

Analyzing the Effectiveness of RANS Turbulence Models for the Holistic Reconstruction of the Inlet Region of the New NIST Neutron Source

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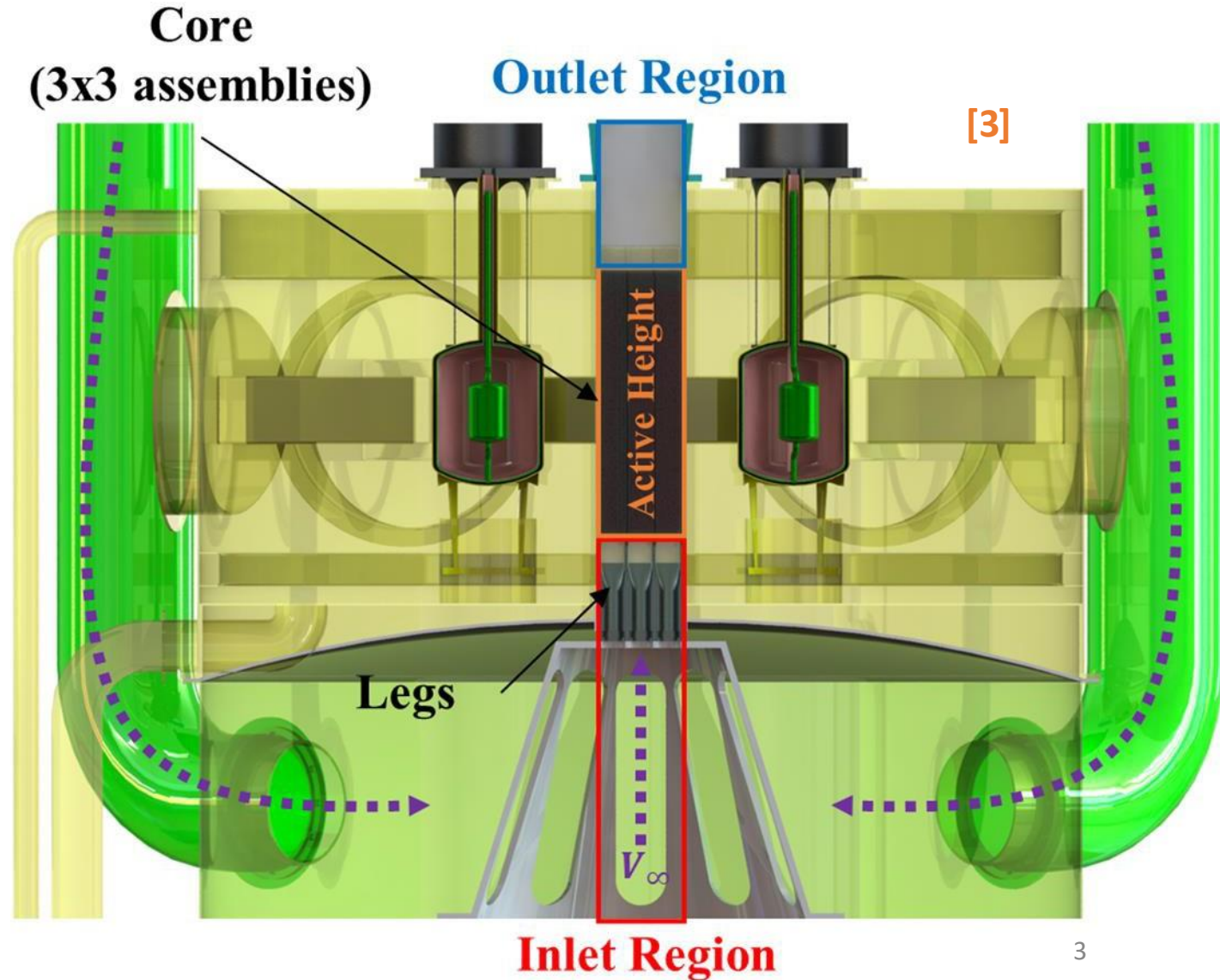
About me

- Evan Bures
- Texas A&M Alumni
- Bachelors of Science in Nuclear Engineering
- Worked in Thermal Hydraulics Verification and Validation Group for more than 2 and half years under Dr. Mark Kimber
- Close to 3 years of experience in Computational Fluid dynamics (CFD)
- Experience in a wide variety of Thermal Hydraulic problems involving molten salt reactors, magnetic confinement fusion, and traditional water based reactors.



NNS Reactor Design

- NIST Neutron Source (NNS)
 - Planned replacement for current reactor (NBSR)
- High power density reactor meant for neutron generation
- Flow modelling centered around:
 - Inlet region (lower plenum)
 - Curved fuel plates with curved fuel channels separating them (Active Height)
 - Outlet region (long stack)

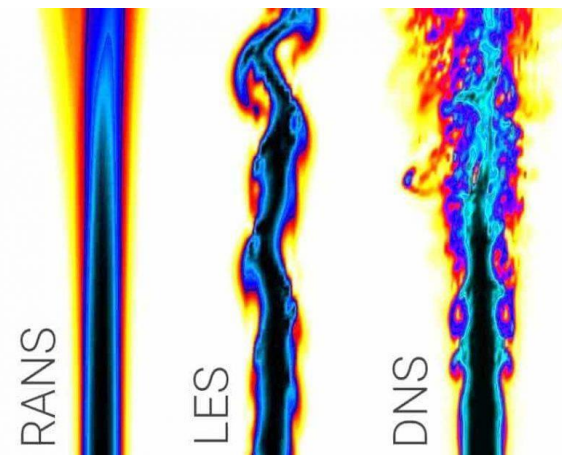


What is Computational Fluid Dynamics?

- We discretize fluid systems into multiple smaller elements known as cells to generate what is known as a “mesh”.
- Once we have our mesh we can attempt to model the Navier Stokes equations in each individual cell to create one larger picture to represent the entire system
- In order to do this efficiently we employ multiple simplifications such as the **Reynolds Averaged Navier Stokes (RANS)** equations, **Large Eddy decomposition equations (LES)**, or even in some cases attempting to directly solve the Navier Stokes equations in what's known as “Direct Numerical Simulation” (DNS)
- Furthermore, turbulent effects must be solved using a separate subset of models known as “turbulence models”.

Navier-Stokes Equation

$$\underbrace{\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j}}_{\text{Gas Pedal}} = - \underbrace{\frac{\partial P}{\partial x_i}}_{\substack{\text{Steering} \\ \text{Wheel}}} + \nu \underbrace{\frac{\partial^2 U_i}{\partial x_j \partial x_i}}_{\text{Brakes}}$$



- Recall the geometry from before:
- Inside this geometry we have a mixing region that comes from 3 parallel channels opening into an empty lower plenum.
- We are interested in determining how much mixing takes place and if the flow will be fully developed by the time it reaches the active height.



- Fortunately for us, we have experimental data extracted by Weiss et al. , this allows us to validate multiple turbulence models to help find a group/set of models we can use to model the mixing region in the NNS.
- We are primarily looking to see just how much fidelity we will need to get an accurate representation of the mixing regions at the bottom of the core. (do we need 3d models? Wall resolved? LES?)



Experimental Thermal and Fluid Science

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[2]

Flow regime and Reynolds number variation effects on the mixing behavior of parallel flows

Abdullah G. Weiss^a, Paul J. Kristo^b, Juan R. Gonzalez^a, Mark L. Kimber^{a, b}  

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Why Computational Fluid Dynamics?

- Computational fluid dynamics provides us an alternative to running complex and expensive experimental setups to provide highly detailed and descriptive data sets involving thermal fluid systems.
- While hand calculations can generally provide us with solid understanding of fluid systems, CFD allows us to drastically reduce the amount of assumptions that are required to problem solve.
- This can further be applied to the comparison to system codes as CFD relies far less on correlations and more on numerical approximations of the Navier-Stokes equations.

Verification and Validation

- Verification and validation is an essential task to understanding the importance of your CFD models.
- Verification Confirms that the computational model is correctly implemented and performs the intended operations according to specifications.
- Validation assesses whether the computational model accurately represents the real world physical system it is intended to simulate.

ASME V&V 20-2009
REAFFIRMED 2021

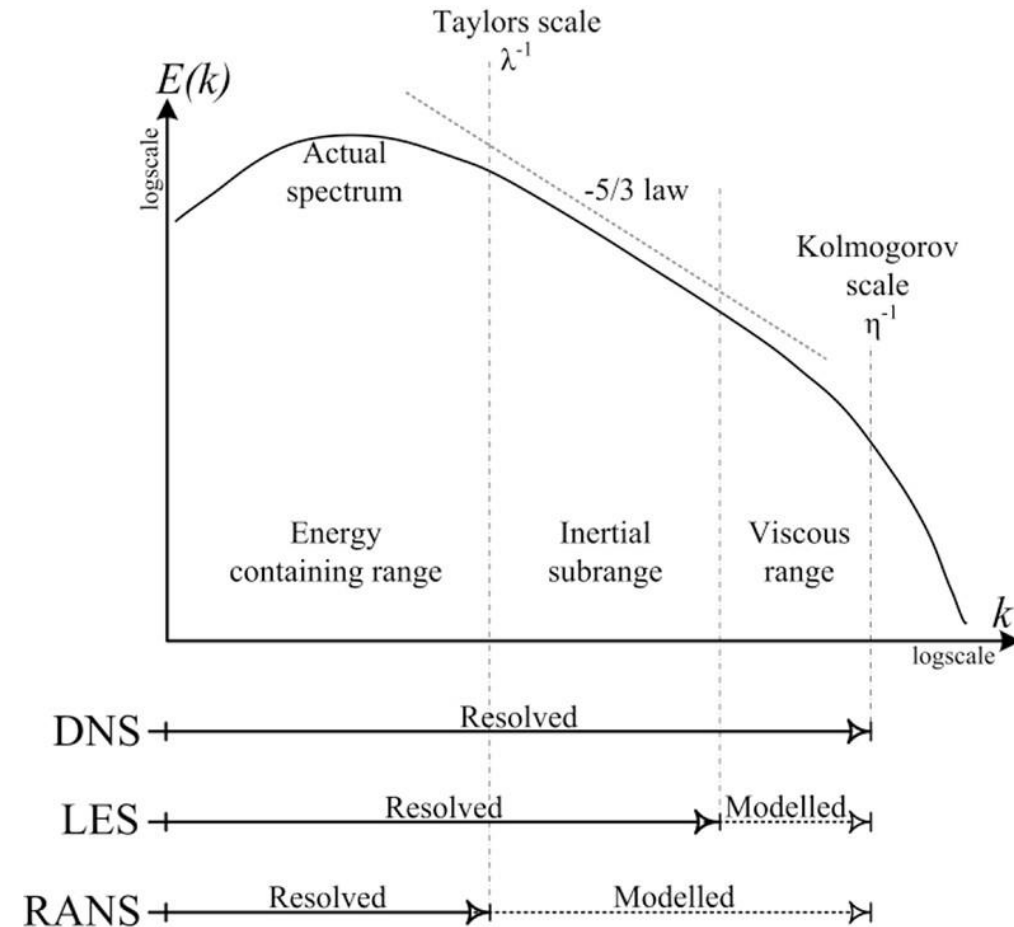
**Standard for
Verification and Validation
in Computational Fluid
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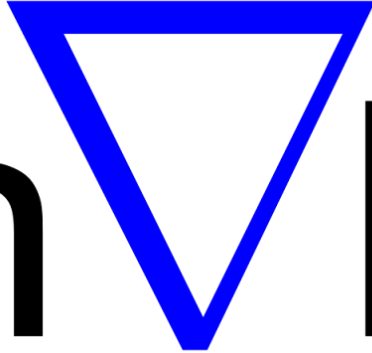
Reynolds Averaged Navier Stokes (RANS)

- RANS Resolves turbulence by creating large, averaged, general approximations for turbulent effects in regions.
- We can use RANS to model simple flows or flows that we want a general idea of how the flow will behave (no super specific values of velocity or pressure)
- RANS is fast!!! Work horse of CFD



- Resolves turbulence at much smaller scales by separating and directly solving large, more influential turbulence scales while modelling smaller scales.
- Much more accurate than RANS
- Significantly more computationally expensive
- Note: as models increase in order of fidelity, more refined meshes of higher cell counts are required so not only are your models becoming more expensive on just an equation basis, but your meshes are needing to increase in size too.

- OpenFOAM is the most popular and commercially standard open source CFD software.
- Provides unequalled amounts of customization due to it being opensource
- Effectively a CFD sandbox.

Open  FOAM ^[4]

- Commercial Meshing software
- Universal meshing software for all range of transport problems
- Entirely structured meshing (meshes that are hand crafted and not automatically generated)



For the purpose of this work, we will focus around 3 models:

1. k - ϵ (2-equation model)
2. k - ϵ Realizable (2-equation model) (A more complex K-epsilon that adds constraints to ensure predictions adhere to physics more closely)
3. k - ω SST (2 equation model)

Example of K-Omega-SST from OpenFOAM User Guide:

The turbulence specific dissipation rate equation is given by:

$$\frac{D}{Dt}(\rho\omega) = \nabla \cdot (\rho D_\omega \nabla \omega) + \frac{\rho\gamma G}{\nu} - \frac{2}{3}\rho\gamma\omega(\nabla \cdot \mathbf{u}) - \rho\beta\omega^2 - \rho(F_1 - 1)CD_{k\omega} + S_\omega, \quad [4]$$

and the turbulence kinetic energy by:

$$\frac{D}{Dt}(\rho k) = \nabla \cdot (\rho D_k \nabla k) + \rho G - \frac{2}{3}\rho k(\nabla \cdot \mathbf{u}) - \rho\beta^* \omega k + S_k.$$

The turbulence viscosity is obtained using:

$$\nu_t = a_1 \frac{k}{\max(a_1\omega, b_1 F_{23} \mathbf{S})}$$

- y^+ is a non-dimensional parameter we use in CFD to represent the ratio of inertial to viscous forces for a fluid near a wall boundary.
- We essentially use this term in grid dependence studies to help determine how much resolution is needed near the wall
- Think of it as just parameter of how many cells need to be near the wall to ensure we are modelling all the effects of that wall.
- So, if y^+ is close to 1 and there's not a lot of cells near the wall, that means the wall functions the model is using are pretty good at modelling the walls
- A high y^+ that has a lot of cells near the wall means wall effects are quite strong and large amounts of cells will be needed near the wall to model the flow accurately

$$y^+ = \frac{u^* y}{\nu}$$

Grid Convergence Study

- 3 meshes are created for each mesh, each with a refinement factor of 1.25 the size of the coarser mesh
- A GCI study is conducted on the points of interest. This is done by taking 3 meshes and comparing them to each other at each cell center.
- Allows us to assign a numerical uncertainty based off grid convergence to our results

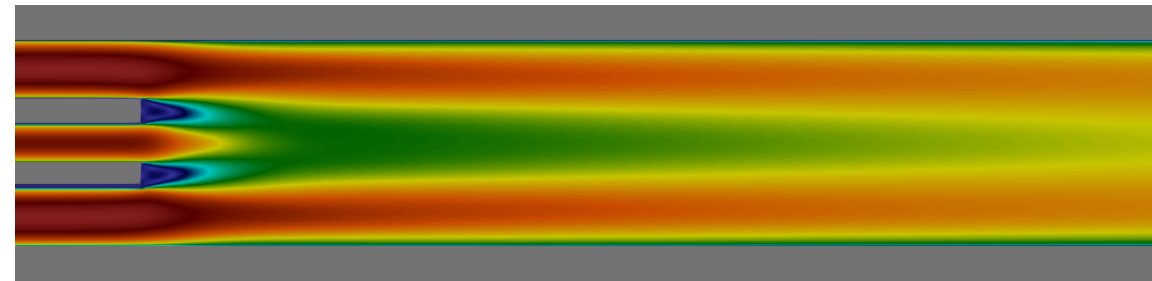
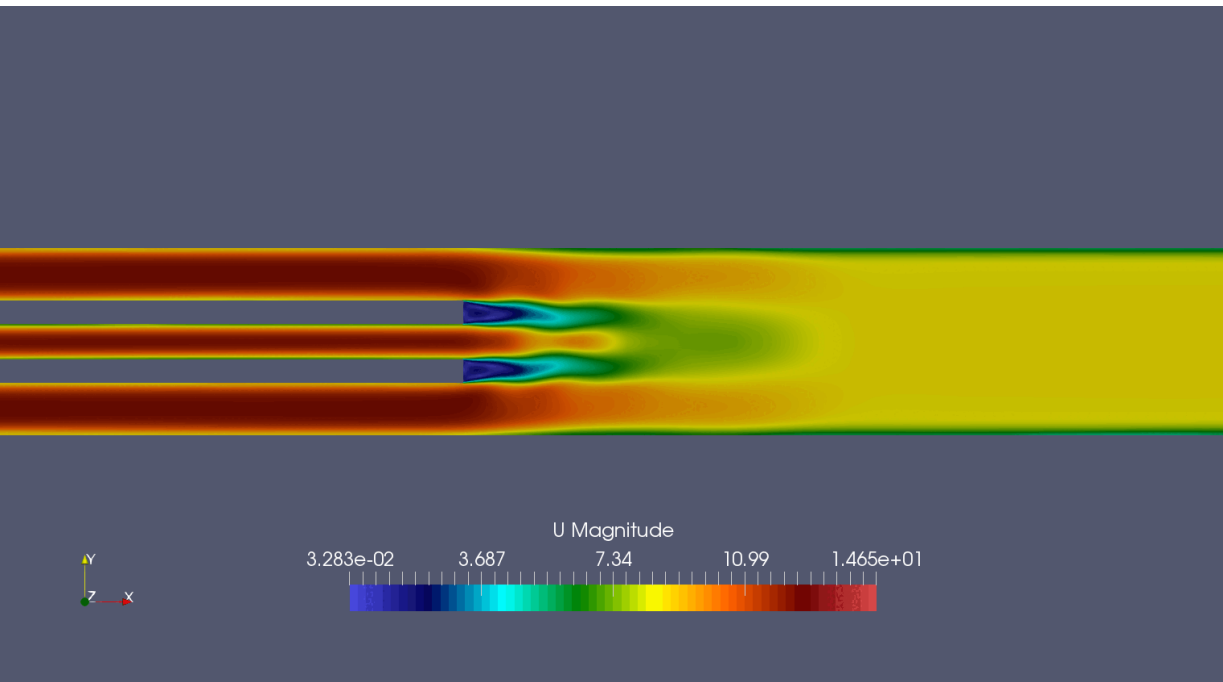
$$F_s \approx 1.25, \quad r = \frac{h_2}{h_1} = \frac{h_3}{h_2}, \quad p \approx \frac{\ln\left(\frac{U_3 - U_2}{U_2 - U_1}\right)}{\ln(r)}$$

$$\delta_{num} \equiv GCI = \frac{F_s}{r^p - 1} |U_2 - U_1|$$

Numerical Uncertainty!

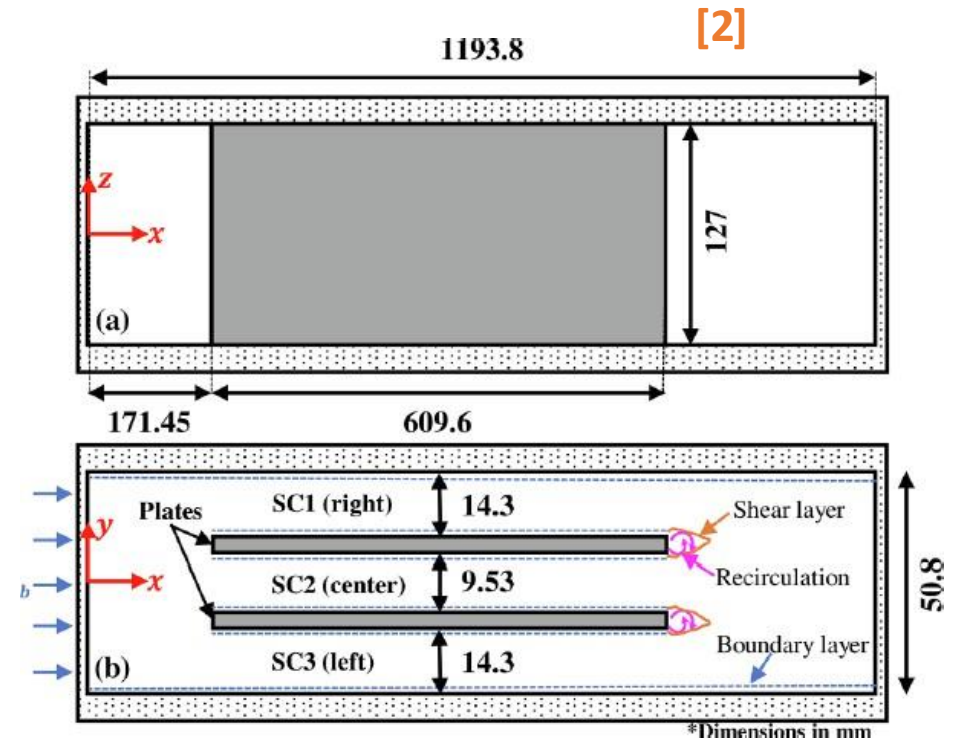
Time Averaging

- Simply put, instead of just using individual time steps, we collect all data points across a given time interval and average them based off of a certain frequency that is based on the write interval of the simulation
- For instance, these mixing studies are analyzed from 1 second after the jet has been turned on to 2 seconds. 100 time steps at an interval of 0.01 seconds are analyzed then averaged together to yield our time averaged profile.



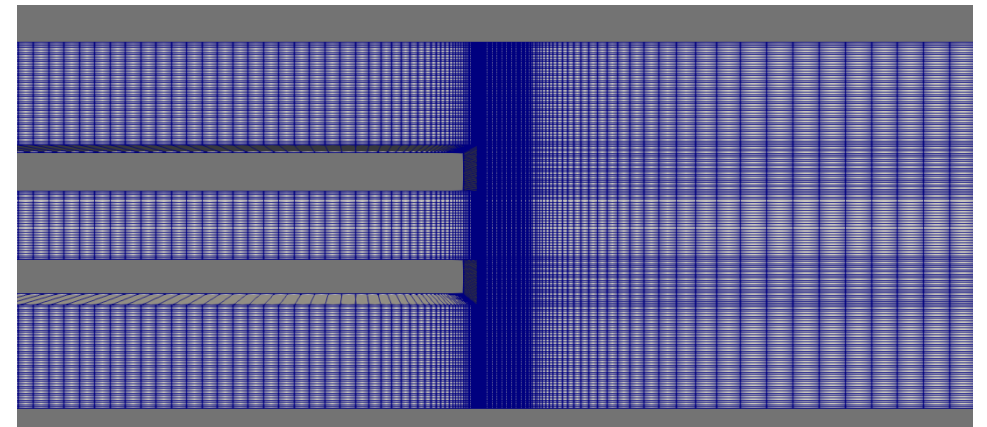
Design Parameters

- 3 Cases studying a mostly laminar flow of bulk inlet velocity 1.08 m/s, a mostly transitional flow velocity 1.88 m/s, and turbulent flow velocity 8.3 m/s.
- ANSYS ICEM is used for Meshing
- OpenFOAM v10 is used for simulation
- Traces are compared at x/D of 10.35.

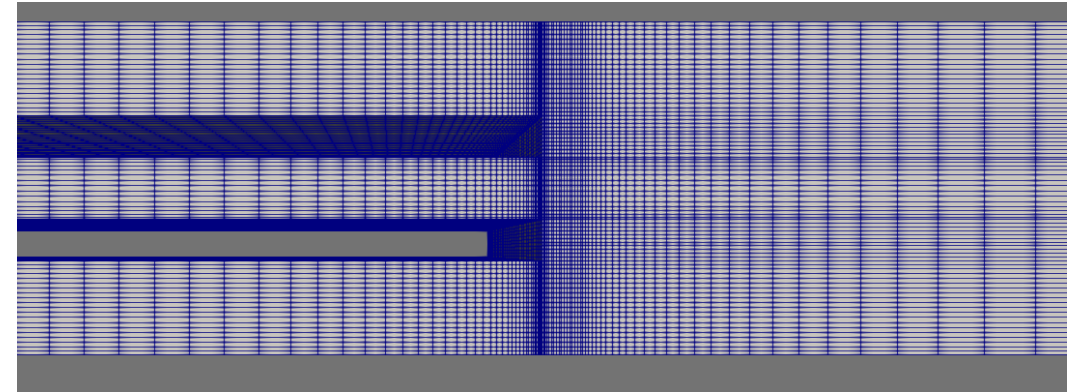


2D Mesh design

- All models are wall modeled for computational efficiency.
- 8 meshes were tested for each turbulence model to determine grid dependence.
- After study was conducted, 3 meshes of sizes ($\sim 82,000$), ($\sim 184,000$), ($\sim 365,000$) cells were chosen for uncertainty analysis and validation ($r = 1.25$)
- Average y^+ across all turbulence models floats around 5.1 with a minimum of 1.02 and a maximum of 8.3.



- All models are wall modeled for computational efficiency.
- 5 meshes were tested for each turbulence model to determine grid dependence.
- After study was conducted, 3 meshes of sizes ($\sim 317,568$), ($\sim 618,750$), ($\sim 1,300,000$) cells were chosen for uncertainty analysis and validation ($r = 1.25$)
- Average y^+ across all turbulence models floats around 7.4 with a minimum of 1.8 and a maximum of 11.6.

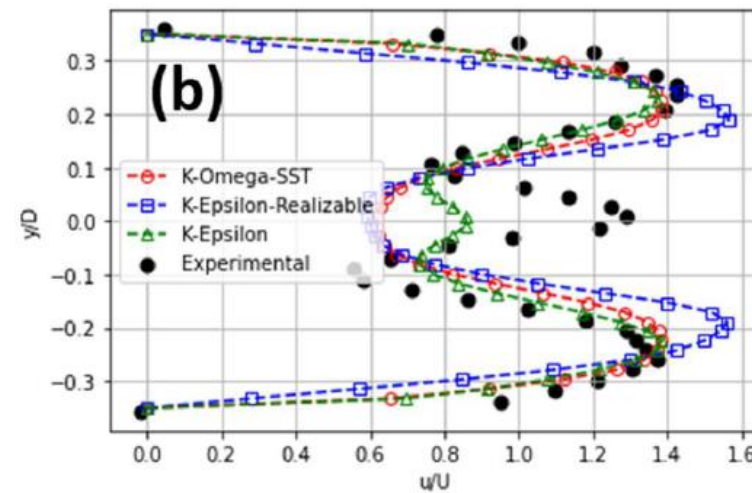
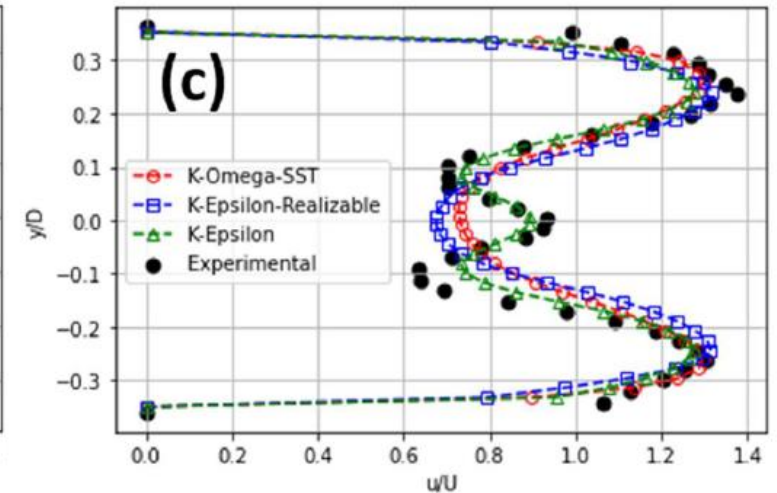
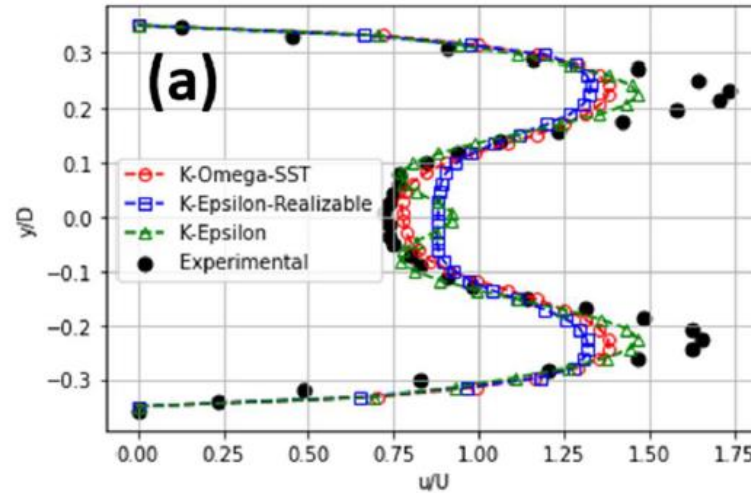


Boundary Conditions

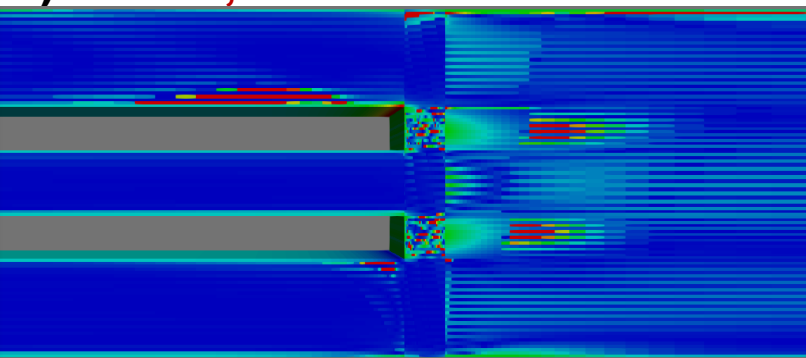
Modeled	u	p	k	ϵ	ω
Inlet	$u = U$	Zero Gradient	Fixed value	Fixed value	Fixed value
Outlet	Zero Gradient	$p = 0$	Zero Gradient	Zero Gradient	Zero Gradient
Walls	No-slip	Zero Gradient	kqR wall function	Epsilon wall function	Omega wall function

2D Results

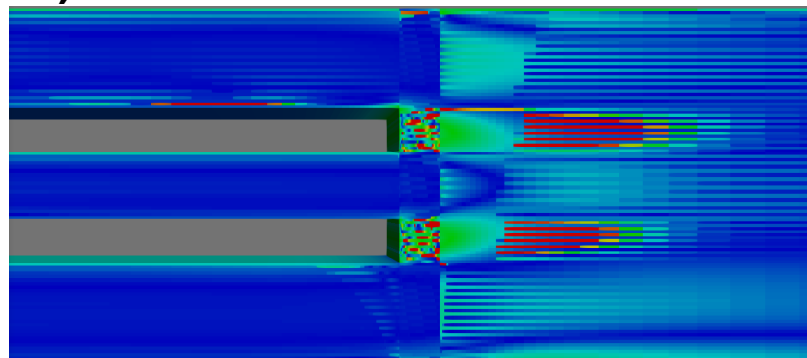
- a) Laminar, b) Transitional, c) Turbulent.
- Solid agreement for laminar cases.
- Interesting behavior by some models particularly in the center band for Transitional and Turbulent



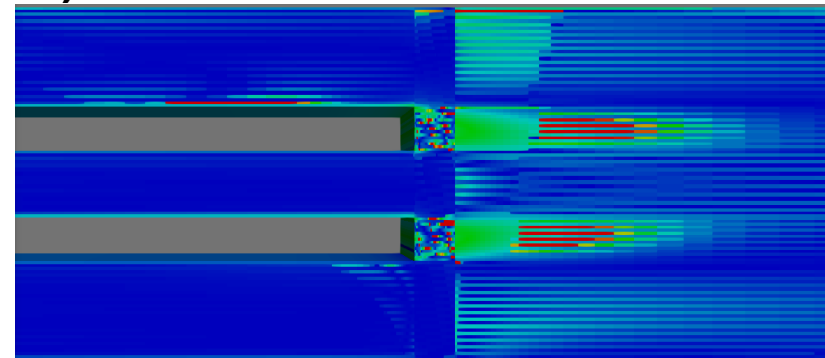
a) Case 1, KOSST



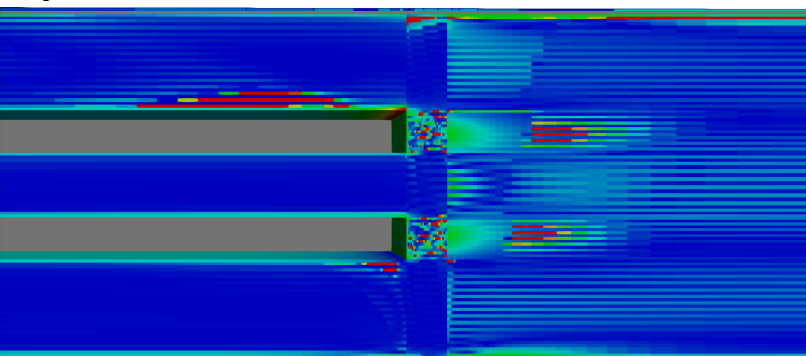
b) KER



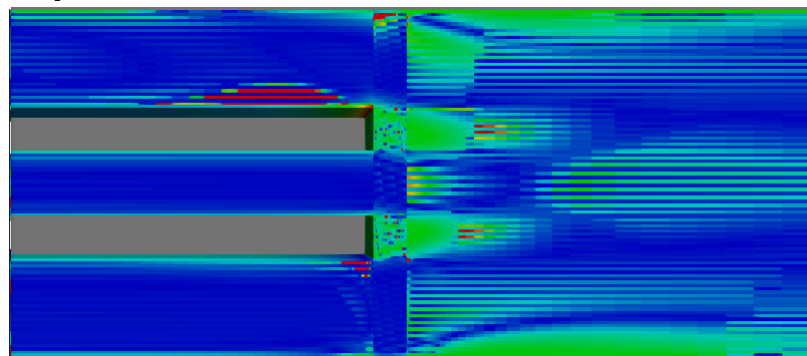
c) KE



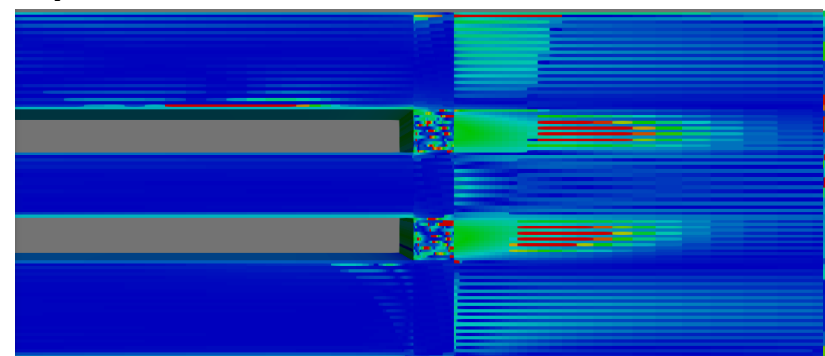
d) Case 2



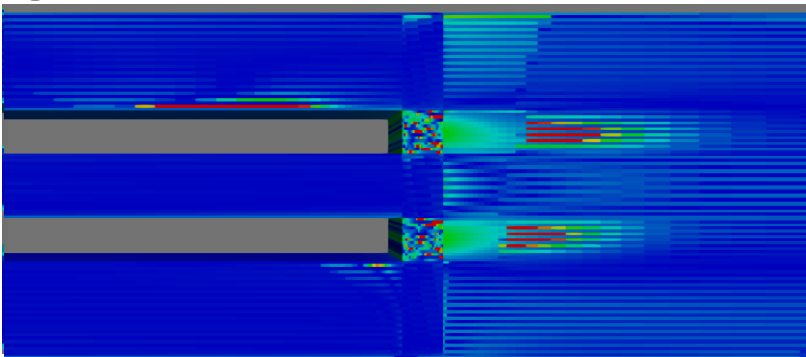
e)



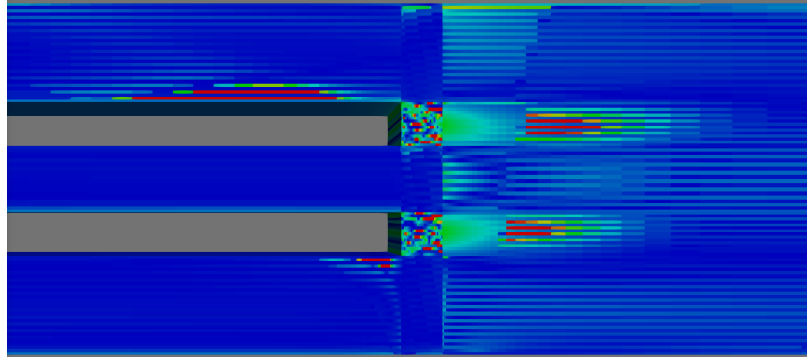
f)



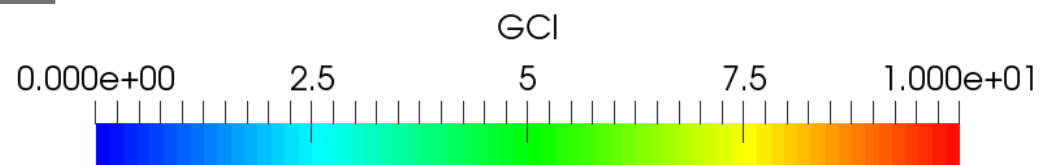
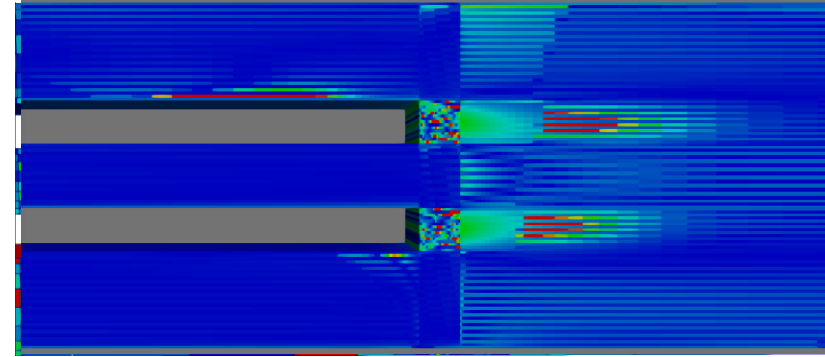
g) Case 3



h)

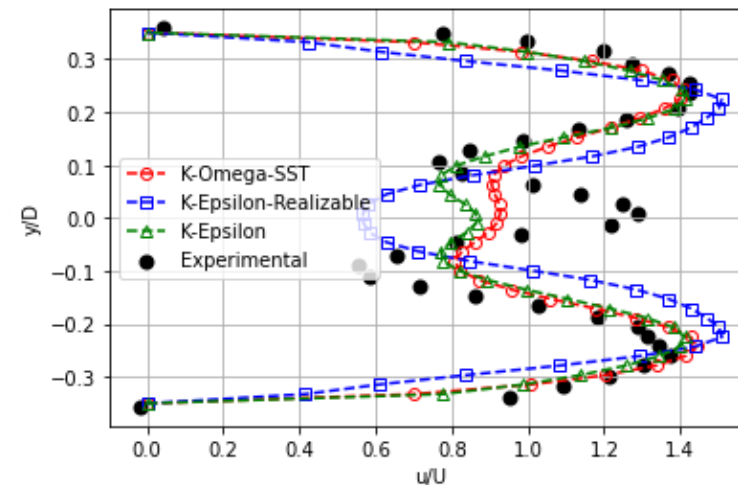
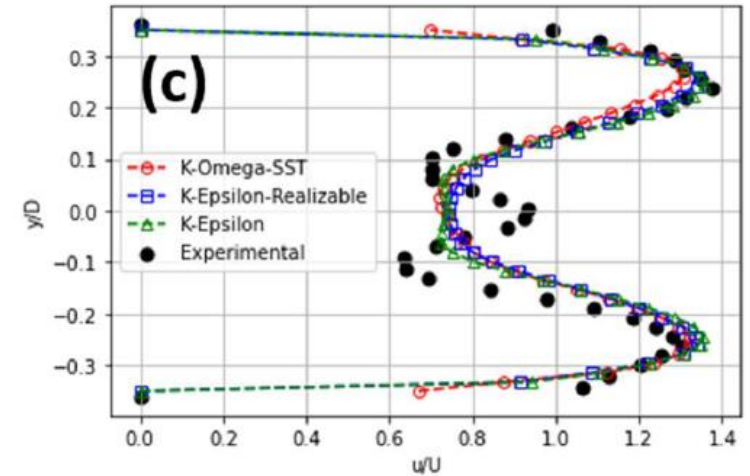
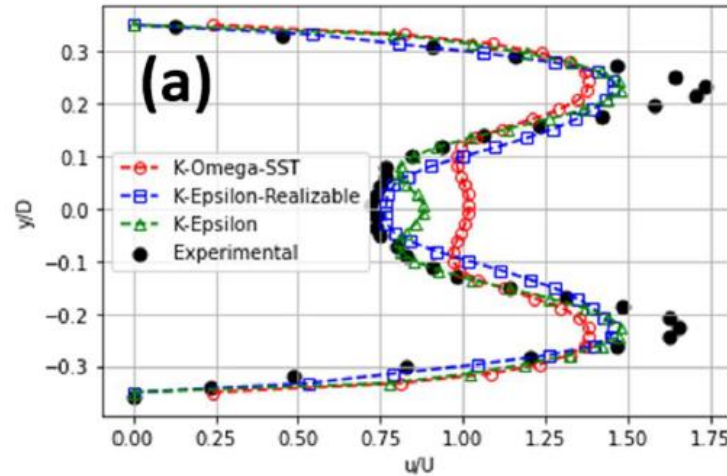


i)

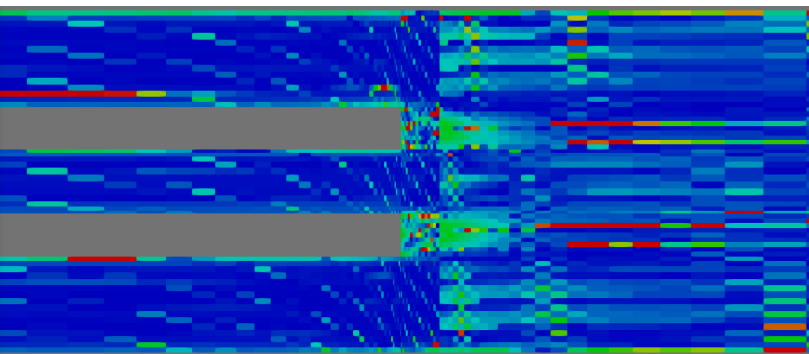


3D Results

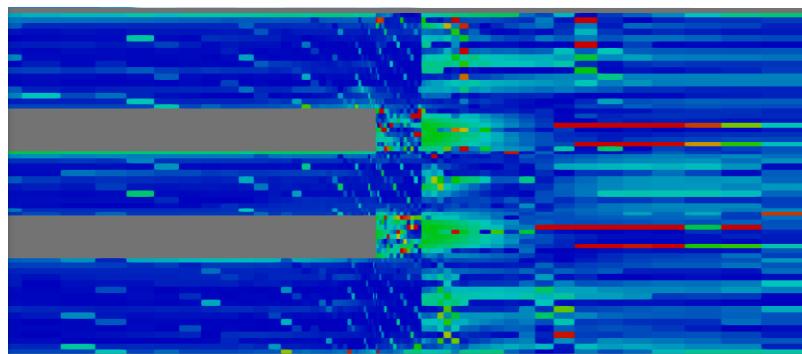
- a) Laminar, b) Transitional, c) Turbulent.
- Much more detached and varied than the 2D models.
- Transitional and Turbulent cases models fail to capture center physics.



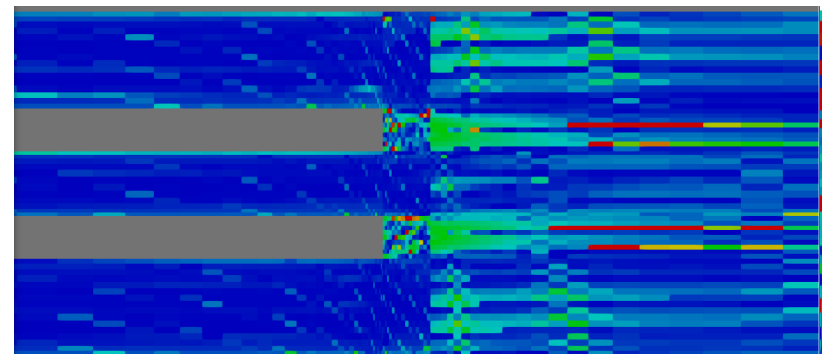
a) Case 1, KOSST



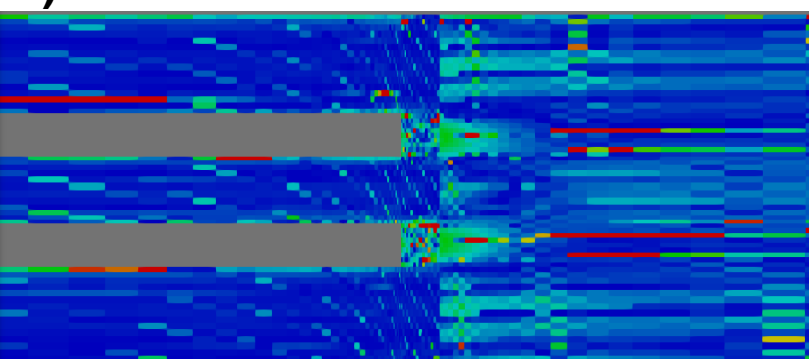
b) KER



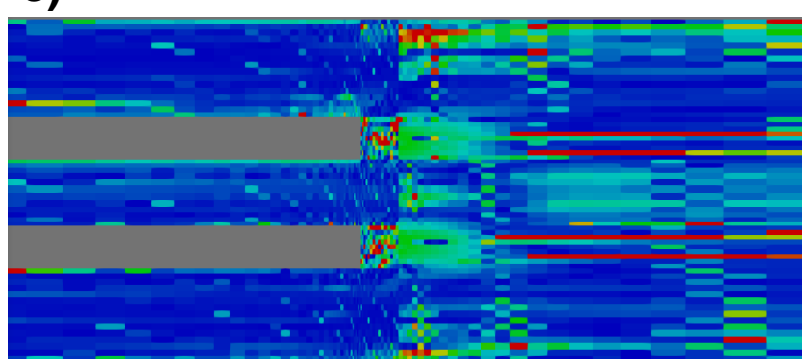
c) KE



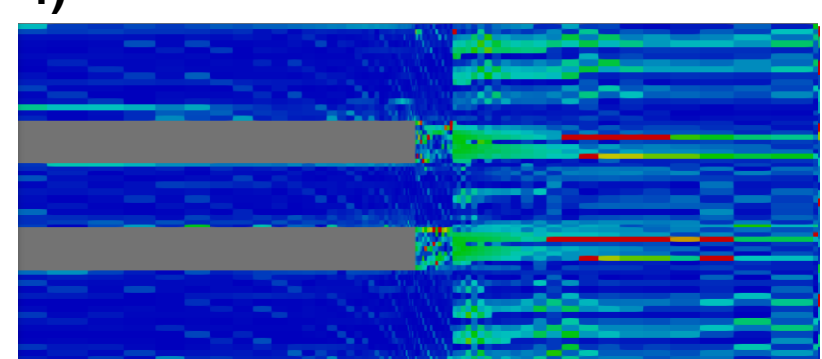
d) Case 2



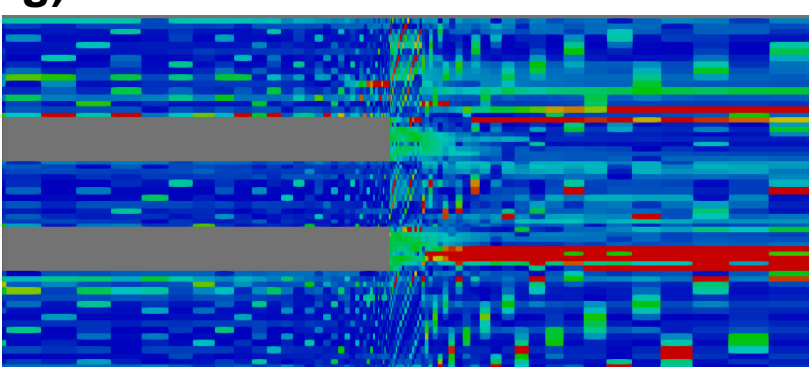
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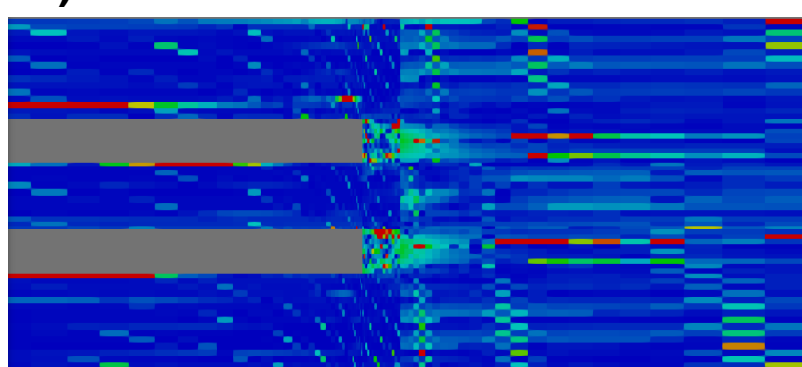
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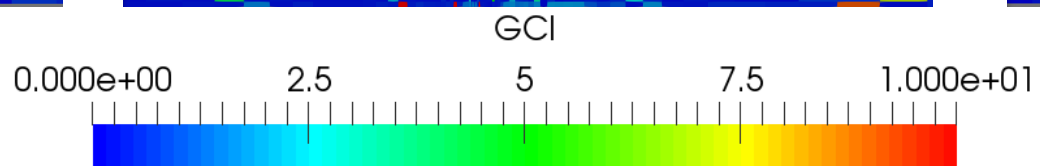
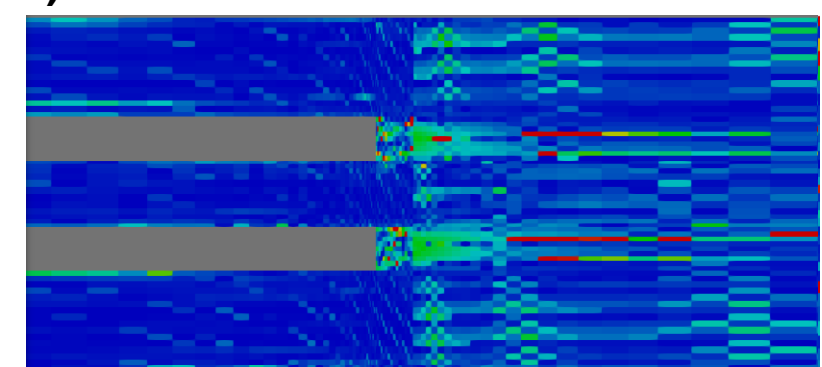
g) Case 3



h)



i)



- Potentially need to increase averaging frequency and average over a longer range of time steps
- Numerical schemes could be causing instabilities in the model leading to offset physics seen in the results
- Wall resolved could be necessary to model splitting effects and near wall instabilities in the mixing region.
- Large eddy simulation or hybrid RANS-LES may need analysis for efficiency.

- 2D and 3D wall modeled RANS models both fail to accurately represent mixing region flow across all cases.
- While some outlier cases exist, every model possesses major drawbacks in some respect when compared to experimental data.
- Even with the potential for future fixes, drastic model changes (Primarily a move to much higher fidelity models) seems more than likely for efforts to model the mixing region/lower plenum of the NNS.

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2. Shen, Joy, et al. "A Turbulence Model Sensitivity Analysis of Thermal-Hydraulic Properties on The Pre-Conceptual NIST Neutron Source Design." *Proceedings of the International Conference on Nuclear Engineering*. 2023.
3. Weiss, Abdullah G., et al. "Flow regime and Reynolds number variation effects on the mixing behavior of parallel flows." *Experimental Thermal and Fluid Science* 134 (2022): 110619.
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Questions?

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