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CASL VMA Milestone Report FY16 (L3:VMA.VUQ.P13.08)

Westinghouse Mixing with STAR-CCM+

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Challenge Problem	Code	VVUQ
CIPS	MAMBA-1D	Code Verification
PCI	BISON	Solution Verification ✓
DNB-CTF	CTF ✓	SET Validation
CILC ✓	MPACT	IET Validation
DNB-CFD ✓	MAMBA-3D	Sensitivity ✓
RIA	STAR-1Phase ✓	Uncertainty ✓
LOCA	STAR-2Phase ✓	Calibration ✓

Outline

- Introduction
  - Hi2Lo and STAR-CCM+ (STAR)
  - Westinghouse Provided Experimental Data
    - Geometry used in WEC experiment
    - Parameters provided in WEC experiment report
    - Translation of inlet values from WEC experiment to input parameters needed for STAR
  - Introduction to STAR Hi2Lo workflow
- Validation of Training Data
- Calibration of Training Data
  - Non-Bayesian Deterministic Calibration
  - Bayesian Statistical Inference Calibration
- Next Steps

Introduction
Hi2Lo: STAR-CCM+

STAR-CCM+ (STAR) is a high-resolution computational fluid dynamics (CFD) code developed by CD-adapco. STAR includes validated physics models and a full suite of turbulence models including ones from the k-ε and k-ω families.

STAR is currently being developed to be able to do two phase flows, but the current focus of the software is single phase flow. STAR can use imported meshes or use the built in meshing software to create computation domains for CFD. Since the solvers generally require a fine mesh for good computational results, the meshes used with STAR tend to number in the millions of cells, with that number growing with simulation and geometry complexity.

The time required to model the flow of a full 5x5 Mixing Vane Grid Assembly (5x5MVG) in the current STAR configuration is on the order of hours, and can be very computationally expensive.

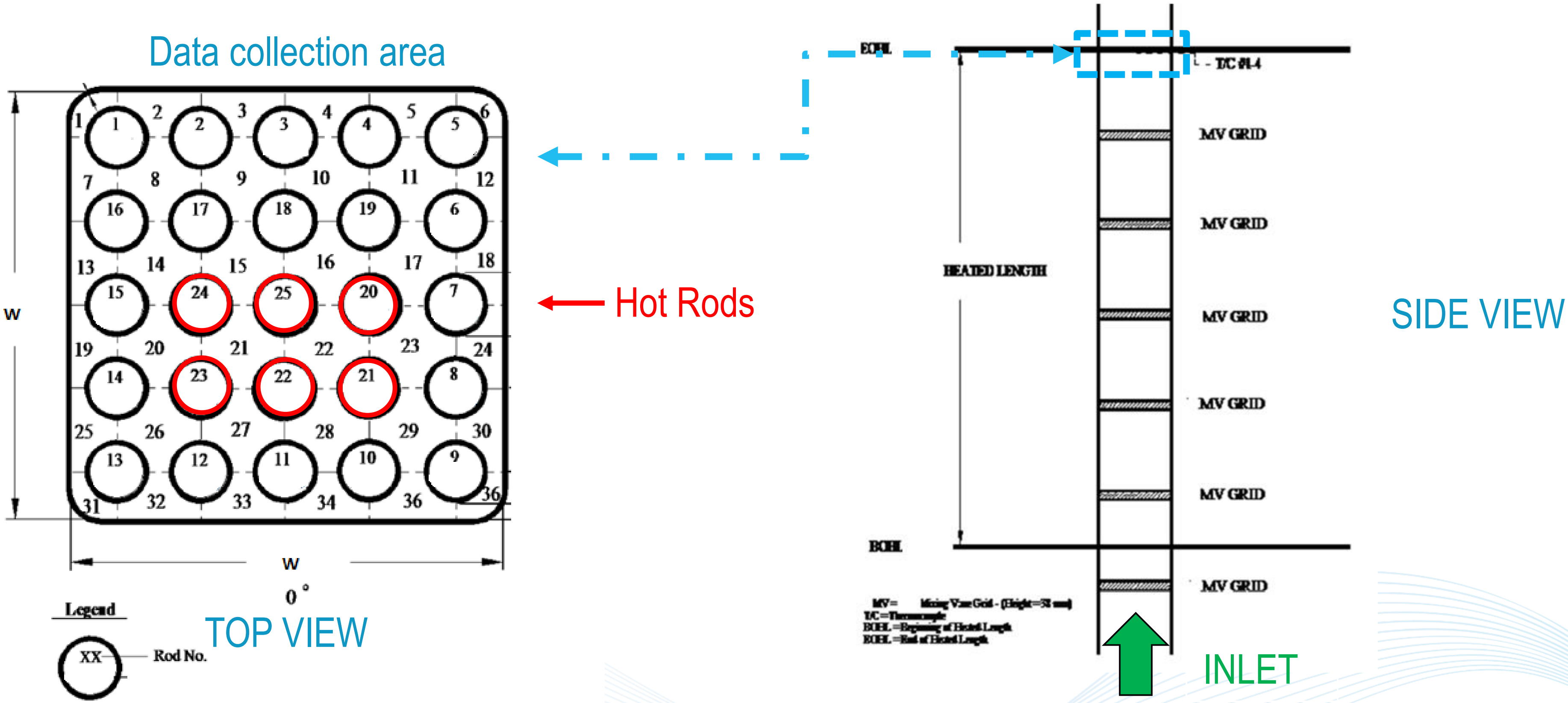
COBRA-TF (CTF) is a low-resolution subchannel code that can be trained using high fidelity data from STAR. CTF does not have turbulence models and instead uses a turbulent mixing coefficient β. With a properly calibrated β, CTF can be used a low-computational cost alternative to expensive full CFD calculations performed with STAR.

During the Hi2Lo work with CTF and STAR, STAR-CCM+ will be used to calibrate β and to provide high-resolution results that can be used in the place of and in addition to experimental results to reduce the uncertainty in the CTF results.

Introduction:

WEC Test Bundle 20 Geometry

The geometry of the Westinghouse (WEC) experimental test bundle 20 contains a 5x5 (25 in total) set of electrically heated rods and 36 subchannels. Of the 25 rods, 6 of them were “hot”, with a higher heat flux than the remaining rods. Thermocouples were placed at the center of each subchannel and used to collect time-averaged temperature data in the blue data collection area highlighted below.



Introduction:
WEC Test Bundle 20 Experimental Data:

Initial Conditions	Exit Measurements
Test Section Exit Pressure	Average Exit Quality
Test Section Inlet Temperature	Exit Temperatures: Subchannels 1-36
Test Section Inlet Enthalpy	
Test Section Volumetric Flow Rate	
Test Section Mass Velocity	
Test Section Power	
Test Section Average Heat Flux	
Test Section Hot Rod Heat Flux	

The initial condition parameters and exit measurements from the experimental testing were provided by WEC document PFT-16-3. The parameters highlighted in blue are the input and output parameters that are relevant to running STAR in Dakota and are used to set initial and boundary conditions. As explained in the next slide, some of these parameters needed additional conversions so they could be used in the STAR input decks for Dakota.

Introduction:
Implementation in STAR-CCM+

NO CONVERSIONS/CALCULATIONS NEEDED:

Test Section Inlet Temperature

Test Section Hot Rod Heat Flux

The above inlet parameters required no further conversions or calculations for the STAR inputs. STAR can use English or SI units. SI units were used for inputs decks.

Initial Conditions → **STAR Input Parameters**

Test Section Volumetric Flow Rate (m^3/h) → Velocity (m/s)

$$Velocity = \frac{Volumetric\ Flow\ Rate\ \left(\frac{m^3}{hr}\right)}{Area\ (m^2)} \times \frac{1hr}{3600sec}$$

Test Section Average Heat Flux

Test Section Hot Rod Heat Flux

→ Test Section Cold Rod Heat Flux

$$Cold\ Rod\ Flux = \frac{(Rod\ Surface\ Area \times Length) \times (25 \times Ave\ Heat\ Flux - 6 \times Hot\ Heat\ Flux)}{Rod\ Surface\ Area \times 19 \times Length}$$

STAR requires unit conversions and calculations to get the needed values for inlet velocity, and the average rod heat flux. The calculations used to find these for the boundary condition values are listed above.

Introduction:

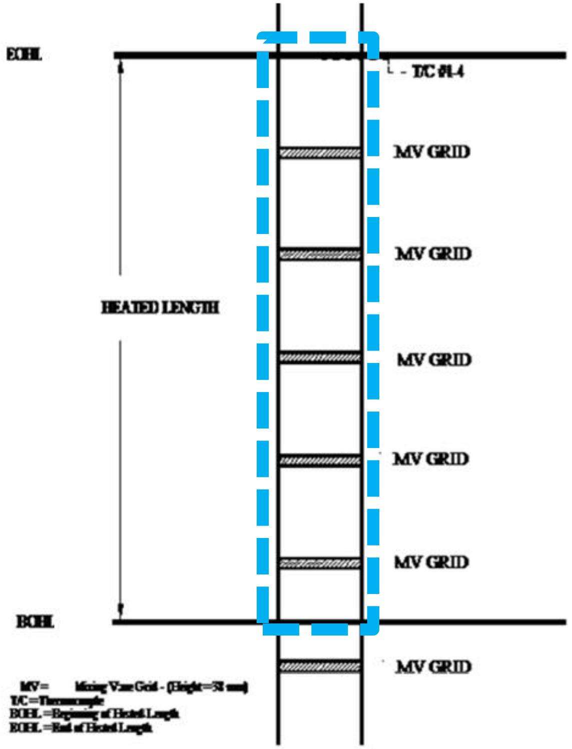
Base CFD Model in STAR-CCM+

The base CFD model in STAR was provided by Emre Tatli (WEC). It consists of a 60M cell base mesh and a full physics parameter setup. The 60M mesh was used because of size and time limitations. Since the STAR simulation needed to be moved from WEC to SNL, we used the finest mesh that could be transmitted (60M cell file ~ 20 GB). Also, due to the long simulation times even for a coarse mesh, it is most practical to implement the Hi2Lo workflow with the current mesh and if desired, repeat the process using a higher cell count in the STAR mesh.

The model contains all the details of the mixing vane grids (springs, dimples and vanes). It contains trimmed hexahedral cells and prism layer cells, created with STAR-CCM+ mesher. Only the fluid domain is included with the base model. Because of this we have a fixed heat flux and are not doing fuller problem of conjugate heat transfer. Solid domains can be added later.

The model has inlet temperature, inlet velocity, and constant heat flux on the rod OD specified as boundary conditions. Density of the water is chosen using a fixed pressure water table (160bar).

FLUID DOMAIN IN STAR-CCM+



Model Assumptions:

- Turbulent
- Steady state
- Variable density (from fixed pressure table)
- Single Phase
- 3D flow
- No gravity

Turbulence Model

- Reynolds-Averaged-Navier-Stokes
- Realizable k-ε turbulence model
- two-layer all y+ wall treatment. Surface average y+ on all mixing vane grids, rods, and chamber walls between 115 and 150.

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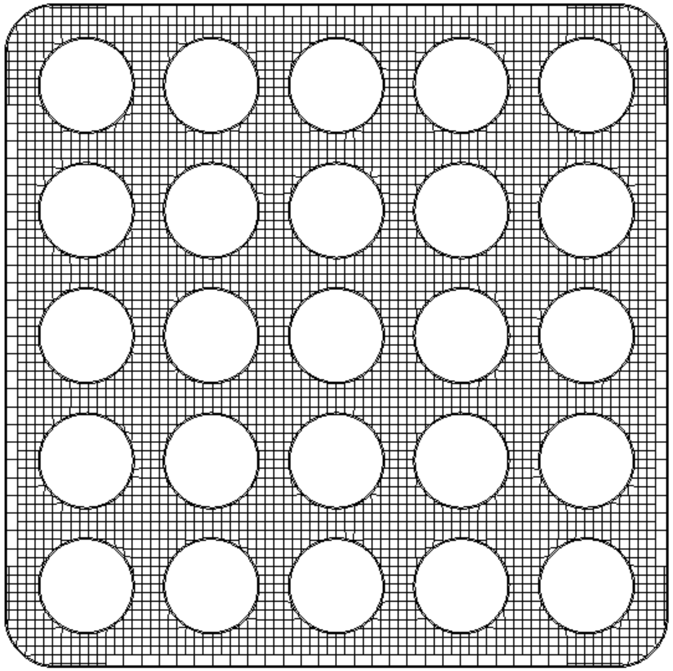
Introduction:

Base CFD Model in STAR-CCM+

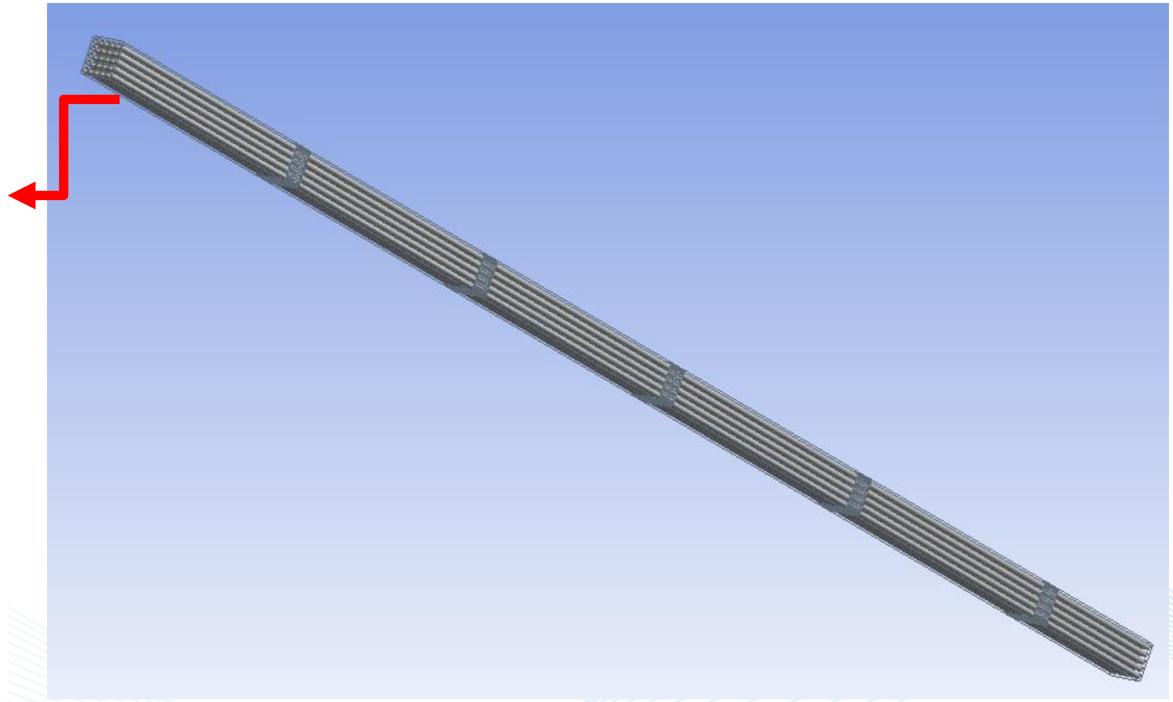
The STAR simulation contains the full length of the heated rods. The data collection site is located near the outlet. 36 probes were placed in the same subchannel center locations as in the experiment. Temperature readings from the probes were not iteration or space averaged over the subchannel. A steady RANS model was used so the temperature results are not a function of time after a steady state condition is reached.

STAR-CCM+ mesh at data collection site



TOP VIEW

STAR-CCM+ simulation full geometry of 5x5 rod bundle



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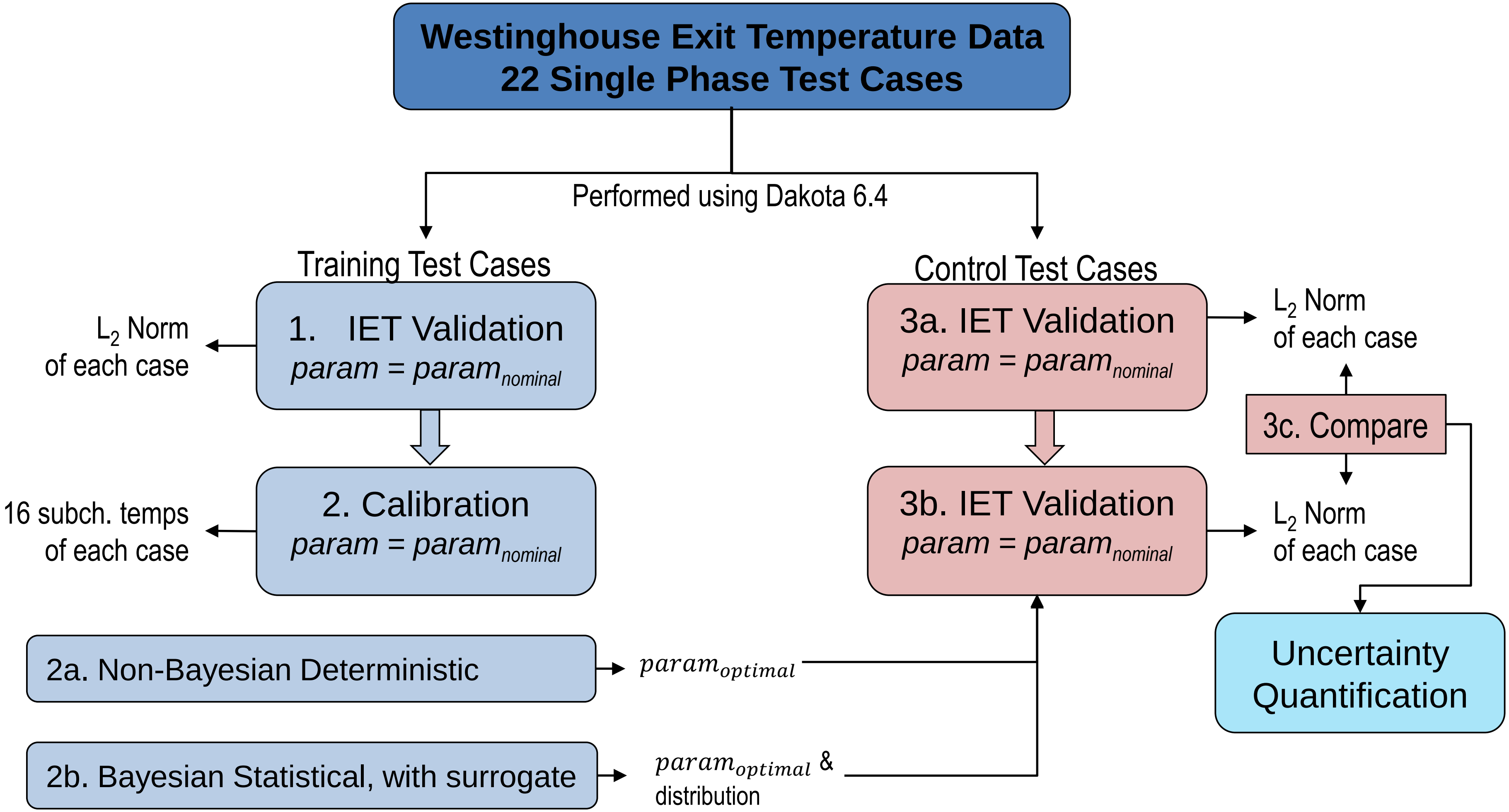
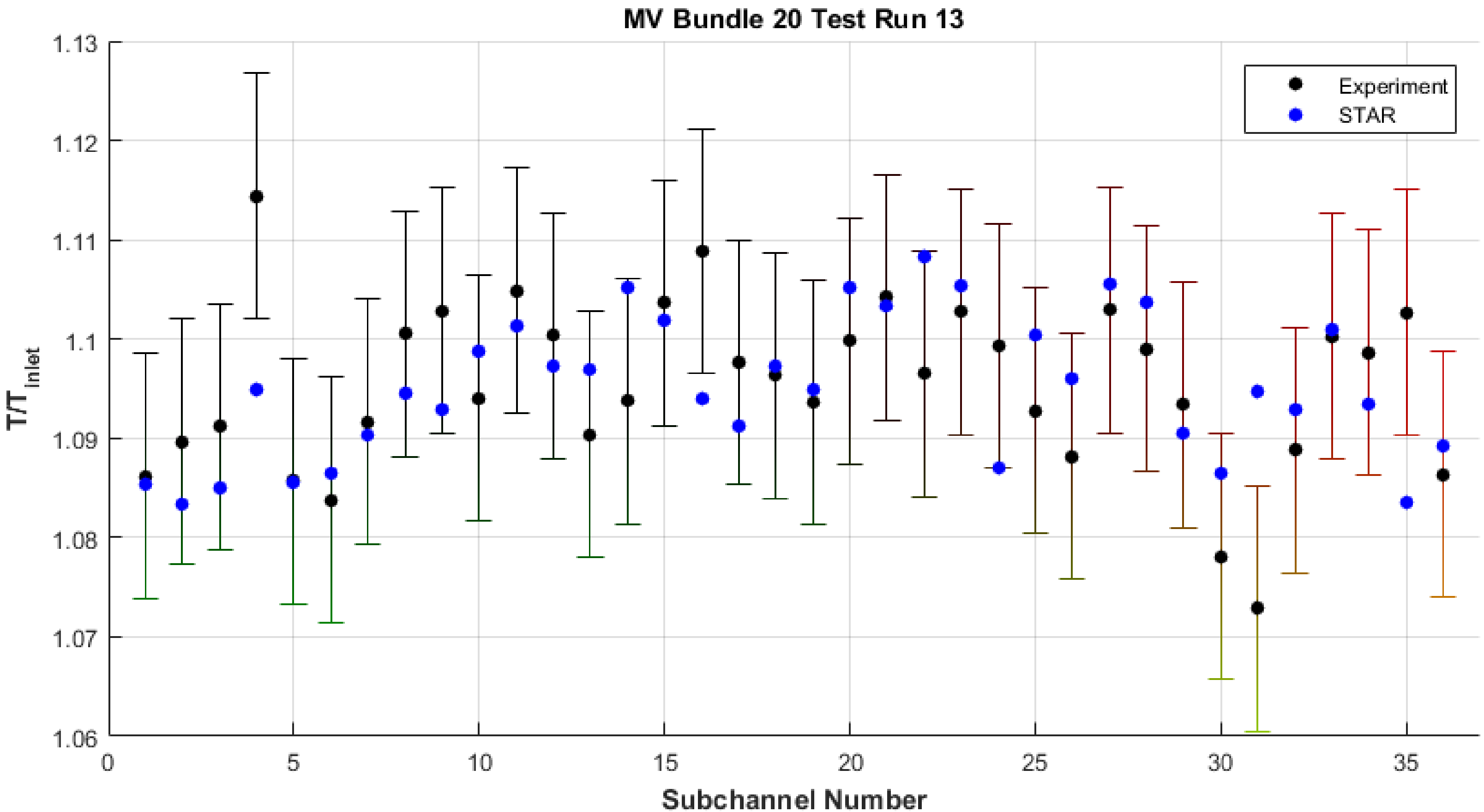
Introduction:
STAR/Experimental Data Workflow



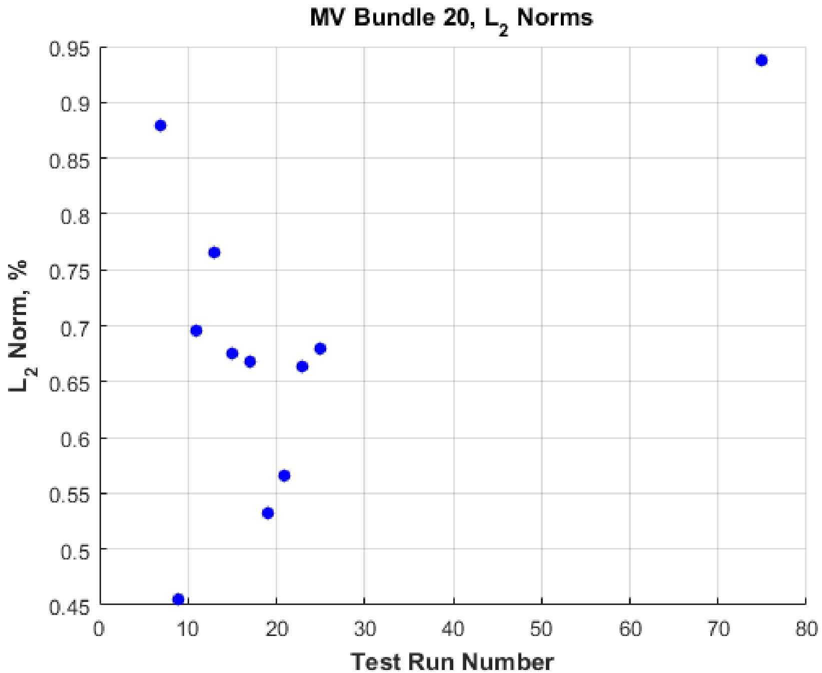
The 22 test cases were split into training and control data. The training data is used to find the optimal values for the calibration parameters in STAR. These values are also used to train a surrogate for Bayesian analysis. The control data is used to confirm that the parameters found during calibration are the optimal values. The L2 norms corresponding to the optimal and nominal parameters will be compared to check that calibration yields results closer to the experiment. After this, uncertainty quantification will be performed with STAR.

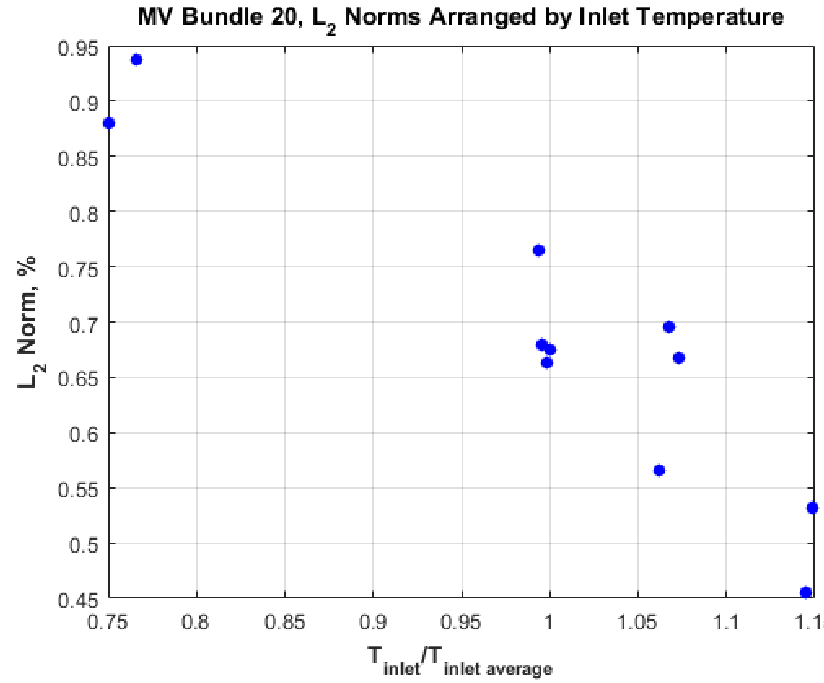
1. Validation of Training Data

The plot below is an example of the one of the STAR validation cases compared to the experiment. The experimental repeatability error was a few degrees Celsius, so it is difficult to completely assess the subchannel temperature accuracy due to the large error bounds, but the STAR results do generally follow the same trends as the experimental results.



1. Validation of Training Data





$$L_2\ Norm = \frac{\sqrt{\Sigma_1^{36}|STAR_{QOI} - exp_{QOI}|^2}}{\sqrt{\Sigma_1^{36}|exp_{QOI}|^2}} \times 100$$

STAR results using the experimental inputs and the "standard" physics models were validated for 11 tests, called the training data. The results use only single phase testing data from WEC. L2 norms were used to evaluate how close the STAR results were to the experimental test data. With the "standard" physics models, the STAR simulation performs very well. The L2 norms are less than 1% for all the training data. The second figure shows that STAR generally performs better (lower L2 norms) for higher temperature tests.

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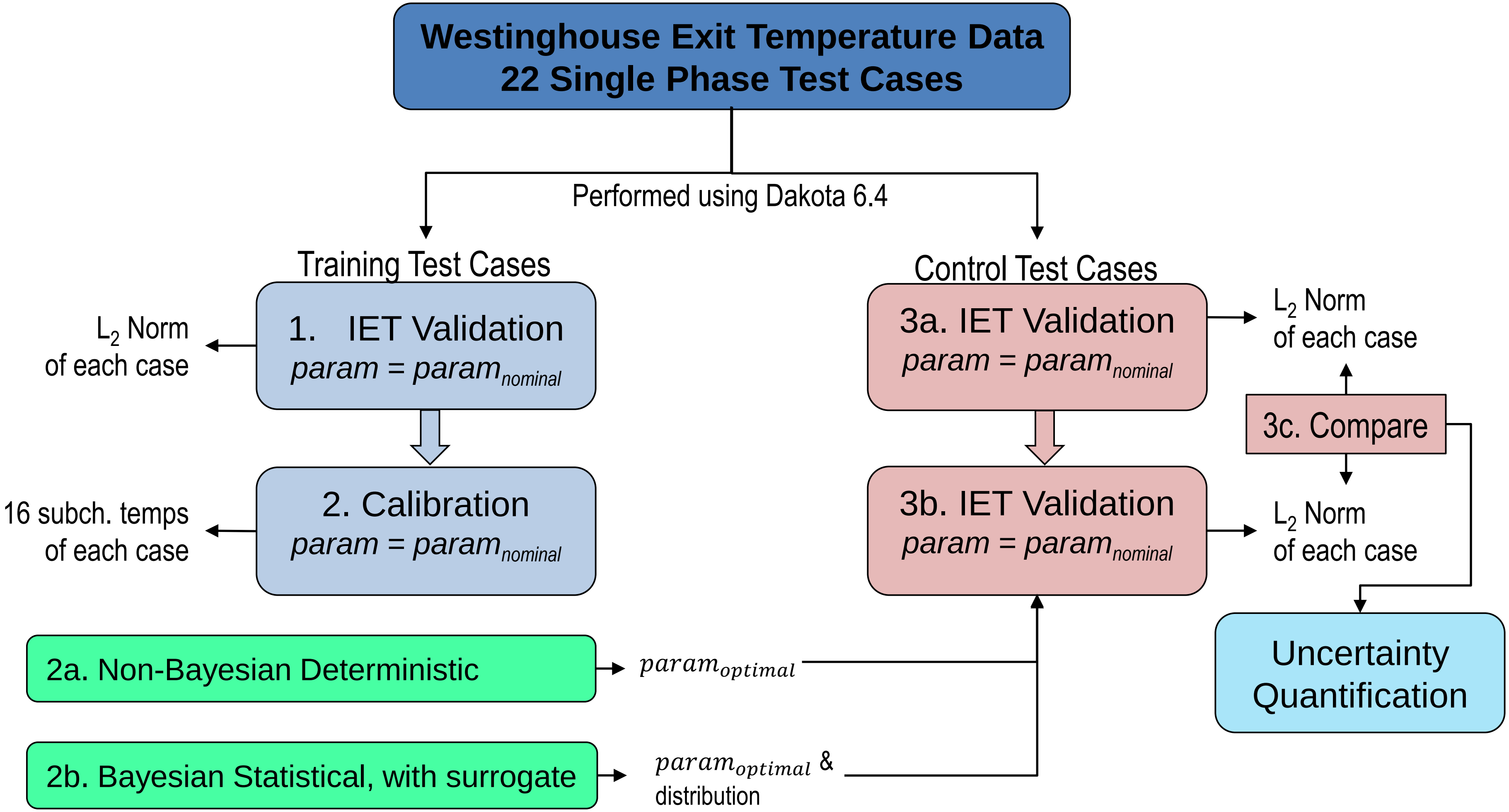
2. Calibration



Calibration is split into two steps, deterministic calibration, and Bayesian analysis with a surrogate. The ncsu_direct method, a derivative-free global optimization method, is being used for the deterministic analysis. Bayesian analysis will be performed using QUESO in Dakota. Steps 2a and 2b (highlighted in green) will be part of the FY17 work for STAR. Since the STAR runs are so computationally expensive, it is impractical to perform Bayesian calibration in the absence of the surrogate, so Bayesian analysis will only be performed with surrogate.

2a. Calibration of Training Data
Non-Bayesian Deterministic Calibration

The first set of calibration tests in STAR consisted of calibrating to an inlet temperature boundary condition. While this is not appropriate for a true calibration parameter selection for STAR, it was a useful exercise that allowed for the framework of calibration to be laid out properly and revealed several difficulties that would have to be addressed and accounted for to move forward with a true calibration study.

Despite use of the steady-state RANS equations, there are some small fluctuations (approximately 0.2°C) in the subchannel temperatures while the simulation is at steady state. This will not significantly affect the accuracy of the STAR simulation (the L2 norms are less than 1% even when accounting for a ± 0.2°C fluctuation), but it will impact future calibration as Dakota will attempt to match the moving iteration dependent STAR solution. In other words, there is a potential issue of Dakota calibrating to noise, especially when the gradients are small.

Due to the long run time of the STAR simulations (1200 core hours for a full simulation from initial conditions and approximately 400 core hours to use a steady simulation as an initial state), most of the calibration process is being trouble-shooted and developed with CTF (run time on order of minutes) before adapting the processes for STAR.

The current plan is to use two separate calibration methods for STAR. The first is a derivative-free, global calibration method, ncsu_direct. Since there are some gradients in the STAR-CCM+ results and STAR does appear to show responsiveness to the input variables, it might also be possible to use nl2sol, a gradient based approach in addition to or to replace the ncsu_direct method calibration in Dakota.

(Cont. on next slide)

2b. Calibration of Training Data
Bayesian Statistical Inference Calibration

Bayesian calibration for STAR will follow direct calibration and be performed using the QUESO solver in Dakota 6.4. Once again, the full STAR calibration is being put on hold until the process has been developed for CTF due to the long STAR simulation times. To ensure that the Bayesian results are not affected by possible experimental error in the outer subchannels in the bundle, only the 16 inner subchannels will be used for calibration. Each analysis will take into account the experimental repeatability error which is a few degrees Celsius.

The Bayesian surrogate work in CTF is on hold until a new feature is implemented into Dakota to handle the surrogate capabilities this problem demands. This new feature will account for the configuration parameters (the boundary conditions) as well as the calibration parameters and will therefore account for the wide range of test conditions used in the experiments.

Bayesian calibration with a surrogate will be essential for STAR due to the long run times for simulations. The surrogate also will help with the issue of noise coming from the STAR results and will not be as sensitive to iteration temperature fluctuations as direct calibration.

Calibration:
Parameter Selection

STAR uses a full set of turbulence models and equations, making calibration parameter selection not a straight forward process. CTF has a beta variable that is used for calibration, but there is no equivalent in STAR. Boundary conditions and material properties are essentially eliminated from consideration for use as calibration parameters due to their wide variance over the tests but will be incorporated into the calibration process as configuration parameters.

Physics settings in STAR will be selected as the calibration parameters.

The turbulence model selection and the associated turbulent parameter ranges are attractive as a calibration metric. For each family of turbulence models, there are coefficients and turbulent parameters that can be used for calibration. Work is currently being done to select appropriate ranges for calibration in STAR.

Some example parameters from the k-ε and k-ω families are below:

k-ε

- Turbulent Kinetic Energy
- Turbulent Dissipation Rate
- Elliptic Function (V2F KE)
- Normal Stress Function (V2F KE)
- Reduced Stress Function (EB KE)
- Turbulence Intensity
- Turbulent Length Scale
- Turbulent Viscosity Ratio

k-ω

- Turbulent Kinetic Energy
- Specific Dissipation Rate
- Turbulence Intensity
- Turbulent Length Scale
- Turbulent Velocity Scale
- Turbulent Viscosity Ratio

Next Steps:

The next step in the STAR Hi2Lo process is to fully prepare the model to complete calibration. The calibration framework for STAR has been laid out and works in Dakota, but the process needs to be tested in CTF before significant computation resources can be dedicated to the STAR calibration process. Direct and Bayesian (with surrogate) calibration will then be started for STAR.

A higher resolution mesh might be developed and used for a second validation study to see if a finer mesh yields results closer to the experiment. However, this would mean further increasing the computation time for a single evaluation in STAR, so if this step will be taken in the near future is currently uncertain.

Work is being done to verify that the turbulence model used for validation is in fact correct the best choice for this simulation. Data smoothing within STAR is another feature that is being currently developed in order to reduce noise in the temperature readings for calibration.

Additionally, it has been suggested that the outer subchannels be removed from consideration in the calculations. This can be fixed in validation by post processing, but will require modifications to the calibration framework to implement currently.

In addition to studying the temperature distributions at the outlet, it might be of interest to perform a Hi2Lo process on the axial temperature distributions of CTF and STAR-CCM+. There is no experimental data in the axial direction for MV Bundle 20, but a Hi2Lo study could be performed between STAR-CCM+ and CTF using STAR data in place of experimental measurements for CTF.

Several other sets of experimental data may also come available for use with STAR. Test Bundle 19 consists of non-mixing tests data, which will be used for another Hi2Lo study between STAR-CCM+ and CTF. The NMV test geometry should be made available to SNL soon. The NESTOR data set is another potential path forward if it is made available. It contains high enough resolution data to perform a full validation for STAR.

STAR-CCM+ Mesh Considerations

One of the possibilities that is currently being investigated is the idea of using a finer mesh for the STAR simulations. The current coarse mesh was chosen due to its fast run times and accurate simulations results (L2 less than 1%). The current mesh consists of 60M cells. Even a small increase in the total resolution has the potential to greatly improve results and simulation stability without significantly impacting run times. The following turbulent parameters can serve as guidelines for mesh selection and design:

Examples from MV Bundle 20, Test 13:

- Reynolds number = 4.92e+05
- Max. mean turbulence velocity = 6.21e+00 m/s
- Entrance length = 4.36e-01 m

- y at y+=1 = 5.34e-07 m
- y at y+=7 = 3.74e-06 m
- y at y+=30 = 1.60e-05 m

- Ratio of turbulent and fluid kinematic viscosities = 1.31e+03
- Turbulence intensity = 3.11e-02
- Turbulence kinetic energy = 3.58e-02 m2/s2
- Eddy dissipation (epsilon) = 7.19e-01 m2/s3
- Kolmogorov eddy size = 7.11e-06 m
- Taylor eddy size = 2.47e-04 m
- Integral eddy size = Integral eddy size = 8.48e-04 m

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STAR-CCM+ Turbulence Model Selection

Selection of a correct turbulence model is key to getting good results for CFD. K-ε is generally the standard "go-to" turbulence model for CFD as it is able to handle a wide range of geometries and flow conditions without running into major numerical errors during calculation. However, even though the current k-ε turbulence model is getting results that resemble the experimental test data, major improvements could be made in terms of stability (noise reduction) and accuracy by using a different turbulence model.

Bob Brewster of WEC suggested the current turbulence models in STAR-CCM+:

1. Realizable k-ε Two-Layer with All-y^+ Wall Treatment (used for all Validation cases)
2. Realizable k-ε with High-y^+ Wall Treatment
3. Standard Linear k-ε with High-y^+ Wall Treatment
4. Standard Quadratic k-ε with High-y^+ Wall Treatment
5. Standard Cubic k-ε with High-y^+ Wall Treatment

Sal Rodriguez of SNL suggested the following additional turbulence models:

6. SST k-ω
7. Wilcox k-ω

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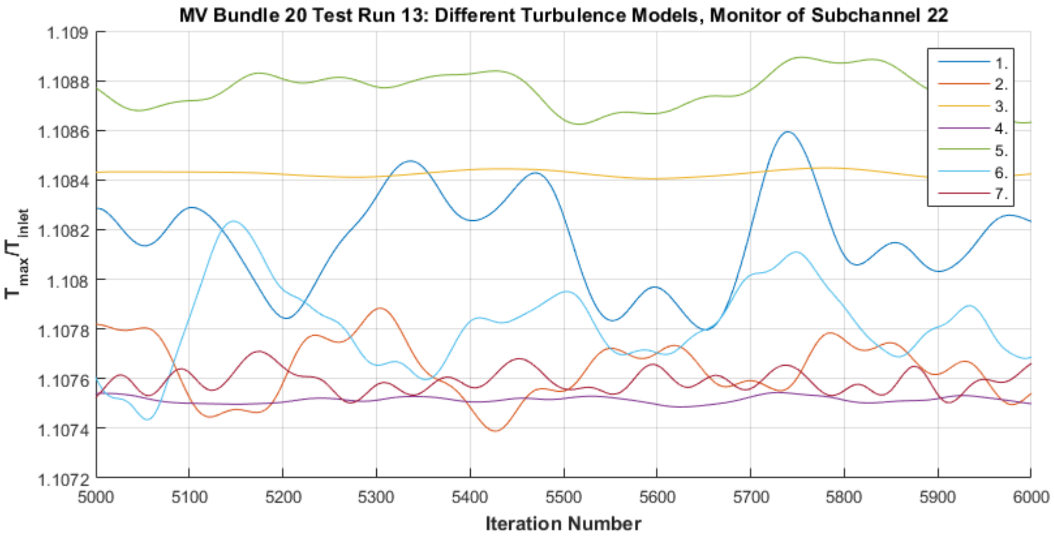
STAR-CCM+ Turbulence Model Selection



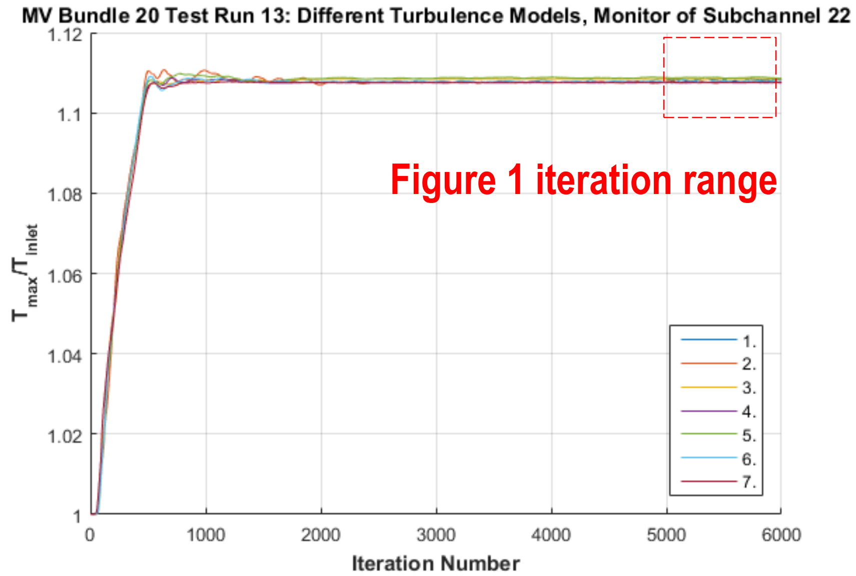


Figure 1 **Legend numbering from previous slide (corresponding to turbulence model)**

Figure 2

This shows a comparison of the STAR selected turbulence models (see numbering on previously slide). To accurately represent this figure, it is very important to note that the seemingly huge fluctuations over 1000 iterations in Figure 1 are a result of the reduced scale. Figure 2 shows the development from initial state to steady state over 6000 iterations. All models take approximately the same amount of time to reach a converged solution for the same test. The fluctuations account for a maximum ±0.1 C° temperature difference at the sub channel collection points.

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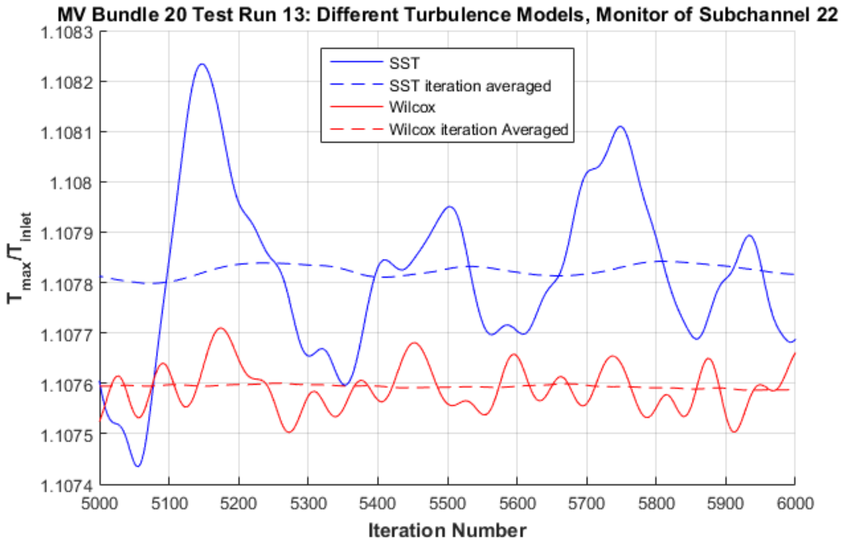
STAR-CCM+ Data Filter

One of the concerns for calibration in STAR-CCM+ is the noise in the simulation results. By changing the calibration parameters by small amounts in their reasonable ranges, we do not expect to see a huge amounts of change in the results, so smoothing the STAR-CCM+ results will be necessary to ensure that we are not just calibrating to noise. The temperature fluctuations are low in magnitude, but their presence indicates that some improvements can be made to the model to improve calibration.

This step will be performed internally in STAR using user-coded libraries. User coded libraries allow for the user to store data from previous iterations internally in STAR, which is not a function built into standard field functions. This step can also be moved external to STAR, but implementation of this would require a very large number of files and space per Dakota iteration.



The above figure shows the difference between the iteration averaged (over 500 iterations) and the instantaneous STAR subchannel graphs for two different turbulence models, SST and Wilcox k-ω. Removing the noise from the STAR temperature subchannels will allow for quicker calibration without the user having to worry that Dakota is calibrating to a point along a fluctuating Temperature/Iteration curve in STAR.

Experimental Concerns

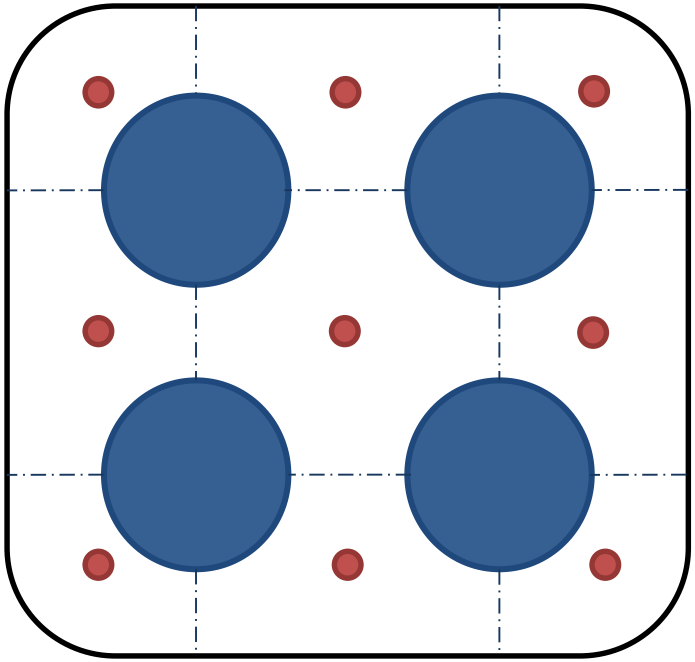


Figure 1

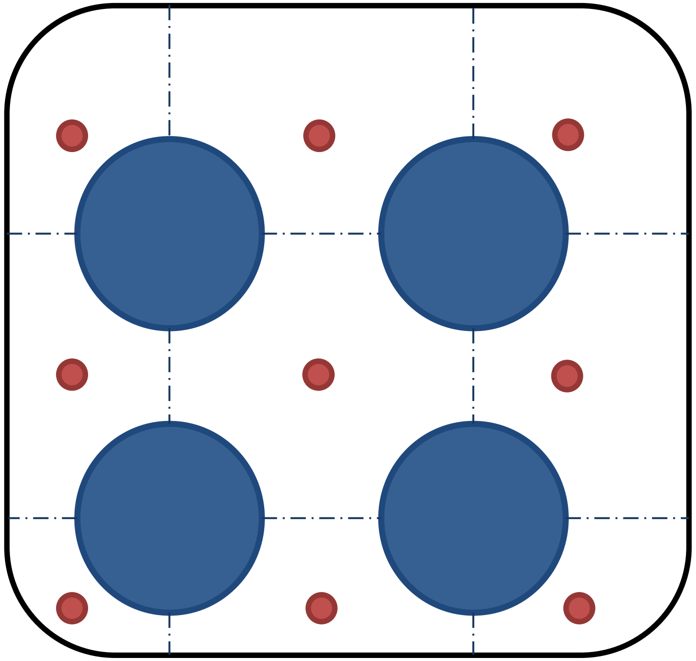


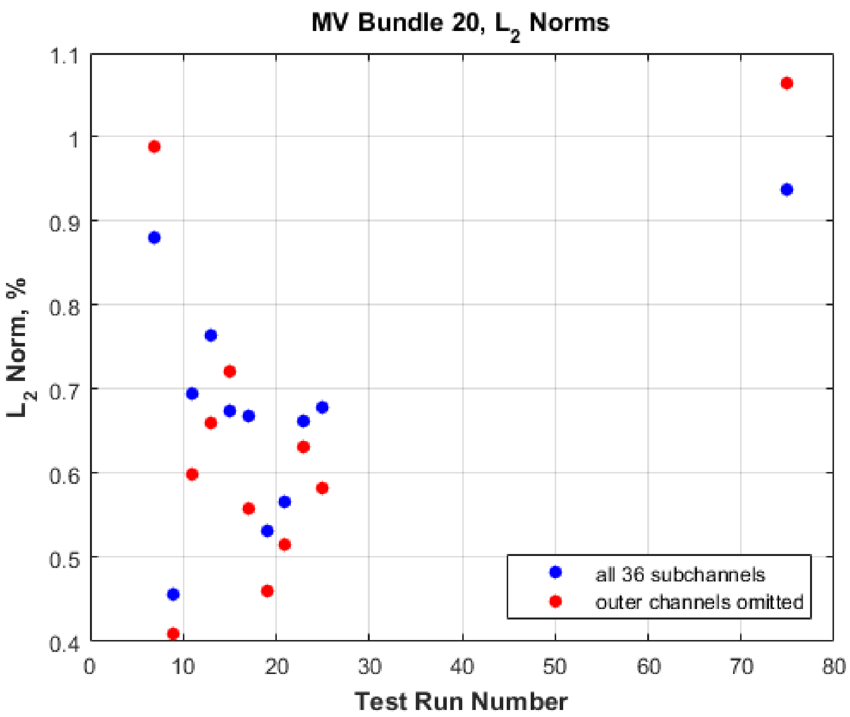
Figure 2

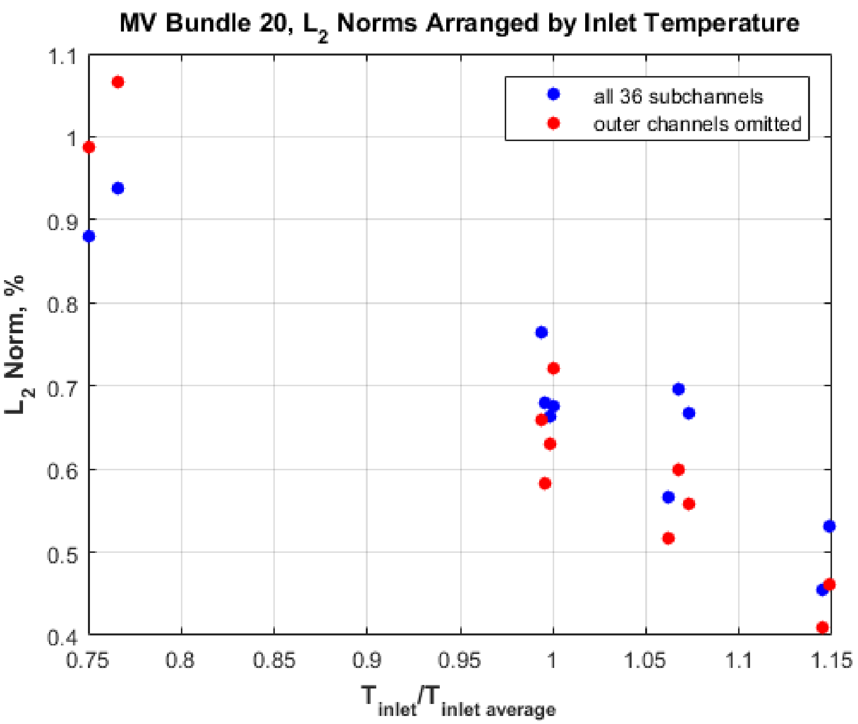
● Location of thermocouples

One concern with the experimental data is that were could be additional experimental error due to the thermocouple alignment shifting in the channels during experiments. This would change the location of the thermocouples relative to the subchannel centers and could effect thermocouple readings. This effect would be especially pronounced in the outer, exterior subchannels since it would change the location of the thermocouples relative to the walls (and associated wall boundary conditions). Figure 2 is exaggerated to show the shift in thermocouple placement that could have occurred near the walls. Westinghouse recommended that we omit the outer subchannels from further analysis since the reliability of the thermocouple placements and measurements are unknown.

Experimental Concerns

Removing the outer subchannels has the following effect on the STAR L2 norms:





The red points represent the omission of the outer subchannels while the blue points represent the results that include all 36 subchannels. Omitting the outer subchannels increases the accuracy of the simulations for 9 out of the 11 training cases. However for the lower temperature simulations, omitting the subchannels has a negative effect on the L2 norms.

Experimental Concerns

STAR generally follows the same symmetry for all tests. The inner subchannels arranged from cold to hot are displayed below for all 11 tests cases for both the experimental and STAR results.

STAR

COLD															HOT
29	8	9	10	11	16	26	17	15	21	28	23	20	27	14	22
29	17	9	8	16	26	10	15	11	21	28	14	23	20	22	27
29	17	9	8	16	26	10	15	11	21	28	14	20	23	22	27
29	17	9	16	8	26	10	11	15	21	28	20	14	23	27	22
29	17	9	16	8	26	10	15	11	21	28	27	20	23	14	22
29	17	9	16	8	26	10	11	15	21	28	20	27	23	14	22
29	17	9	16	8	26	10	11	15	21	28	20	23	27	14	22
29	8	9	16	17	10	26	11	27	15	21	20	28	23	14	22
29	8	9	10	16	11	26	17	15	27	21	28	20	23	14	22
29	17	9	16	8	26	10	11	15	21	28	27	23	20	14	22
29	8	9	10	16	11	26	17	21	15	28	23	20	14	27	22

Experiment

COLD															HOT
28	14	20	8	29	22	10	9	11	15	23	27	26	17	21	16
14	29	26	8	20	9	28	11	22	27	15	17	10	23	21	16
26	14	10	29	22	17	8	28	20	27	23	9	15	21	11	16
26	29	14	10	22	17	28	20	8	23	9	27	15	21	11	16
8	11	9	20	14	28	29	15	22	26	27	23	16	21	17	10
26	10	29	14	22	17	8	28	20	23	9	27	15	21	11	16
26	14	29	10	22	20	28	8	17	9	27	15	23	11	21	16
26	14	29	8	9	20	28	22	23	17	15	10	27	11	21	16
26	14	29	8	20	22	28	9	11	17	15	23	27	10	21	16
26	10	29	14	22	17	28	20	23	8	9	27	21	15	11	16
28	14	8	11	15	20	9	22	23	29	16	27	21	17	26	10

Experimental Concerns

An alternative way of displaying this data is to sum all temperature readings per subchannel and nondimensionalize by a common factor (sum of the inlet temperatures).

$$result_i = \frac{\sum_{j=1}^{j=11} T_{sc_{i,j}}}{\sum_{j=1}^{j=11} T_{inlet_j}}$$ where i is the subchannel number and j is the test number.

STAR peak temperature occurs at subchannel 22. The experimental data has the peak temperature at subchannel 16. These subchannels are located next to each other. The STAR peak temperature occurs where we would predict it to just by looking at the hot/cold rod arrangement (subchannel 21 or 22) on slide 5.

STAR-CCM+

	1	2	3	4	5	6
1						
2		1.08728101	1.087707	1.092043	1.094451	
3		1.09891634	1.095179	1.090276	1.088949	
4		1.09844267	1.096238	1.101693	1.098428	
5		1.09179796	1.098503	1.097354	1.084978	
6						

Experiment

	1	2	3	4	5	6
1						
2		1.09005355	1.092259	1.092221	1.09351	
3		1.08663982	1.093623	1.098073	1.093017	
4		1.0907468	1.096113	1.090282	1.093758	
5		1.0861598	1.093875	1.089906	1.088077	
6						

MV Test 20 Run 7 Relative Percent Error: STAR and CTF

CTF: Beta = 0.4 (Nominal)

	1	2	3	4	5	6
1						
2		1.084	1.042	0.909	1.925	
3		5.230	1.295	4.927	2.866	
4		4.112	3.803	0.201	1.740	
5		2.651	1.800	6.477	0.902	
6						

CTF: Beta = 0.2

	1	2	3	4	5	6
1						
2		1.004	0.901	0.766	1.999	
3		5.513	0.712	4.363	2.597	
4		4.526	3.061	0.977	1.338	
5		2.478	1.334	6.985	1.093	
6						

CTF: Beta = 0.15

	1	2	3	4	5	6
1						
2		0.951	0.808	0.673	2.047	
3		5.699	0.328	3.992	2.420	
4		4.799	2.572	1.488	1.074	
5		2.364	1.028	7.319	1.219	
6						

STAR-CCM+

	1	2	3	4	5	6
1						
2		6.276	3.920	0.797	0.052	
3		13.629	1.908	3.568	0.009	
4		11.454	0.859	12.061	4.648	
5		0.196	5.486	12.484	6.701	
6						

% Error max

0.008926
0.01
0.05
0.1
0.25
0.5
1
2
4
6
8
10
12
13.62851

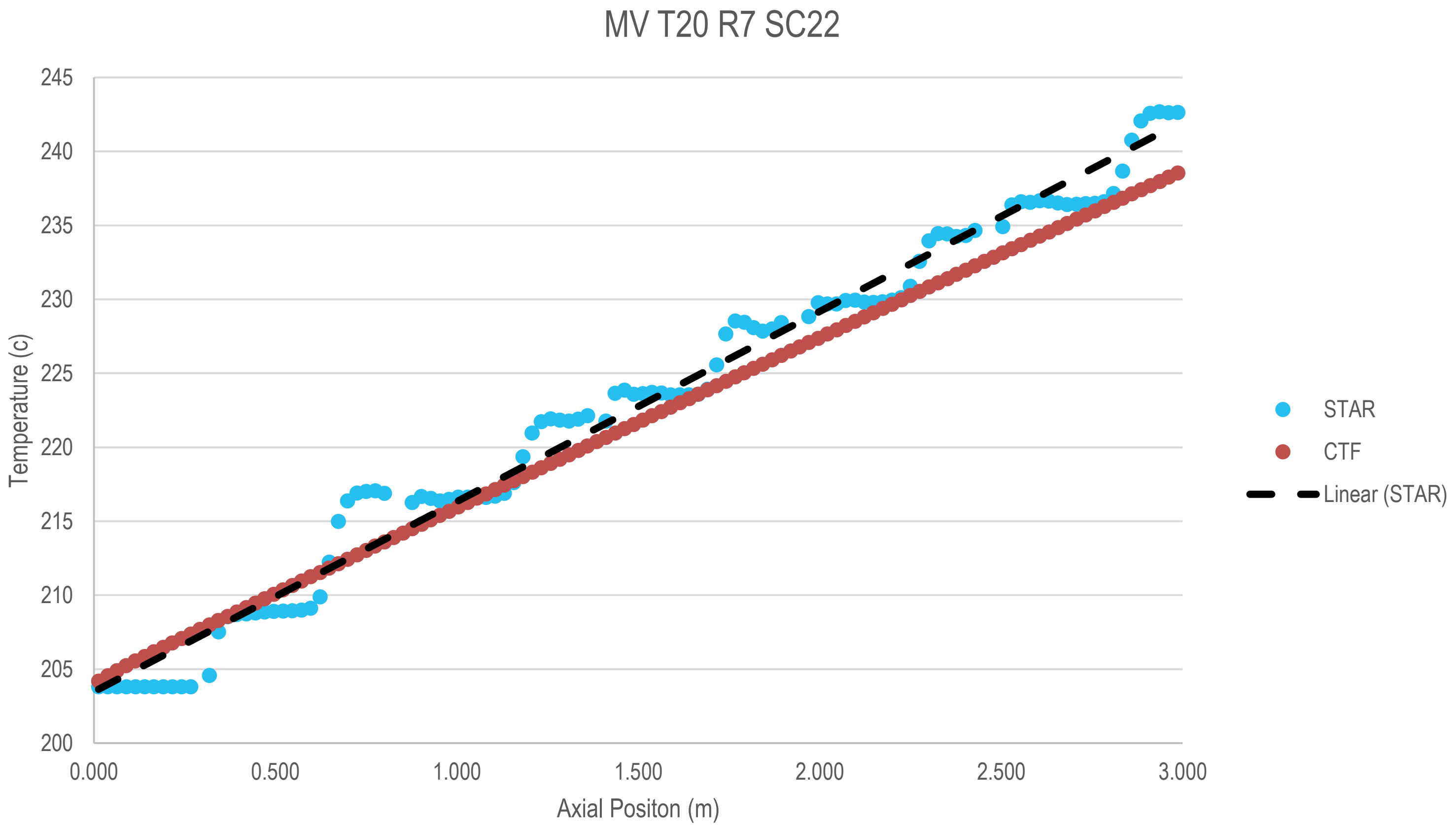
% Error min

$$\%\ error\ from\ experiment = \frac{(T_{CTF,i} - T_{EXP,i})}{(T_{EXP,i} - T_{EXP\_inlet})} \times 100$$

Differences in temperature distributions between the experiment and STAR-CCM+/CTF can impact the percent error significantly. STAR-CCM+ predicts temperatures closer to the experimental measurements for certain subchannels and further away for other subchannels even after omission of the outer subchannels. CTF has a much flatter temperature profile, which is why the STAR error appears to be so high when compared to CTF. This is also one of the tests with the highest L2 norms in STAR, meaning it is further from the experiments than 9 out of the 11 tests.

Despite the larger errors for certain subchannels, the STAR L2 norms are lower than the CTF results for validation (typically 2%), and are below 1%.

Potential Path: Axial Temperature



The hot channel (SC22) axial temperatures were used to compare results from STAR-CCM+ and CTF. While CTF does not model the mixing grids explicitly, the CTF temperature profile should still show a step-like temperature pattern as a function of axial position down the channel. The CTF results however are linear (with no steps) while the STAR results show a step pattern axially. If a trend line is drawn for the STAR results, it closely matches CTF until approximately 1.5 m downstream of the bundle inlet. The STAR line has a higher slope than the CTF results and predicts higher temperatures in the last half of the channel than the CTF calculation. This is an alternative Hi2Lo exercise that might be interesting to demonstrate for CTF and STAR.

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