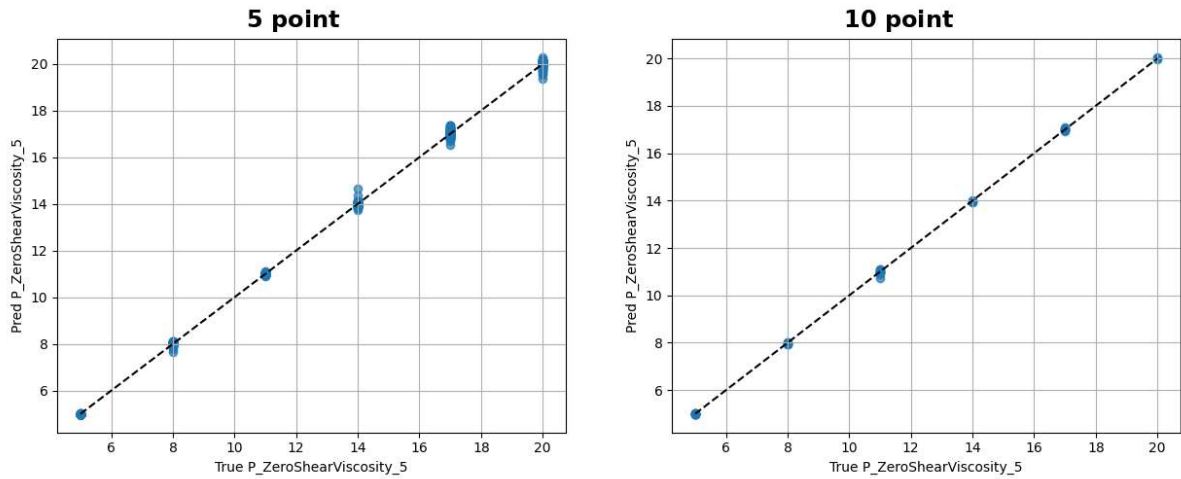


Figure 53: Parity plots for zero-shear viscosity prediction using the 5-point model (left) and the 10-point model (right). Both models show strong agreement with the 1:1 parity line, with the 10-point model exhibiting slightly lower scatter at intermediate and high values.

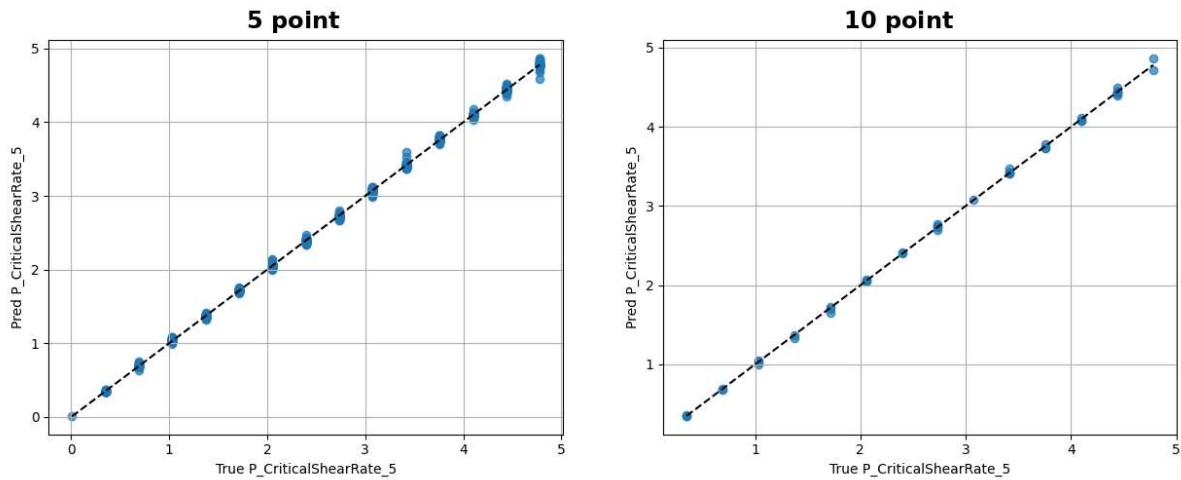


Figure 54: Parity plots for critical shear rate prediction using the 5-point model (left) and the 10-point model (right). Predicted values closely follow the ideal parity line for both models, although the 5-point model shows slightly larger scatter at the highest values.

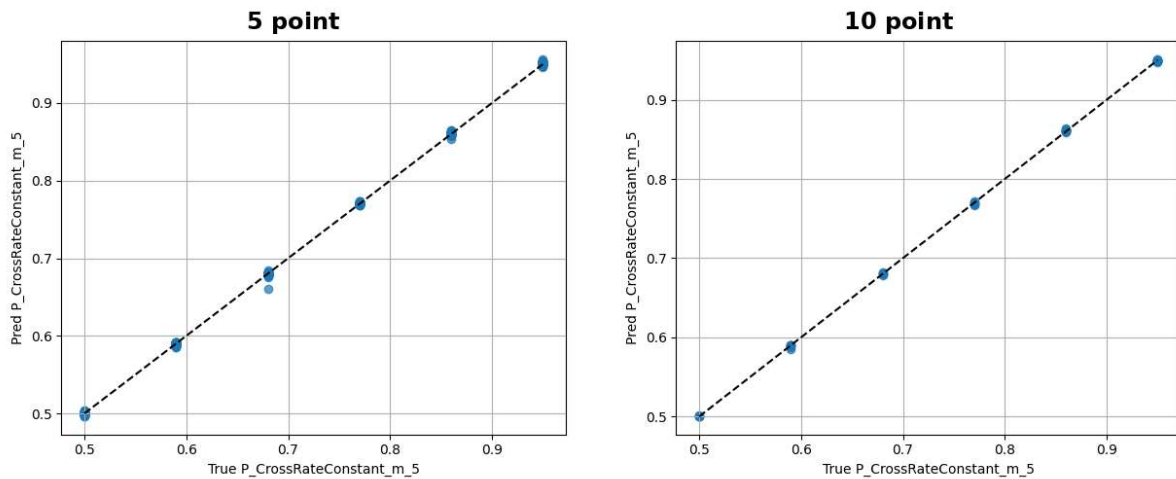


Figure 55: Parity plots for Cross rate constant prediction using the 5-point model (left) and the 10-point model (right). Both models achieve near-perfect agreement with the parity line, with the 10-point model showing the tightest clustering of points.

A likely explanation for the stronger performance of the 10-point model for certain parameters is that the additional input points provide a more complete description of the underlying rheological curve. This is particularly relevant for parameters such as critical shear rate, which are not determined by a single part of the curve, but rather by how the full shape develops across the transition from low to higher shear rates. When only five points are used, the model must infer this transition from more limited information. Given that RV5 torque data correspond to a relatively broad shear rate span rather than a sharply localized measurement region, the relationship between input points and the resulting rheological curve is not always straightforward. As discussed previously in *Section 6.1.2*, this makes it more difficult for the AI to reconstruct the correct curve shape from only a few observations. The 10-point model therefore likely benefits from having access to more of the curve structure directly, reducing ambiguity in the prediction task.

Key takeaways here are that the predictive models have a high degree of predictive accuracy when tested on the unseen data in the dataset split based on CFD data. The 10 point model has a higher accuracy, possibly due to it having more datapoints to base its predictions on, but the overall results on unseen CFD data shows good predictive accuracy.

6.4.2 Comparison of AI-Predicted Parameters with CC27-Based Regression

To evaluate how well the finalized AI model reproduced the rheological behaviour beyond the predicted Cross model parameters, Power Law parameters K and n were obtained by fitting the AI-predicted Cross model to the shear rate range of $20\text{--}720\text{ s}^{-1}$, using the same shear rate points as those measured with the RheolabQC.

The AI predicted Cross and Power Law parameters were compared with the regressed model parameter values obtained from the CC27 regressions, an example of the regressions can be seen in *Table 19* in *Section 6.1.2*, and the remainder of which can be found in the *Appendix B3 and B4*. For the 5-point model, the reported results represent the mean values obtained by iterating over the ten measured Brookfield points, while the complete set of individual predictions together with their standard deviations is provided in *Appendix D2*. The corresponding full results for the 10-point model are reported in *Appendix D3*. A summarized version of all the parameter predictions for both models can be seen in *Table 27*.

Table 27: Mean AI-predicted Cross parameters and their corresponding extrapolated Power Law parameters, for each CMC concentration. Full individual predictions are given in Appendix D2 and D3. $\pm$ calculated by (max-min)/2

CMC concentration	AI model	Zero-shear viscosity (mPa·s)	Critical shear rate (s ⁻¹)	Cross rate constant	K (Pa·s ⁿ)	n
1.0 wt%	5-point	6160 $\pm$ 25	0.949 $\pm$ 0.024	0.5995 $\pm$ 0.0020	4.730 $\pm$ 0.054	0.4350 $\pm$ 0.0017
1.0 wt%	10-point	6013 $\pm$ 118	1.087 $\pm$ 0.082	0.597 $\pm$ 0.00759	4.917 $\pm$ 0.1	0.4389 $\pm$ 0.0068
1.4 wt%	5-point	22590 $\pm$ 1292	0.728 $\pm$ 0.057	0.6494 $\pm$ 0.0034	15.252 $\pm$ 0.269	0.3754 $\pm$ 0.0026
1.4 wt%	10-point	23612 $\pm$ 1622	0.595 $\pm$ 0.088	0.6521 $\pm$ 0.004	14.4637 $\pm$ 0.2	0.3708 $\pm$ 0.0023

An example of the comparisons between the AI predictions and the parameters obtained through regression from CC27 data in excel can be found in *Table 28* for predictions of 1wt% dataset without any points removed. Comparisons for 1wt% 1 point removed and the subsequent comparisons for 1.4wt% no points and one point removed can be found in the *Appendix E1*. Calculated by (AI-lab)/lab.

Table 28: Comparison between AI prediction and excel regression for 1wt% average no points removed and with or without end effects correction taken into account for the CC27 regression.

Parameter	AI 5 vs With end effects	AI 10 vs With end effects	AI 5 vs Without end effects	AI 10 vs Without end effects
ZeroShear (Pa·s)	+11.94%	+9.26%	+16.60%	+13.81%
CriticalShearRate (/s)	-47.23%	-39.56%	-53.26%	-46.46%
CrossrateConstant	-8.87%	-9.20%	-8.18%	-8.51%
K (Pa·s ⁿ)	-22.24%	-19.16%	-23.41%	-20.37%
n	+13.45%	+15.01%	+11.12%	+12.64%

What becomes clear from the comparison in *Table 28* is that the AI predictions are systematically shifted relative to the CC27-based regressions rather than randomly scattered around them. This is seen for both the Cross model parameters and the derived Power Law parameters. In particular, the AI tends to overpredict zero-shear viscosity, underpredict critical shear rate, and underpredict the Cross rate constant relative to the reference values obtained through physical measurements in the CC27 system and regression of those measurements. A visual representation of this mismatch between the AI 10-point prediction for 1wt% CMC30000 at 21.3 °C vs measured CC27 data (no points excluded) and its subsequent regression is shown in *Figure 56* below.

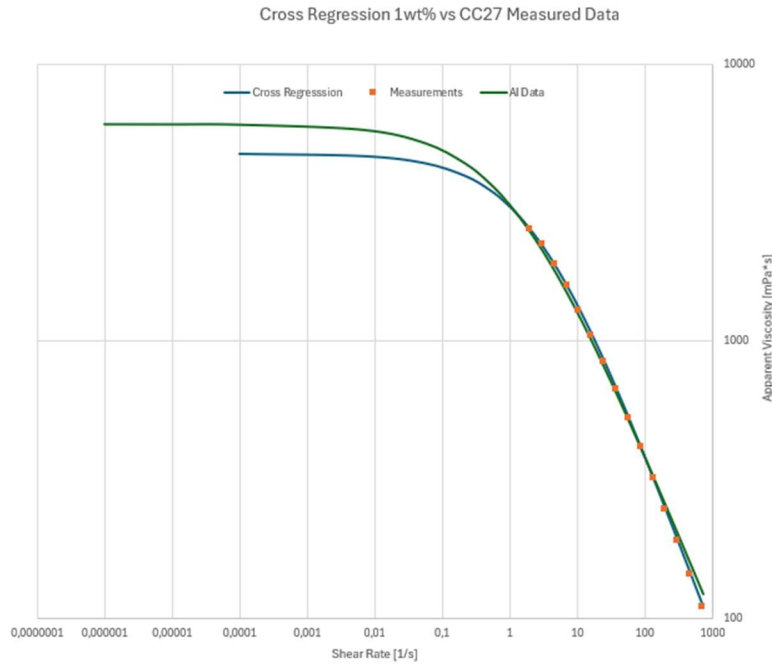


Figure 56: Example plot for cross parameters obtained through excel (blue) and AI (green) with the CC27 measurement points as represented by orange dots.

The behaviour of the Cross rate constant is especially noteworthy because it is the most consistent of the Cross-model parameters across all the comparisons. In *Table 28*, For 1 wt%, the deviations are tightly clustered around -8% to -9% for both the 5-point and 10-point models, regardless of whether the comparison is made against the with or without end effects case, and regardless of whether one Brookfield point was removed. The same is true for 1.4 wt%, where the Cross rate constant deviations remain close to -8% to -9% throughout. This is in strong contrast to the critical shear rate, which differs by approximately -38% to -63%, and to the zero-shear viscosity, which differs by approximately +11% to +55% depending on concentration and comparison case.

This suggests that, among the Cross parameters, the AI is able to reproduce the Cross rate constant with relatively good consistency, while the agreement for the other Cross parameters is clearly weaker. The stable behaviour of the Cross rate constant suggests that the model captures the general curvature of the shear-thinning region more reliably than the exact location of the transition region or the magnitude of the zero-shear plateau.

A similar comparison to the one in *Table 28* can be made using the viscosity at 100 s^{-1} , as shown in *Table 29*. Since no direct experimental measurements were taken at this shear rate, the reference viscosities were calculated from Cross model regressions using different data treatments: without point exclusion (i), with one point excluded and end-effect correction included (ii), and with one point excluded but without end-effect correction (iii).

Table 29: Viscosity comparison for CMC 30000 between the two different AI models and the measured viscosities at 100/s. Difference is calculated with $100 \times (\text{Measured-AI})/\text{AI}$. Regression strategies according to (i, ii and iii).

Conc.	Treatment	AI 10 Viscosity @100/s Relative Error	AI 5 Viscosity @100/s Relative Error
1.0 wt%	No exclusion, no end-effect corr.	0.105%	7.12%
	1 point excluded, no end- effect corr.	0.206%	7.23%
	1 point excluded, with end- effect corr.	-5.00%	1.66%
1.4 wt%	No exclusion, no end-effect corr.	-5.26%	-12.37%
	1 point excluded, no end- effect corr.	-5.05%	-12.18%
	1 point excluded, with end- effect corr.	-11.20%	-17.86%

As shown in Table 29, both AI models reproduce viscosity in the shear-thinning region with good practical accuracy. For initial fluid understanding, Tetra Pak's allowed viscosity error is $<20\%$. At 100 s^{-1} , all predictions from both the 5-point and 10-point models are well within this requirement. The full $20\text{-}720 \text{ s}^{-1}$ comparison is provided in Appendix E1, where all 10-point predictions remain within 20% except one case at 720 s^{-1} , which deviates by -20.18% .

This shows that Brookfield-measured torque can be used as input to the AI model trained with the workflow developed in this work to predict viscosities within Tetra Pak's initial understanding requirements. The predictions should therefore be viewed as useful first estimates in the shear-thinning region, rather than absolute rheological values. The deviations also depend on the chosen regression treatment, with the end-effect corrected reference generally giving more negative deviations.

The remaining discrepancies are likely related to the limited low-shear resolution of the RV5 measurements. Since the RV5 response is based on torque over a broad and indirect shear rate distribution, the AI may not fully resolve the transition region, mainly affecting the critical shear rate while still giving practically useful viscosity estimates. In addition, the CC27 regression itself is sensitive to low-shear data, and different parameter combinations can produce similar curve shapes within the measured range.

The noise formulation used during training may also contribute to the discrepancies. The ANN was trained using a 1% relative noise, whereas Brookfield uncertainty is linked to the instrument's full-scale range and may vary with torque level, particularly at low values. As a result, the model may perform well on CFD-generated data while being less robust when applied to experimental measurements.

Key takeaway: The AI-predicted Cross parameters do not fully match the CC27-based regressions, but the resulting viscosity predictions are practically useful. At 100 s^{-1} , all predictions are within Tetra Pak's $<20\%$ requirement for initial fluid understanding, and the 10-point model stays within this limit across $20\text{-}720 \text{ s}^{-1}$ except for one case at -20.18% . This indicates that Brookfield-measured torque can be used with the developed CFD-AI workflow to provide useful first viscosity estimates, while the remaining parameter discrepancies are mainly related to limited low-shear information and measurement-uncertainty differences.

6.4.3 CFD simulation of torque with AI predicted parameters

To further evaluate the practical usefulness of the finalized AI models, we wanted to investigate if the AI-predicted Cross parameters could recreate the real torque from the Brookfield measurements in CFD.

The AI-predicted Cross parameters from each different CMC concentration batch and temperature sample were used as input to new CFD simulations. The resulting torque were compared with the corresponding RV5 temperature and batch laboratory measurements. This analysis is particularly relevant since the previous *Section 6.4.2* showed that the AI-predicted parameter values did not always agree closely with the CC27-derived regression parameters. Especially not for zero-shear viscosity and critical shear rate. The present comparison therefore addresses a more application-oriented question. Even if the predicted parameters differ from the regression-derived values, can they still reproduce the measured torque response with sufficient accuracy?

Table 30 shows the mean torque deviations (Mean dev. Column) for the 5-point and 10-point AI models at 1.0 wt% and 1.4 wt% CMC30000. All values in the table are CFD predicted torque with our AI-parameters vs laboratory torque. The *Table 30* further includes deviation trend across the RPM range, and Min/Max deviation.

Table 30: CFD torque deviations using AI-predicted Cross parameter.. The deviations compare average CFD-simulated Brookfield RV5 torque with measured Brookfield torque for the 5-point and 10-point AI models. Deviation trends across low, mid and high operating regions are shown as defined in Section 5.5, Table 8. The full table with individual data for each sample can be seen in Appendix E2.

wt%	AI Model	Mean dev. (%)	Dev. trend Low→Mid Mid→High	Low mean dev. (%)	Mid mean dev. (%)	High mean dev. (%)	Min dev. (%) [RPM]	Max dev. (%) [RPM]
1.0 wt%	5-point	-4.75	↑ ↑	-3.79	-4.84	-5.41	-1.75 [10]	-6.30 [100]
	10-point	-0.56	≈ ≈	-0.67	-0.50	-0.52	-0.008 [40]	-1.32 [80]
1.4 wt%	5-point	+6.06	↑ ≈	+5.01	+6.30	+6.67	+2.48 [10]	+8.72 [100]
	10-point	-0.97	≈ ≈	-0.60	-0.96	-1.27	-0.05 [60]	-1.72 [80]

The results in *Table 30* show a clear difference between the 5-point and 10-point AI models. For 1 wt%, the CFD simulations based on the 5-point AI-model, consistently slightly underpredict the measured torque, with mean deviation -4.75%. The deviation becomes more negative with increasing RPM, as indicated by the ↑ | ↑ trend, and can be seen in Low, Mid and High mean deviation columns. When the Cross parameters are instead predicted by the 10-point AI-model, the mean deviation is reduced to -0.56%. A much flatter, less systematic deviation trend is shown.

Similarly for the 1.4wt% batch, the 5-point AI-model produces an acceptable torque prediction that deviated +6.06% from the measured Brookfield RV5 laboratory torque and a slightly increasing deviation trend is shown (↑ | ≈). An even better prediction is shown from the 10-point AI-model, which predicted again predicted Cross parameters that resulted in spot on torque prediction (-0.97%) from the CFD.

An additional important observation is that the 10-point AI model does not simply shift the predicted torque in one consistent direction, but rather corrects the prediction in opposite directions for the two investigated batches. This behaviour strongly suggests that the 10-point model is not merely introducing an arbitrary offset in torque, but is instead capturing more detailed information about the shape of the underlying Cross parameter curve and its influence on the torque response. Furthermore, it is particularly noteworthy that the resulting torque predictions for 10 points AI-model both batches, fall within the typical experimental uncertainty of the Brookfield measurements ($\pm 1\%T_m$). This indicates that the CFD-AI workflow is able to reproduce the measured torque at a level comparable to the intrinsic measurement accuracy.

Taken together, the CFD results show that the 10-point AI model provides a clearly better torque reconstruction than the 5-point model for both investigated concentrations. This is a significant observation because, in the previous section, the AI-predicted Cross parameters did not always agree particularly well with the CC27-derived regression values. In spite of that, the CFD simulations based on the AI predictions, especially those from the 10-point model, still reproduce the measured Brookfield torque well. This indicates that agreement with the CC27 regression parameters is not the only relevant measure of usefulness. Even when the parameter values differ noticeably from the rheological reference values, they may still form a parameter combination that reproduces the measured torque effectively within the CFD framework.

One likely reason for this is that the AI model was developed entirely within a CFD-generated dataset, meaning that it learned how different combinations of Cross parameters affect the torque response in that specific simulation environment. It is therefore expected that the predicted parameters will perform relatively well when they are returned to the same CFD framework. In that sense, the AI does not necessarily recover the exact rheological parameters that would be obtained from a separate regression on measured rheometry data, but rather identifies effective parameter sets that yield the correct torque behavior in the Brookfield-CFD context. This is also consistent with the observation that large deviations in individual parameters, such as critical shear rate, do not automatically result in equally large deviations in the simulated torque.

These findings suggest that the current AI approach may be useful as a torque-matching tool, even if it is not yet a fully reliable method for recovering physically exact rheological parameters. From an industrial perspective, this may still be valuable if the main objective is to generate a CFD model that reproduces Brookfield torque with reasonable accuracy. In that context, the 10-point model appears promising, whereas the 5-point model still shows too large and systematic deviations to be equally reliable.

At the same time, the results also indicate that more work is needed before the method can be considered robust for broader rheological characterization. One possible explanation for the difference between the models is that the 10-point model receives more information about the measured torque curve and therefore has a better basis for identifying parameter combinations that reproduce the full response. Another possibility is that the current CFD training dataset defines a relatively tight parameter landscape, which may encourage the model to learn locally accurate but not necessarily broadly generalizable mappings. If the dataset were expanded to include a wider range of rheological behaviours and parameter combinations, the AI might be able to generate predictions that are both more stable and more physically representative. Such an expansion could also reduce the risk of overfitting to a narrow CFD response space.

Key takeaways from this section is that the CFD simulations using AI-predicted Cross parameters showed that the developed CFD-AI workflow can reproduce measured RV5 torque with very good accuracy, especially for the 10-point model. This is a promising proof-of-concept, as it demonstrates that Brookfield measurements can be combined with CFD-generated training data and AI-based inverse prediction to obtain CFD-usable parameter estimates. The 10-point model outperformed the 5-point model, giving smaller and less systematic torque deviations for both 1.0 wt% and 1.4 wt% CMC30000. Although the predicted parameters did not fully match the CC27-regressed values, the good torque agreement suggests that the method is valuable as a torque-reproduction tool and has clear potential for further development with broader validation and improved uncertainty handling.

7. Conclusion

This thesis developed and evaluated a CFD-AI based method for linking Brookfield DV2T-RV with RV5 spindle measurements to rheological model parameters that can be used in initial understanding of fluid behaviour and process dimensioning. In practice, the workflow consisted of measuring torque and apparent viscosity with the RV5, performing controlled Anton Paar RheolabQC (CC27) measurements at matching temperatures, fitting Cross model parameters from the CC27 data, validating these parameters in CFD, generating CFD-based RV5 torque datasets, and training AI models to predict Cross parameters from Brookfield-type input data.

The initial Power Law-based CFD-AI approach provided a useful proof-of-concept, showing that AI could learn the relationship between CFD-generated Brookfield torque data and rheological model parameters. However, comparison with laboratory data showed that the Power Law model was too limited for reliable transfer between the RV5 and CC27 geometries, mainly because it cannot capture the low-shear plateau or transition region of shear-thinning fluids. The shear rate analysis showed that the CC27 and Brookfield RV5 geometries only partly overlap in the sampled shear rate range and do not probe equivalent regions of the viscosity curve. This means that direct transfer of rheological parameters between the instruments involves uncertainty, especially in the low-shear region relevant to the RV5.

CFD validation showed that the Cross model provided a substantially more coherent description of both measurement geometries than the Power Law model. In the CC27 geometry, applying end-effect correction reduced the systematic torque mismatch and improved agreement between CFD and experiment to approximately 1%, showing that the Cross model implementation could reproduce torque well within the fitted shear rate region. When the same CC27-derived parameters were transferred to the Brookfield RV5 geometry, systematic concentration-dependent deviations remained. These deviations were mainly attributed to the broader and lower shear rate range of the RV5 geometry and the limited low-shear information available from the CC27 regression.

The AI models trained on CFD-generated Cross model data showed high predictive accuracy on unseen synthetic test data. The 10-point model performed better than the 5-point model, likely because it used more of the Brookfield measurement curve and therefore contained more information about the overall viscosity behaviour. Although the AI-predicted Cross parameters did not always match the CC27-regressed parameters, especially for zero-shear viscosity and critical shear rate, CFD simulations using the AI-predicted parameters reproduced measured Brookfield torque with good accuracy. This was especially clear for the 10-point model, which produced much smaller and less systematic torque deviations than the 5-point model for both 1.0 wt% and 1.4 wt% CMC30000.

The practical use of the measurement input required for the AI models was not discussed in detail, but a basic comparison between the two input approaches can still be made. The 10-point model gave the most accurate torque and viscosity reconstruction, as it used a larger part of the Brookfield measurement curve and therefore captured more information about the fluid behaviour. However, this approach requires an increased quantity of controlled Brookfield measurements from the customer. This may make it less practical in industrial use, as proper viscometer handling is not always the case. In comparison, the 5-point model is simpler and more flexible, since it requires fewer measurements. Although its predictions were less accurate than those of the 10-point model, it still reproduced the Brookfield torque with a mean deviation within 6% across the measurement series. This indicates that the 5-point model can still provide a useful and practical first estimate for further calculations, especially when measurement time or available data are limited.

Overall, the developed method shows that Brookfield measurements can be successfully combined with CFD-generated training data and AI-based inverse prediction to estimate usable Cross model parameters. The method therefore partly bridges the gap between relative Brookfield measurements and the absolute rheological parameters required for CFD-based process calculations and is a promising tool for early-stage fluid characterization and process dimensioning. In particular, a controlled Brookfield measurement series, such as ten RPM points at a known temperature, can provide enough information to generate parameter estimates that reproduce Brookfield torque with good accuracy in CFD. These

estimates can also provide an initial understanding of the fluid's viscosity behaviour. The predictive reliability goal was therefore achieved for Brookfield torque reproduction, especially for the 10-point model, but only partly achieved for independent recovery of physically unique Cross parameters. Thus, the method represents a valuable step toward making simple rotational viscosity measurements more useful for advanced modelling.

8. Future Work

Future work should focus on improving measurement reliability, expanding the CFD-AI dataset, and validating the method for a wider range of fluids and geometries.

First, the Brookfield RV5 measurement method should be investigated more systematically. The influence of spindle alignment, fill volume, immersion depth, sample loading, temperature gradients, and measurement time should be quantified. This would make it possible to identify the dominant sources of Brookfield measurement uncertainty and improve the reliability of the AI input data.

Second, the low-shear region should be measured more accurately. The Cross model regression was sensitive to the lowest CC27 shear rate points, which affect the fitted zero-shear viscosity and critical shear rate. Although 60 s stabilization improved the measurements, torque-versus-time tests or measurements with a more sensitive rheometer, such as an Anton Paar MCR, would help confirm whether the low-shear measurements are fully steady-state.

Third, Future AI training should use a more realistic Brookfield noise model. In the current implementation, the same relative perturbation is applied to several measurement points, whereas real Brookfield uncertainty may vary between individual RPM points. A future model could therefore apply an individually sampled, normally distributed torque-percentage error to each RPM point in every training row. This would better represent absolute Brookfield torque uncertainty, especially at low torque values where the relative impact of measurement error is larger.

The CFD-generated training dataset should be expanded to cover wider Cross-parameter ranges and more Brookfield spindles to cover all possible shear thinning fluids exhibiting a zero-shear plateau. Validations on other shear thinning fluids should be performed to determine whether the strong performance of the 10-point model remains valid outside the CMC30000 cases studied here.

Finally, the method should be tested on other fluid models, including fluids with yield-stress behaviour, shear-thickening behaviour and time-dependent effects such as thixotropy. The long term goal is to cover all possible fluids that can be measured in the Brookfield viscometer and finalize the parameter estimation tool that translates Brookfield measurements into useful rheological data.

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Appendix

Note on decimal notation:

Due to the Swedish regional settings of the Excel version used in this work, decimal values in the appendix may use either commas (,) or periods (.) as decimal separators. Both notations should be interpreted equivalently as decimal values.

Appendix A – Experimental Measurement Data

A.1 Brookfield RV5 raw data

Table 31: Summary table of Brookfield measurements. Average percent of torque max, average apparent viscosity and temperature span for each batch (concentration of CMC solution), with variation included.

RPM	1.0 wt% Temp. span (°C)	1.0 wt% Torque (%)	1.0 wt% Viscosity (mPa*s)	1.4 wt% Temp. span (°C)	1.4 wt% Torque (%)	1.4 wt% Viscosity (mPa*s)	1.5 wt% Temp. span (°C)	1.5 wt% Torque (%)	1.5 wt% Viscosity (mPa*s)
10	21,0–21,3	7,0 ± 0,1	2780 ± 23	20,4–20,8	20,8 ± 0,5	8320 ± 188	21,0–21,3	24,3 ± 1,3	9720 ± 513
20	21,0–21,4	10,8 ± 0,1	2160 ± 23	20,4–20,8	30,0 ± 0,5	6000 ± 91	21,0–21,2	34,8 ± 2,0	6965 ± 392
30	21,0–21,4	13,7 ± 0,1	1826 ± 16	20,4–20,8	36,7 ± 0,4	4890 ± 60	21,0–21,3	42,5 ± 2,3	5666 ± 310
40	21,0–21,4	16,1 ± 0,1	1610 ± 12	20,4–20,8	42,0 ± 0,5	4198 ± 46	21,0–21,3	48,9 ± 2,7	4888 ± 274
50	21,0–21,4	18,2 ± 0,1	1456 ± 9	20,4–20,8	46,6 ± 0,4	3726 ± 33	21,0–21,3	54,1 ± 3,1	4328 ± 248
60	21,0–21,4	20,1 ± 0,1	1338 ± 10	20,4–20,8	50,5 ± 0,6	3366 ± 36	21,0–21,2	58,6 ± 3,2	3908 ± 211
70	21,0–21,4	21,8 ± 0,2	1242 ± 10	20,4–20,8	54,1 ± 0,5	3090 ± 29	21,0–21,2	62,5 ± 3,4	3574 ± 197
80	21,0–21,4	23,4 ± 0,2	1168 ± 9	20,4–20,8	57,2 ± 0,5	2860 ± 27	21,0–21,3	66,1 ± 3,5	3306 ± 176
90	21,0–21,4	24,8 ± 0,2	1100 ± 8	20,4–20,8	60,2 ± 0,5	2674 ± 23	20,9–21,3	69,3 ± 3,6	3080 ± 162
100	21,0–21,4	26,1 ± 0,2	1045 ± 8	20,4–20,8	62,9 ± 0,5	2515 ± 21	21,0–21,2	72,2 ± 3,8	2889 ± 152

CMC30000 1w% utan spindle guard															
sample	spindle	time	rpm	temp C	torque%	viscosity		sample	spindle	time	rpm	temp C	torque%	viscosity	
1.1	RV5	60s	10	21.0	7.0	2800		1.2	RV5	60s	10	21.0	7.0	2800	
			20	21.0	10.9	2180					20	21.0	10.9	2180	
			30	21.0	13.8	1840					30	21.0	13.8	1840	
			40	21.0	16.2	1620					40	21.0	16.2	1620	
			50	21.0	18.3	1464					50	21.0	18.3	1464	
			60	21.0	20.2	1347					60	21.0	20.2	1347	
			70	21.0	21.9	1251					70	21.0	21.9	1251	
			80	21.0	23.5	1175					80	21.0	23.5	1175	
			90	21.0	24.9	1107					90	21.0	24.9	1107	
			100	21.0	26.3	1052					100	21.0	26.3	1052	
sample	spindle	time	rpm	temp C	torque%	viscosity		sample	spindle	time	rpm	temp C	torque%	viscosity	
2.1	RV5	60s	10	21.3	6.9	2760		2.2	RV5	60s	10	21.3	6.9	2760	
			20	21.3	10.7	2140					20	21.4	10.7	2140	
			30	21.3	13.6	1813					30	21.4	13.6	1813	
			40	21.3	16	1600					40	21.4	16.0	1600	
			50	21.3	18.1	1448					50	21.4	18.1	1448	
			60	21.3	19.9	1327					60	21.4	20.0	1333	
			70	21.3	21.6	1234					70	21.4	21.6	1234	
			80	21.3	23.2	1160					80	21.4	23.2	1160	
			90	21.3	24.6	1093					90	21.4	24.6	1093	
			100	21.3	25.9	1036					100	21.4	26.0	1040	

Figure 57: Brookfield RV5 laboratory data for batch 1wt% CMC30000, with presented temperature, percent of torque max and apparent viscosity for each measurement, RPMs 10-100.

CMC30000 1.4w% utan spindle guard															
sample	spindle	time	rpm	temp C	torque%	viscosity		sample	spindle	time	rpm	temp C	torque%	viscosity	
1.1	RV5	60s	10	20.8	20.2	8080		1.2	RV5	60s	10	20.8	21.0	8400	
			20	20.8	29.5	5900					20	20.8	30.0	6000	
			30	20.8	36.1	4813					30	20.7/20.8	36.7	4893	
			40	20.8	41.4	4140					40	20.7/20.8	41.9	4190	
			50	20.8	46.1	3688					50	20.8	46.5	3720	
			60	20.8	49.9	3327					60	20.8	50.3	3353	
			70	20.8	53.5	3057					70	20.8	53.9	3080	
			80	20.8	56.6	2830					80	20.8	56.9	2845	
			90	20.8	59.7	2653					90	20.8	59.8	2658	
			100	20.8	62.3	2492					100	20.8	62.6	2504	
sample	spindle	time	rpm	temp C	torque%	viscosity		sample	spindle	time	rpm	temp C	torque%	viscosity	
2.1	RV5	60s	10	20.5	20.7	8280		2.2	RV5	60s	10	20.4/20.5	21.3	8520	
			20	20.5	29.9	5980					20	20.4	30.6	6120	
			30	20.5	36.7	4893					30	20.4	37.2	4960	
			40	20.5	42.1	4210					40	20.4	42.5	4250	
			50	20.5	46.6	3728					50	20.4	47.1	3768	
			60	20.5	50.7	3373					60	20.4	51.2	3413	
			70	20.5	54.2	3097					70	20.4	54.7	3126	
			80	20.5	57.5	2875					80	20.4	57.8	2890	
			90	20.5	60.4	2684					90	20.4	60.8	2702	
			100	20.5	63.1	2524					100	20.4	63.5	2540	

Figure 58: Brookfield RV5 laboratory data for batch 1.4wt% CMC30000, with presented temperature, percent of torque max and apparent viscosity for each measurement, RPMs 10-100.

CMC30000 1.5wt% utan spindle guard															
sample	spindle	time	rpm	temp C	torque%	viscosity		sample	spindle	time	rpm	temp C	torque%	viscosity	
1.1	RV5	60s		10	21.0	24.2	9680	1.2	RV5	60s		10	21.0	26.1	10440
				20	21.0	35.2	7040					20	21.0	37.4	7480
				30	21.0	43.5	5800					30	21.0	45.3	6040
				40	21.0	50.7	5070					40	21.1	51.7	5170
				50	21.1	56.2	4496					50	21.0	57.3	4584
				60	21.1	60.7	4047					60	21.0	61.9	4127
				70	21.0/21.1	65.0	3714					70	21.0	66.0	3771
				80	21.0	68.8	3440					80	21.0	69.5	3475
				90	21.0	72.2	3209					90	20.9/21.0	72.7	3231
				100	21.0	75.4	3016					100	21.0	75.6	3024
sample	spindle	time	rpm	temp C	torque%	viscosity		sample	spindle	time	rpm	temp C	torque%	viscosity	
2.1	RV5	60s		10	21.3	23.1	9240	2.2	RV5	60s		10	21.2	23.8	9520
				20	21.2	32.9	6580					20	21.2	33.8	6760
				30	21.3	40.3	5373					30	21.2	40.9	5453
				40	21.3	46.1	4610					40	21.2	47.0	4700
				50	21.2/21.3	51.1	4088					50	21.2	51.8	4144
				60	21.2	55.4	3693					60	21.2	56.5	3767
				70	21.2	59.2	3383					70	21.2	60.0	3429
				80	21.3	62.7	3135					80	21.2	63.5	3175
				90	21.3	65.9	2929					90	21.2	66.4	2951
				100	21.2	68.6	2744					100	21.2	69.3	2772

Figure 59: Brookfield RV5 laboratory data for batch 1.5wt% CMC30000, with presented temperature, percent of torque max and apparent viscosity for each measurement, RPMs 10-100.

A.2 RheolabQC CC27 raw data

Table 32: Summary table of Anton Paar RheolabQC CC27 measurements. Average torque, average viscosity and temperature span for each batch (concentration of CMC solution), with variation included.

Shear rate (1/s)	RPM	Temp 1wt% (°C)	Torque 1wt% (mN*m)	Viscosity 1wt% (mPa*s)	Temp 1.4wt% (°C)	Torque 1.4wt% (mN*m)	Viscosity 1.4wt% (mPa*s)
2	1,55	21-21,3	0,280469 ±0,012104	2640,567 ±113,9667	20.5-20.8	0,759255 ±0,012665	7151,217 ±116,4167
3,05	2,36	21-21,3	0,368105 ±0,006395	2276,075 ±39,525	20.5-20.8	0,956088 ±0,010935	5911,667 ±67,66667
4,64	3,60	21-21,3	0,470717 ±0,002057	1911,533 ±8,333333	20.5-20.8	1,187767 ±0,015633	4823,35 ±63,45
7,06	5,47	21-21,3	0,59721 ±0,00426	1592,75 ±11,35	20.5-20.8	1,452117 ±0,01755	3872,783 ±46,85
10,7	8,33	21-21,3	0,74265 ±0,00256	1300,825 ±4,475	20.5-20.8	1,754967 ±0,020833	3073,967 ±36,5
16,4	12,69	21-21,3	0,91588 ±0,00161	1053,592 ±1,841667	20.5-20.8	2,096617 ±0,02285	2411,9 ±26,3
24,9	19,32	21-21,3	1,118625 ±0,002075	845,1442 ±1,559167	20.5-20.8	2,479767 ±0,025233	1873,5 ± 19,06667
37,9	29,42	21-21,3	1,350683 ±0,003183	670,2025 ±1,5875	20.5-20.8	2,91075 ±0,02905	1444,283 ±14,41667
57,8	44,79	21-21,3	1,620867 ±0,003567	528,2042 ±1,169167	20.5-20.8	3,38835 ±0,032883	1104,2 ±10,7
88	68,20	21-21,3	1,937933 ±0,000467	414,7717 ±0,098333	20.5-20.8	3,91845 ±0,036883	838,65 ±7,893333

Shear rate (1/s)	RPM	Temp 1wt% (°C)	Torque 1wt% (mN*m)	Viscosity 1wt% (mPa*s)	Temp 1.4wt% (°C)	Torque 1.4wt% (mN*m)	Viscosity 1.4wt% (mPa*s)
134	103,85	21-21,3	2,282042 ±0,002208	320,7725 ±0,3125	20.5-20.8	4,493717 ±0,037217	631,6583 ±5,231667
204	158,12	21-21,3	2,6764 ±2,22E-16	247,0775 ±0,0025	20.5-20.8	5,136 ±0,0408	474,1383 ±3,765
311	240,76	21-21,3	3,124242 ±0,001592	189,4225 ±0,0975	20.5-20.8	5,834083 ±0,043583	353,7217 ±2,645
473	366,58	21-21,3	3,610725 ±0,002175	143,7783 ±0,088333	20.5-20.8	6,6025 ±0,045433	262,91 ±1,806667
720	558,17	21-21,3	4,1929 ±0,0142	109,6517 ±0,371667	20.5-20.8	7,445933 ±0,0418	194,725 ±1,091667

Table 33: Summary table of Anton Paar RheolabQC CC27 CMC30000 measurements. Average torque, average viscosity and temperature span for each batch (concentration of CMC solution), with variation included

Shear rate (1/s)	RPM	Temp 1.5wt% (°C)	Torque 1wt% (mN*m)	Viscosity 1wt% (mPa*s)
0,499	0,39	21-21,3	0,266493 ±0,009734	10052,1 ±368,450852
0,84	0,65	21-21,3	0,46497 ±0,002315	10416,666667 ±50,520623
1,41	1,09	21-21,3	0,68607 ±0,006567	9142,266667 ±85,209761
2,38	1,85	21-21,3	0,953633 ±0,003405	7558,266667 ±26,933684
3,99	3,09	21-21,3	1,288467 ±0,023066	6075,4 ±109,468534
6,72	5,21	21-21,3	1,655067 ±0,011912	4641,533333 ±33,019136
11,3	8,76	21-21,3	2,070233 ±0,002779	3453,7 ±4,592385
19	14,73	21-21,3	2,553567 ±0,002344	2534,1 ±2,457641
31,9	24,73	21-21,3	3,1143 ±0,011285	1838,4 ±6,596211
53,6	41,55	21-21,3	3,739733 ±0,005297	1313,233333 ±1,858315
90,1	69,85	21-21,3	4,452033 ±0,005164	929,926667 ±1,078255
152	117,84	21-21,3	5,231433 ±0,002676	650 ±0,334215
255	197,69	21-21,3	6,118433 ±0,005689	452,206667 ±0,418609
428	331,80	21-21,3	7,115433 ±0,012851	312,826667 ±0,565007
720	558,17	21-21,3	8,230167 ±0,013903	215,233333 ±0,367741

Table 34: 1wt% 21°C triplicate measurement

Shear rate (1/s)	Torque (mN·m)	STDev Torque (mN·m)	Viscosity (mPa·s)	STDev Viscosity (mPa·s)
2	0,292573	0,031936	2754,533	300,8283

Shear rate (1/s)	Torque (mN·m)	STDev Torque (mN·m)	Viscosity (mPa·s)	STDev Viscosity (mPa·s)
3,05	0,3745	0,006477	2315,6	40,05209
4,64	0,472773	0,007538	1919,867	30,64055
7,06	0,60147	0,008419	1604,1	22,42253
10,7	0,74521	0,009647	1305,3	16,92365
16,4	0,91749	0,008691	1055,433	10,00467
24,9	1,1207	0,009071	846,7033	6,861088
37,9	1,353867	0,010981	671,79	5,452366
57,8	1,624433	0,010275	529,3733	3,345001
88	1,937467	0,012404	414,6733	2,658596
134	2,279833	0,017436	320,46	2,442192
204	2,6764	0,01652	247,08	1,52915
311	3,125833	0,019225	189,52	1,16529
473	3,6129	0,015418	143,8667	0,613297
720	4,2071	0,027402	110,0233	0,717031

Table 35: 1wt% 21.3°C triplicate measurement

Shear rate (1/s)	Torque (mN·m)	STDev Torque (mN·m)	Viscosity (mPa·s)	STDev Viscosity (mPa·s)
2	0,268365	0,000304	2526,6	2,969848
3,05	0,36171	0,002531	2236,55	15,76848
4,64	0,46866	0,003479	1903,2	14,14214
7,06	0,59295	0,00116	1581,4	3,11127
10,7	0,74009	0,000226	1296,35	0,353553
16,4	0,91427	0,000764	1051,75	0,919239
24,9	1,11655	0,003606	843,585	2,736503
37,9	1,3475	0,002121	668,615	1,039447
57,8	1,6173	0,002121	527,035	0,685894
88	1,9384	0,008344	414,87	1,781909
134	2,28425	0,003182	321,085	0,445477
204	2,6764	0,010465	247,075	0,968736
311	3,12265	0,009122	189,325	0,558614
473	3,60855	0,004172	143,69	0,169706
720	4,1787	0,004667	109,28	0,127279

Table 36: 1.4wt% 20.5°C triplicate measurement

Shear rate (1/s)	Torque (mN·m)	STDev Torque (mN·m)	Viscosity (mPa·s)	STDev Viscosity (mPa·s)
2	0,77192	0,02456	7267,633	231,3014
3,05	0,967023	0,008052	5979,333	49,7121
4,64	1,2034	0,010928	4886,8	44,41092
7,06	1,469667	0,013062	3919,633	34,74152
10,7	1,7758	0,017433	3110,467	30,49989
16,4	2,119467	0,018127	2438,2	20,8113
24,9	2,505	0,020201	1892,567	15,24675
37,9	2,9398	0,026062	1458,7	12,94566
57,8	3,421233	0,030223	1114,9	9,819878
88	3,955333	0,036345	846,5433	7,782964
134	4,530933	0,036728	636,89	5,16247
204	5,1768	0,040451	477,9033	3,734251
311	5,877667	0,045129	356,3667	2,736866
473	6,647933	0,051624	264,7167	2,055075
720	7,487733	0,041426	195,8167	1,082143

Table 37: 1.4wt% 20.8°C triplicate measurement

Shear rate (1/s)	Torque (mN·m)	STDev Torque (mN·m)	Viscosity (mPa·s)	STDev Viscosity (mPa·s)
2	0,74659	0,023217	7034,8	228,1331
3,05	0,945153	0,007215	5844	44,62152
4,64	1,172133	0,004966	4759,9	20,01025
7,06	1,434567	0,006555	3825,933	17,52836
10,7	1,734133	0,006962	3037,467	12,18866
16,4	2,073767	0,009418	2385,6	10,86692
24,9	2,454533	0,010992	1854,433	8,306825
37,9	2,8817	0,010579	1429,867	5,215681
57,8	3,355467	0,014973	1093,5	4,856954
88	3,881567	0,015908	830,7567	3,411749
134	4,4565	0,015935	626,4267	2,241926
204	5,0952	0,018923	470,3733	1,750438
311	5,7905	0,023145	351,0767	1,407563
473	6,557067	0,020158	261,1033	0,803264

Shear rate (1/s)	Torque (mN·m)	STDev Torque (mN·m)	Viscosity (mPa·s)	STDev Viscosity (mPa·s)
720	7,404133	0,024501	193,6333	0,640026

Table 38: 1.5wt% 21°C triplicate measurement

Shear rate (1/s)	Torque (mN·m)	STDev Torque (mN·m)	Viscosity (mPa·s)	STDev Viscosity (mPa·s)
0,498	0,26406	0,009093	9969,85	366,493445
0,84	0,464135	0,018802	10405	425,678282
1,41	0,67927	0,004667	9049,4	63,215346
2,38	0,94761	0,004964	7511,85	39,103005
3,99	1,25895	0,01987	5936,05	93,974491
6,71	1,6592	0,067317	4653,35	189,716749
11,3	2,06685	0,018173	3448,3	29,839906
19	2,5484	0,045538	2529,1	45,113413
31,9	3,08895	0,03981	1823,5	23,617366
53,6	3,71645	0,041649	1305,05	14,63711
90,1	4,4252	0,051336	924,33	10,719739
152	5,1924	0,0577	645,15	7,170063
255	6,07595	0,059468	449,065	4,391133
428	7,07015	0,066822	310,83	2,941564
720	8,1899	0,078913	214,18	2,064752

Table 39: 1.5wt% 21.3°C triplicate measurement

Shear rate (1/s)	Torque (mN·m)	STDev Torque (mN·m)	Viscosity (mPa·s)	STDev Viscosity (mPa·s)
0,499	0,266493	0,009734	10052,1	368,450852
0,84	0,46497	0,002315	10416,66667	50,520623

Shear rate (1/s)	Torque (mN·m)	STDev Torque (mN·m)	Viscosity (mPa·s)	STDev Viscosity (mPa·s)
1,41	0,68607	0,006567	9142,266667	85,209761
2,38	0,953633	0,003405	7558,266667	26,933684
3,99	1,288467	0,023066	6075,4	109,468534
6,72	1,655067	0,011912	4641,533333	33,019136
11,3	2,070233	0,002779	3453,7	4,592385
19	2,553567	0,002344	2534,1	2,457641
31,9	3,1143	0,011285	1838,4	6,596211
53,6	3,739733	0,005297	1313,233333	1,858315
90,1	4,452033	0,005164	929,926667	1,078255
152	5,231433	0,002676	650	0,334215
255	6,118433	0,005689	452,206667	0,418609
428	7,115433	0,012851	312,826667	0,565007
720	8,230167	0,013903	215,233333	0,367741

Appendix B – Cross Model Regression

B.1 Excel Solver setup

Figure 60: Excel Solver setup used for fitting the Cross model parameters. The Solver objective cell was set to minimize the total squared error between the measured and calculated viscosity values. The variable cells corresponded to the fitted Cross model parameters: the zero-shear viscosity, η_0 , the time constant, a , and the Cross rate constant, c . Parameter constraints were applied to keep the fitted values within physically reasonable limits

B.2 Parameter constraints and guesses

	A	B	C	D	E	F
1	Shear rate	apparent viscosity		SE		1 n(inf)
2	2	7267,633333	7048,287358	48112,7	15498,63617	n(0)
3	3,05	5979,333333	5923,321782	3137,3	0,646097483	a
4	4,64	4886,8	4880,103197	44,8	0,708291028	c
5	7,06	3919,633333	3944,629111	624,8	1,547754056	critshear(1/a)
6	10,7	3110,466667	3142,537586	1028,5	53368,2	SSE
7	16,4	2438,2	2452,268123	197,9	0,000709533	SMSE
8	24,9	1892,566667	1901,608626	81,8	2323,1	Avg
9	37,9	1458,7	1458,472506	0,1		
10	57,8	1114,9	1108,802364	37,2	71022007,1	sstot
11	88	846,5433333	838,9703077	57,4		
12	134	636,89	631,9140085	24,8	0,999248567978243	R2
13	204	477,9033333	474,4401708	12,0		
14	311	356,3666667	354,9930514	1,9		
15	473	264,7166667	265,5884277	0,8		
16	720	195,8166667	198,3516336	6,4		

Figure 61: Example of the Excel calculation sheet used for Cross model parameter fitting. Column A contains the measured shear rate values, column B contains the measured apparent viscosity values, and column C contains the viscosity values calculated using the fitted Cross model. The squared error between the measured and calculated viscosity values was used to define the optimization objective for the Solver

B.3 Regression results: all points included

Table 40: Cross Regression Excel sheet values without end effect correction no points removed, K and n taken from 20-720 /s, viscosity at 100/s calculated using cross model.

Regression	K (Pa*s ⁿ)	n	Infinite shear (mPa*s)	Zeroshear (mPa*s)	Crossrate constant	Critical Shear rate (s ⁻¹)	Viscosity @ 100/s (mPa*s)
CMC 30000 21_3 1wt%	6,165789	0,391618	1	4772,942	0,659715	2,440387	380,2399
CMC 30000 21 1wt%	6,184538	0,39144	1	5793,452	0,646167	1,621884	378,5419
CMC 30000 20_5 1.4wt%	17,09814	0,324518	1	16510,79	0,704276	1,370724	768,3115
CMC 30000 20_8 1.4wt%	16,59661	0,327174	1	16108,33	0,701707	1,363764	754,9416

Table 41: Cross Regression Excel sheet values with end effect correction no points removed, K and n taken from 20-720 /s, viscosity at 100/s calculated using cross model.

Regression	K (Pa*s ⁿ)	n	Infinite shear (mPa*s)	Zeroshear (mPa*s)	Crossrate constant	Critical Shear rate (s ⁻¹)	Viscosity @ 100/s (mPa*s)
CMC 30000 21_3 1wt%	6,097155	0,382814	1	4946,473	0,665297	2,180475	360,7884
CMC 30000 21 1wt%	6,067313	0,384114	1	6059,917	0,650475	1,417615	358,7647
CMC 30000 20_5 1.4wt%	16,56876	0,316992	1	17502,32	0,709012	1,172695	718,6552
CMC 30000 20_8 1.4wt%	16,09354	0,319618	1	17072,88	0,706487	1,167598	706,5366

B.4 Regression results: lowest shear rate point excluded

Table 42: Cross regression Excel sheet values without end effect correction one points removed, K and n taken from 20-720 /s, viscosity at 100/s calculated using cross model.

Regression	K (Pa*s ⁿ)	n	Infinite shear (mPa*s)	Zeroshear (mPa*s)	Crossrate constant	Critical Shear rate (s ⁻¹)	Viscosity @ 100/s (mPa*s)
CMC 30000 21_3 1wt%	6,165789	0,391618	1	4881,947	0,657694	2,3204	379,8404
CMC 30000 21 1wt%	6,184538	0,39144	1	5364,662	0,652054	1,920174	379,7097
CMC 30000 20_5 1.4wt%	17,09814	0,324518	1	15498,81	0,70829	1,547731	770,0349
CMC 30000 20_8 1.4wt%	16,59661	0,327174	1	15210,01	0,705338	1,52327	756,4708

Table 43: Cross regression Excel sheet values with end effect correction one points removed, , K and n taken from 20-720 /s, viscosity at 100/s calculated using cross model.

Regression	K (Pa*s ⁿ)	n	Infinite shear (mPa*s)	Zeroshear (mPa*s)	Crossrate constant	Critical Shear rate (s ⁻¹)	Viscosity @ 100/s (mPa*s)
CMC 30000 21_3 1wt%	6,097155	0,382814	1	5091,131	0,662905	2,047972	360,3373
CMC 30000 21 1wt%	6,067313	0,384114	1	5614,005	0,655848	1,669697	359,7807
CMC 30000 20_5 1.4wt%	16,56876	0,316992	1	16501,55	0,712364	1,309034	720,007
CMC 30000 20_8 1.4wt%	16,09354	0,319618	1	16203,56	0,709452	1,287786	707,7084

B.5 Measured vs fitted Cross model plots



Figure 62: $R^2=0.99998$, regression with 2 points excluded 1.5wt%

Appendix C – CFD Setup and Mesh Sensitivity

C.1 CFD setup



Figure 63: RV5 0.40mm base size final production mesh.

C.2 Shear rate profile

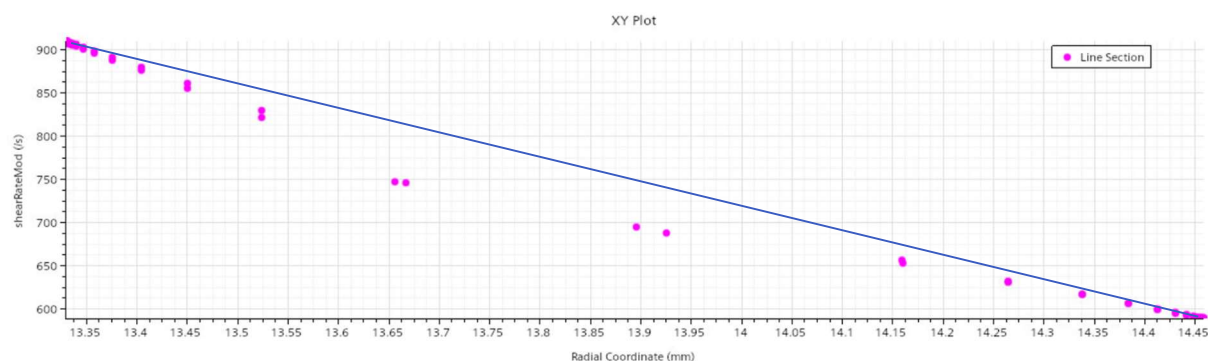


Figure 64: CC27 shear rate profile in the gap depicted as purple measurement points for each cell, with function $ShearRateMod$ against Radial coordinate. A blue linear curve is drawn as the theoretical approximation. For 1.0 wt% CMC30000 at 21.0 °C using regressed Cross parameters at 558.17 RPM, corresponding to the 720 s^{-1} data point.

Appendix D – Neural Network Details

D.1 Hyperparameter sweep results

Table 44: Hyperparameter sweep 5 point model, 10 best models

Rank	Trial	Hidden trunk	Loss weights	Optimizer	LR sched. patience	Early stop patience	Batch	Max err 0 %	Max err 1 %	Max err 2 %
1	24	(512, 512, 512, 256)	(1.0, 2.0, 1.0)	adamw	30	50	64	4.803	9.839	2.784
2	15	(512, 512, 512, 256)	(1.0, 1.0, 1.0)	adam	30	50	32	5.334	10.088	1.295
3	13	(512, 512, 512, 256)	(1.0, 1.0, 1.0)	adam	30	40	32	5.334	10.088	1.295
4	93	(512, 512, 512, 128)	(1.0, 3.0, 1.0)	adam	30	40	32	4.936	10.421	1.180
5	119	(512, 512, 512, 512)	(1.0, 2.0, 1.0)	adamw	30	50	32	6.002	10.629	1.042
6	117	(512, 512, 512, 512)	(1.0, 2.0, 1.0)	adamw	30	40	32	6.002	10.629	1.042

7	95	(512, 512, 512, 128)	(1.0, 3.0, 1.0)	adam	30	50	32	4.59 4	10.66 8	1.15 5
8	25	(512, 512, 512, 256)	(1.0, 2.0, 1.0)	adam	20	40	32	6.31 0	10.90 3	1.13 9
9	27	(512, 512, 512, 256)	(1.0, 2.0, 1.0)	adam	20	50	32	6.31 0	10.90 3	1.13 9
10	31	(512, 512, 512, 256)	(1.0, 2.0, 1.0)	adam	30	50	32	5.70 4	11.12 6	0.93 7

Table 45: Hyperparameter sweep results 10 point model, 10 best models

Ran k	Tri al	Hidde n trunk	Loss weigh ts	Optimiz er	LR sched. patien ce	Early stop patien ce	Batc h	Best epoc h	Ma x err 0 %	Ma x err 1 %	Ma x err 2 %
1	55	(512, 512, 512, 512)	(1.0, 1.0, 1.0)	adamw	30	50	32	216	2.84 0	2.45 7	0.44 1
2	53	(512, 512, 512, 512)	(1.0, 1.0, 1.0)	adamw	30	40	32	216	2.84 0	2.45 7	0.44 1
3	96	(512, 512, 512, 512)	(1.0, 3.0, 1.0)	adam	30	50	64	430	2.37 3	3.42 9	0.79 3
4	41	(512, 512, 512, 256)	(1.0, 3.0, 1.0)	adam	20	40	32	173	4.00 4	3.65 0	0.59 5
5	51	(512, 512, 512, 512)	(1.0, 1.0, 1.0)	adamw	20	50	32	290	2.02 9	3.76 3	0.42 3
6	49	(512, 512, 512, 512)	(1.0, 1.0, 1.0)	adamw	20	40	32	290	2.02 9	3.76 3	0.42 3

7	87	(512, 512, 512, 512)	(1.0, 3.0, 1.0)	adamw	30	50	32	201	4.36 7	3.80 5	0.50 3
8	35	(512, 512, 512, 256)	(1.0, 3.0, 1.0)	adamw	20	50	32	182	2.23 5	3.84 3	0.50 2
9	33	(512, 512, 512, 256)	(1.0, 3.0, 1.0)	adamw	20	40	32	182	2.23 5	3.84 3	0.50 2
10	69	(512, 512, 512, 512)	(1.0, 2.0, 1.0)	adamw	30	40	32	270	4.38 7	3.88 5	0.50 9

D.2 Final 5-point model results

Table 46: Results AI(1)(5 point) (average summarized)

CMC wt%	Sample	ZeroShear (Pa*s)	CriticalShearRate (/s)	CrossrateConstant	K (Pa*s ⁿ)	n	Viscosity @100/s (m*Pa*s)
1	S11	6.1687	0.9444	0.5991	4.7312	0.4354	354.9265
1	S12	6.1687	0.9444	0.5991	4.7312	0.4354	354.9265
1	S21	6.1241	0.9831	0.6023	4.7939	0.4327	355.3308
1	S22	6.1803	0.9253	0.5975	4.6620	0.4367	351.5243
1.4	S11	21.1623	0.7903	0.6522	14.9361	0.3737	844.2523
1.4	S12	23.7470	0.6651	0.6459	15.3029	0.3780	882.8067
1.4	S21	21.8310	0.7582	0.6526	15.1846	0.3728	854.1505
1.4	S22	23.6181	0.6979	0.6471	15.5845	0.3772	895.1693
1.5	S11	19.8994	1.5664	0.6930	20.3837	0.3419	993.9087
1.5	S12	22.5492	1.3760	0.6996	21.8347	0.3321	1020.5321
1.5	S21	23.0956	0.9628	0.6624	17.7368	0.3655	966.0633
1.5	S22	23.2894	1.0976	0.6740	18.8839	0.3549	981.1765

Table 47: AI 5 point model predictions based on Brookfield measurements of CMC 30000

Sample	Parameter	Median	Mean	Std.dev (σ)	CV (%)
10wtS11	Zero Shear Visc (Pa·s)	6.1553	6.1687	0.4434	7.19%
	Crit. Shear Rate (1/s)	0.9336	0.9444	0.1283	13.58%

Sample	Parameter	Median	Mean	Std.dev (σ)	CV (%)
	Cross Constant (m)	0.5984	0.5991	0.0087	1.44%
	Viscosity @ 100/s	350.4747	354.9265	21.8908	6.17%
	Power Law index (n)	0.4360	0.4354	0.0077	1.76%
	Consistency index (K)(Pa*s ⁿ)	4.6878	4.7312	0.2889	6.11%
10wtS12	Zero Shear Visc (Pa·s)	6.1553	6.1687	0.4434	7.19%
	Crit. Shear Rate (1/s)	0.9336	0.9444	0.1283	13.58%
	Cross Constant (m)	0.5984	0.5991	0.0087	1.44%
	Viscosity @ 100/s	350.4747	354.9265	21.8908	6.17%
	Power Law index (n)	0.4360	0.4354	0.0077	1.76%
	Consistency index (K)(Pa*s ⁿ)	4.6878	4.7312	0.2889	6.11%
10wtS21	Zero Shear Visc (Pa·s)	6.1295	6.1241	0.4578	7.48%
	Crit. Shear Rate (1/s)	0.9716	0.9831	0.1434	14.58%
	Cross Constant (m)	0.5988	0.6023	0.0143	2.37%
	Cross viscosity @ 100/s	354.2319	355.3308	23.3633	6.58%
	Power Law index (n)	0.4365	0.4327	0.0132	3.06%
	Consistency index (K) (Pa*s ⁿ)	4.7929	4.7939	0.2856	5.96%
10wtS22	Zero Shear Visc (Pa·s)	6.0886	6.1803	0.6741	10.91%
	Crit. Shear Rate (1/s)	0.9228	0.9253	0.1626	17.57%
	Cross Constant (m)	0.5969	0.5975	0.0123	2.07%
	Cross viscosity @ 100/s	346.8752	351.5243	23.4298	6.67%
	Power Law index (n)	0.4377	0.4367	0.0105	2.40%
	Consistency index (K) (Pa*s ⁿ)	4.6303	4.6620	0.3508	7.53%
14wtS11	Zero Shear Visc (Pa·s)	21.4500	21.1623	2.4838	11.74%
	Crit. Shear Rate (1/s)	0.7049	0.7903	0.2655	33.60%
	Cross Constant (m)	0.6518	0.6522	0.0267	4.09%
	Cross viscosity @ 100/s	825.5561	844.2523	73.7740	8.74%
	Power Law index (n)	0.3730	0.3737	0.0246	6.57%
	Consistency index (K) (Pa*s ⁿ)	14.6730	14.9361	0.6579	4.40%
14wtS12	Zero Shear Visc (Pa·s)	23.9004	23.7470	2.6487	11.15%
	Crit. Shear Rate (1/s)	0.6227	0.6651	0.1918	28.84%
	Cross Constant (m)	0.6419	0.6459	0.0241	3.74%
	Cross viscosity @ 100/s	889.9231	882.8067	82.5386	9.35%
	Power Law index (n)	0.3813	0.3780	0.0227	6.01%
	Consistency index (K) (Pa*s ⁿ)	15.2523	15.3029	0.4249	2.78%
14wtS21	Zero Shear Visc (Pa·s)	22.1439	21.8310	2.0801	9.53%

Sample	Parameter	Median	Mean	Std.dev (σ)	CV (%)
	Crit. Shear Rate (1/s)	0.7010	0.7582	0.2153	28.40%
	Cross Constant (m)	0.6502	0.6526	0.0223	3.42%
	Cross viscosity @ 100/s	844.6341	854.1505	63.7797	7.47%
	Power Law index (n)	0.3738	0.3728	0.0207	5.56%
	Consistency index (K) (Pa*s ⁿ)	15.0047	15.1846	0.4899	3.23%
14wtS22	Zero Shear Visc (Pa·s)	24.1352	23.6181	2.5790	10.92%
	Crit. Shear Rate (1/s)	0.6351	0.6979	0.2272	32.56%
	Cross Constant (m)	0.6418	0.6471	0.0224	3.46%
	Cross viscosity @ 100/s	901.6336	895.1693	72.0018	8.04%
	Power Law index (n)	0.3820	0.3772	0.0207	5.49%
	Consistency index (K) (Pa*s ⁿ)	15.5043	15.5845	0.4398	2.82%
15wtS11	Zero Shear Visc (Pa·s)	20.8195	19.8994	3.3783	16.98%
	Crit. Shear Rate (1/s)	1.2498	1.5664	0.7664	48.93%
	Cross Constant (m)	0.6808	0.6930	0.0371	5.35%
	Cross viscosity @ 100/s	985.6970	993.9087	66.3763	6.68%
	Power Law index (n)	0.3499	0.3419	0.0308	8.99%
	Consistency index (K) (Pa*s ⁿ)	19.7655	20.3837	2.0855	10.23%
15wtS12	Zero Shear Visc (Pa·s)	23.4036	22.5492	3.5837	15.89%
	Crit. Shear Rate (1/s)	1.1443	1.3760	0.6258	45.48%
	Cross Constant (m)	0.6848	0.6996	0.0379	5.42%
	Cross viscosity @ 100/s	1031.4415	1020.5321	91.1965	8.94%
	Power Law index (n)	0.3448	0.3321	0.0329	9.91%
	Consistency index (K) (Pa*s ⁿ)	21.3720	21.8347	1.6862	7.72%
15wtS21	Zero Shear Visc (Pa·s)	22.9195	23.0956	3.9157	16.95%
	Crit. Shear Rate (1/s)	0.8650	0.9628	0.4810	49.96%
	Cross Constant (m)	0.6657	0.6624	0.0333	5.03%
	Cross viscosity @ 100/s	938.8670	966.0633	85.8294	8.88%
	Power Law index (n)	0.3594	0.3655	0.0288	7.89%
	Consistency index (K) (Pa*s ⁿ)	17.4662	17.7368	1.0269	5.79%
15wtS22	Zero Shear Visc (Pa·s)	24.0211	23.2894	4.8769	20.94%
	Crit. Shear Rate (1/s)	0.8779	1.0976	0.7028	64.03%
	Cross Constant (m)	0.6800	0.6740	0.0426	6.33%
	Cross viscosity @ 100/s	940.9735	981.1765	110.6766	11.28%
	Power Law index (n)	0.3489	0.3549	0.0368	10.38%
	Consistency index (K) (Pa*s ⁿ)	18.5816	18.8839	1.5418	8.16%

D.3 Final 10-point model results

Table 48: AI 10 point model predictions based on Brookfield Measurements of CMC 30000

Sample	ZeroShear (Pa*s)	Critical Shear Rate (s ⁻¹)	Crossrate constant	Viscosity @ 100/s	Derived PowerLaw n	Derived PowerLaw K (Pa*s ⁿ)
10wt_S11	6.074195	1.063982	0.595943	380.784271	0.442127	4.915554
10wt_S12	6.074195	1.063982	0.595943	380.784271	0.442127	4.915554
10wt_S21	5.837580	1.193568	0.606372	373.697388	0.433224	5.022845
10wt_S22	6.066440	1.027876	0.591200	380.705109	0.446582	4.815539
14wt_S11	21.816881	0.689786	0.655776	804.803406	0.369055	14.586856
14wt_S12	25.061096	0.513356	0.647707	798.906189	0.373635	14.196360
14wt_S21	22.881121	0.624461	0.652439	805.657532	0.371185	14.466443
14wt_S22	24.690905	0.554834	0.652646	806.116272	0.369359	14.605178
15wt_S11	22.196640	1.034271	0.672565	981.307739	0.357577	18.709750
15wt_S12	25.656876	0.912416	0.693465	952.141724	0.332962	20.355038
15wt_S21	26.019564	0.616682	0.657405	886.958191	0.365608	16.342257
15wt_S22	26.082769	0.639314	0.666169	871.619751	0.356771	16.725831

Appendix E – Validation and Supplementary Results

E.1 AI-predicted parameter comparison

Table 49: Comparison between Ai prediction and excel regression for 1.4wt% no points removed

Parameter	AI 5 vs With end effects	AI 10 vs With end effects	AI 5 vs Without end effects	AI 10 vs Without end effects
ZeroShear (Pa*s)	+30.67%	+36.59%	+38.51%	+44.78%
CriticalShearRate (/s)	-37.80%	-49.1%	-46.76%	-56.44%
CrossrateConstant	-8.24%	-7.85%	-7.62%	-7.23%
K (Pa*s ⁿ)	-6.61%	-11.43%	-9.47%	-14.15%
n	+17.95%	+16.50%	+15.22%	+13.80%

Table 50: Comparison between Ai prediction and excel regression for 1wt% with one point removed

Parameter	AI 5 vs With end effects	AI 10 vs With end effects	AI 5 vs Without end effects	AI 10 vs Without end effects
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ZeroShear (Pa·s)	+15.09%	+12.34%	+20.24%	+17.36%
CriticalShearRate (/s)	-48.93%	-41.50%	-55.23%	-48.72%
CrossrateConstant	-9.08%	-9.40%	-8.46%	-8.78%
K (Pa·sⁿ)	-22.24%	-19.15%	-23.41%	-20.37%
n	+13.45%	+15.00%	+11.12%	+12.63%

Table 51: Comparison between Ai prediction and excel regression for 1.4wt% with one point removed

Parameter	AI 5 vs With end effects	AI 10 vs With end effects	AI 5 vs Without end effects	AI 10 vs Without end effects
ZeroShear (Pa·s)	+38.14%	+44.40%	+47.12%	+53.78%
CriticalShearRate (/s)	-43.94%	-54.13%	-52.60%	-61.21%
CrossrateConstant	-8.65%	-8.26%	-8.12%	-7.74%
K (Pa·sⁿ)	-6.61%	-11.45%	-9.47%	-14.15%
n	+17.95%	+16.50%	+15.22%	+13.80%

Table 52: Viscosity comparison for CMC 30000 between the two different AI models and the measured viscosities at 100/s. Difference is calculated with $100 \cdot (\text{Measured-AI})/\text{AI}$. Regression strategies according to (i, ii and iii).

Conc.	Treatment	AI 10 Viscosity @20/s Relative Error	AI 5 Viscosity @20/s Relative Error	AI 10 Viscosity @100/s Relative Error	AI 5 Viscosity @100/s Relative Error	AI 10 Viscosity @720/s Relative Error	AI 5 Viscosity @720/s Relative Error
1.0 wt%	No exclusion, no end- effect corr.	6.28	11.74	0.105%	7.12%	-9.39	-3.00
	1 point excluded, no end- effect corr.	6.35	11.82	0.206%	7.23%	-9.51	-3.13
	1 point excluded, with end- effect corr.	2.58	7.85	-5.00%	1.66%	-15.35	-9.39
1.4 wt%	No exclusion, no end- effect corr.	-0.42	-8.51	-5.26%	-12.37%	-13.34	-22.08
	1 point excluded, no end- effect corr.	-0.25	-8.36	-5.05%	-12.18%	-13.59	-22.31
	1 point excluded, with end- effect corr.	-5.07	-12.78	-11.20%	-17.86%	-20.18	-28.23

E.2 Torque reconstruction using AI parameters

Table 53: CFD torque deviations using AI-predicted Cross parameters. The deviations compare CFD-simulated Brookfield RV5 torque with measured Brookfield torque for the 5-point and 10-point AI models. Trends show how the deviation changes from low to mid and mid to high RPM.

wt%	CFD simulation case	Mean deviat ion (%)	Deviat ion trend (Low →Mid Mid→ High)	Best deviation (%) [RPM]	Worst deviation (%) [RPM]	Low mean deviat ion (%)	Mid mean deviat ion (%)	High mean deviat ion (%)
1 wt%	S11 5 point	-5.47	↑ ↑	-3.76 [10]	-6.29 [100]	-4.62	-5.48	-6.11
	S12 5 point	-5.47	↑ ↑	-3.76 [10]	-6.29 [100]	-4.62	-5.48	-6.11

wt%	CFD simulation case	Mean deviation (%)	Deviation trend (Low → Mid Mid → High)	Best deviation (%) [RPM]	Worst deviation (%) [RPM]	Low mean deviation (%)	Mid mean deviation (%)	High mean deviation (%)
	S21 5 point	-3.48	↑ ↑	-1.75 [10]	-4.33 [80]	-2.42	-3.60	-4.20
	S22 5 point	-4.56	↑ ↑	-2.72 [10]	-5.51 [100]	-3.46	-4.79	-5.22
	S11 10 point	-0.88	≈ ≈	-0.68 [90]	-1.32 [20]	-1.10	-0.76	-0.81
	S12 10 point	-0.88	≈ ≈	-0.68 [90]	-1.32 [20]	-1.10	-0.76	-0.81
	S21 10 point	-0.11	≈ ≈	-0.008 [40]	-0.31 [90]	+0.02	-0.05	-0.26
	S22 10 point	-0.37	≈ ≈	-0.10 [90]	-0.64 [10]	-0.53	-0.46	-0.20
1.4 wt%	S11 5 point	+3.92	↑ ≈	+3.51 [10]	+5.42 [100]	+4.27	+5.09	+5.29
	S12 5 point	+7.44	↑ ≈	+4.48 [10]	+8.42 [90]	+6.11	+7.71	+8.25
	S21 5 point	+4.27	↑ ≈	+2.48 [10]	+4.77 [100]	+3.62	+4.46	+4.63
	S22 5 point	+7.61	↑ ≈	+4.43 [10]	+8.72 [100]	+6.07	+7.95	+8.50
	S11 10 point	+0.02	↓ ≈	-0.05 [60]	+0.69 [10]	+0.54	+0.02	-0.36
	S12 10 point	-1.28	≈ ≈	-0.60 [20]	-1.60 [70]	-1.04	-1.28	-1.46
	S21 10 point	-1.28	≈ ≈	-0.44 [20]	-1.73 [80]	-0.78	-1.30	-1.64
	S22 10 point	-1.38	≈ ≈	-0.94 [30]	-1.68 [90]	-1.12	-1.30	-1.64