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M-Star® Software Test and Verification for Impeller Mixing in a Tank

M. R. Poirier

S. R. Noble

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M-Star® Modeling of SME Mixing with Three Impeller Blades

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November 2022

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REVIEWS AND APPROVALS

AUTHORS:

____

M. R. Poirier, Chem Flowsheet Dev Date

____

S. R. Noble, Chem Flowsheet Dev Date

TECHNICAL REVIEW:

____

E. K. Hansen, Chem Flowsheet Dev, Reviewed per E7 2.60 Date

APPROVAL:

____

G. A. Morgan, Manager, Chemical Flowsheet Development Date

____

F. M. Pennebaker, Director, Chemical Processing & Characterization Date

____

R. M. Hoeppel, H. P. Boyd, DWPF/Saltstone Facility Engineering Date

EXECUTIVE SUMMARY

Before a sample of the Slurry Mix Evaporator (SME) can be taken, the SME product sampling procedure requires that the agitator power be stable between 20 and 30 kW for at least one hour. The SME transfer to Melter Feed Tank (MFT) procedure also requires the SME agitator power be stabilized between 20 and 30 kW prior to transfer. These requirements are specified to ensure samples are homogeneous, as discussed in the Waste Form Qualification Report. During SME Batch 804, the agitator power dropped to 19 kW and struggled to achieve and maintain 20 kW. It was later discovered that the cause of the power drop was due to one of the bottom blades of the agitator breaking off. Both the sample and the transfer occurred without the power stabilizing between 20 and 30 kW. Therefore, the quality of SME Batch 804 is indeterminate, and homogeneity was questionable.

To evaluate mixing in the SME with a broken agitator containing only three blades (90 degrees apart with space for a missing blade) on the bottom impeller, the Savannah River National Laboratory (SRNL) was requested to perform computer simulations of impeller mixing in the SME using M-Star® software. The simulations will be used to determine if SME Batch 804 was well mixed and satisfies homogeneity requirements.

The M-Star® software is currently classified as Level D in Software Classification Document X-SWCD-A-00011 in accordance with the latest revision of Manual 1Q Procedure 20-1. The M-Star® software needs to be qualified to Level C software to satisfy the Waste Form Affecting (WFA) requirements within Manual 1Q Procedure 20-1, Attachment 8.2.

M-Star® software was used previously to develop and qualify a model that accurately calculated the release rate of retained hydrogen from benchtop vessels during Sludge Batch (SB) 3 and SB5 qualification testing. This model was then used to simulate hydrogen release from DWPF process vessels.

Various Quality Assurance (QA) software tests including, but not limited to agitator power number calculations and mixing cavern size, were performed to test the accuracy and reliability of the M-Star® software. This document describes the work performed to validate the software as Level C, Waste Form Affecting. The M-Star® simulation results acceptance criteria compared to literature data is 20% for impeller power number and 30% for the cavern diameter.

The conclusions from the work follow.

- The comparisons of impeller power number with Newtonian fluids shows the M-Star® produced power numbers within 10% of the experimental power number when the Reynolds number is greater than or equal to 15.
- The comparisons of impeller power number with Bingham plastic fluids shows the M-Star® produced power number to be within 5% of the experimental power number.
- Cavern mixing tests showed the M-Star® simulation prediction of cavern diameter to be within 30% of the cavern diameter from literature data and literature correlations in all tests, and within 10% for most of the tests.
- Based on the results of the software testing, the M-Star® software meets the requirements for level C, Waste Form Affecting for impellerc mixing of Newtonian and non-Newtonian Fluids in a tank.

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LIST OF ABBREVIATIONS

CFD	Computational Fluid Dynamics
DWPF	Defense Waste Processing Facility
EN	Elson – Nienow
HB	Herschel Bulkley
LES	Large Eddy Simulation
MFT	Melter Feed Tank
PBT	Pitch Blade Turbine
QA	Quality Assurance
RANS	Reynolds Averaged Navier-Stokes
Re	Reynolds number
RPM	Revolutions per minute
SB	Sludge Batch
SME	Slurry Mix Evaporator
SRAT	Sludge Receipt and Adjustment Tank
SRMC	Savannah River Mission Completion
SRNL	Savannah River National Laboratory
SWCD	Software Classification Document
TTR	Technical Task Request
WFA	Waste Form Affecting

1.0 Introduction

Before a sample of the Slurry Mix Evaporator (SME) can be taken, the SME product sampling procedure requires that the agitator power be stable between 20 and 30 kW for at least one hour.[1] The SME transfer to Melter Feed Tank (MFT) procedure also requires the SME agitator power be stabilized between 20 and 30 kW prior to transfer.[2] These requirements are specified to ensure samples are homogeneous, as discussed in the Waste Form Qualification Report.[3, 4] During SME Batch 804, the agitator power dropped to 19 kW and struggled to achieve and maintain 20 kW. It was later discovered that the cause of the power drop was one of the bottom blades of the agitator breaking off. Both the sample and the transfer occurred without the power stabilizing between 20 and 30 kW. Therefore, the quality of SME Batch 804 is indeterminate, and homogeneity was questionable.[5, 6]

To evaluate mixing in the SME with a broken agitator containing only three blades (90 degrees apart with space for a missing blade) on the bottom impeller, the Savannah River National Laboratory (SRNL) was requested to perform computer simulations of impeller mixing in the SME using M-Star® software, per Technical Task Request (TTR) X-TTR-S-00089 issued by Savannah River Mission Completion (SRMC).[5] The simulations will be used to determine if SME Batch 804 was well mixed and satisfies homogeneity requirements. The simulation results will be used to support the disposition of 2021-NCR-05-0033.[6]

The M-Star® software is currently classified as Level D in Software Classification Document X-SWCD-A-00011 in accordance with the latest revision of Manual 1Q Procedure 20-1. This software is currently being validated as Level B software for the Defense Waste Processing Facility (DWPF) Retained Hydrogen program contribution to the accident analysis.[7] However, for this TTR, the M-Star® software need only be qualified to Level C software to satisfy the Waste Form Affecting (WFA) requirements within Manual 1Q Procedure 20-1, Attachment 8.2. The first task described in X-TTR-S-00089 is to reclassify the M-Star® software to Level C, WFA which will include updating the Software Quality Assurance Plan (SQAP), B-SQP-A-00097 and performing software tests to validate the software performance prior to use.

M-Star® software is a computational fluid dynamics (CFD) program that utilizes the lattice-Boltzmann method rather than the traditional Reynolds-averaged Navier–Stokes (RANS) approach. This allows for simulations to be run quickly while delivering results accurately. The user interface allows the user to focus on the system and the process instead of the small nuances like other CFD software.

M-Star® software was used previously to develop and qualify a model that accurately calculated the release rate of retained hydrogen from benchtop vessels during Sludge Batch (SB) 3 and SB5 qualification testing. This model was then used to simulate hydrogen release from DWPF process vessels.[8]

Various Quality Assurance (QA) software tests including but not limited to impeller power number and mixing cavern diameter size calculations, were performed to test the accuracy of the M-Star® software. This document describes the work performed to validate the software as Level C, Waste Form Affecting.

2.0 Approach

SRMC Defense Waste Processing Facility Engineering requested SRNL to upgrade the M-Star® software to QA Level C, WFA. Because the results from the software are required for the DWPF Waste Acceptance process, the software will be WFA and must be classified as Level C on the Software Classification Document (SWCD) and must follow the appropriate level of rigor per the "WFA" column of Attachment 8.2 within Manual 1Q Procedure 20-1. The software will also be subject to the requirements of DOE/RW-0333P Supplement I, "Software".[9]

2.1 Software Verification

The slurry in the SME is considered a Bingham plastic fluid, and the mixing is performed with dual impellers on a single shaft. A parameter used for designing, understanding, and modeling impeller mixed tanks is the impeller power number. Simulations of impeller mixed tanks were performed, the impeller power number determined, and results compared with power numbers in technical literature. These simulations were performed for both Newtonian and non-Newtonian fluids.

Mixing of Bingham plastic fluids is often described by the cavern model, in which the tank contains a well-mixed cavern near the impeller where the shear stresses produced by the impeller exceed the yield stress of the fluid. The region outside of the cavern, where the fluid yield stress exceeds the shear stress generated by the impeller, is stagnant. This application will assess the ability of the code to model how stresses generated by the impeller can be limited by the yield stress, hence impacting mixing.

2.1.1 Software Testing for Impeller Power Number Calculations and Comparison with Literature Data

Ma provides an extensive set of data describing power numbers for different types of impellers and a wide range of operating parameters.[10] This data set is used by M-Star® to test and verify the software. Simulations of mixing in tanks with Rushton impellers, pitch blade impellers, and hydrofoils were performed, and the calculated power numbers compared with this data.

In addition, Nagata, et. al. measured the power number of a number of impeller types during the mixing of Bingham plastic fluids.[11] Their data set included Rushton impellers and flat blade turbines. Simulations of mixing of Bingham plastic fluids under turbulent conditions as those used by Nagata, et. al. was performed, and the power numbers compared with this work.

The acceptance criteria for the power number tests are for the M-Star® predictions to be within 20% of the experimental data. This criterion comes from the software test plan group 2 problems for the work to upgrade the software for safety applications.[12]

2.1.2 Software Testing for Cavern Mixing Calculations and Comparisons with Literature Results

Cavern mixing occurs in vessels with non-Newtonian fluids, such as the fluids in the DWPF Slurry Receipt and Adjustment Tank (SRAT) and SME. Simulations of mixing with non-Newtonian fluids, including Bingham plastic and Herschel-Bulkley fluids were performed using M-Star® and the cavern sizes from the simulations were compared with cavern sizes measured by Elson et al[13], Adams and Barigou[14], and correlations developed by Elson et. al.[13] Since the sludge slurries in the DWPF process vessels behave as non-Newtonian fluids, this comparison will provide data to assess the ability of the M-Star® software to simulate mixing of non-Newtonian fluids in these vessels.

The acceptance criteria for the cavern mixing tests is for the M-Star® predictions to be within 30% of the experimental and literature data. This criterion comes from the software test plan group 3 problems for the work to upgrade the software for safety applications.[12]

2.2 Quality Assurance

Requirements for performing reviews of technical reports and the extent of review are established in manual E7 2.60. SRNL documents the extent and type of review using the SRNL Technical Report Design Checklist contained in WSRC-IM-2002-00011, Rev. 2.

The requested work is described in TTR X-TTR-S-00089 and directed by TTQAP SRNL-RP-2021-05004.[5,15] The Functional Classification of this task is Production Support. SME homogeneity is waste form affecting and needs to follow the quality assurance requirements of RW-0333P.[9] Requirements for performing reviews of technical reports and the extent of review are established in Manual E7 2.60. This document, including calculations, was reviewed by Design Verification. SRNL documents the Design Verification using the SRNL Technical Report Design Checklist contained in WSRC-IM-2002-00011, Rev. 2. The Design Checklists for this report are stored in electronic laboratory notebook experiment Y5714-00412.

3.0 Results and Discussion

3.1 Software Test Problems

3.1.1 Impeller Power Number

The impeller power number is an important application for mixing equipment suppliers. Knowing the power allows one to determine the power draw and to size the motor/gearbox for the agitator. It also allows for optimizing the impeller diameter and impeller speed. In addition, many correlations for parameters such as blend time, cavern diameter, gas bubble size, liquid droplet size, and mass transfer coefficient depend on the agitator power.[16]

Simulations with rotating impellers were performed to validate the hydrodynamic forces induced by the impeller as measured by the torque on the shaft against measured data over a range of Reynolds numbers. Each test case considered a single Rushton, 45° pitch blade turbine (PBT), or hydrofoil impeller in a baffled 1 m diameter tank with an impeller diameter and rotational speed specified in Table A 1. The impellers were centered in the vessel with a one-diameter off-bottom clearance. The viscosity of the fluid was assumed to be constant but varied between simulations to sweep over a range Reynolds number. All simulations were performed using a lattice spacing of 250 points across the vessel diameter. As suggested by our previous investigations, this resolution is expected to generate grid-independent power numbers. The Courant number was set to 0.01, a value sufficient to keep lattice density variations below 1% across the vessel.

In Figure 1, we present the variation in predicted power number versus Reynolds number for all three impellers. For each condition, the Reynolds number Re is defined by:

$$Re = \frac{ND^2}{\nu} \quad [1]$$

where *N* is the impeller speed (in revolutions per second), *D* is the impeller diameter, and ν is the kinematic viscosity. The impeller power number is defined by equation [2]

$$P = \rho \, N_p \, N^3 \, D^5 \quad [2]$$

where P is the applied power, ρ is the fluid density, N_p is the impeller power number, N is the impeller speed, and D is the impeller diameter.[16]

The predicted power numbers and measured power numbers for each impeller at each Reynolds number are shown in Table A 1 in the Appendix. The general trends are consistent between the two data sets: at low Reynolds numbers (Re<100), the power number increases with decreasing Reynolds number. At high Reynolds numbers (Re>10000), the power number for an impeller becomes constant. Between these two extremes, around Re = 1000, there is a transitional regime with a small local minimum in power draw. The kinematic viscosity, Reynolds number, and the measured and predicted power number for each impeller type are provided in Table A 1. The predicted power numbers are within 20% of the measured values.

In the DWPF facility, the SME and Melter feed vessels consist of impellers with a diameter of 3 ft, a maximum shaft speed of 130 rpm, a slurry density of 1.2 g/mL, and a consistency of 50 cP, resulting in a Reynolds number of ~43,000. This value is within the range of the values tested. The test of the M-Star®

software at determining the impeller power number during impeller mixing of a Newtonian fluid is determined to be successful.

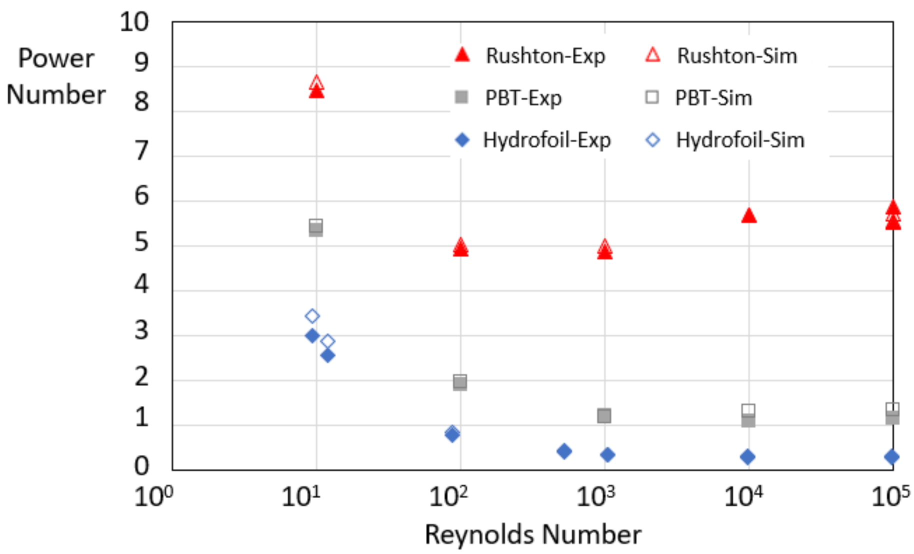

Figure 1. Simulation predicted (Sim) versus experimentally measured (Exp) power numbers for multiple impellers across a range of Reynolds numbers.

Because many processes at SRS involve the mixing of non-Newtonian fluids with impellers. Additional tests of the M-Star® software were performed to calculate the power number of impellers in this application.

Nagata, et. al. measured the power number of a number of impeller types during the mixing of Bingham plastic fluids.[11] Their data set included Rushton impellers and flat blade paddles. The configuration used in M-Star® for the verification of the power number is a tank with a diameter and height of 1 m containing a impeller/tank diameter ratio of 0.5 and four standard baffles. The slurry density was 1330 kg/m^3, the yield stress was 15 Pa, and the consistency was 40 cP. The turbine rotated at 130 rpm. These parameters were selected to match the design of the SME. The Reynolds number for this simulation is 18,000. Figure 2 shows the layout of the vessels used in the simulation with a 6-blade paddle and Rushton turbine. Simulations of mixing of Bingham plastic fluids under turbulent conditions as those used by Nagata et al were performed, and the power numbers are shown in Table 1. The power numbers from the M-Star® simulations agree with the data of Nagata et al within 5%. Nagata states that the power number in turbulent mixing conditions for Newtonian or non-Newtonian fluids yield close agreement, something that is expected. The test of the M-Star® software at determining the impeller power number during impeller mixing of a Bingham plastic fluid is determined to be successful.

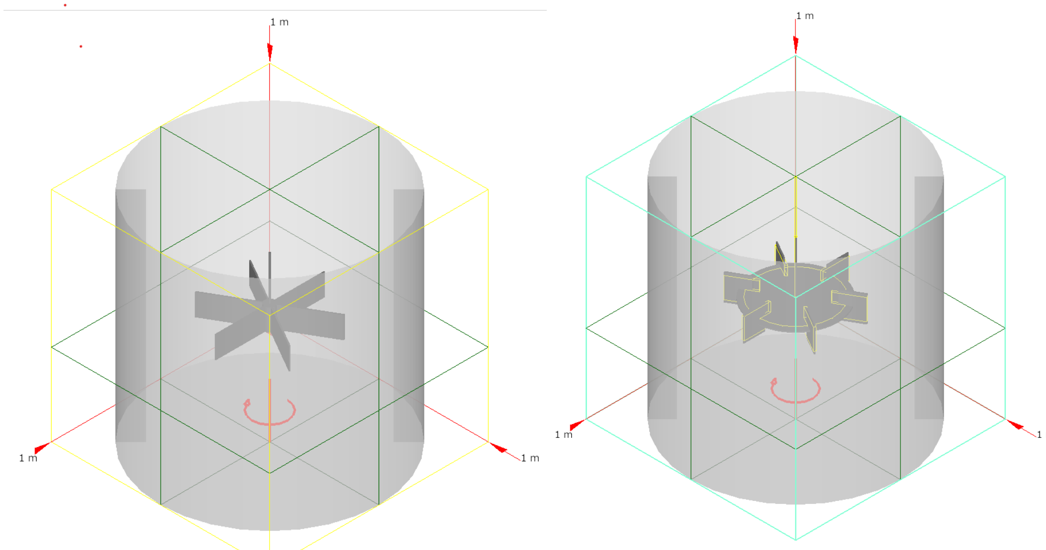

Figure 2. Vessel Layout for Bingham Plastic Mixing Simulations

Table 1. Impeller Power Number during Mixing of Non-Newtonian Fluids

Impeller	Nagata et al	M-Star®	Ratio	Differencxe
Rushton	5.5	5.38	0.98	-2%
6 Blade Paddle	4.5	4.68	1.04	4%

3.1.2 Cavern Mixing

Cavern mixing occurs in vessels with non-Newtonian fluids. Given that the DWPF SRAT and SME contain non-Newtonian (i.e., Bingham plastic) fluids, demonstrating the ability of the M-Star® software to simulate impeller mixing with non-Newtonian fluids will verify that it can simulate mixing in these vessels.

Although many constitutive relationships are available for describing the relationship between stress and strain in non-Newtonian fluids, one particularly general framework is the Herschel–Bulkley (HB) model:

$$\tau = K\dot{\gamma}^n + \tau_y \qquad [3]$$

where τ is the shear stress, $\dot{\gamma}$ is the shear rate, K is the consistency, n is the flow index, and τ_y is the yield stress.[17] If the HB model is parameterized using a zero-yield stress and a flow index equal to 1, it recovers the Newtonian (constant viscosity) model. If the HB model is parameterized using a zero-yield stress, it recovers the power-law fluid model. If parameterized with a non-zero yield stress but a flow index equal to 1, it recovers the Bingham plastic model. These last two parameterizations are particularly relevant to cavern mixing.

Simulations of cavern mixing were performed comparing the cavern diameter with the empirical model developed by Elson et. al. (EN), and with experimental data from work done by Elson et. al. and Adams and Barigou.[13, 14] The EN model is an empirically developed model based on a right cylinder centered on and coaxial with an Rushton impeller, with a height equal to 40% of the diameter, and the yield stresses from the non-Newtonian fluids were obtained using a Casson rheological model. The EN model is described by equation [4]

$$(D_c/D)^3 = (1.36\, N_p/\pi^2)\,(\rho\, N^2\, D^2/\tau_y) \qquad [4]$$

where D_c is the cavern diameter. This equation is applicable when the cavern diameter is larger than the impeller diameter but smaller than the tank diameter, i.e. when $D \leq D_C \leq T$. The EN model can be used with other rheological models. The EN model will only be compared to the M-Star® simulation where the cavern diameter is smaller than the tank diameter.

3.1.2.1 M-Star® Cavern Mixing Compared to Experimental Results from Elson

The experiments performed to develop the EN model were modeled in M-Star® to confirm if M-Star® could yield similar mixing caverns to Elson's original experiments.[13, 14] M-Star® derived cavern diameter, dimensionless cavern diameter, and cavern height to diameter ratio were compered to Elson's original experimental results. The cavern diameters calculated in M-Star® were determined by the maximum diameter across the cavern where the velocity is above 0.001 m/s after the system reaches steady state after 2 seconds and the maximum diameter in which a miscible scalar added near the impeller was well mixed in the fluid. The tank simulated in this comparison is a flat bottom tank with a diameter of 0.071 m meter with baffles. A Ruston impeller with a diameter of 0.0355 meters was used so that the model could be directly comparable to the 0.5 D/T experiments. The mixing speeds chosen were 480, 1020, and 1620 rpm to get caverns with diameters near the blade, between the blade and the wall, and at the vessel wall.

Elson described the rheology of the 3% xanthan gum solution with Casson and power law models.[13, 14] The Casson model was used to determine the yield stress. The power law fluid was used to determine the Reynolds number. Elson used the Herschel-Bulkley model, but they determined yield stress gave values far removed from the residual stresses obtained from the rheometer, hence these results were not used. To support the M-Star® simulation, a single rheological model such as the HB is required to cover the yield stress and higher shear rates. Elson's rheological data was fitted to the HB model using Microsoft EXCEL and the results are shown in Table 2 and Figure 3. The density of the fluid is 987 kg/m^3.

Table 2. Elson Experiment Rheology Parameters

	Power Law	Casson	Herschel-Bulkley
Yield Stress (Pa)	n/a	20	11
K	40.3	2.73	28.5
n	0.143	n/a	0.195

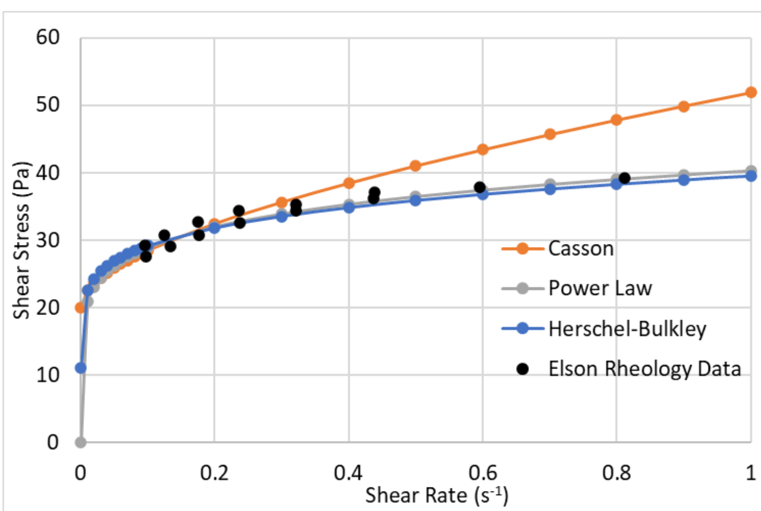

Figure 3. Elson Experiment Rheology

The results of the simulation matched closely to those of Elson. The cavern diameters measured in M-Star® are all within 10% of those measured by Elson when using both velocity and miscible scalar to describe the mixing cavern as shown in Table 3. Both velocity and miscible scalar were used as parameters to show how closely the two matched each other. The miscible scalar emulates what was done experimentally but takes more than 20 seconds of simulated time to mix to the edges of the cavern in some cases. The cavern fully develops and is steady within 5 seconds of simulated time in most cases so using velocity as a parameter for cavern diameter is much quicker than using a miscible scalar to determine cavern diameter. The Reynolds numbers were calculated using the Metzner and Otto method shown below in equation[18-21] [5] for Bingham plastics and Equation [6] for Herschel-Bulkley Fluids.

$$Re = \frac{\rho k_s N^2 D^2}{\tau_y + \eta_b k_s N} \quad [5]$$

$$Re = \frac{\rho k_s N^2 D^2}{\tau_y + K(k_s N)^n} \quad [6]$$

In equations [5] and [6], k_s is the Metzner and Otto constant, assumed to be 11 for this work for all impeller types[22], and η_b is the plastic viscosity.

The comparison of dimensionless cavern diameter as a function of Reynolds number was studied by Elson as a way to compare the experiments independent of the impeller diameter used.[13, 14] Dimensionless cavern diameter is the ratio of the cavern diameter to the diameter of the impeller blade. Figure 4 A shows that the dimensionless cavern diameter measured in M-Star® closely matches those measured experimentally well within the target 30% threshold. Elson also studied the ratio of the cavern height to diameter and even used his results in developing the EN model.[13, 14] Elson found that when the cavern diameter is smaller than the vessel diameter the ratio of cavern height to diameter is between 0.35 and 0.45. The M-Star® miscible scalar results closely matched the experimental ratios shown in Figure 4 B since they recreated the scalar behavior as the dye did in Elson's experiment. On the other hand, the M-Star® velocity ratios are larger than the experimental and scalar ratios. This is primarily due to the motion of the fluid in the middle of the vessel directly above the impeller. Although the fluid is in motion, the miscible scalar will not travel to that region and become well mixed there. Overall M-Star® was able to proficiently model the mixing of this yield stress fluid with cavern diameters within 10% of experimental values.

Table 3. Elson experiments cavern diameter results.

Impeller speed (rpm)	Re	N_p	D_C Elson (m)	D_C M-Star® (m) Velocity	D_C M-Star® (m) Scalar	D_C% difference Velocity	D_C% difference Scalar
480	11.1	14.7	0.043	0.045	0.044	5.0 %	2.3 %
1080	43.9	4.4	0.057	0.055	0.051	-3.2 %	-10.3 %
1620	102.3	1.7	0.071*	0.068	0.069	-4.6 %	-3.0 %

*The cavern has reached the wall of the vessel

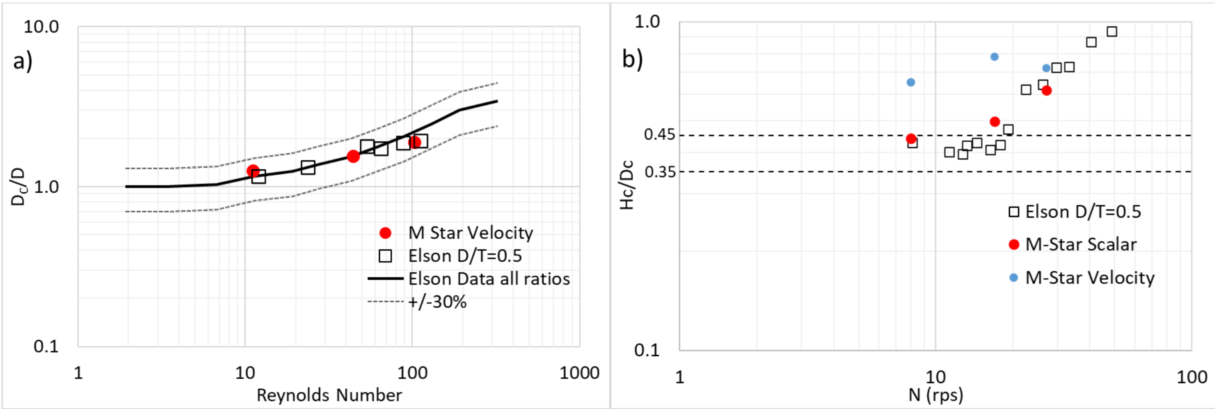

Figure 4. M-Star® results compared to experimental a) dimensionless cavern diameter as a function of Reynolds number b) cavern height to diameter ratio as a function of mixing speed

3.1.2.2 Cavern Mixing of Herschel-Bulkley Fluid

The system used to compare M-Star® simulations with the EN model is comprised of an unbaffled flat bottom cylindrical tank with a diameter of 1 m and a height of 1 m. The impeller used is a 6 bladed Rushton turbine with a diameter of 0.1485 m and centrally located 0.5 m from the bottom of the tank. The physical properties of the HB fluids are shown in Table 4. The N_p in equation [4] was determined using M-Star® simulations for each impeller speed and rheological condition and the results are also provided in Table 4. The cavern diameter from M-Star® was defined as the maximum radial region where the fluid velocity is above 0.001 m/s and was constant after approximately two seconds of simulated time as shown in Figure A 1. Table 4 shows the M-Star® cavern diameter results, which are compared to cavern diameters calculated using equation [4].

The M-Star® results were within 20% of the EN model results. The M-Star® cavern diameters for the 1.79 Pa yield stress where within 10% of the EN model, and as the agitator speed increased, this difference increased resulting in a larger cavern diameter. For the 5.25 Pa yield stress, M-Star® results were within 20% of the EN model. In this case, as the impeller speed increased, the difference went from a lowest negative to the greatest positive differences. For both yield stress conditions, as the impeller speed increased, M-Star® consistently predicts larger cavern diameters compared to the EN model. Amanullah showed that when comparing the EN model to experimental results the EN model predicted smaller caverns in the range of 20%-45% smaller than experimental results at Reynolds number above 20.[23] In Amanullah's work the difference in cavern diameter estimated by the EN model when compared to experimental values increases with increasing Re. This same trend was observed using M-Star®.

Table 4. Cavern diameter results using Herschel Bulkley Fluid properties from M-Star® and the EN model

Impeller speed (rpm)	Re	N_p	Yield stress (Pa)	K ($Nm^{-2}s^{n}$)	n	Density (kg/m^3)	D_C EN (m)	D_C M-Star® (m)	D_C% difference
75	65	6.86	1.79	3	0.11	997.4	0.39	0.39	0%
100	115	7.0	1.79	3	0.11	997.4	0.48	0.52	8.8%
150	247	7.49	1.79	3	0.11	997.4	0.64	0.70	9.7%
75	23	6.6	5.25	8	0.12	991.8	0.27	0.24	-10.7%
100	41	6.23	5.25	8	0.12	991.8	0.32	0.31	-3.3%
150	88	7.0	5.25	8	0.12	991.8	0.44	0.49	12.7%
200	153	7.3	5.25	8	0.12	991.8	0.53	0.64	19.8%

3.1.2.3 Cavern Mixing of Bingham Plastic

The cavern diameter calculated by M-Star® and the EN equation are determined using a Bingham plastic fluid. The tank and impeller used in these experiments are the same as those used in the Elson literature experiments. The Bingham plastic properties are similar to the fluids in the DWPF facility with a yield stress of 5-15 Pa and a consistency of 50-100 cP. The cavern diameters calculated in M-Star® were determined by the maximum diameter across the cavern where the velocity is above 0.001 m/s after the system reaches steady state after 2 seconds. The tank simulated in this comparison is a flat bottom tank with a diameter of 0.071 m meter with baffles. A Rushton turbine with a diameter of 0.0266 meters was used. The mixing speed was varied from 50-500 rpm. Table 5 shows the M-Star® cavern diameter results are well within 30% of the EN calculations. For both 5 Pa and 15 Pa yield stress fluid comparison, the cavern sizes calculated in M-Star® are all larger than those calculated using the EN model except for 1 which is consistent with the findings of Amanullah where the actual caver diameter is larger than that calculated using the EN model when the cavern diameter is smaller than the tank diameter.[23] However over the wide range of mixing speeds the difference in cavern size is no larger than 12% which is well within the target threshold.

Table 5. Cavern diameter results using Bingham plastic properties from M-Star® and the EN model

Impeller Speed (rpm)	Re	N_p	Yield Stress (Pa)	Consistency (cP)	Density (kg/m^3)	D_C EN (m)	D_C M-Star® (m)	D_C% difference
50	1.5	130	5	50	1460	0.0365	0.0387	6.0%
100	5.3	35	5	50	1460	0.0374	0.0340	-9.1%
500	82.5	3.5	5	50	1460	0.0508	0.0560	10.3%
50	0.5	365	15	100	1460	0.0357	0.0399	11.8%
100	1.9	98	15	100	1460	0.0366	0.0400	9.4%
500	32.7	4	15	100	1460	0.0368	0.0388	5.4%

3.1.2.4 M-Star® Cavern Mixing Compared to Experimental Results from Adams and Barigou

The use of models to predict cavern size comes with inherent uncertainties. Therefore, comparison between experimental data and M-Star® simulations were performed. The work performed by Adams and Barigou[14] was chosen as the experimental data. The 0.1% Carbopol solution used in the experiment was characterized as a HB fluid with the fluid properties shown in Table 6. Table 6 also provides the Re and impellers speeds tested by Adams and Barigou. The vessel used in M-Star® is the same as in the literature; vessel diameter of 0.148 m, 4 baffles of width 0.0148 m and thickness of 0.00148 m. The solution was agitated using a 6 bladed 45° down-pumping PBT with a diameter of 0.0493 m and an off-bottom clearance of 0.0493 m. The liquid height was 0.148 m. The lattice spacing for the M-Star® experiments modeled after the experiments performed by Adams and Barigou was 0.00074 m giving 200 lattice points across the diameter of the tank. The Courant number used was 0.001.

Table 6. Rheological properties of Carbopol solution

Re	Impeller speed (rpm)	N_p	Yield stress (Pa)	K (Pa s^n)	n	Density (kg/m^3)
7.3	69	12.3	2.625	0.541	0.555	997
20.4	95	4.7	1.413	0.373	0.572	997
70.3	194	2.8	1.289	0.348	0.573	997
86.6	246	2.7	1.558	0.446	0.551	997

The Adams and Barigou measured cavern diameters (D_C Adams) as stated in Table 7 were found using planar laser induced fluorescence to visualize and measure the caverns.[14] The M-Star® cavern diameters are provided in Table 7 and were determined from the M-Star® simulations where the steady state fluid velocity is greater than 0.001 m/s in the radial direction (D_C M-Star® Velocity). The cavern diameter as determined by scalar (D_C M-Star® Scalar) was determined by measuring the distance the scalar had traveled in the radial direction after mixing for an extended time between 20-40 seconds. In all cases the cavern diameter, when measured using fluid velocity, was constant after two seconds of simulated time as shown in Figure A 2. The percent difference between the M-Star® velocity and Adam's cavern diameters are within 20% in all cases and in all cases predicted a smaller diameter other than at the smallest agitator speed. The M-Star® velocity is used to calculate the % difference for three reasons. The first is that the cavern diameter defined by velocity and by scalar are very close so either would be sufficient, however the velocity profile of the cavern was established much more quickly. The velocity profile was established within seconds of while the scalar takes tens of seconds to fill the cavern. The velocity profile is also very stable once the fluid reaches steady state while the scalar can continue to diffuse outward even after filling the cavern. Lastly Amanullah established that a suitable velocity boundary condition for a cavern is 0.001 m/s.[23]

The steady state velocity field and dye concentration for all cases between 20-40 seconds of agitation in M-Star® is shown in Figure 5. Longer times were needed for the scalar to fill the cavern at the higher mixing speeds. At this point, both the velocity and scalar (dye) concentration fields are stable and form a well-defined cavern. The fluid velocity inside the cavern shows a mixed fluid and is stagnant outside the cavern. The cavern profile generated by M-Star® using either the velocity or scalar field yields similar cavern diameter shapes, with larger differences in the height of the cavern. Although the simulation appears to underpredict cavern formation just above the impeller, the overall shape and extent of the predicted cavern is in-line with the directly measured data. The axial growth of the cavern using M-star® is conservative.

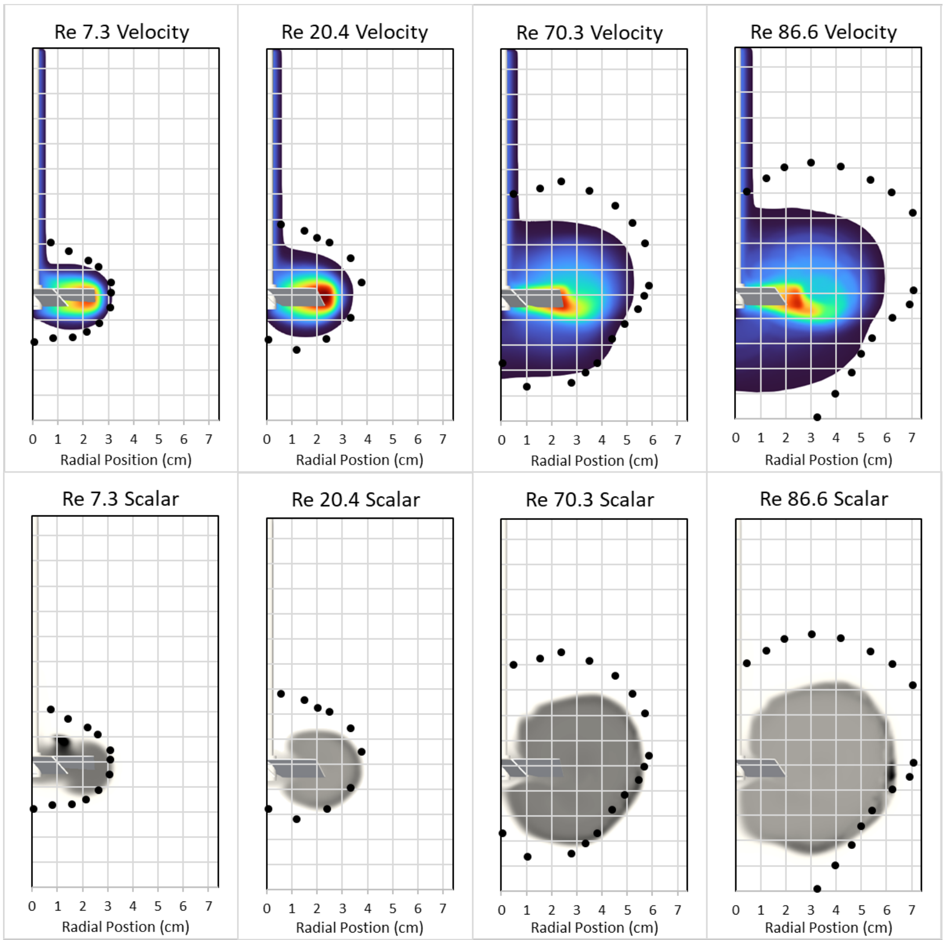

Figure 5. Comparing the predicted mixing cavern, as characterized using (i) velocity field and (ii) scalar concertation, to the measured data (points)

Table 7. Comparison of results of Cavern mixing of Carbopol Solution from M-Star® and Literature

Re	D_C Adams	D_C M-Star® Velocity	D_C M-Star® Scalar	D_C EN	% dif Adams	% dif EN
7.3	0.062	0.064	0.067	0.063	2.6%	1.1%
20.4	0.074	0.071	0.077	0.070	-4.7%	1.1%
70.3	0.117	0.108	0.114	0.097	-7.7%	11.2%
86.6	0.148	0.120	0.129	0.105	-18.9%	14.3%

The tests of cavern mixing are determined to be successful.

4.0 Conclusions

The conclusions from the work follow.

- The comparisons of impeller power number with Newtonian fluids shows the M-Star® produced power numbers within 10% of the experimental power number when the Reynolds number is greater than or equal to 15.
- The comparisons of impeller power number with Bingham plastic fluids shows the M-Star® produced power number to be within 5% of the experimental power number.
- Cavern mixing tests showed the M-Star® simulation prediction of cavern diameter to be within 30% of the cavern diameter from literature data and literature correlations in all tests, and within 10% for most of the tests.
- Based on the results of the software testing, the M-Star® software meets the requirements for level C, Waste Form Affecting for impellerc mixing of Newtonian and non-Newtonian Fluids in a tank.

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6.0 Appendix

Table A 1 Power Number Data from Experimental Data and M-Star® Simulations

Impeller	D (m)	N (rpm)	Viscosity (m^2/s)	Re	N_p Experimental	N_p M-Star®	Ratio	Difference (%)
Rushton	0.33	300	5.45E-05	9991	5.68	5.68	1.00	0.0
Rushton	0.33	30	5.45E-05	999	4.88	5.0	1.02	2.5
Rushton	0.33	3	5.45E-05	100	4.94	5.03	1.02	1.8
Rushton	0.33	3	5.45E-04	10	8.46	8.65	1.02	2.2
Rushton	0.33	300	5.45E-06	99908	5.53	5.57	1.01	0.7
Rushton	0.33	3000	5.45E-05	99908	5.87	5.7	0.97	-2.9
PBT	0.33	300	5.45E-06	99908	1.15	1.32	1.15	14.8
PBT	0.33	300	5.45E-05	9991	1.08	1.3	1.20	20.4
PBT	0.33	30	5.45E-05	999	1.21	1.19	0.98	-1.7
PBT	0.33	3	5.45E-05	100	1.91	1.95	1.02	2.1
PBT	0.33	3	5.45E-04	10	5.35	5.42	1.01	1.3
PBT	0.33	0.3	5.45E-04	1	26.90	26.94	1.00	0.1
Hydrofoil	0.242	450.2	5.11E-06	97250	0.31	0.28	0.90	-9.7
Hydrofoil	0.242	391	4.92E-05	9668	0.31	0.27	0.87	-12.9
Hydrofoil	0.242	419	5.25E-04	1041	0.34	0.34	1.00	0.0
Hydrofoil	0.242	559	1.43E-03	523	0.40	0.42	1.05	5.0
Hydrofoil	0.242	259	3.95E-03	88	0.78	0.82	1.05	5.1
Hydrofoil	0.242	75	1.10E-02	9	3.00	3.43	1.14	14.3
Hydrofoil	0.242	95	1.10E-02	12	2.54	2.88	1.13	13.4

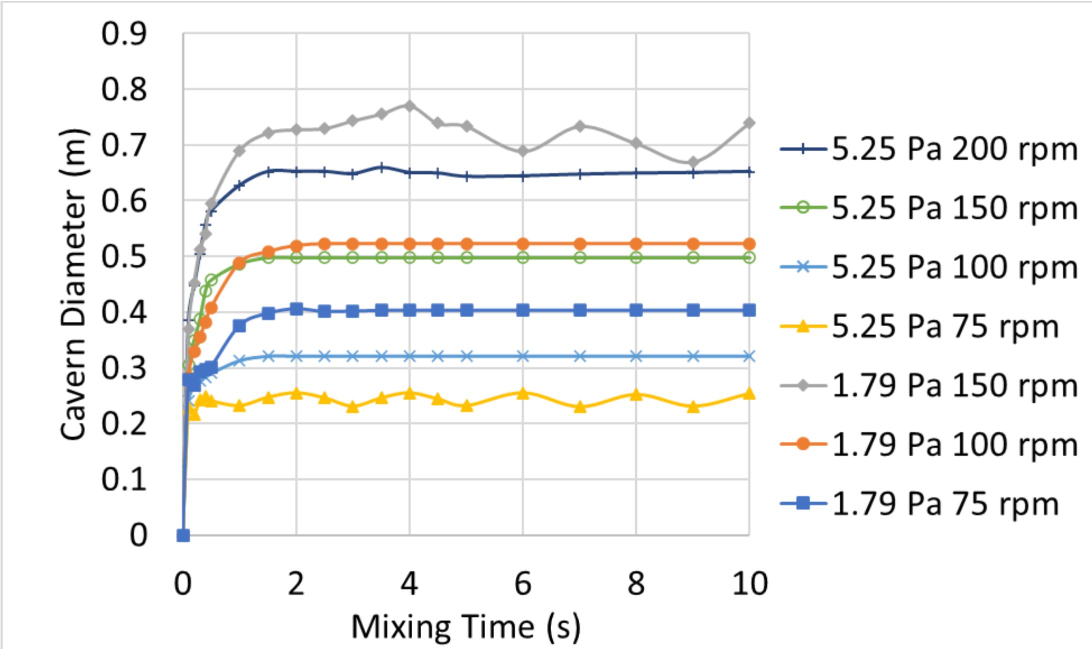

Figure A 1 Cavern Diameter as a Function of Mixing Time for M-Star® Herschel-Bulkley Fluids

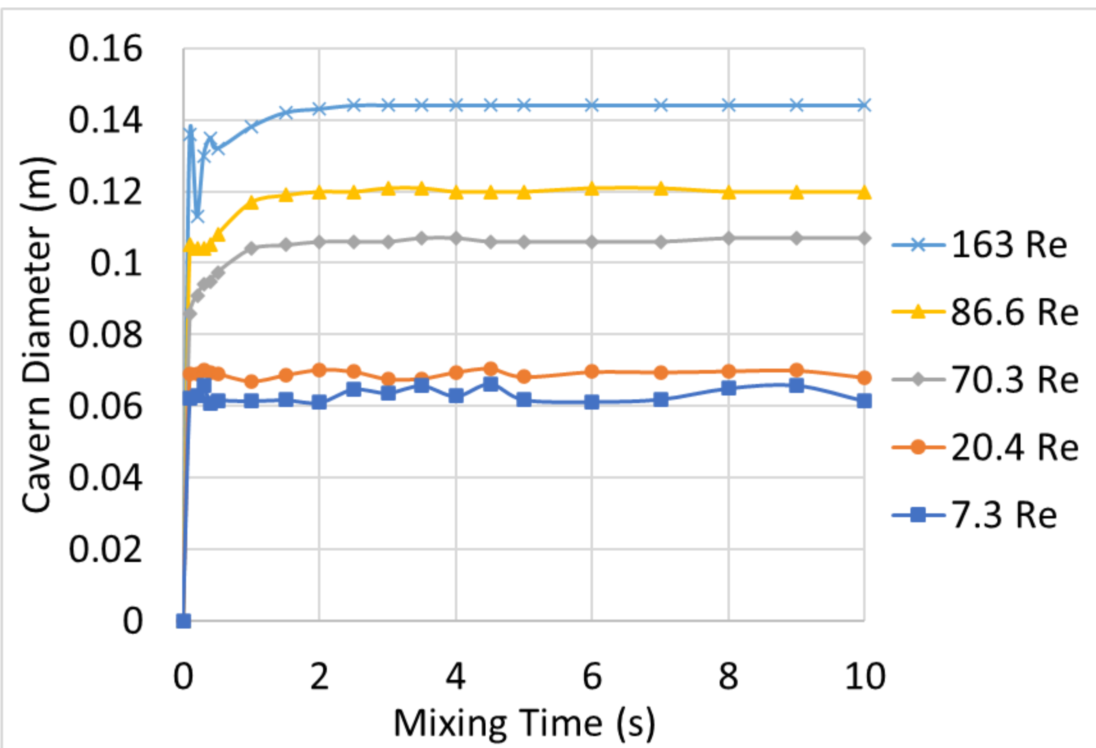

Figure A 2 Cavern Diameter as a Function of Mixing Time for M-Star® Adams Comparison

Distribution:

C. C. Herman
F. M. Pennebaker
G. A. Morgan
B. J. Wiedenman
E. K. Hansen
A. S. Choi
D. J. Baxter
J. W. Ray
P. E. Fogelman
R. M. Hoeppel
H. P. Boyd