HPC4EnergyInnovation Final Report

Project Title: Compact Diffusion Bonded Heat Exchanger Fatigue Life Simulations

Short Project Description:

Compact diffusion bonded heat exchangers are essential for high pressure heat exchange, but they are subject to thermal fatigue and ramp rate limitations. Simulation of these geometries is challenging with a large range of length and time scales from thousands of mm-sized microchannels inside a m-sized heat exchanger. Multi-physics simulations including thermal, fluid, and solid mechanics components are being used to predict stress within the heat exchangers under these conditions. These predictions can then be used to understand thermal ramp rate limitations while keeping maximum stresses low as well as fatigue life predictions from well-known empirical models.

Company Name: Vacuum Process Engineering, Inc.

Company Sector: Manufacturing

Process Category: Diffusion Bonding

HPC4EI Program (HPC4Mfg or HPC4Mtls): HPC4Mtls

CRADA Agreement ID: 01921.00

MPO ID (if applicable): B628318

Approved/Costed Budget: $300k

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Computational Resources used for Project:

System	Time (MCH)	Largest # of cores used	Commercial Software	Custom Software
TLCC2	0.2	1000	NA	Sierra/TF
TLCC2	0.2	3000	NA	Sierra/SM

Briefly describe any algorithm development. How and to what extent will this development be disseminated internally and/or externally?

This work utilized several Sandia-developed codes within the Sierra environment that are available internally and licensed to select external partners. While no algorithms were developed specifically for this project, technical issues in implementing the physics codes resulted in code improvements and bug fixes which will benefit the broader Sierra user community. The simulations performed for this project required large memory resources and 64-bit node numbering that resulted in a few code modifications related to improving efficiency and handling large node counts.

For instance, significant improvements were made to memory usage efficiency in Krino, a Sandia-developed conformal decomposition finite element method to generating tetrahedral meshes that conform to complex geometry. Because the node count of the meshes required 64-bit numbering, a code modification was required for surface creation in Sierra/Thermal-Fluid.

Executive Summary

Compact microchannel heat exchangers (MCHEs) are an essential component to several clean energy technologies including hydrogen fueling stations and supercritical carbon dioxide (sCO_2) Brayton cycles. MCHEs have exceptional thermal performance, high pressure containment capability, low cost, and compact size. However, the mechanical lifetime of MCHEs is challenging to predict due to the large variety of potential configurations and extreme operating conditions. While studies have attempted to establish guidelines for mechanical lifetime using analytical, experimental, and computational techniques, the computational cost of the coupled multi-physics simulations has limited their practicality. Recent advancements in high performance computing (HPC) resources and code capabilities have enabled coupled thermal-mechanical simulations of a full-scale MCHE geometry to gain insights into localized mechanical stresses due to combined loading from pressure, thermal gradients, and transient operational conditions. The insights gained from these simulations will improve design sophistication and MCHE reliability, reduce construction material waste, and increase thermal operating efficiencies which will support a hydrogen economy and reduce the cost of electrical power production.

In this project, a one-way coupled model is developed within Sandia's Sierra code suite of the thermal and mechanical performance of an MCHE. This model uses 1D reduced-order elements to model heat transfer within individual channels coupled to full 3D thermal and mechanical resolution within the remainder of the MCHE. Steady-state simulation analysis is presented for a full-scale prototype MCHE and compared against thermal test data to validate the modeling approach. Transient analyses are also performed to evaluate the development of internal stresses during combined thermal-pressure-flow rate changes that relate to nominal load following and rapid disruptions. This predictive modeling capability provides excellent insight into transient best practices of sCO_2 power cycles.

Introduction

(1) Problem Description:

The purpose of this project is to use multi-physics simulations to gain the first known, first-principles predictions of fatigue and ramp limitations for safe and reliable operation. VPE shared heat exchanger designs, manufacturing knowledge, application understanding, and expert review of simulation predictions. Sandia developed geometry from designs, meshes, simulation workflows, prediction visualization, and fatigue life predictions. The simulations have the greatest known fidelity of any previously published for microchannel heat exchangers. The results include predicted fluid and solid temperatures as well as mechanical stress distributions through the entire volume of the heat exchangers. Fatigue life for various transient scenarios can be predicted using the internal stress response of the MCHE and empirical standards from the American Society of Mechanical Engineers' (ASME) Boiler and Pressure Vessel Code (BPVC) [ASME].

(2) Motivation:

Microchannel heat exchangers (MCHEs) are critical components of sCO_2 power cycles and other heat exchanger applications, especially at high pressure. A representative MCHE is shown in Figure 1 with semi-circular, external headers. The diagram shows the large range of scales involved from approximately mm-sized channels to multiple-cm-sized nozzles that make them a challenge for multi-physics modeling. The channel counts are easily in the hundreds or thousands for benchtop scale units with much larger units in operation.

MCHEs have been shown to work reliably over years of steady state and slow ramping conditions in a variety of research applications across the world. Several manufacturers including Heatric and Kobe Steel have tested them in pressure fatigue to 100,000 cycles or more with excellent lifetime performance [Kobe]. Nevertheless, this testing was limited to pressure fatigue only. Thermal ramping and fatigue life limits are a much more challenging area and have received little attention as observed from the known literature.

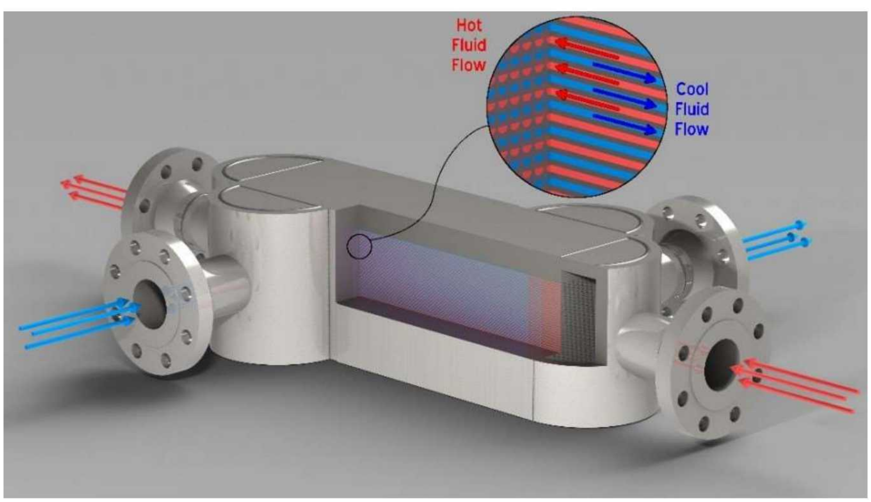

Figure 1. Schematic of microchannel heat exchanger with external headers. Cut-away view shows internal core structure with alternating hot and cool layers. Courtesy of Vacuum Process Engineering, Inc. (VPE).

Pra et al. published a very relevant paper investigating thermal ramping of a MCHE with both simulations and experiments [Pra]. They performed coupled computational fluid dynamic (CFD) and finite element analysis (FEA) on a prototype under thermal shock conditions and predicted the stress distribution as a function of time. The thermal shock consisted of a very fast air temperature ramp from 510 to 180°C in 5 seconds that represents a loss of offsite power with turbine trip for a nuclear application. The testing consisted of 100 cycles with no observed failure. While this is the most comprehensive published work known on transient predictions and testing, it has several shortcomings. The microchannels were not resolved but were modeled as a porous media in an infinite stack using symmetric boundary conditions and air as the working fluid. While stress concentrations at the internal header corners were resolved, the potential stress increase from differential thermal expansion in the channel ribs and corners was not captured. Additionally, any interaction between the microchannel core and the thick top and bottom plates was not captured with the symmetry condition in this direction.

Moisseytsev and Sienicki investigated severe accidents in a complete sCO_2 Brayton cycle coupled to a Sodium Fast Reactor and their impact to MCHE wall thermal ramp rates [Moisseytsev]. Their complete system model allowed for transient analysis while the MCHE model was discretized with 5 axial nodes for the reactor (primary) heat exchanger, high and low temperature recuperators, and a cooling heat exchanger. The transients investigated ranged from gradual and high frequency load following to very rapid but low probability severe accidents. While it presents realistic system transient conditions, the MCHE model has been simplified and does not resolve stress concentrations and other geometrical effects. Nevertheless, it has great value in providing inputs to a higher fidelity model that are representative of a complete system. Since the paper presented mainly the reactor heat exchanger wall temperature time histories, the authors were consulted and shared sCO_2 fluid conditions throughout the system as a function of time for transient modeling in this work.

The current work builds on these previously published studies and is the highest fidelity MCHE model known for either steady or transient conditions. It is expected to provide detailed insight into stress concentrations, header effects, and differential thermal expansion and their impact on mechanical lifetimes.

(3) Modeling and Simulation Approach:

The capability to numerically model the transient thermal/mechanical response of an MCHE has been developed within Sandia's Sierra code suite. This capability utilizes a workflow that consists of geometry discretization, thermal simulations, and solid mechanics simulations. Each of these steps is discussed in further detail in the following subsections.

MCHE Geometry and Discretization

In this paper, the Sierra/Aria software [Sierra] used for these simulations uses finite element solutions of the thermal diffusion equation and quasi-static equations of motion. Therefore, a numerically discretized representation of the MCHE geometry is required. A prototype MCHE geometry (see Figure 2) is considered with alternating layers of Z and straight microchannels that represents a typical design. This represents an actual heat exchanger that was designed by Sandia and manufactured by VPE in 2015 with a straight channel profile. The design is not proprietary and has semi-circular channels with a diameter of 0.06" with the center 0.01" below the plate surface. The rib width is 0.06". The plate width is 6" and length is 18". Each plate contains 33 channels and the full geometry consists of 40 channel layers (20 each of Z and straight channels) along with end caps and headers.

Figure 2. Prototype geometry used for the simulations and for validation testing.

For computational efficiency, the simulations herein contain five pairs of layers that constitute one fourth of the full stack height. A hexahedral mesh was generated in CUBIT [CUBIT Team] that conforms to this simplified geometry and is shown in Figure 3. This mesh contains 28.8 million elements and 30.8 million nodes. Scaling up to the full height is desirable but proved a challenge to even modern HPC hardware. Initial mesh refinement studies indicate that further refinement is necessary, but results are convergent. Specifically, only three elements are currently included between channels both horizontally and vertically, which may not be suitable to fully capture gradients that exist between heat transfer layers.

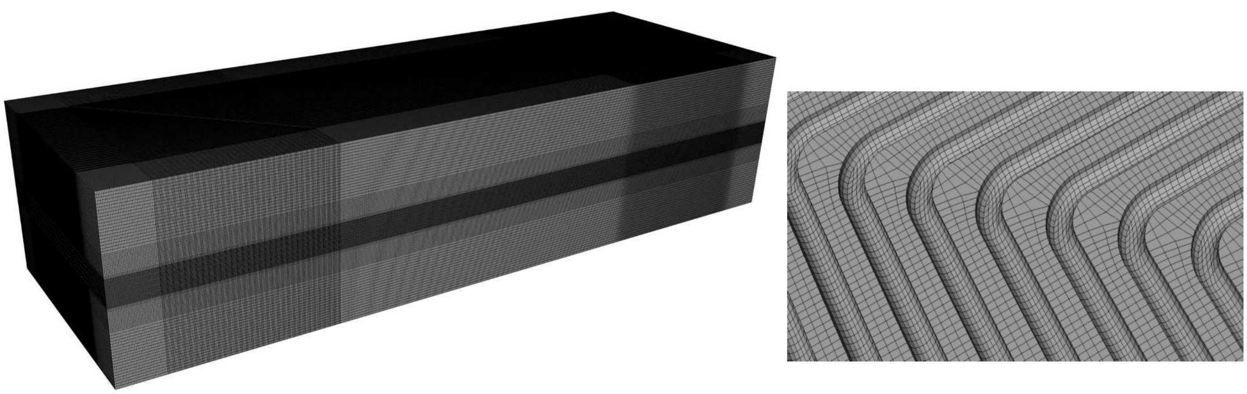

Figure 3. Computational mesh for simplified MCHE core geometry consisting of 5 heat transfer layer pairs. The full core (left) mesh shows refined elements near heat transfer layers and coarser elements in end caps. Close-up image of mesh around Z channel corners (right) illustrates channel resolution with some lower quality elements that occur near complex geometric features.

Thermal Model

To simulate the thermal response of a MCHE, the temperature field is determined by solving the thermal transient advection-diffusion equation:

$$\rho C_p\left(\frac{\partial T}{\partial t}+v\cdot\nabla T\right)=\nabla\cdot(k\nabla T)+Q \tag{1}$$

where ρ is density, C_p is specific heat, T is temperature, t is time, v is the fluid (advection) velocity, k is thermal conductivity, and Q is a heat source. The advection term is only used in the microchannels. Closure of the thermal diffusion equation requires an initial temperature.

Several conditions are applied to account for the heat transfer mechanisms at the boundaries of the computational domain. The exterior surfaces of the MCHE interact with a $T_{\mathrm{ref}} = 300$ K (26.85°C) environment reference temperature via radiation and natural convection. The radiative flux is determined by:

$$q=\varepsilon\sigma\left(T^4-T_{ref}^4\right) \tag{2}$$

where ε is the emissivity of the overwrap and σ is the Stefan-Boltzmann constant. For this work, $\varepsilon = 0.3$ and $\sigma = 5.67\times10^{-8}$ W/(m^2·K^4). Convection around the MCHE core is approximated by assuming laminar natural convection occurs from vertical sides for which the laminar natural convection coefficient, h, in air can be estimated as:

$$h=1.42\left(\frac{\Delta T}{L_y}\right)^{1/4} \tag{3}$$

and laminar natural convection from the top flat surface is given by:

$$h=1.32\left(\frac{\Delta T}{L_x}\right)^{1/4} \tag{4}$$

and laminar natural convection from the bottom flat surface is given by:

$$h=0.61\left(\frac{\Delta T}{L_x^2}\right)^{1/5} \tag{5}$$

where L_x and L_y refer to the MCHE length and height [Sierra].

Boundary conditions must be also applied to allow heat exchange between the MCHE core and the working fluid as it flows through the microchannels. For the geometry considered here, there are 33 channels in each layer which each requires a convective boundary condition. Thus, there are 165 (straight) channels on the hot side and 165 (Z) channels on the cold side. The heat transfer coefficients in each of these boundary conditions are determined from the Dittus-Boelter correlation which is defined as follows:

$$h=\frac{k}{D_h}\mathrm{Nu} \tag{6}$$

$$\mathrm{Nu}=0.023\,\mathrm{Re}^{0.8}\,\mathrm{Pr}^{0.4} \tag{7}$$

where D_h is the hydraulic diameter, Nu is the Nusselt number, Re is the Reynolds number, and Pr is the Prandtl number. The hydraulic diameter is determined by $D_h = 4\,A/P$, where A is the cross-sectional area of the microchannel and P is the wetted perimeter of the microchannel. Re is given by $\mathrm{Re} = \rho v D_h/\mu$, and Pr is defined by $\mathrm{Pr} = C_p\mu/k$, where μ is the dynamic viscosity of the coolant.

As discussed above, heat transfer from the MCHE core to the working fluid is inherently dependent upon the velocity of the fluid in the channels. Additionally, the material properties of the fluid depend on temperature, which requires coupling the convective boundary condition for each channel to a model of the fluid flow. Because high-fidelity fluid dynamics simulations for flow in each channel would be computationally too expensive, a one-dimensional, steady state, fully developed flow model is instead constructed for each channel and coupled to the thermal diffusion equation. This approach is implemented within the Sierra/Aria code (Sierra Team) using a feature called an advective bar, in which the continuity equation ($\dot{m} = \rho A v = const.$) is solved on a one-dimensional bar element with nodal mapping to surface elements on the solid mesh. In this simple formulation, the mass flow rate at the inlet must be specified along with the cross-sectional area along the length of the channel.

Mechanical Model

The mechanical response of the MCHE is determined in the three-dimensional elements by solving the discrete equations of motion for the displacement field using the Sierra/Solid-Mechanics code as in

$$\nabla \cdot \boldsymbol{T} + f = \rho \frac{\partial^2 d}{\partial t^2} \qquad (8)$$

where $\boldsymbol{T}$ is the Cauchy stress tensor, f are the distributed body forces, and d is the displacement field. Initial and boundary conditions are required to close the system. Here, the pressure in each channel is applied to the channel walls. Additionally, the mechanical simulations are one-way coupled to the thermal results, such that the temperature field is solved and then imported to the mechanical simulation to determine thermal strains internal to the core. Additionally, boundary conditions were imposed on three sides to constrain the six degrees of freedom for rigid body rotation.

MCHEs are generally manufactured with stainless steel 316/316L that is dual certified for metal content and strength. A linear elastic material model was used with a Young's modulus of 200 GPa and a Poisson's ratio of 0.265. Thermal strain is specified as a temperature dependent function ranging from 0 m/(m·K) at 293 K to 0.00864 m/(m·K) at 773 K. Stresses were calculated at the solid elements using a strongly objective formulation that integrates stress with a mean quadrature rule.

Results

A. VALIDATION OF STEADY-STATE THERMAL RESPONSE

Experiments conducted using the prototype geometry were performed under a parallel project and made available for comparison to thermal simulation results. The experimental data included sCO_2 properties (mass flow rate, temperature, and pressure) at the inlets and outlets of the MCHE. Using the inlet conditions as boundary conditions in the simulation, average steady state outlet flow temperatures were predicted using the thermal model. Table 1 summarizes these conditions and the simulation results. On the hot circuit of the MCHE, the thermal simulation agrees very well with the average outlet temperature of the experiments with a prediction error of the inlet-outlet temperature change very close to -2%. However, the comparisons are not as good on the cold side with a prediction error of -18%. This is likely due to the cold inlet flow being near the critical point of CO_2, at which material properties change drastically and are therefore more uncertain and harder to resolve. Nevertheless, this validation comparison does provide a level of confidence in the temperature predictions.

Table 1. Prototype MCHE validation study conditions and results

	Inlet Conditions			Outlet Conditions		
HX Circuit	**Per Channel Flow Rate [kg/s]**	**Pressure [MPa]**	**Temp. [K]**	**Experimental Temp. [K]**	**Simulation Temp. [K]**	**Temp. Change Error [%]**
Cold	9.2×10^{-5}	8.56	311.9	416.6	397.7	-18.05
Hot	8.8×10^{-5}	8.54	505.5	337.0	340.4	-2.02

B. TRANSIENT RESPONSE

The following discussion presents results from a specific transient event to demonstrate the capability of the thermal/mechanical modeling developed under this project. The large pipe break scenario detailed below is only one scenario of interest to VPE but consists of steep gradients in pressure and temperature. Other transient conditions of interest to VPE include start-up, load-following, and shut-down scenarios in which the changes to the temperatures and pressures are more gradual than those experienced in the large pipe break scenario considered here.

The transient simulations shown here use the reduced prototype geometry (5 repeated heat transfer layers) and use the conditions from Figure 4 and Figure 6 to model the thermal/mechanical response of the MCHE to a large pipe break event in which the mass flow rate, channel pressure, and inlet temperatures are transient functions. These conditions, which are scaled to represent the predictions from Moisseytsev and Sienicki's work, indicate that the pressure and mass flow rates in the channels decrease rapidly, while the inlet temperatures (shown in Figure 6) increase on the hot side and decrease slightly on the cold side [Moisseytsev]. In the prototype geometry considered here, the cold and hot working fluids are in counterflow.

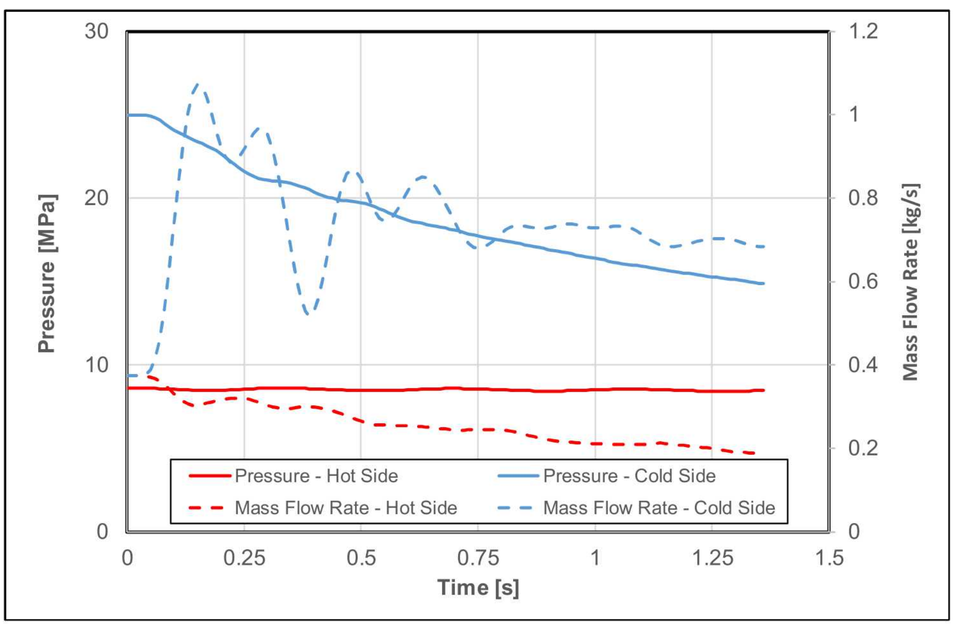

Figure 4. Large pipe break pressure and mass flow rate conditions

The thermal and mechanical simulations are solved for steady state behavior for the initial transient conditions to establish steady temperature and stress fields prior to the transient simulations. Both transient thermal and mechanical simulations were run on 256 processors and required approximately 4 hours run time to complete the 1.36 s transient event with 0.1 s timesteps.

THERMAL RESPONSE

Results of transient thermal simulations of the MCHE response to a large pipe break event are presented in Figure 5 and Figure 6. In Figure 5, qualitative temperature distributions are visualized for the MCHE core. Cold fluid enters the Z channels on the left front of the MCHE and exits out of view in the rear right of these images. Hot fluid enters the straight channels on the right side and exits the left side of these images. In the cutaway views, the one-dimensional fluid elements are exposed showing the temperature distribution of the microchannels. Three-dimensional temperature effects are observed in these images, stemming from the fact that the MCHE is asymmetric vertically. Essentially, cold layers on top of hot layers results in the top end cap being cooler than the bottom. Likewise, the Z channel configuration creates a lateral asymmetry making the front, left corner of this MCHE the coolest section of the core.

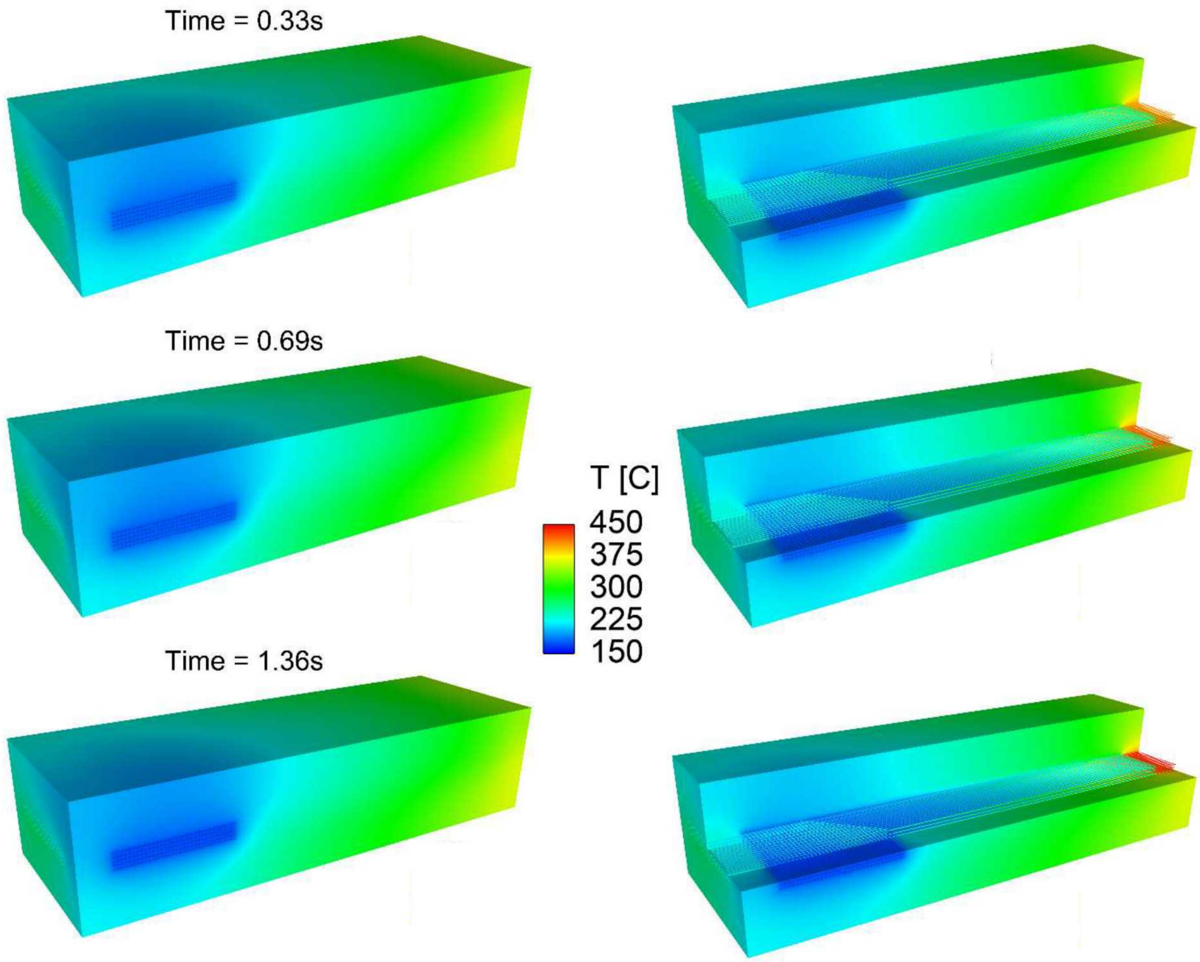

Figure 5. MCHE core temperatures at several times following a large pipe break event. Shown at each time is the full three-dimensional core (left) and a cutaway to show internal core and channel temperatures (right).

Figure 5 also indicates the transient thermal behavior during the large pipe break scenario modeled here. Although the temperatures in the bulk of the core do not change significantly over the short 1.36s duration simulated here, there are a couple of changes that occur. Primarily, the hot inlet temperature increase during the event and therefore the steel core heats up around the hot inlet channels, especially where there is no cold channel nearby to move the heat out of the system. This heat does not appear to propagate deeply into the core, most likely due to the short duration of these simulations.

Figure 6 provides a line plot of channel-average temperatures at the inlets and outlets for both the cold and hot sides. Note that because the fluids are in counterflow, it is possible that the outlet temperature for the cold side is hotter than the hot side outlet. Another interesting result is that although the hot side inlet temperature increases, the outlet temperatures for both sides are generally unchanged. This is likely due to the mass flow rate on the hot side decreasing more rapidly than that on the cold side. The unchanged outlet temperatures indicate that the excess heat is conducted into the MCHE core and over the short duration of this simulation has not fully diffused into the cold channels for removal, which would appear as an increase in the cold side outlet temperature.

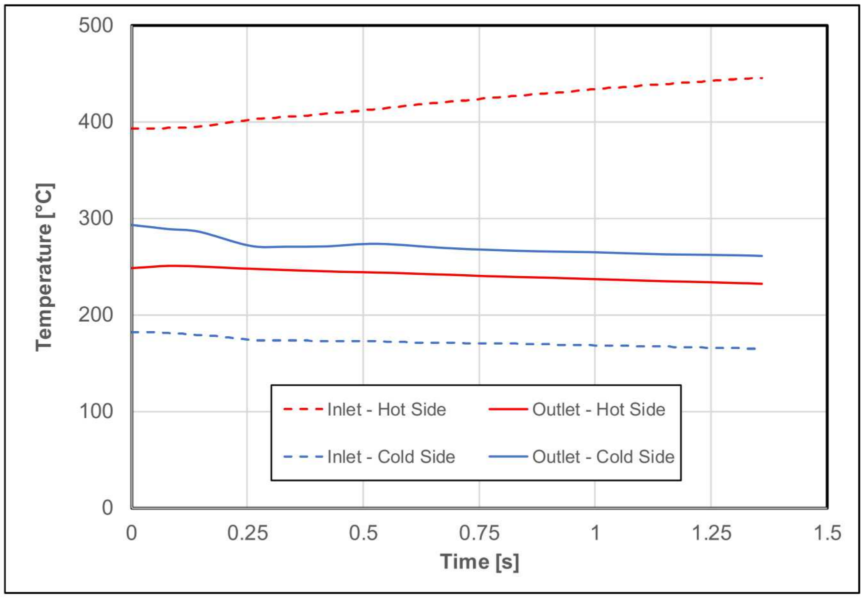

Figure 6. Average transient channel inlet and outlet temperatures following a large pipe break.

MECHANICAL RESPONSE

Using the transient thermal response, transient mechanical simulations were conducted to determine the internal stress state of the MCHE during the large pipe break transient. The results of these simulations are provided in Figure 7 through Figure 9. The qualitative images showing the von Mises stress field in Figure 7 and Figure 8 indicate that the stress is largest at the channel surfaces, with concentrations at the sharp corners that exist between layers as well as in the bottom of the channels. It is apparent that the von Mises stress is nearly uniform along the central length of the MCHE and does not significantly change between layers. This evidence could be used to claim that the 5 layers used here is sufficient to model the internal stresses for this particular geometry, since adding heat transfer layers would unlikely change the internal stress state. The transient mechanical response is observable in that the stress increases not only along the channel walls but also in the MCHE core, especially near the initial intersection of the hot side channels with the cold side channels. This increase in stress is due primarily to thermal strains developing in the MCHE core as hot circuit channel temperatures increase while the pressure is nearly constant during the transient. Therefore, along the entrance length of the hot circuit channels, increased stress on the channel walls propagates further into the core due to thermal diffusion.

Figure 11

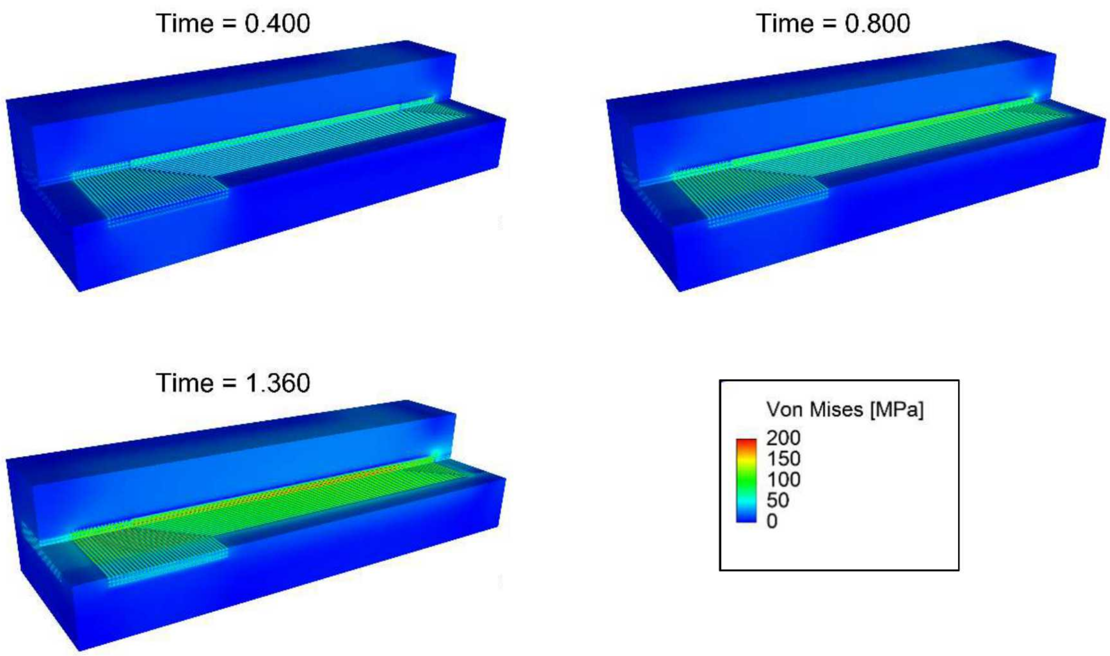

Figure 7. Cutaway view of MCHE core showing the von Mises stress at various times to illustrate the mechanical response to the large pipe break event.

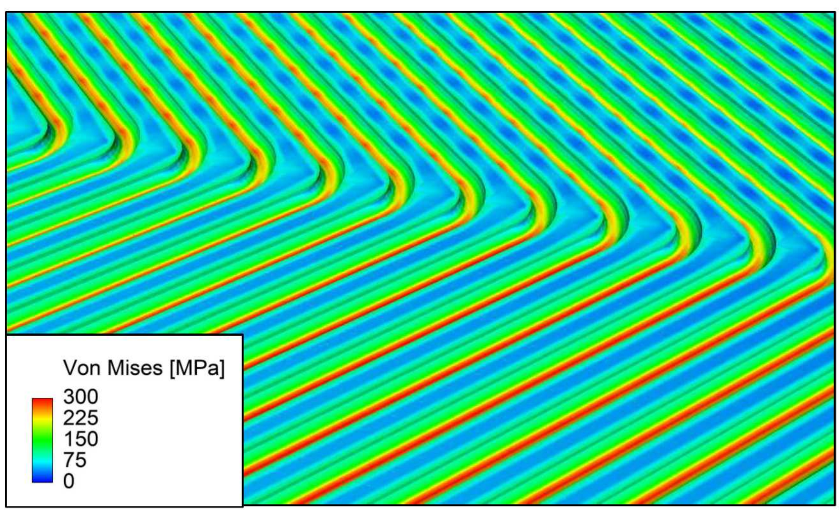

Figure 8. Magnified view showing location of maximum stress at the bottom of the microchannels. Note the steady stress on the channels in bottom of the image and the periodic stress in the top due to the adjacent set of channels below that are all straight.

Figure 9 shows the maximum von Mises stress in the MCHE during the large pipe break event. Although the maximum stress is perhaps not the best indicator of performance as it can be subject to localized simulations conditions, it is used here to illustrate the changing state of the MCHE. The maximum stress occurs in the bottom hot side along the entrance length prior to exchanging heat with cold channels. The stress increases here due to the constant hot side pressure and increasing inlet temperature. It is worthwhile to note that the maximum stress shown in this plot exceeds the nominal yield stress for 316/316L, which is not entirely unexpected for MCHEs as local yielding of the very ductile material is expected to relax and reduce stress concentrations, but does indicate that the linear elastic material model may be insufficient for similar simulations in the future.

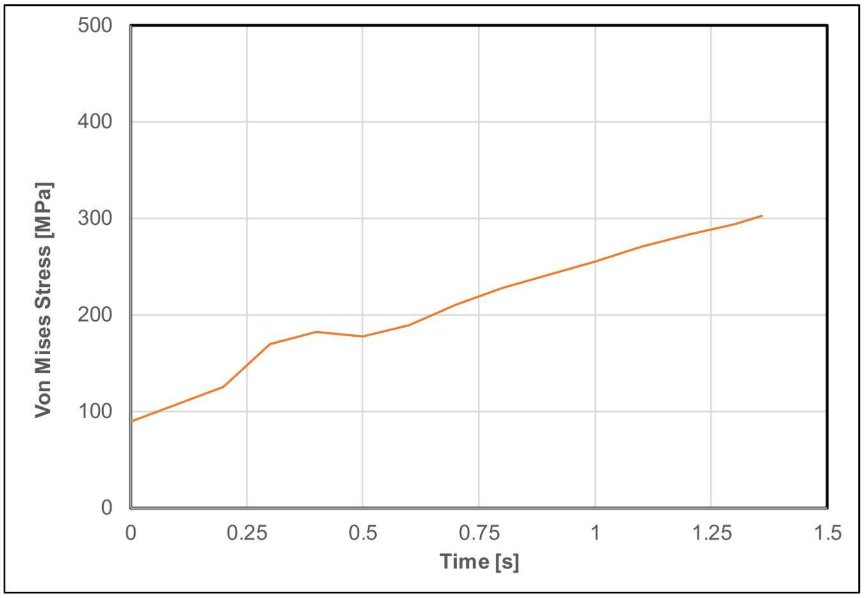

Figure 9. Maximum von Mises stress in MCHE core during response to large pipe break transient.

FATIGUE LIFE PREDICTIONS

The maximum von Mises stress cyclic amplitude can be used to predict the number of design cycles with the help of the ASME BPVC [ASME], assuming the same transient was repeated. The BPVC, Section VIII, Division 2 contains rules for fatigue life predictions given a material, temperature, and stress amplitude. There is specific guidance in ANNEX 3-F, Design Fatigue Curves, 3-F.1.2(b) for Series 3XX High Alloy Steels for temperatures not exceeding 427°C. A calculator was developed from the equations to predict the design fatigue life with the results shown in Figure 10. The curve is the theoretical design life in number of cycles given a stress amplitude (though the curve shifts based on temperature). The average inlet temperature of the hot circuit of 325°C was used as well as the stress amplitude of 105 MPa (half of the predicted stress range from Figure 9). The result is a design fatigue life of about 700,000 cycles shown in Figure 10 as a box, much higher than anticipated for such rapid transient conditions. Of general note, the fatigue life through the entire curve is surprisingly higher than expected from the perspective of ramp-type transients where the stress amplitude is taken as half of the range. Perhaps the curves were developed assuming purely oscillatory behavior with a zero mean stress, but they are the best known method for mapping predicted stress transients to fatigue life. The current application of these methods needs to be verified.

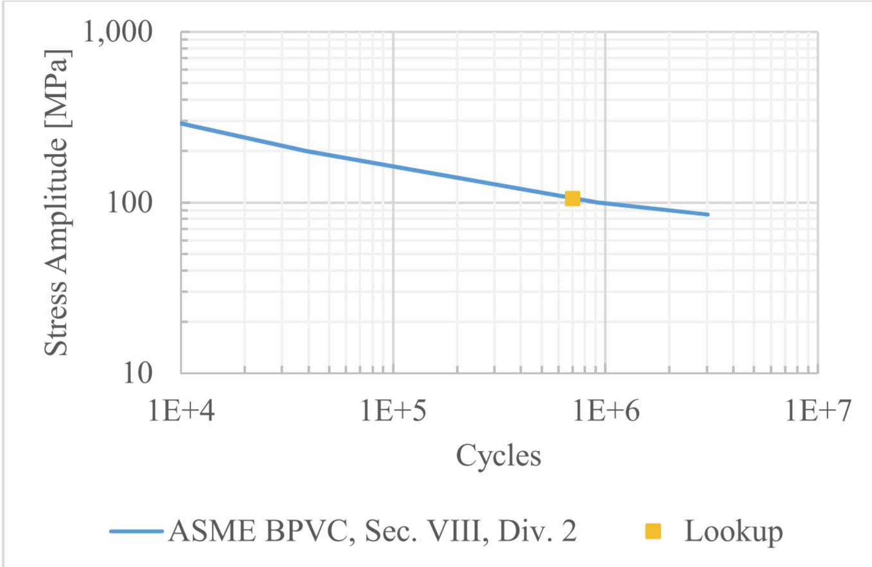

Figure 10. Design fatigue life curve from the ASME BPVC for 3XX Series stainless steels

Discussion

This work contains the highest fidelity simulations known in terms of multi-physics and geometrical features represented for the challenging problem of MCHE modeling in steady state conditions, not including the added complexity of transient modeling. It is the first step to provide first-principles informed guidance for MCHE ramp rate and fatigue life best practices where no other information exists. The original goal was to predict fatigue life for a fast transient (such as the large pipe break described herein), an electric grid load-following case, and a parameter study to determine the ramp rate required for (practically) infinite fatigue life. The fast transient was selected first as it was expected to be the worst-case scenario. The load-following case was attempted but not possible with the challenges encountered and the infinite fatigue life was not possible.

The predicted fatigue life with the large pipe break transient was 700,000 cycles, much higher than expected. Given the rare occurrence of this event, the initial results suggest that it is not a limiting case for fatigue life. But the lack of full geometry, including headers where higher stress amplitudes are likely, limits this to only a partial conclusion.

The magnitude of the maximum stresses was higher than expected. The predicted values are a localized quantity that may be artificially high from a single low-quality element and don't account for yielding over a small area. This behavior was initially concerning but talks with project partner VPE helped the Sandia team understand practical design principles. MCHEs are carefully designed according to ASME BPVC requirements that dictate the allowable stress levels in the bulk material [ASME]. Maximum stresses tend to relax and be spread over an area such that the stress through the thickness of the pressure vessel will remain within allowable limits.

Implementation

The project was divided into phases where physical phenomena are incrementally modeled and compared against experimental data until the full application is simulated. VPE and Sandia participated in monthly conference calls for progress updates and information exchange. Additionally, the results will be made available to VPE for continued post-processing and analysis after project completion. The planned tasks are outlined below:

Task 1: Define Simulation Conditions
Planned Activity: VPE defines problem statement and physical conditions to be modelled and Sandia verifies understanding
Status: Complete
Explanation: VPE and Sandia agreed upon geometry, physical properties, and operational scenarios early in the project. Regular information exchange facilitated changes in scope as the project progressed.

Task 2: Steady-state Thermal Analysis
Planned Activity: Sandia performs thermal simulations to replicate 1) experimental conditions for validation study and 2) VPE application conditions to test scalability of models
Status: Complete using reduced geometry
Explanation: The goal of this task was to conduct thermal simulations of a full scale MCHE geometry with integrated headers. However, the full-scale simulations were not completed due to computer memory issues encountered implementing the model in the Sierra/TF code. A reduced geometry representing 5 heat transfer layers was used instead to complete this task. Available experimental data consisted of an average of the channel outlet temperatures and was compared to simulation results with scaled mass flow rates for validation purposes.

Task 2a: Steady-state Thermal Analysis Verification
Added Activity: Small-scale geometry mesh resolution studies.
Explanation: Due to early issues in modeling full-scale geometries, attempts were made to better understand the meshing requirements for the problem. A quarter geometry MCHE with a reduced number of channels was modeled to assess the impact of element size on solutions and guided the mesh resolution for larger scale simulations.

Task 3: Steady-state Mechanical Stress Analysis
Planned Activity: Sandia performs mechanical stress simulations to replicate 1) experimental conditions for validation and 2) VPE application conditions to test scalability of models
Status: Complete using reduced geometry
Explanation: Because the mechanical simulations required one-way coupling with the thermal simulations, the same reduced geometry was used to complete this task. Another variation from the desired outcome was that convergence of the numerical solution could not be obtained unless the boundary conditions were overly constrained which resulted in internal stresses that were larger than expected. Validation of the mechanical simulations was not performed due to time constraints.

Task 4: Header and Microchannel Turbulent Flow Analysis

Planned Activity: Sandia performs computational fluid dynamics simulations to replicate 1) experimental conditions for validation and 2) VPE application conditions to test scalability of models
Status: Incomplete
Explanation: Due to the difficulty to model the full geometry with integrated headers and other setbacks, this task was not possible.

Task 5: High Fidelity Transient Multi-physics Analysis
Planned Activity: Sandia performs full transient multi-physics simulations coupling independent models to replicate VPE application conditions
Status: Complete using reduced geometry
Explanation: This analysis was completed with reduced geometry using conditions from a large pipe break severe accident scenario. The thermal and mechanical predictions suggest that the MCHE can survive many cycles under these conditions.

Task 6: Document Research
Planned Activity: Sandia documents results for full simulation and describes project activities
Status: Complete
Explanation: A draft paper was submitted and accepted to the sCO_2 Power Cycles Symposium and will be presented when the meeting occurs in February 2021.

Issues or Challenges

This project encountered several challenges and issues during its execution. Perhaps the biggest impact to the project was staff availability at Sandia. The original timeline and funding were enough to dedicate a single staff member at over a half-time for a year. Unfortunately, staff were overloaded and could not commit to that level of effort. To mitigate this, the project period of performance was extended twice so that this project lasted nearly two and a half years. It is possible that this extended schedule added some inefficiencies associated with working on several projects concurrently.

Additionally, some technical barriers existed and were not fully overcome. The element count required to capture the mm-scale microchannels in a tens/hundreds of cm-sized MCHE was and remains a challenge. The magnitude of the simulations attempted here encountered memory issues on all codes used. Through user support tickets, direct interaction with developers, and reduction of simulation scales, useful models were developed. By working with the code teams, several bugs were identified and fixed, some memory issues were resolved, and much was learned about how to approach a large-scale problem like MCHE thermal/mechanical response.

Impact

Company Impact: *Describe the economic, energy, and/or material consumption impacts your company expects to realize due to this project. Impact examples include energy and material savings, increased competitiveness, job creation or enhanced job stability.*

The knowledge gained by Sandia and VPE will be used to ensure confidence in transient operation of microchannel heat exchangers. Additionally, as the project results will be shared with a wider audience at an industry conference, the benefits will be wider reaching. The greater understanding of best practices will likely improve customer confidence and lead to greater adoption of these novel heat exchanger designs. VPE, as the lead domestic manufacturer of microchannel heat exchangers, will benefit by increased sales that will increase revenue and create jobs. Currently VPE is expanding their workforce and manufacturing capabilities to keep up with unprecedented demand. The consumer can likely realize lower product costs such as lower electricity prices through more efficient and compact power cycles and reduced hydrogen vehicle fuel costs.

Describe how collaborating with the National Laboratories has impacted your organization's operations and competitiveness. Descriptions can be qualitative or quantitative in nature as appropriate.

Small companies such a Vacuum Process Engineering, Inc., are inherently at a competitive disadvantage when the business model is capital intensive. Even with a strong management-belief in the value of research and development, a lack of adequate financial resources can starve innovation.

The value that the National Laboratories brought to VPE is considerable. A hand-in-glove fit of VPE's needs with the technical assets and intellectual capital of the National Laboratories, has multiplied the output and successes with what we were struggling to accomplish on our own.

Our relationship with National Laboratories has:

- Made available the technical (staff, facility and plant) resources to enable us to problem solve, test, and validate our designs
- Enabled VPE to recruit the technical talent needed to foster invention
- Helped VPE grow revenue by roughly 120%, and our number of employees by 90%, since our initial collaboration
- Contributed to introduction of our product line of COTS (Commercial off-the-shelf) microchannel heat exchangers. These MCHEs are now sold worldwide, supporting Hydrogen-based transportation infrastructure, energy efficiency mandates, renewable energy, aviation, defense, etc.
- Enabled us to speak with and meet, scientific staff who provided important insights into problem solving in areas where our own technical staff lacked specific expertise
- Assisted in the development and demonstration of new product features that will contribute to VPE growing reputation as an innovative company
- Helped us discover funding opportunities that fit our R&D initiatives and market growth strategy.

National impact: Describe how the results of this project can or will lead to national scale impacts. What economic, energy, and/or material impacts be to your industry? Examples include energy and material savings, increased competitiveness, job creation or enhanced job security or stability.

The Department of Energy is likely to benefit from this work that built confidence in microchannel heat exchangers and attempted to develop best practices. The benefits will likely be realized in several industries including electricity production with sCO_2 and gas turbine power cycles, transportation energy with hydrogen fuel cell vehicle filling stations, liquified natural gas processing, and others. The simulation capabilities developed in this work are likely to be used for further development and application to numerous MCHEs in a variety of industries. One direct example of this is that the modeling approaches developed here will be applied to a currently funded ARPA-E project led by VPE to develop design optimization tools for high pressure and high temperature heat exchanger applications.

Future Work

For even more complex channel geometries, like zig-zag or serpentine channels, a standard meshing tool like CUBIT is insufficient to develop a fully conformal mesh. Meshes on these geometries require a more novel approach like the Conformal Decomposition Finite Element Method (CDFEM), which combines a description of the channel boundaries and a background mesh to create a mesh conformal to the geometric description.

As illustrated in Figure 11, the CDFEM workflow takes a tetrahedral mesh of the core, superimposes the channel definitions to define level set fields on the background mesh which are then used to decompose the mesh into sub-elements that conform to the channel boundaries. To demonstrate the utility of the CDFEM method, a mesh has been created for the full prototype geometry and is shown in Figure 12.

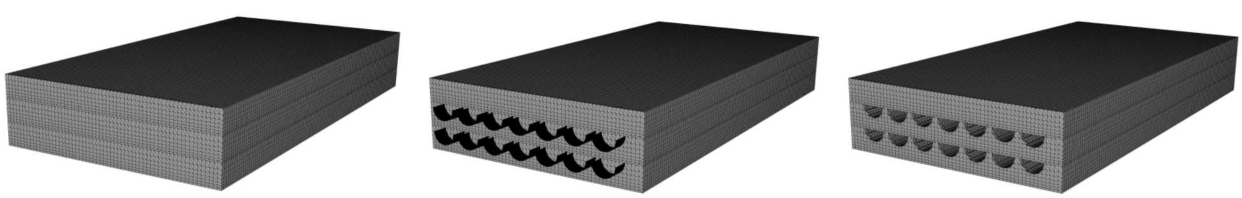

Figure 11. Schematic illustrating CDFEM workflow with background mesh (left), microchannel definition (center), and resulting mesh (right).

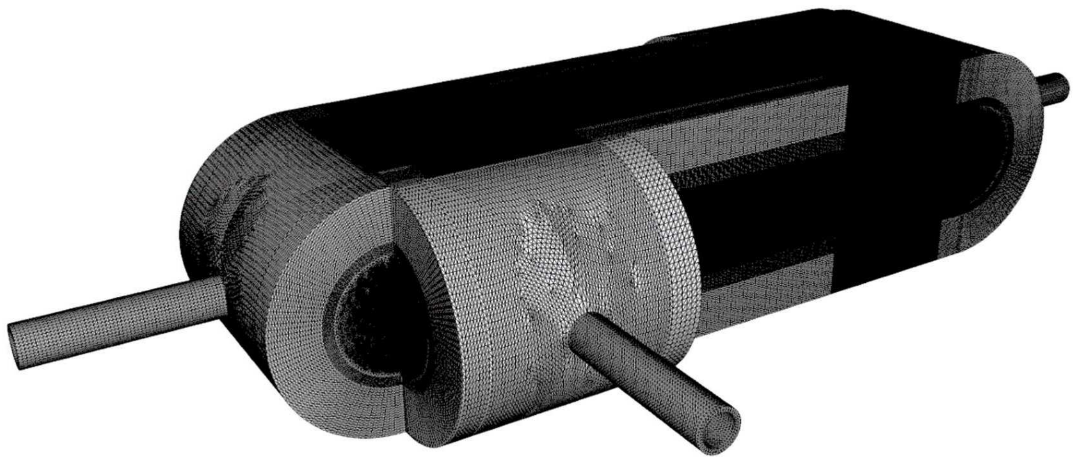

Figure 12. Schematic showing the full-scale mesh of the prototype MCHE with headers.

The work shown here is still developing and much more work is required before the MCHE simulations can be considered predictive. First, a significant effort in verification and validation of the model must be completed. Solution verification activities including mesh refinement studies to establish credibility that the solutions are convergent and work to ensure that linear tetrahedral elements are sufficient for the mechanical analysis are required. Additionally, the validation study using data from recently performed sCO_2 experiments suggests that the model should be developed further to reduce thermal prediction errors and increase model confidence for transient cases or geometries that are not feasibly tested.

Furthermore, the preliminary results shown here can be extended in many ways. For instance, by increasing the duration of the simulations, the long-time response following a transient event can be captured to better understand MCHE performance. Also, using the full-scale geometry for future simulations will enable analysis of the mechanical and thermal behavior in the headers, a likely location of fatigue under duty cycling. Finally, by performing simulations of cyclic operation of the MCHE, estimates of MCHE fatigue can be developed and used to improve future designs in order to minimize acceptance testing for MCHEs with sCO_2.

Pictures for Publication:

Figure 1 and Figure 8 and their captions are excellent for publication.

Laboratory PI Experience Feedback

(1) Why were you interested in working with the HPC4EI program?

I was excited to work with the program to obtain funding to support the collaborative R&D that our industry partner VPE desired. They attempted to develop simulations on their own with commercial software and soon realized that the HPC resources of the national labs were required to simulate their challenging application. The model of funding national labs to support industry applications is very powerful.

(2) Was your overall experience as part of the HPC4 Energy Innovation Program positive, neutral, or negative? Why?

The program experience was very positive as the funding was sizable, the model for collaborative R&D with industry was effective, and the feedback was constructive.

(3) Did your experience as an HPC4EI PI help build your capabilities and expertise? How?

The experience strongly built our capabilities for both program and personnel management as well as technical simulation capabilities. This has been my largest project as PI and allowed me to work with other staff in a positive way. The group was able to develop the highest-fidelity simulation workflows for multi-physics simulations of microchannel heat exchangers known.

(4) How can the HPC4 Energy Innovation program be improved?

We could have benefitted from feedback on our quarterly reports to provide a wider perspective with unique ideas to improve our work.

Company Experience Feedback

(1) Have you already or do you intend to submit a Phase 2 proposal for this project?

a. If yes, when?

We intend to submit Phase 2 proposal for this project, in the fourth quarter of 2020.

b. If no, why not?

(2) Is this your first project funded through the HPC4 Energy Innovation Program? If not, with how many previous projects have you been involved?

This is our first project that was funded through HPC4 Energy Innovation Program.

(3) Was your overall experience as part of the HPC4 Energy Innovation Program positive, neutral, or negative? Why?

Our overall experience with the HPC4 Energy was very positive. Key aspects of the project were accomplished and contributed to the understanding of best to model computationally complex monolithic microchannel heat exchangers. Heretofore, VPE tried using sophisticated commercial modeling software and computation services. However, memory and processing speed challenges were promptly found, and our work stopped. In addition to designing a computation strategy, we obtained results of commercial value. Specifically, our MCHE Hydrogen Precooler, which was designed using ASME design guidelines, was found to be within working stress criteria when operated at approximately 1000 bar. These findings are an important commercially competitive advantage that other foreign manufacturers do not have. I'm positive that the findings will expand our market in the EU, Canada, South Korea and possibly in MENA.

(4) Are you interested in working with one or more HPC4EI affiliated laboratories on one or more future HPC4EI projects? On one or more future projects outside of the HPC4EI program?

Yes, including AM (3-d printing or other AM concepts that VPE is developing). Yes. We are also interested in determining the effects of temperature (in addition to pressure) on the service life of complex monolithic MCHE for high temperature and high-pressure applications. Also, the results of this work are extremely useful for our future work in manufacturing AM advanced heat exchangers using powder and possibly other material forms. The program should enable us to use expensive materials more efficiently by not overdesigning to compensate for a lack of actual operational stresses.

(5) How can the HPC4 Energy Innovation program be improved or augmented to better serve your needs?

No comment

Acknowledgements

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