Multi-Fluid, Thermal Flow Simulation of Geometrical-induced Effects on a TPMS-UHTC Heat Exchanger

Using UHTC for Corrosive, High Temperature-Pressure Conditions

MED MATERIALS ENGINEERING DIVISION

CHRES CONSORTIUM OF HYBRID RESILIENT ENERGY SYSTEMS DE-NA0003982

GEM THE NATIONAL GEM CONSORTIUM

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Lawrence Livermore National Laboratory

Self-introduction

- Mechanical Engineering Masters student at UPRM on the thermal science field.
  - Future Ph.D. MechE student at CUNY-CCNY
- Summer experience at LLNL:
  - Collaborative environment culture in the lab
  - Many researchers are open to show you their work
  - Lots of positive encouragement towards networking

Molten Salts – Hostile and Corrosive Environment

- Certain benefits can be obtained from the properties of molten salts
  - e.g., good thermal conductivity, heat capacity, and thermal storage capacity with low melting point (in some cases)
- The problem is that, in high temperatures and pressures, unpurified molten salts become very corrosive [Bell et al. '19]
  - This makes the use of metals an unpractical and expensive choice
- Ceramics often have lower thermal conductivities than metals, but could be able to withstand the extreme environment [Opila et al. '99]

Molten Salts – Hostile and Corrosive Environment

- Ultra-High Temperature Ceramics (UHTCs) are a special group of ceramics that possess relatively high thermal conductivities and have great corrosion resistance
  - Some even have thermal conductivities comparable to Ni, which is higher that some stainless-steel alloys
  - Higher temperatures lead to higher efficiencies, if the material can handle it

- Additionally, inner geometry of the heat exchanger could be modified to maximize heat transfer
  - How thin can you make the channel walls of a heat exchanger before corrosion damage on the system becomes a problem (i.e. low structural integrity)?
  - How does corrosion affect the performance of the system?

Triply Periodic Minimal Surfaces (TPMS)

- Triply Periodic Minimal Surfaces (TPMS) are intricate geometries where the mean curvature (half of the sum of two principal curvatures of a surface) is zero
  - This means that all points in said surface is equally convex and concave [Hydes et al.]

- The “triply periodic” part means that it has a pattern that repeats indefinitely in all three spatial dimensions

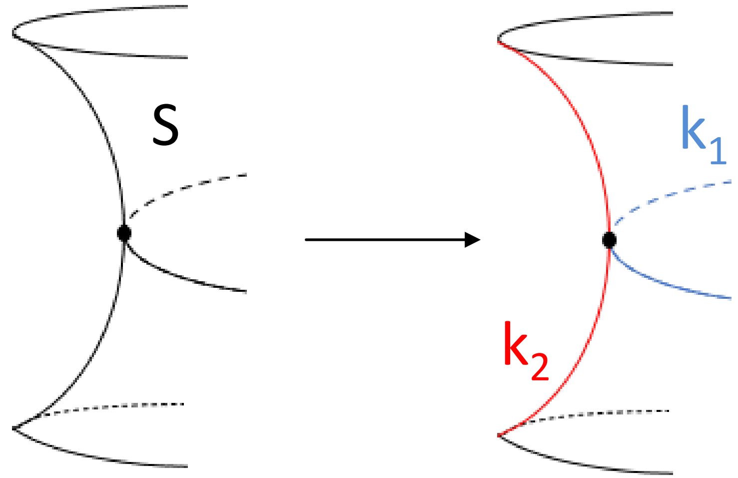


Fig. 1 – Principal curvatures k_1 and k_2 of a surface S. Image adapted from [O’neill ’06].

$$H = \frac{1}{2}(k_1 + k_2) = 0$$

TPMS with Corrosion

- Past research has shown that these geometries enhance thermal and hydraulic properties in simulated systems, such as heat exchangers [Iyer et al. '22]
- Yet, if those benefits are maintained even in corrosive environments is yet to be studied
  - Environments with high temperatures and pressure along with corrosion are present in components such as heat exchangers in Molten Salt Small Modular Reactors (SMRs) and in Concentrated Solar Power (CSP) plants

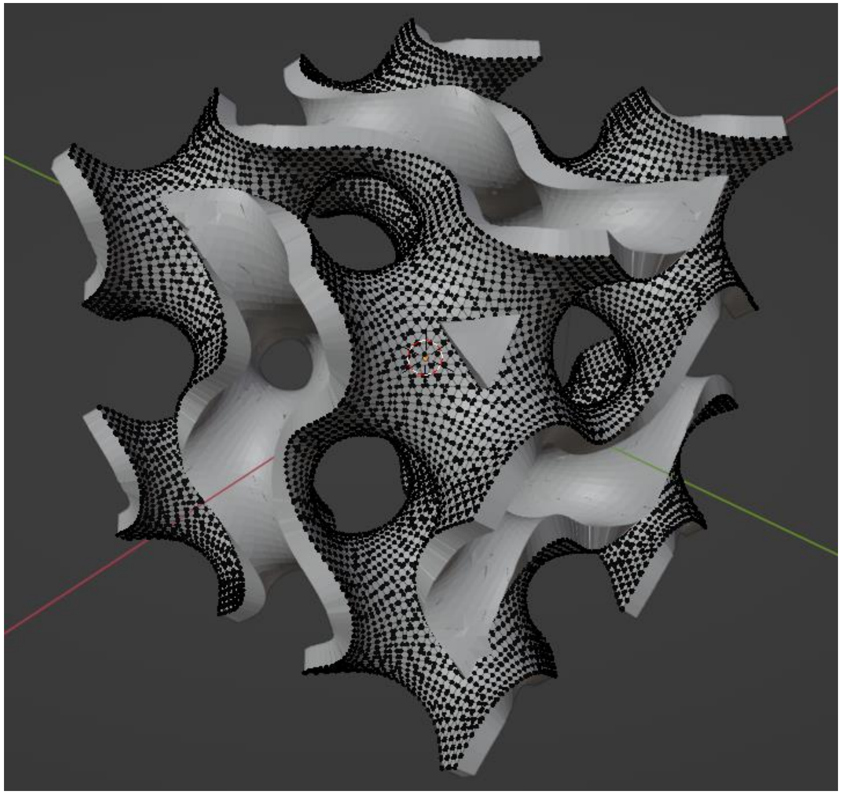


Fig. 2 – A TPMS example named gyroid, generated using MathMod and modeled in Blender

Scope and Key Factors

- Develop a general model for a heat exchanger with an inner TPMS geometry under high temperature and pressure where the effects of geometrical changes representing corrosion damage can be shown
  - Factors such as material, fluids, pressure/temperature, are to be chosen by the user and the model should be able to produce results

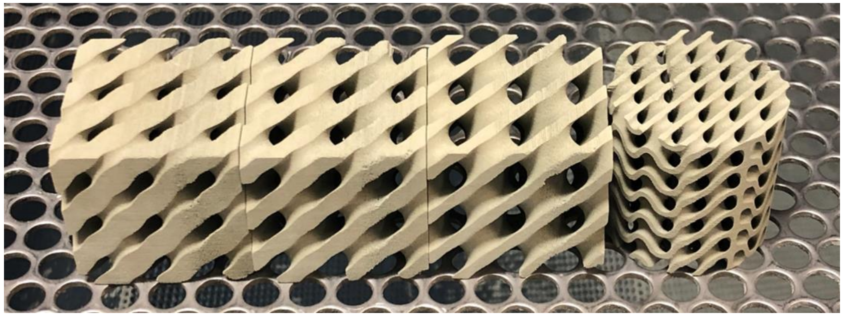
- Relevant initial conditions:
  - Temperature: 600°C - 1500°C
  - Pressure: 40 bar - 200 bar

- Materials of interest:
  - Ultra-High Temperature Ceramics
    - Titanium Diboride (TiB_2)
    - Tungsten Carbide (WC)
    - Zirconium Diboride (ZrB_2)

Fig. 3 – ZrB_2 sample and details

TPMS-UHTC Heat Exchanger Background

- Additive Manufacturing (AM) with Binder Jet printer
- Pressure-less sintering to near full density, near net shape
  - Post-sintering Hot Isostatic Pressing (sinter-HIP) can increase density from ~93v% to ~99% if needed
- AM printing of UHTC-TPMS structures is an enabling technology to produce ceramic TPMS structures



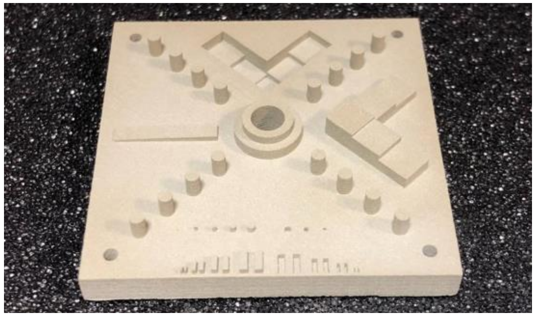


Fig. 4 – Ceramic AM samples. Images by [Kelly J. et al.]

Strategy – Indirect Measurement of Corrosion Damage

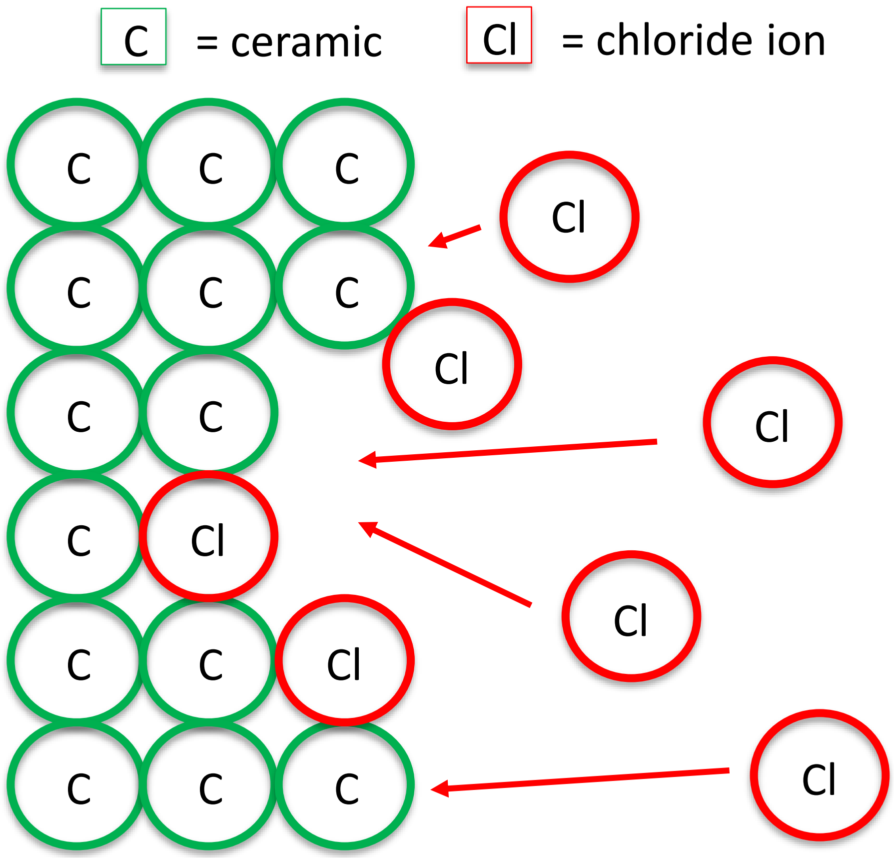


Fig. 5 – Simplified representation of corrosion on a non-oxide ceramic due to a KCl-$MgCl_2$ salt. Image adapted from [Bell et al. '19]

- Implementing corrosion models from differential equations is very challenging, hence an indirect measurement strategy will be used
- As corrosion occurs, the walls of the TPMS will decrease in thickness
  - Hence, we can consider the wall thickness as an independent variable and perform a parametric sweep

Thermal Simulations Workflow

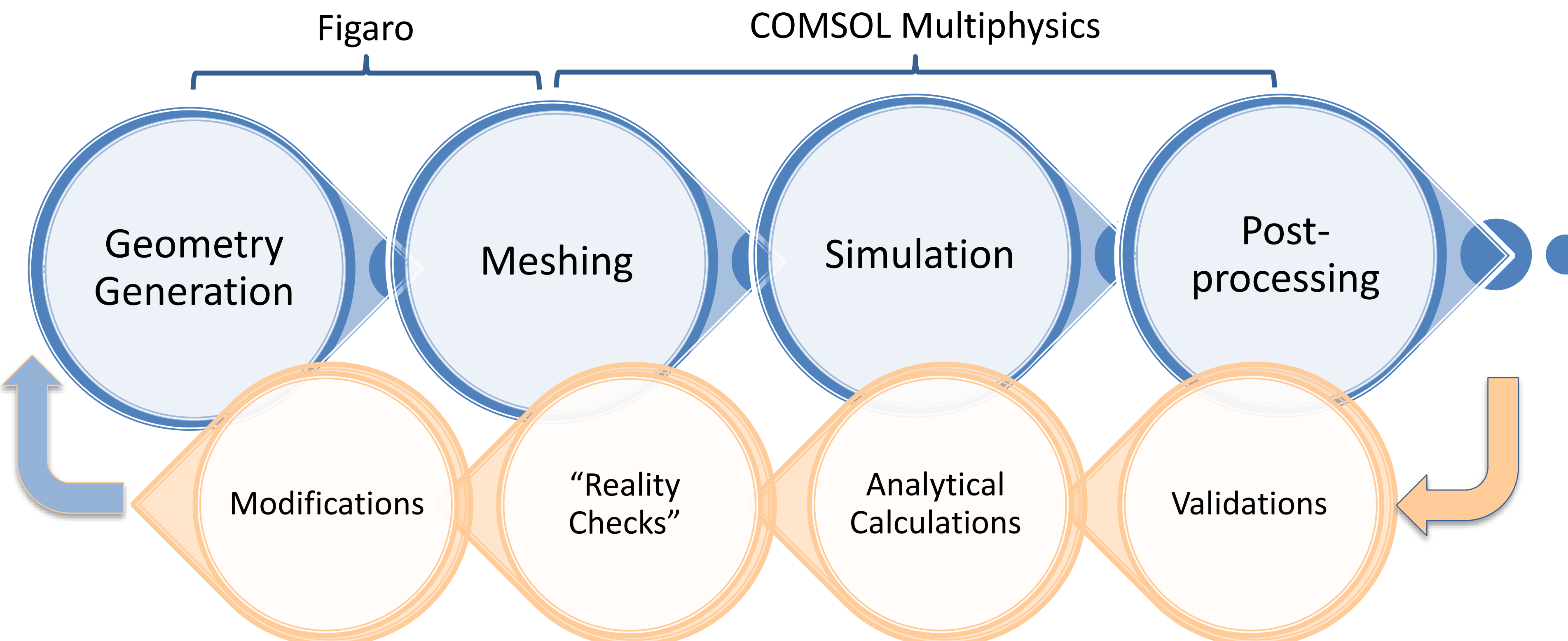


Fig. 6 – General steps which shows the process for making simulations

Preliminary Results – Velocity Profile for a Single-Phase Fluid from a simplified simulation

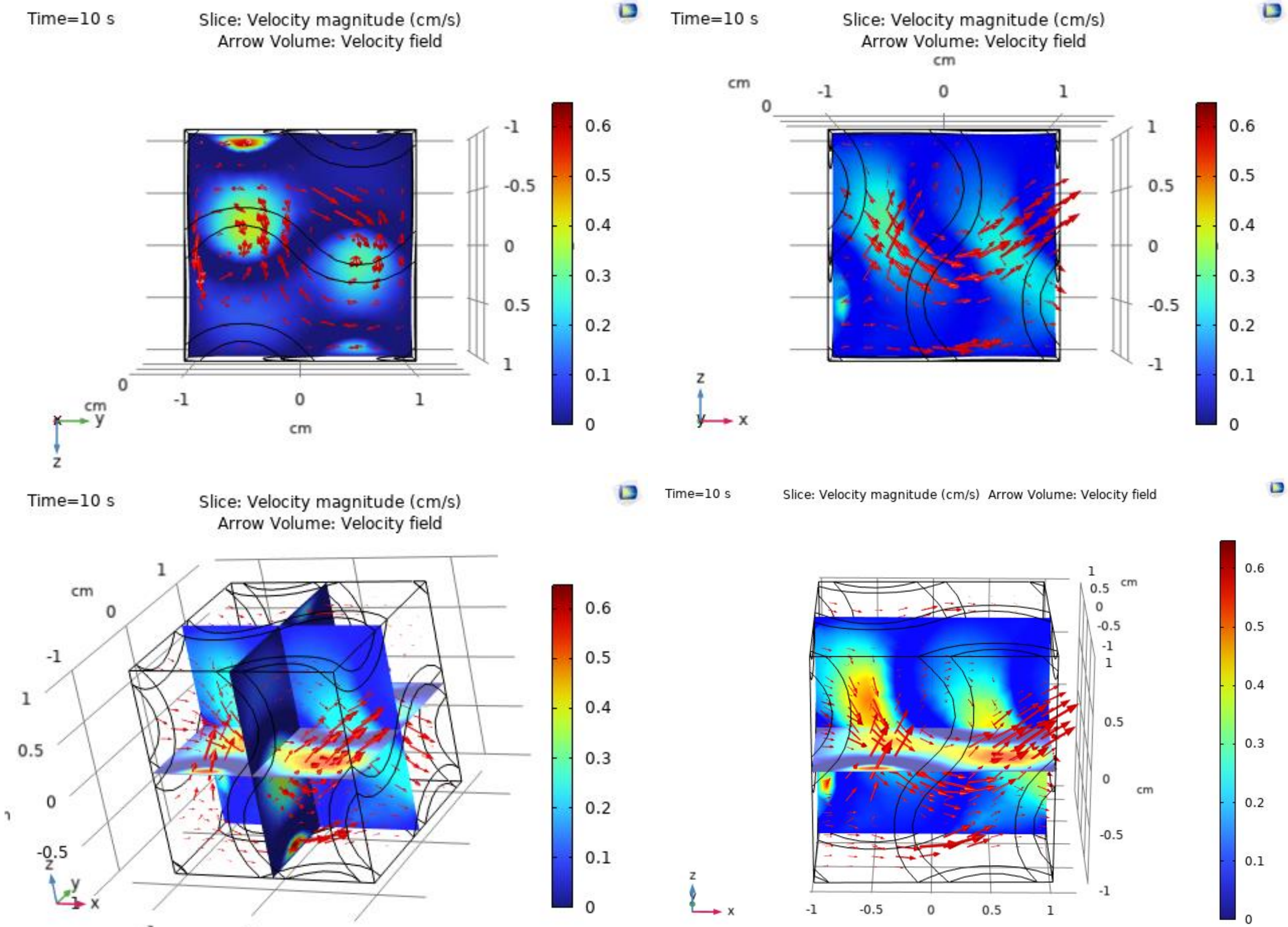
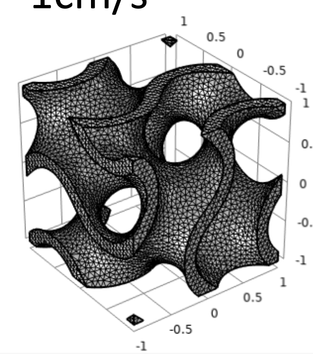


Fig. 7 – (a) Preliminary velocity profile results.

- Profile for a fluid with properties similar to water.
- TPMS size is a 2 x 2 x 2 cm^3
- Initial conditions:
  - Velocity: 1cm/s



Preliminary Results – Fluid Flow inside the TPMS

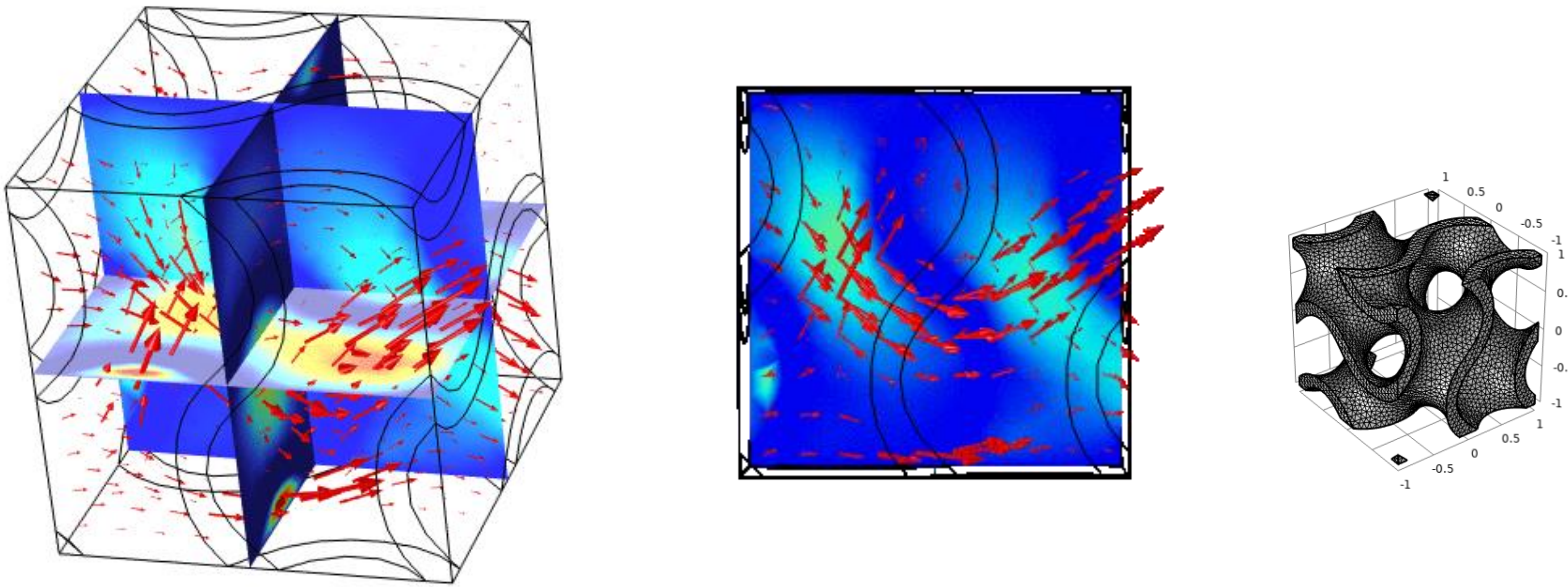


Fig. 7 – (b) Preliminary velocity profile results.

- The arrows represent the velocity magnitude and direction of the fluid flow within the 3D volume
- As the geometry rotates, a sense of how the fluid flow changes depending on the location inside the TPMS is depicted

Multi-fluid simulation: 3x3x3 and 3x1x1 models

- Stationary thermal flow physics modules were implemented and preliminary temperature profiles were obtained from 3x3x3 and 3x1x1 unit cells geometries
- Tungsten carbide (WC), 68.2 KCl - 31.8 MgCl2 (mol%) binary salt (hot reservoir) and steam (cold reservoir) material models were applied

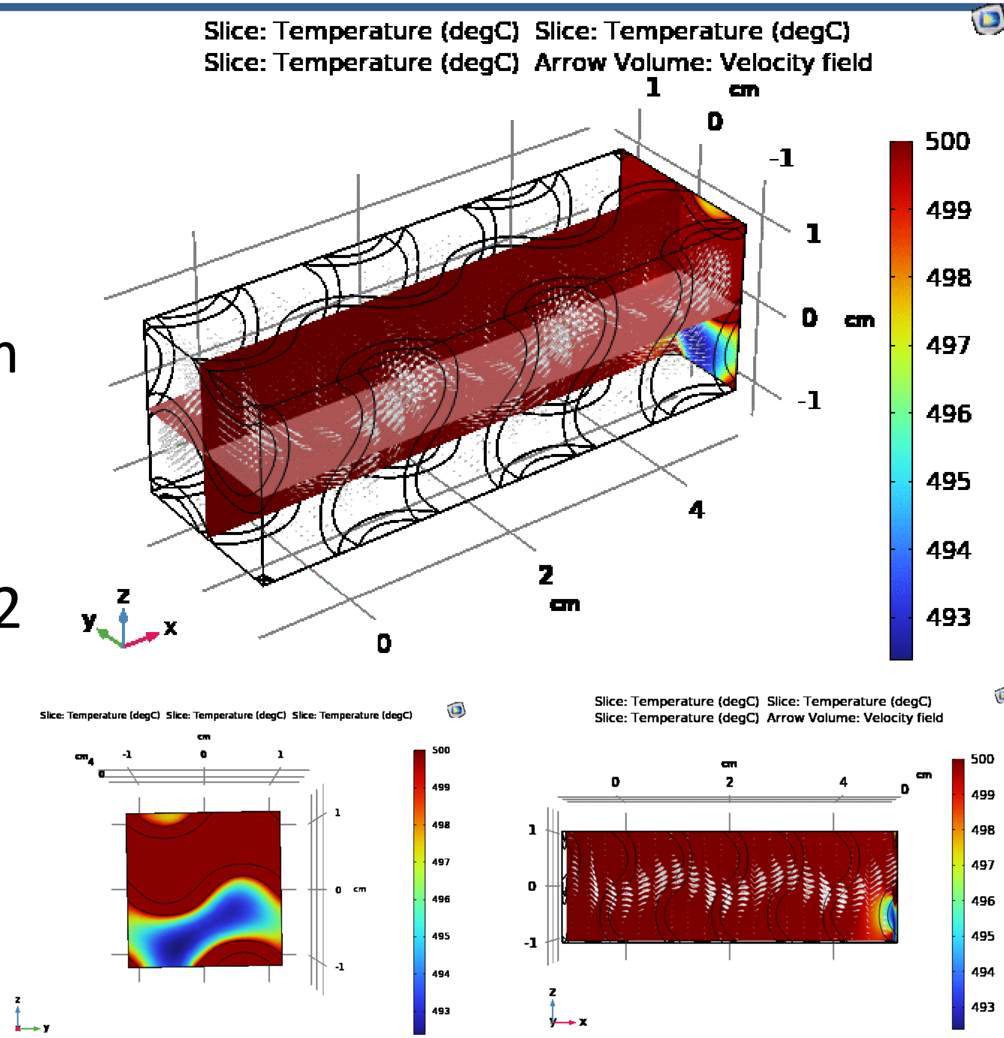


Fig. 8 – (a) Preliminary temperature profile results on a 3x1x1 HX model.

Multi-fluid simulation: 3x3x3 and 3x1x1 models

- Mass and energy balance were checked to confirm conservation on the simulation
- COMSOL expressions that evaluate conservation on the model were utilized
  - 3x3x3 model is conserved within 0.55W
  - 3x1x1 model is conserved within 0.04W
- Heat flux measurements are currently being validated

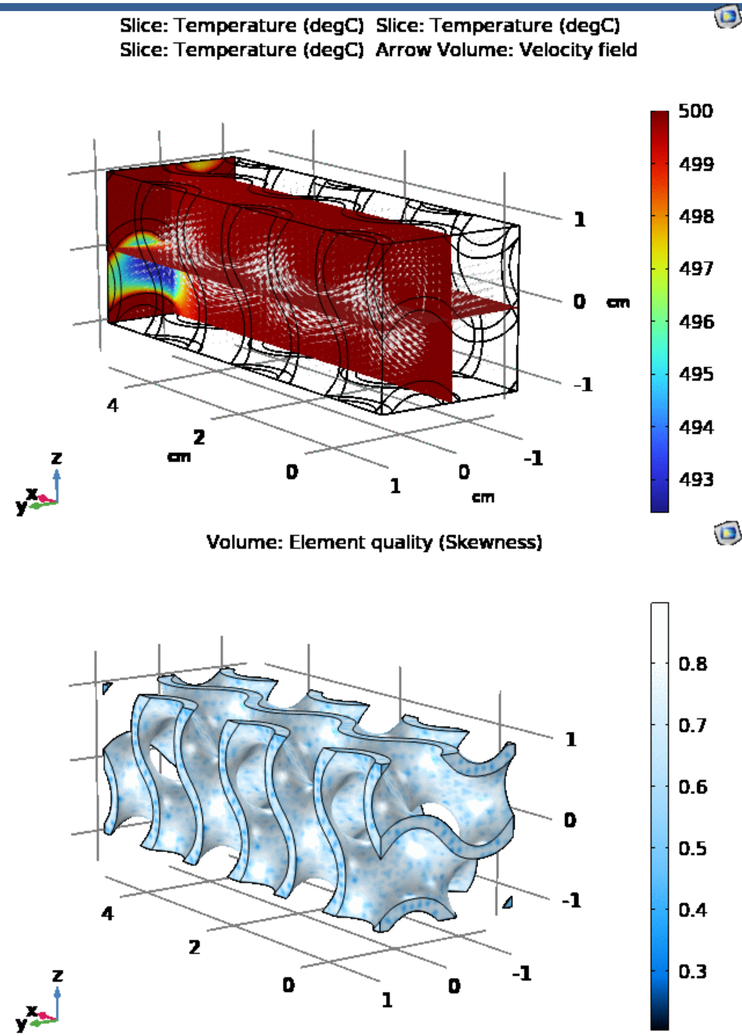


Fig. 8 – (b) Preliminary temperature profile results on a 3x1x1 HX model.

Next Steps

- Validate heat transfer rate by comparing it to energy balance result to obtain numerical error
- Estimate average overall heat transfer coefficient for a single TPMS model
- Perform parametric sweep to estimate overall heat transfer coefficient for different cases

$$U_{th_i} = f(T_i, P_i)$$

$U_{th_i} \equiv$ overall heat transfer coefficient for the i-th thickness
$T_i \equiv$ Temperature on the i-th iteration
$P_i \equiv$ Pressure on the i-th iteration

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