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Marshall Space Flight Center Faculty Fellowship Program

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PUBLICATION OVERVIEW

The 2021 Marshall Faculty Fellowship Program involved 4 faculty virtually working in the laboratories and departments at Marshall Space Flight Center. These faculty engineers and scientists worked with NASA collaborators on NASA projects, bringing new perspectives and solutions to bear. This Technical Memorandum is a compilation of the research reports of the 2021 Marshall Faculty Fellowship program, along with the Program Announcement (Appendix A) and the Program Description (Appendix B).

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Performance Prediction of Coolant Chamber in Rocket Engines Using GFSSP

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ABSTRACT

This paper presents a model for flow and heat transfer in a regenerative coolant chamber used in rocket engine. One of the key features in this model is to include the surface roughness of the coolant channels as obtained from the test data. The model based on Generalized Fluid System Simulation Software (GFSSP) includes friction loss due to surface roughness, inertia, manifold loss, and conjugate heat transfer. The model predicted flow rates are compared with the test data.

I. Introduction

Metal Additive Manufacturing has become a cost effective and popular manufacturing process for building various complex components such as liquid rocket engine combustion chambers and nozzles¹. However, one of the main concerns is the higher surface roughness of the pipe walls as compared with the traditional machining process. GRCo-84 and GRCo-42 are two popular alloys used for manufacturing these components. Reduction of hot wall surface finish is a primary post-processing technique for alteration of heat transfer performance in liquid rocket chamber liners. As the surface finish, or the friction factor along the wall, is reduced the total heat added to the coolant and the pressure drop in the coolant are also reduced. The combustion group at NASA Marshall Space Center has been studying the effect of these different processing techniques on the heat transfer performance. One such application is the study of heat transfer performance in a regenerative coolant chamber used in rocket engines.

A schematic of a typical regenerative coolant chamber is shown in figure 1 below. As shown in the figure, the coolant (liquid hydrogen) flows through the rectangular channels within the thrust chamber wall, and the hot combustion gases pass through the combustion chambers. In the current study, the coolant used is water as testing has been conducted using water. There are 55 rectangular channels along the periphery of the wall, and the inner surface is rough. The coolant flow and heat transfer between the coolant and the hot gas across the channel walls is studied using a suitable model in GFSSP.

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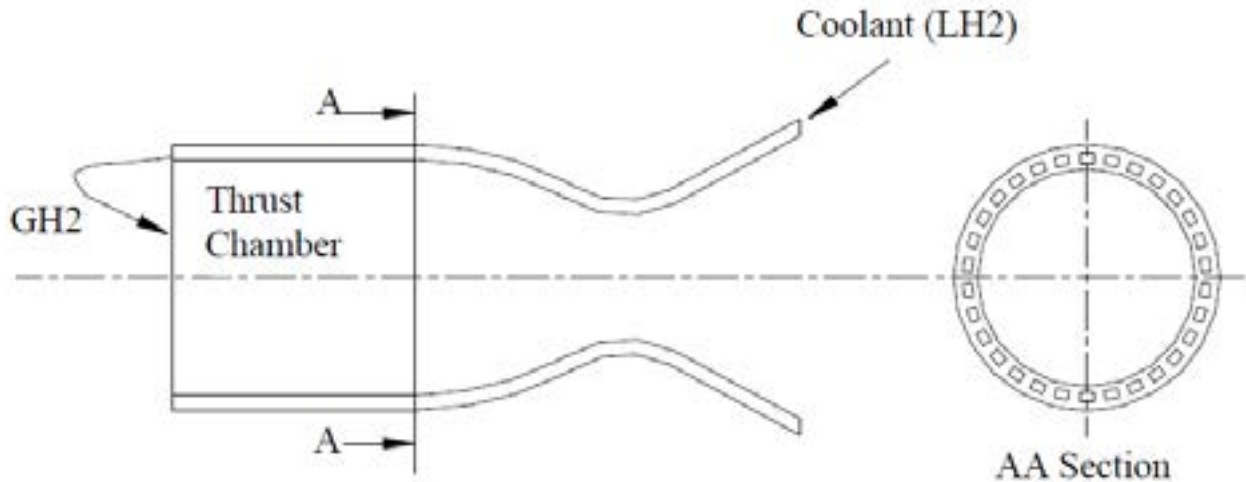


Figure 1. Schematic of a typical regenerative cooled Rocket Thrust Chamber and Nozzle

II. Problem Description and Computational Model

The testing of the combustion chamber coolant flow and heat transfer has been done at the MSFC combustion group using different type of wall finishing of the coolant channel wall. The coolant used is pressurized water and not LH2. Figure 2(a) shows the schematic diagram of the coolant flow along with hot gas passing through the thrust chamber. Figure 2(b) shows the detail of the cooling channels and the wall coating along the periphery of the wall. In order to model the coolant flow through these channels, considering symmetry, only one channel is modelled for the flow and heat transfer computation.

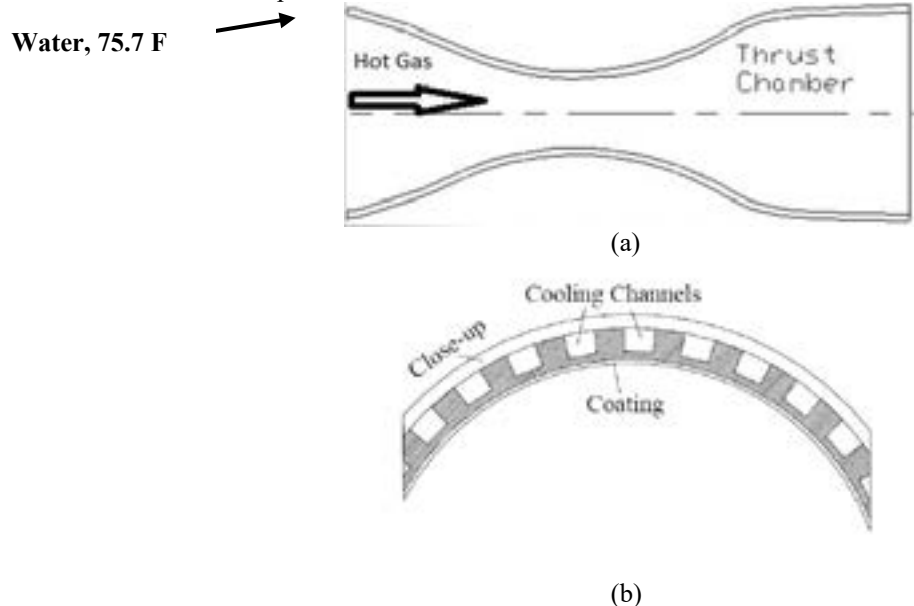


Figure 2. Schematic of the (a) Thrust Chamber and (b) Rectangular Coolant Channels within the wall.

The nozzle is about 1.44 inches long in the converging part and 7.35 inches long in the divergent part. The nozzle internal diameter varies from 2.5 inches at the inlet to 1.2 inches at the throat and about 2.2 inches at the exit. The cross-sectional dimension for each of the rectangular channels also vary along the length, the width varies from 0.072 inches at the inlet to 0.04 inches at the throat and 0.08 inches at the exit, height also varies slightly from 0.1 inches at the inlet to 0.08 inches at the throat area and 0.1 inches again at the exit. The hot wall thickness is 0.05 inches. All the dimensions are according to test data provided by MSFC Combustion group.

Computational Model:

Considering symmetry in the problem, only one rectangular channel along the wall of the entire thrust chamber is modeled using GFSSP². Both the fluid flow and conjugate heat transfer from the hot gas to the coolant are considered for the modeling. Due to varying geometry along the axial direction, the entire channel is split into 25 fluid nodes as shown below. The branches represent the segmental rectangular channels, area of which is not necessarily the same, and areas are computed as given by the test data. At the inlet and exit, to account for the loss in the entrance and exit manifolds, sudden contraction and sudden expansion branches are added at the entrance and exit respectively. Conjugate heat transfer is turned on and convection between coolant fluid and wall and conduction in the solid wall are accounted for. Nodes 26 through 50 represent the solid nodes next to the fluid nodes (coolant side) and nodes 51 through 74 represent the solid nodes next to the thrust chamber. The heat flux as obtained from the test data (from the chamber hot gas) is applied directly to these outer nodes as heat source. The heat flux applied is not constant and varies along the nozzle axial direction.

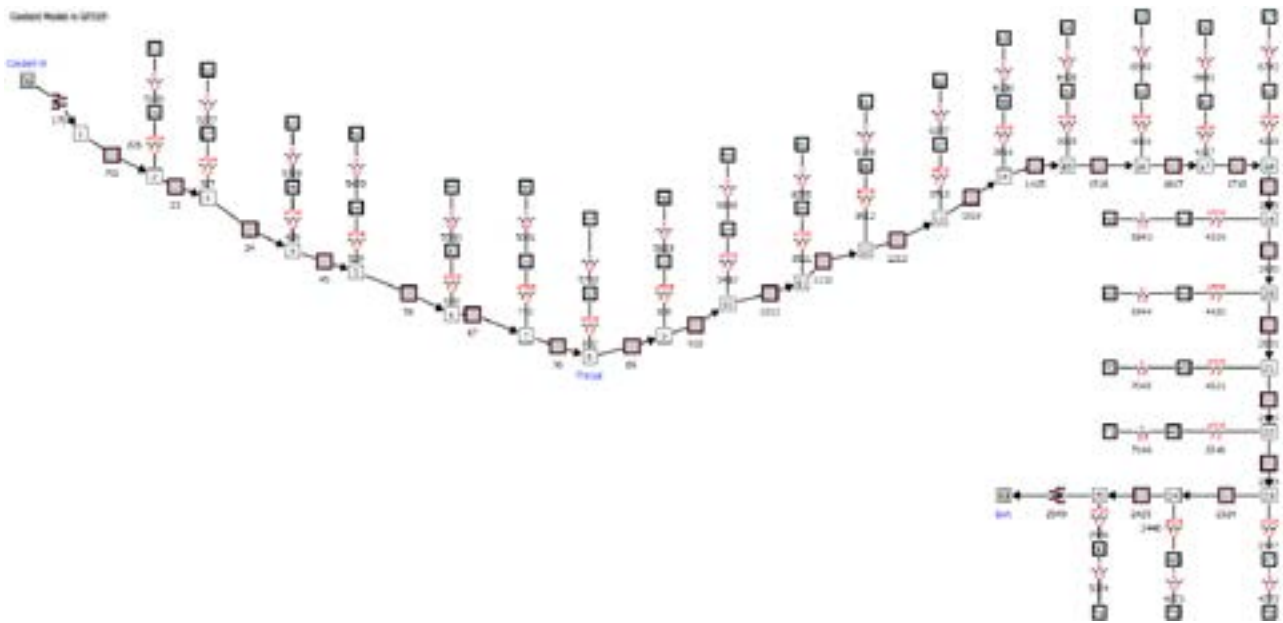


Figure 3. Computational Model for Coolant Channel Model using GFSSP

For the flow modeling, both the friction and inertia forces are considered along with pressure drop. The friction loss computation is based on Colebrook equation, for non-circular ducts². The surface roughness parameter is assumed to be constant along the coolant duct wall. The sudden expansion and sudden contraction at the inlet and exit are to account for the manifold loss. The pressure along the axial direction in the channel and the temperatures of the fluid, and in the solid wall region are computed using the model. The operating conditions are as per the test data as given in table 1 below. This table shows the measured flow rates (in all 55 coolant channels) in three tests, where the geometry remains the same, but the surface roughness parameter varies from 933 micro-inches to 300 micro-inches. The inlet and exit pressure values are also not the same in each case.

Case No	p _{in} (psi)	p _{exit} (psi)	Surface Roughness (micro-inches)	Flow Rate (lb _m /s)
1	2056	1377	933	6.86
2	2036	1754	540	7.61
3	2013	1833	300	8.09

Table 1. Test Data with three different surface roughness values of the coolant channel

The surface heat flux at the hot wall (thrust chamber side) varies as shown in figure 4 below. The heat flux is maximum near the throat region. The green line shows the variation of the coolant flow area along the nozzle axis.

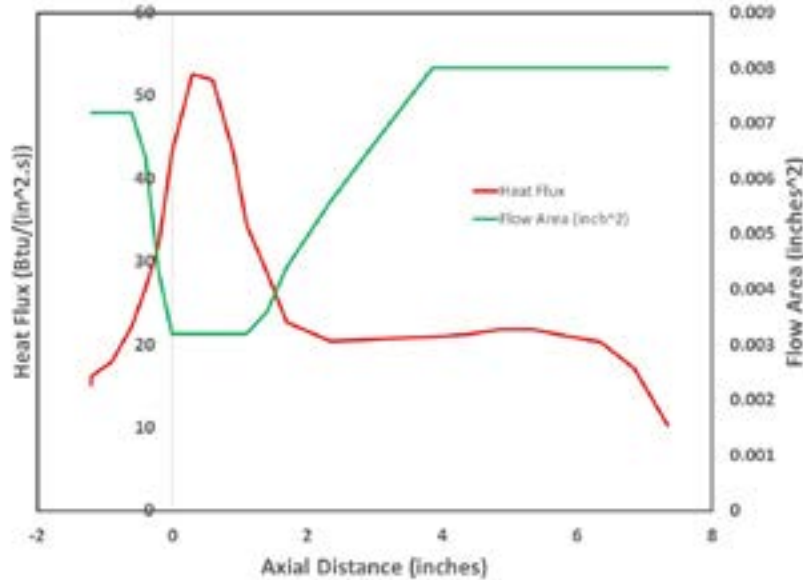


Figure 4. Heat Flux and Flow area Distribution along the axial direction

The thermal conductivity (k) and the specific heat (C_p) of the wall material varies as a function of temperature and this is given in table 2 shown below.

Temp (R)	k (Btu/(s.ft.R))	Temp (R)	C_p (Btu/(lbm.R))
260	0.04458	536.67	0.091
460	0.045	671.67	0.094
533	0.04611	851.67	0.0967
581	0.04657	1031	0.09888
671	0.04693	1211	0.10079
851	0.04724	1391	0.102226
1031	0.04716	1571	0.103659
1211	0.04691	1751	0.104615
1391	0.04672		
1481	0.04638		

Table 2. Thermal Properties of the Nozzle Wall

The convective heat transfer between the coolant and the wall can be computed using the built-in forced convection heat transfer correlation models in GFSSP. There are various heat transfer correlation models available. For the current study, the Dittus-Boelter² heat transfer correlations are used, as this predicts the lowest heat transfer coefficient as compared to the other models (Sieder-Tate, Gnielinsky, and Petukhov models) used in this study, to

get conservative design, as this predicts maximum wall temperature. This is discussed more in the results and discussion section.

III. Results and Discussion

The coolant flow modeling through the rectangular channel in GFSSP has been conducted under two different boundary conditions: (a) By keeping the pressure drop across the channel same as given in the test data for each of three cases (fixed_DP case) and (b) By adjusting the exit pressure to match the flow rate as in the case of test data (fixed_M case). In the first case, the flow rate computed from the model is being compared against the test data and in the second case, the pressure drop is compared with that of the test data. Figure 5 shows the plot of pressure drop along the channel length and as shown two different flow rates with fixed_DP and fixed_M case. This figure shows the result of rough channel with surface roughness parameter of 933. The flow rates shown in these plots are the total flow rate across all 55 channels. Hence, the flow rate as obtained from the model of a single channel is multiplied by 55 to obtain the values shown in these plots.

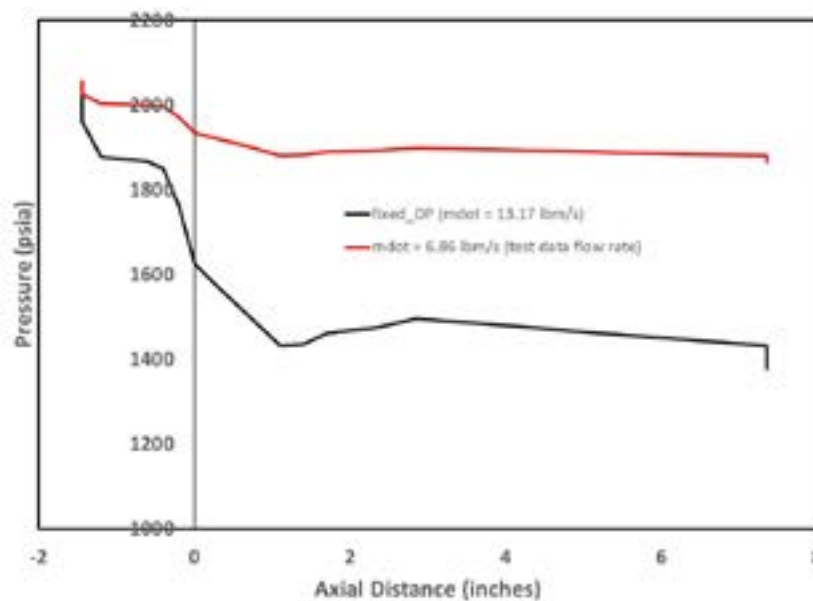


Figure 5. Pressure Distribution Along the length of the channel with surface roughness = 933

In this plot, the sudden drop of pressure at the inlet and exit is due to the sudden contraction and expansion. The black line indicates the correct pressure drop applied across the inlet and exit (as given in test data), and GFSSP predicts a flow rate of 13.17 lbm/s, and this is much higher as compared to that of the test data (6.86 lbm/s). On the other hand, to match the flow rate of 6.86 lbm/s, the exit pressure must be changed to 1865 psia as opposed to 1377 psia as given in the test data. The huge discrepancy may be due to the fact that the Colebrook equation used for friction modeling in GFSSP is inaccurate, and the relative surface roughness (roughness to hydraulic diameter ratio) is approximately 0.02 in this case, which is quite high, and the flow is turbulent. There may be other factors, such as assumption of constant surface roughness in the model. The pressure distribution for all the three different surface roughness cases under the fixed_DP and fixed_M approaches is being shown in figure 6 below. The solid lines indicate applying the correct pressure drop as given in the test data, and the dotted lines indicate the correct flow rate as the test data but adjusting the exit pressure (inlet pressure kept same as the test data). It has been shown in this plot, that case 2 when surface roughness is 540 micro-inches, the GFSSP predicted values match reasonably well with that of the test conditions (shown in black color solid and dotted lines respectively). The case with surface roughness of 300 micro-inches on the other hand shows an under prediction of the flow rate when correct pressure drop is used, as compared to that of the test data.

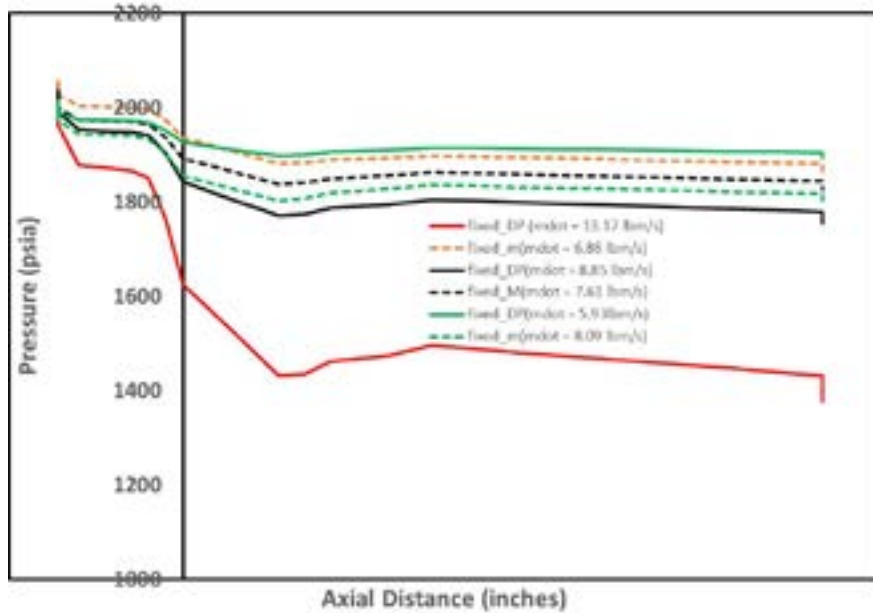


Figure 6. Pressure Distribution for all three cases of surface roughness

Four different heat transfer correlations are used to compare the wall temperature distribution in the wall next to the coolant. These are Dittus-Boelter² (DB), Gnielinski³(Gn), Sieder-Tate⁴ (ST) and Petukhov⁵ (PT) model. All these models are built-in in GFSSP software. Figure 7 and 8 show the heat transfer coefficient between the coolant and the solid wall along the axial direction. These predictions are by using single solid node for each fluid node. However, results do not vary much by using two solid nodes for each solid node.

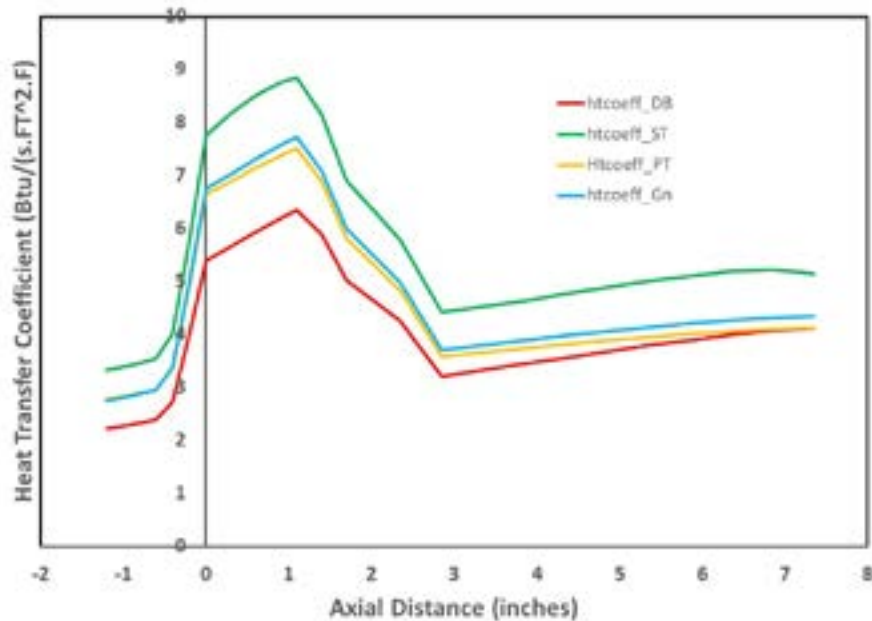


Figure 7. Comparison of Heat Transfer Coefficient using various models: Gnielinski (Gn), Sieder-Tate (ST), Petukhov (PT) and Dittus-Boelter (DB)

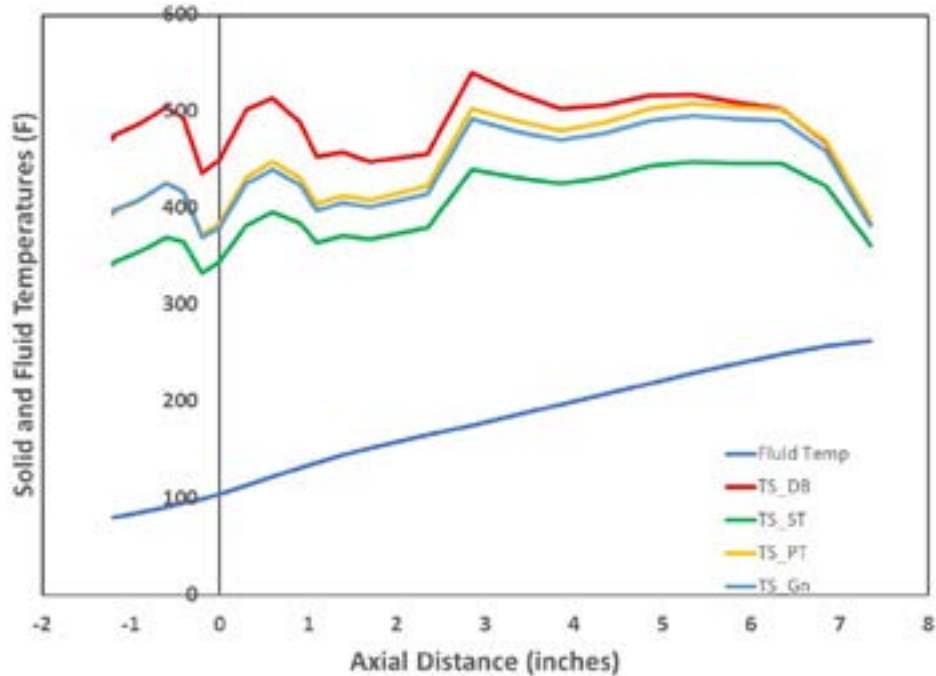


Figure 8. Wall Temperature Distribution using different convective heat transfer correlations.

Figure 7 shows that the maximum heat transfer coefficient is near the nozzle throat area, and this effect is because flow velocity is maximum near that region due to area change in the coolant channel as shown in figure 4. Figures 7 and 8 support each other, and show physically realistic results, as using Dittus-Boelter the heat transfer coefficient is the lowest as compared to the other models, and hence predicts maximum wall temperature. For the subsequent studies with two solid nodes per fluid node to capture the effect of conduction through the hot wall, for the conjugate heat transfer, the Dittus-Boelter model is used, to have conservative design. It has also been observed in this study, that increasing number of solid nodes in the coolant wall does not change the result appreciably. Hence, two solid nodes per fluid node seem to be enough for this study.

Figures 9, 10 and 11 show the axial temperature distribution of the fluid, cold wall (wall next to coolant) and the hot wall (wall next to gas chamber) for the three different cases (Surface roughness = 933, 540 and 300 micro-inches) respectively. In each study, two different flow rates are shown as for each case fixed_DP (green line) and fixed_DM (fixing the mass flow rate to test data, as given in redline) are shown. As observed in figure 9 (most rough coolant channel), the wall temperature is a strong function of the flow rate and higher the flow rate, lower the temperature of the wall, as expected. The temperature difference between the maximum hot wall temperature and the maximum cold wall temperature is about 600 F.

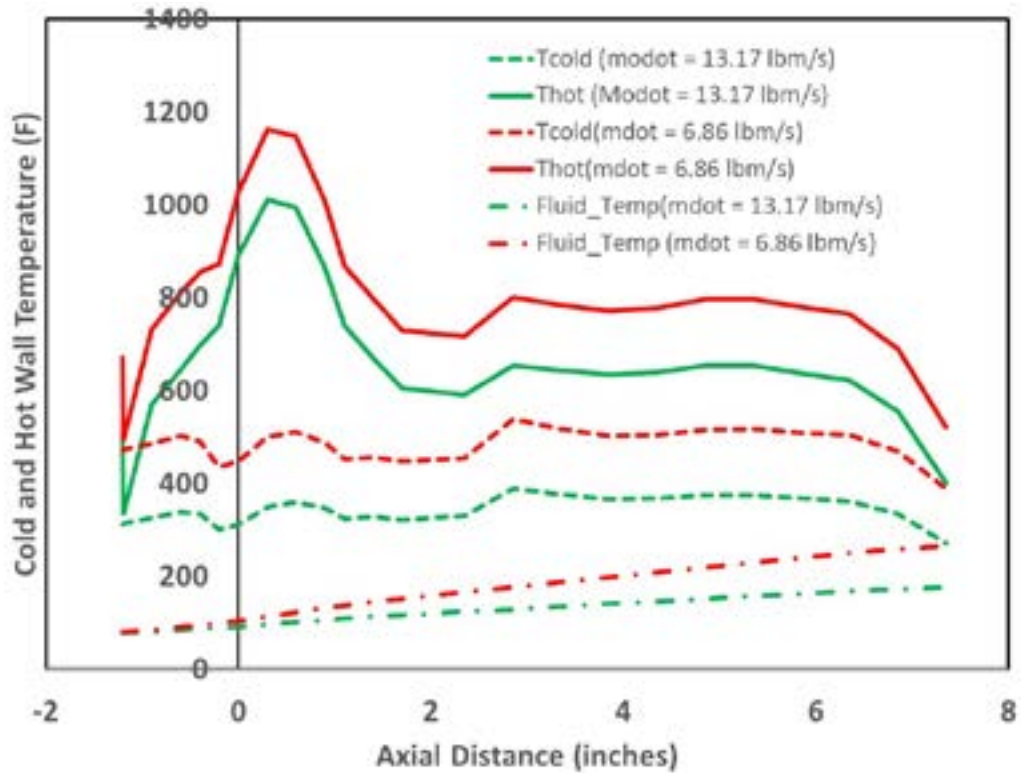


Figure 9. Fluid and Wall Temperature Distribution for surface roughness = 933 μ inches

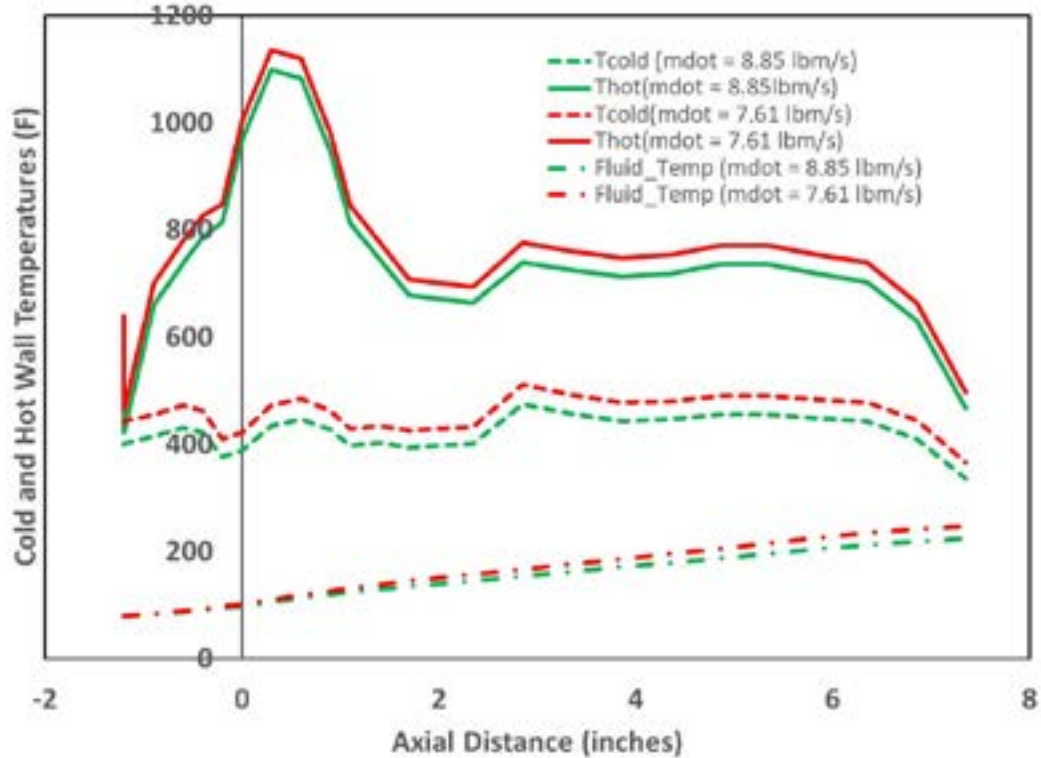


Figure 10. Fluid and Wall Temperature Distribution for surface roughness = 540 μ inches

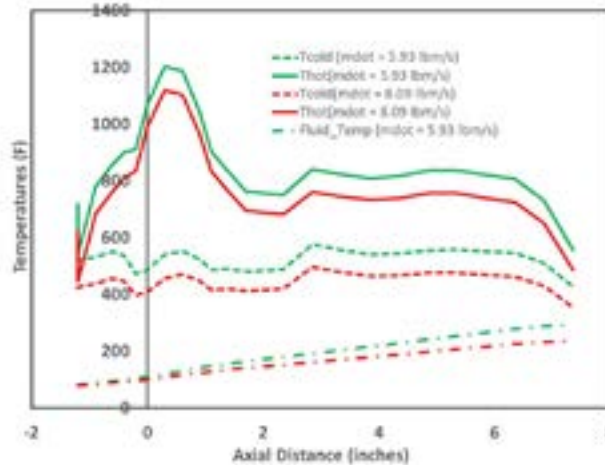


Figure 11. Fluid and Wall Temperature Distribution for surface roughness = 300 μ inches

IV. Conclusion

It has been observed from the results that friction losses due to surface roughness plays a very important part in the computation of flow rate. The GFSSP predicted flow rates match reasonably well for relatively lower surface roughness (case 2, surface roughness of 540 microinches), but at higher surface roughness, the predicted value of the flow rate (by applying the same pressure drop as the test data) is quite-off from the test data (more than 100 %). This can be attributed to several factors, such as assumption of the validity of the Colebrook equation at high surface roughness, assumption of uniform flow (same flow rate in each of the 55 channels), and also uncertainty in the measurement of the surface roughness parameter. The surface roughness parameter assumed in this model is constant throughout the length of the coolant channel, whereas it actually varies along the length, and one needs accurate surface roughness test data to incorporate into the model. This can be thought of as future work.

Acknowledgments

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ANSYS Fluent and CFX Techniques to Predict Temporal and Spatial Temperature Distribution in a Cryogenic Storage Tank

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Stored cryogenics are essential for long-term space travel. Due to external heating from the environment, ullage temperature increases, and with it, pressure. When ullage pressure reaches a specified limit, strategies including venting must be employed to reduce the pressure. Various modeling techniques were attempted using the ANSYS suite of analysis tools. Reasonable spatial gradients, as compared to experimental data, were obtained with the Transient Thermal Solver. This was, however at lower than observed heat leak values. Efforts are ongoing to develop a valid model using Fluent VOF modeling as well as UDF, or User Defined Functions as an improvement on the Lee model of evaporation used in VOF modeling.

I. Nomenclature

A	=	area
h	=	convective coefficient
I	=	electrical current
k	=	conductive coefficient
L	=	length of conductive path for conductive resistance calculation
Q	=	heat power
R_{cond}	=	conductive thermal resistance
R_{conv}	=	convective thermal resistance
T_w	=	temperature of warm radiating body
T_c	=	temperature of cold radiating body
ϵ_w	=	emissivity of warm radiating body
ϵ_c	=	emissivity of cold radiating body
σ	=	Stefan-Boltzman constant

II. Introduction

For long-term space travel, cryogenics need to be stored over long periods of time. The cryogenics are stored at a low enough temperature, typically in the low 20s K, that heat tends to flow from the environment into the cryogen. The dominant mode of heat transfer in the absence of significant gaseous atmosphere for convection, is radiative heat transfer. The cryogen will reach saturation temperature and pressure due to the heat leak, and the gaseous phase in the

headspace (Ullage) will continue to increase in temperature and pressure until the physical limits of the container are reached. This necessitates strategies for maintaining the pressure at or below the safe structural limit of the vessel (Ref. 1, 2) Ultimately, the pressure must be released by venting, which causes loss of the cryogen and possibly an unwanted thrust vector (Ref. 2).

Past studies have focused on characterizing and modeling the insulation properties, therefore minimization of heat leak (Ref. 3,4,5). The current study attempts to model the temperature increase at given points with time as well as the spatial temperature distribution also as a function of time. Three-dimensional models using ANSYS Workbench were attempted. Specifically ANSYS Transient Thermal module with both the CFX solver and Fluent solver being tried, as well as the Fluent module with VOF.

III. Procedure

CREO version 6.0 was used to create solid model files. The 3-D solid models were based on the dimensions of the Multipurpose Hydrogen Test Bed (MHTB), which is located at the Marshall Space Flight Center (MSFC), in Alabama. (Ref. 1, 2, 3). Hydrogen was assumed to be the cryogen although the models can be easily adapted to other cryogenics and ullage mixtures. The solid models were only the contents of the tank and did not include the tank walls. For the Transient Thermal module, two solids were created. One solid represented the 90% fluid fraction and the other represented the 10% ullage fraction. For the Fluent module, one solid representing the entire tank was modeled as the mesh was partitioned within Fluent to represent 90% liquid and 10% ullage.

Solid models were imported into ANSYS Space Claim, meshed, and then preprocessed in the appropriate module. Figure 1 shows solid model imported into Space Claim, Figure 2 shows mesh for Fluent VOF Model (similar to Transient Thermal model Mesh), and Figure 3 shows partitioned mesh for liquid portion of Fluent VOF model.

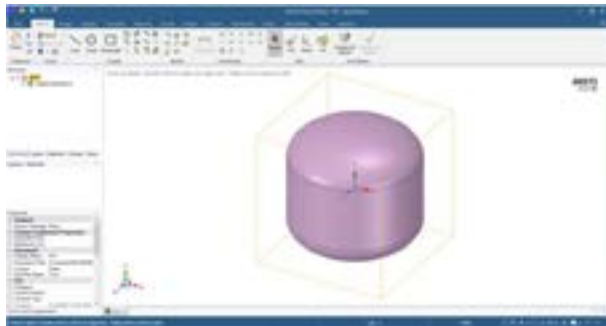


Figure 1. CREO Solid Model Imported into Space Claim.

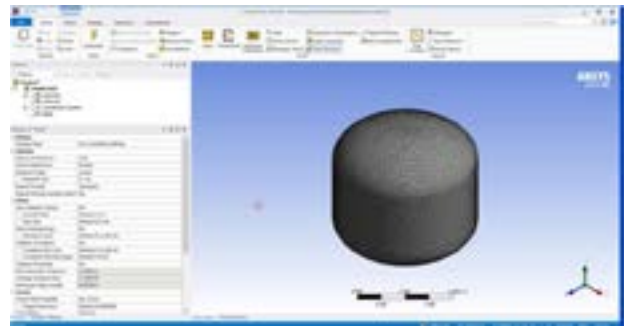


Figure 2. Fluent VOF Model Mesh

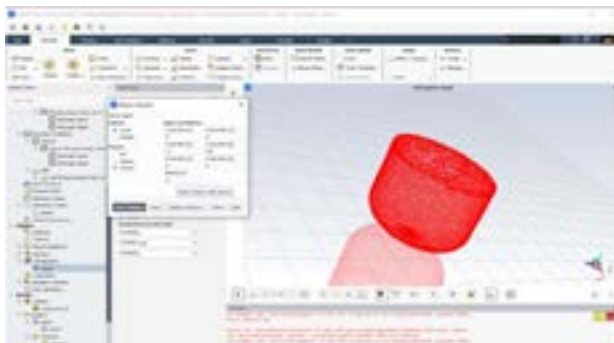


Figure 3. Fluent VOF Liquid Partition of Mesh

To simulate heat leak, a heat flux boundary condition was applied to the outer surface in all models. Modeled results were compared to dataset P263981d and mhtblh2_02thru10merge.p2472. Dataset P263981d is hydrogen liquid and hydrogen ullage, whereas mhtblh2_02thru10merge.p2472 has data from hydrogen liquid/hydrogen Ullage as well as hydrogen liquid with an ullage mixture of hydrogen and helium.

While pressure is the property of concern, temperature distribution is a better comparison to the datasets and better indicator of the validity of the model as there is no significant pressure distribution in the tank. There are, however many temperature probes. The pressure is, of course related to temperature and easily determined from the FLUENT model, or calculated from thermodynamic

tables and compared to the datasets. Since the heat enters the tank from all sides, the temperature would increase well past the point where the tank would burst, the model would not be useful if allowed to find steady state. As well, the increase in temperature over time is the important metric. Therefore, a transient solver was used in all cases. Outer iterations simulated 1000 s, 1500s, or 1800 s depending on the overall solve time and limitations of the computer, while inner iterations were set at a maximum of 250 while allowing the solver to terminate based on residuals.

IV. Results

Figure 4 shows the modeled spatial temperature distribution as modeled with ANSYS Transient Thermal Solver. Figure 5 compares temporal variation of temperature in the same model, at one point, with data at that corresponding point in dataset p263981d. At the times graphed in Figure 5 from the dataset, the ullage volume was around 10% of the total volume. Three time slices are shown where the temperature increased from about 21.3 C to around 23.2 C. Total time to increase in temperature was 1800 s. The graph shows that at a modeled heat leak of 28W, the modeled temperature increased at the same rate, at the same point in the tank.

Figure 6 shows a similar comparison of the same ANSYS model data to actual data from the combined dataset.

While the Transient Thermal solver could predict the rate of change and distribution of temperature for 10% hydrogen ullage, it did so at around half of the known heat leak. It was decided to concentrate efforts on the Fluent solver using VOF (Volume of Fluid).

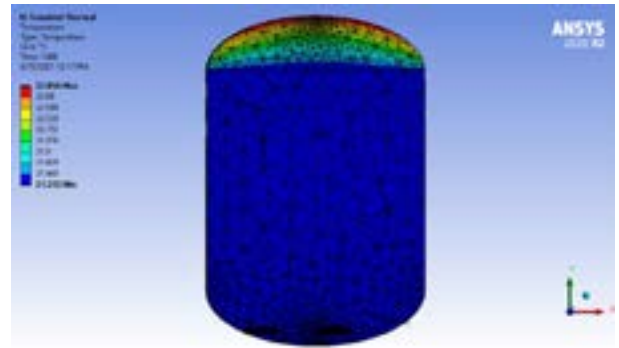


Figure 4. Calculated and actual temperatures assuming $k=0.000866$ W/mK

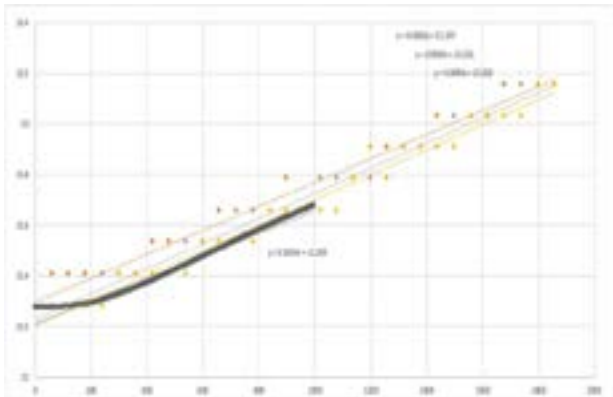


Figure 5. Comparison of modeled temperature increase at 28W heat leak to dataset p263981d

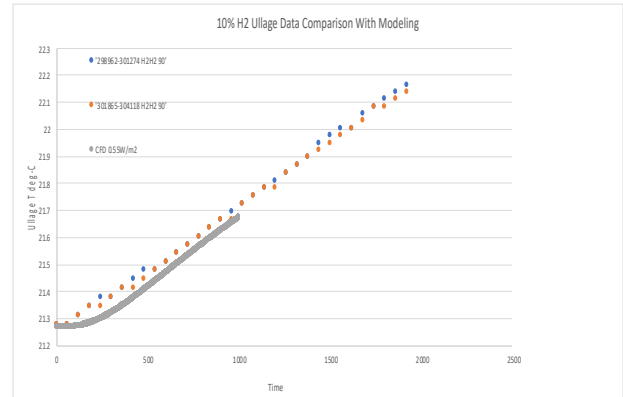


Figure 6. Comparison of modeled temperature increase at 28W heat leak to merged dataset (H2H2 10%)

Preliminary results from the Fluent solver using VOF are shown in Figure 7. Relative temperature profiles are shown rather than comparisons to data as modeling is on-going. Stratification is not what was expected so further investigation into the datasets is necessary, as well as scrutiny of the modeling technique. Figure 8 shows temporal variation in temperature at one point for 10% hydrogen ullage, 10% hydrogen/helium mixture ullage, and 50% hydrogen/helium mixture ullage. Further analysis needs to be done to compare spatial variation at several time intervals, for each mixture case. What the current analysis shows in Figures 5, 6, and 8 is that the slope and therefore the rate of change is consistent for each volume fraction and mixture for a given heat leak.

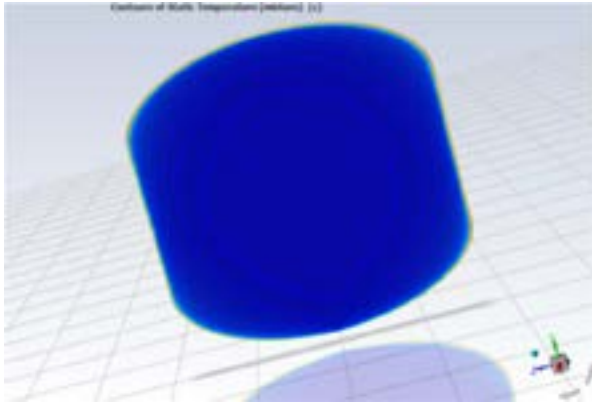


Figure 7. ANSYS Fluent VOF model, relative temperature contours.

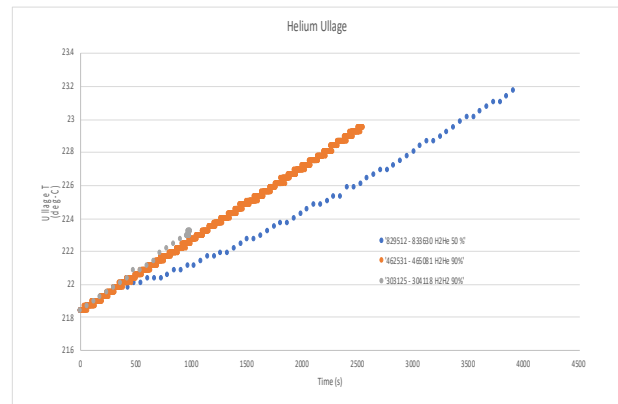


Figure 8. Combined dataset comparison of varying ullage volume and mixture.

V. Conclusion

Further investigation is needed using FLUENT with VOF, as well as investigation into the datasets used in this work. While the Transient Thermal Solver yielded a thermal profile that appeared more reasonable, more virtual thermal probes would have to be modeled in the same location as actual probes, and each compared at various points in time. Since it is computationally intensive, and not expected to address the inconsistency in the heat leak, this would not be a good use of time and resource. Rather, it would be a better use of time to continue developing the Fluent model.

The VOF methodology in Fluent has a possible shortcoming in that the “Lee” model for interface energy exchange may not be optimal for this type of modeling (fluid at saturation in a sealed vessel). After further modeling with VOF and comparison to data, a User Defined Function (UDF) should be investigated in-place of the Lee model

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Infrared Immersion Grating Testing

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In this paper we describe the results of the summer 2021 fellowship taken by Professor Chris Packham at NASA MSFC. The fellowship occurred during the Covid-19 pandemic, and hence was completed in a totally virtual modality. Nevertheless, the key twin aims of the fellowship were broadly met, but of course future work remains.

I. Nomenclature

UTSA	=	University of Texas at San Antonio
NASA	=	National Aeronautics and Space Administration
MSFC	=	Marshall Space Flight Center
IR	=	Infrared
IG	=	Immersion Grating
MUREP	=	Minority University Research and Education Project
TIR	=	Thermal Infrared
TMT	=	Thirty Meter Telescope
MICHI	=	Mid-IR Camera, High Disperser, and IFU spectrograph
HDS	=	High-Dispersion Spectrometer
MSI	=	Minority Serving Institute
URM	=	underrepresented minorities
HSI	=	Hispanic Serving Institute
STEM	=	Science Technology Engineering Mathematics

II. Introduction

In this paper, we describe the results of a summer 2021 fellowship at NASA MSFC. One of the goals of this 6 week program is to team NASA personnel with academics in other universities. For this work, we had two primary goals to achieve during this collaboration: (1) preparation for testing of an IR IG, and (2) submission of a NASA MUREP proposal. In this paper we describe the science drivers and testing preparations for the IR IG in section 3, the goals of our MUREP proposal in section 4, and discuss conclusions and future work in section 5.

III. Science Cases & Testing Preparation for an IR IG

[The science case text is heavily based on that published by Packham et al., 2018¹].

With the imminent launch of the JWST, the field of (TIR) astronomy will enjoy a revolution. It is easy to imagine that all areas of IR astronomy will be greatly advanced, but perhaps impossible to conceive of the new vistas that will be opened. To allow both follow-up JWST observations and a continuance of work started on the ground-based 8m's, we continue to plan the science cases and instrument design for a TIR imager and spectrometer for early operation on the TMT. We present here selected high spectral resolution science cases which will complement the advanced afforded by the high sensitivity JWST observations..

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A TIR HDS affords high-resolution spectroscopy of exoplanets and offers unique insights into the atmospheric dynamics, composition, and chemistry of these objects; and in a few cases, into their spin and orbital angular momenta, and aspects of their global weather patterns.

MICHI could become TMT's workhorse instrument for estimating atmospheric metallicity through O and C measurements and the ratio of these two elements (C/O). The L band accesses strong H₂O absorption, and this wavelength range has provided the bulk of the high-resolution detections of this molecule in short-period exoplanets (Birkby et al. 2013², 2017³, Lockwood et al. 2014⁴, Piskorz et al. 2016⁵, 2017⁶). Furthermore, in Solar-abundance atmospheres H₂O is expected to be the most abundant species after H₂ (Heng & Kitzmann, 2017⁷), suggesting that L band measurements of H₂O will form a large part of MICHI's exoplanet work. The L band also hosts the strongest CH₄ feature easily accessible from the ground, a molecule that is yet to be detected in any short-period transiting planet. When L band H₂O and CH₄ measurements are combined with the strong CO and CO₂ absorption lines in the M band, MICHI will be poised to measure the abundances of all major O- and C-bearing molecules; if higher-order hydrocarbons such as C₂H₂ are present, MICHI will also be able to measure their abundance (de Kok et al. 2014⁸), constraining models of hydrocarbon "soot" haze formation in exoplanet atmosphere (Morley et al. 2015⁹, Kawashima & Ikoma 2018¹⁰). Both metallicity and C/O provide strong constraints on the formation method and location of the observed planets (e.g., Mordasini et al. 2016¹¹).

One of the most exciting prospects with TMT/MICHI is advancing photon constrained observations of the rotation of exoplanets (Fig. 1), pioneered on the VLT. The β Pic b planet rotation rate of 8.1 ± 1 hours was determined by observations of CO emission lines. Whilst this type of measurement was repeated for ~ 10 objects, TMT/MICHI will extend this to $\sim$ several 10s of objects, enabling a detailed sample of the rotational properties of exoplanets and how they obtained their angular momentum during formation. For numerous highly irradiated planets, detailed line profiles will probe upper atmosphere wind speeds and circulation patterns, advancing high spectral resolution results that previously measured the day-to-night winds speeds on hot Jupiters HD209458 b (-2 ± 1 kms⁻¹; Snellen et al. 2010¹²) and HD 189733 b (-1.7 ± 1.2 kms⁻¹; Brogi et al. 2016¹³). Such properties are uniquely determined at high-spectral resolution.

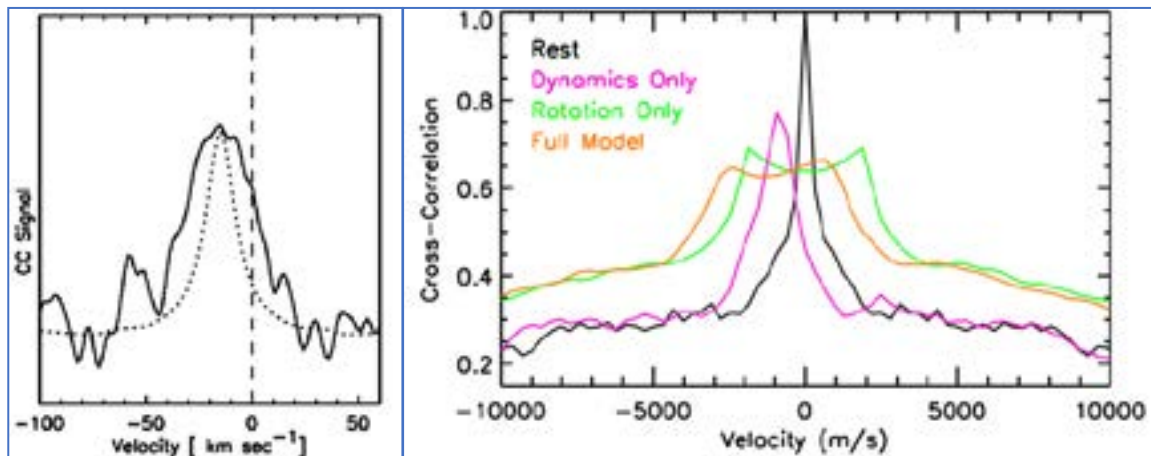


Figure 1. First measurement of an exoplanet rotation (left) showing the rotationally-broadened cross-correlation profile of the giant exoplanet β Pic b (Snellen et al. 2014¹⁴). The dotted line shows the expected profile without planetary rotation. Examples (right) of the predicted profile of rotation (green line) and winds (purple line) on the cross-correlation profile of exoplanet atmospheres (Kempton & Rauscher 2012¹⁵; Showman et al. 2013¹⁶).

More broadly, MICHI high spectral resolution observations will accomplish groundbreaking science on multiple fronts, exemplified by these selected highlights:

- Detect atmospheres of the nearest neighboring rocky worlds via high-dispersion spectroscopy and medium-resolution IFU observations (Snellen et al. 2015¹⁷, Lovis et al. 2017¹⁸, Hoeijmakers et al. 2018¹⁹)
- Detect giant storms on the surfaces of widely-separated giant planets via Doppler imaging (Crossfield 2014²⁰);
- Atmospheric chemistry of exoplanets, from (super-)Earths to hot Jupiters, and production of 1D photochemistry maps as a function of longitude. This will lead to the first measurements of low-abundance species, e.g. isotopic ratios connected to evolutionary history (e.g. HDO, ^{13}CO);
- Measure true masses of non-transiting (super-)Earths around nearby bright stars.

The prospects for the formation of planetary systems and the development of life are pre-determined in protoplanetary disks. Whether planets have the necessary chemical ingredients to generate and nurture life depends on the chemical and physical disk structures from which they form. Time-dependent theoretical models of the physical and chemical evolution of the disk (e.g. Aikawa et al. 2002²¹) have been tested through observations of disk chemistry and structure (Fig. 2). Particularly the snow lines of water and other volatile molecules (e.g. Blevins et al. 2016²², Notsu et al. 2017²³) play a vital role in planetary formation, and subsequently the chances for life. As noted above, such observations are optimally performed at TIR wavelengths due to the greatly improved CR. TMT/MICHI will be capable of spatially and spectrally resolving the snow lines of these species by making use of gas emission lines and ice absorption features (e.g. Honda et al. 2016²⁴). Disk thermal structure evolution can also be measured by tracing the spatial distribution of crystalline silicate material in the disk. TMT/MICHI affords a unique opportunity to uncover both mineralogical evolution and transport of solid material within a disk by spatially-resolved MIR spectroscopy (e.g. Okamoto et al. 2004²⁵, and Fig. 2). Existing 8m's and JWST do not afford the combination of high sensitivity and spatial/spectral resolution, leaving a large and crucial parameter space to be filled by TMT/MICHI.

TMT/MICHI will also be a powerful tool to obtain emission/absorption line profiles of a number of molecular (e.g. CO, OH, H₂O, H₂, CH₄, C₂H₂), atomic (e.g. H lines), and ionic (e.g. [Ne II], [Fe II]) lines in the TIR. Molecular lines are excellent tracers of temperature and abundance, and their spatial location obtained by MICHI will help our understanding of disk chemical/physical structures and evolution (e.g. Salyk et al. 2008²⁶; Banzatti et al. 2017²⁷). CH₄ and C₂H₂ lines are useful to trace the distribution of the C/O ratio, are only available in the TIR. Atomic and ionic lines in the TIR provide powerful diagnostics of mass inflows, outflows and physical processes (e.g. Neufeld & Hollenbach 1994²⁸, Pascucci et al. 2011²⁹, Edwards et al. 2013³⁰, Watson et al. 2016³¹). As multiple processes can produce these lines (e.g. Herczeg et al. 2012³²) it is critical to have both high spatial ($< 0.1''$) and spectral ($R > 60,000$) resolution observations to disentangle contributions from infall, accretion, and outflows to assess mass flow rates. JWST/MIRI will not resolve these lines spectrally nor spatially, but TMT/MICHI will. This makes it possible for the first time to audit mass flow rates in protostars & disks, providing fundamental insights into the physical processes that assemble protoplanetary disks.

Growing protoplanets are also important targets to fill in the evolutionary gap between the disk and planets. MICHI will be able to detect these objects in two ways with IFU spectral images. First, spiral waves created by accreting planets should be detectable in CO and other molecules (Regaly et al. 2015³³). Second, a growing giant planet may have a circumplanetary/proto-lunar disk, with a chemical and physical structure analogous to the much larger parent circumstellar disk. Evidence for a planet has already been seen in CO spectroastrometry in a ~ 10 AU planet around HD 100546 (Brittain et al. 2014³⁴); TMT/MICHI will push these detections to within an AU, where planets are more prevalent.

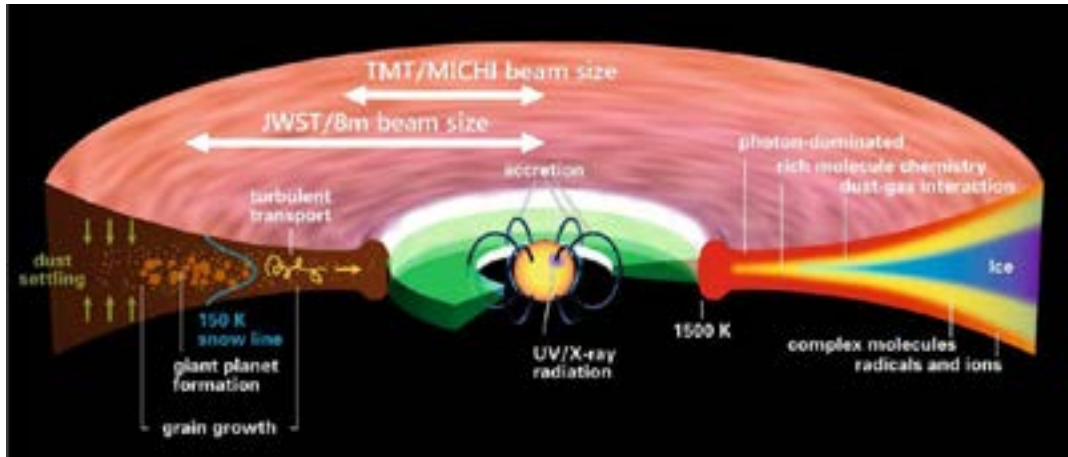


Figure 2. Cartoon of the chemical structure, including the H₂O snow line and planet formation in a typical protoplanetary disk around a solar-mass star (adapted from Henning & Semenov 2013³⁵).

To achieve the high spectral dispersion required by these science cases, we could use a traditional reflecting grating, or an IG. An IG has the grating ‘carved into’ a crystalline substrate, hence the term IG, and the spectral dispersion is increased by the index of refraction of the substrate. This can be as high as ~4, which can thus either be thought of reducing the necessary pupil size by that value as compared to a reflection grating, or increasing the dispersion by that factor. Reducing the pupil size in a cryogenic instrument is highly attractive and could reduce the instrument size, complexity, and cost. In the paragraphs below, we discuss the test setup for an IR IG.

An IG is available from Canon (Japan), and we need to build a holder to permit IR testing of the IG. The following requirements for the testing at level 0 and 1 were set:

Level 0

The test holder shall permit infrared spectrometric testing of immersion gratings (IGs) at both room (300K) and LN₂ (76K) temperatures.

Level 1

1.1 Mechanical Stability

1.1.1 The holder shall permit the IGs to be oriented at any incoming angle to the incident beam in the horizontal plane

1.1.2 The holder shall permit the IGs to be oriented and stable to <<1 degree in both the horizontal and vertical planes

1.1.3 The holder shall mount the IGs at both room (300K) and LN₂ temperatures (76K) without any damage (i.e. due to differential thermal contraction)

1.1.3.1 The IGs are made from high quality, high-purity InP (Indium phosphide) and Ge (Germanium)

1.1.4 The holders shall mount the IGs as detailed in the design drawings provided by Canon for the InP and Ge devices.

1.2 Optical Testing

1.2.1 The IGs shall be tested within the wavelength ranges: InP 1.5-9.0μm, Ge 1-14μm

1.2.2 Optical tests should be performed at both room (300K) and LN₂ temperatures (76K).

1.2.3 The polarization of the incident beam should be modulated (i.e. change the position angle of polarization)

1.2.4 Optical measurements shall be:

1.2.4.1 Measure the resultant flux in the diffracted line

1.2.4.2 Measure the width of the diffracted line

1.2.4.3 Measure (for each occurrence) the flux within any ghost or scattered images

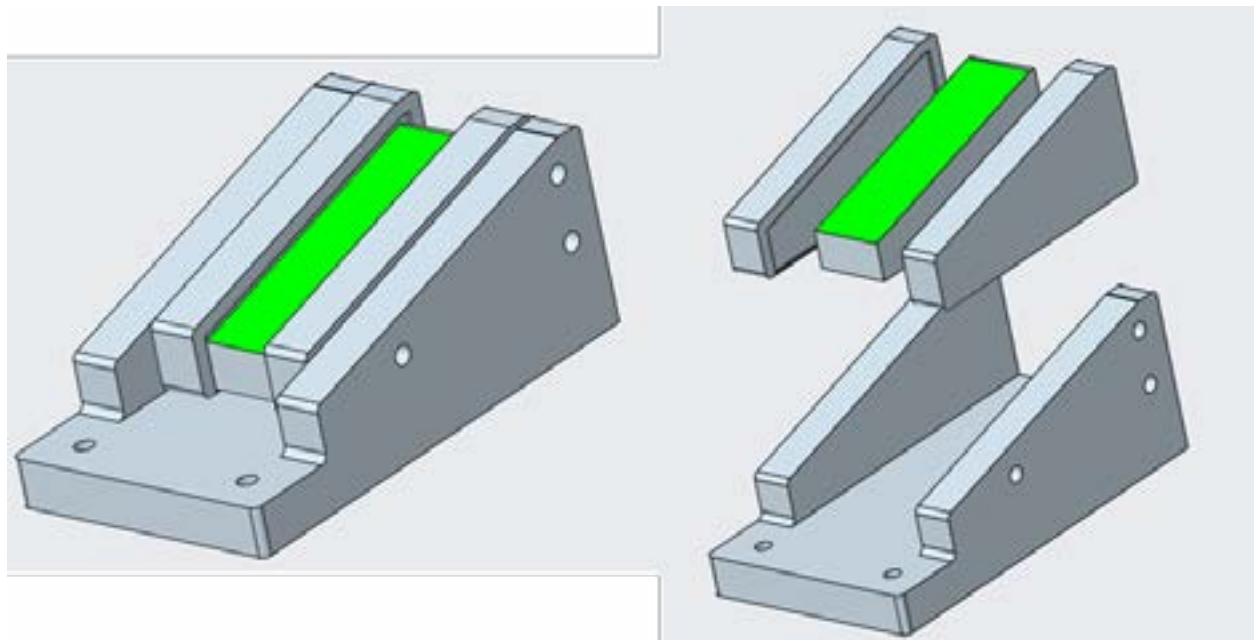
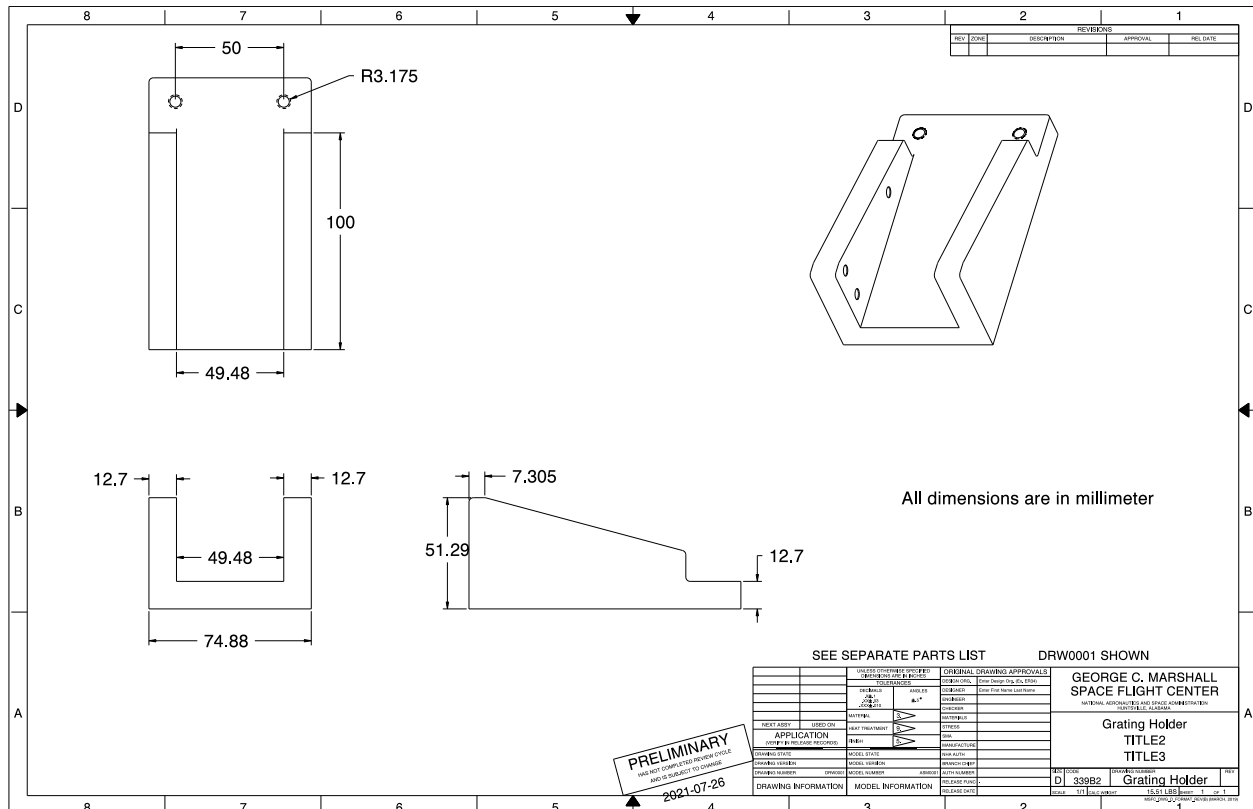
1.2.4.4 Measure (for each occurrence) the flux within any ‘grass’ images

1.3 Transportation

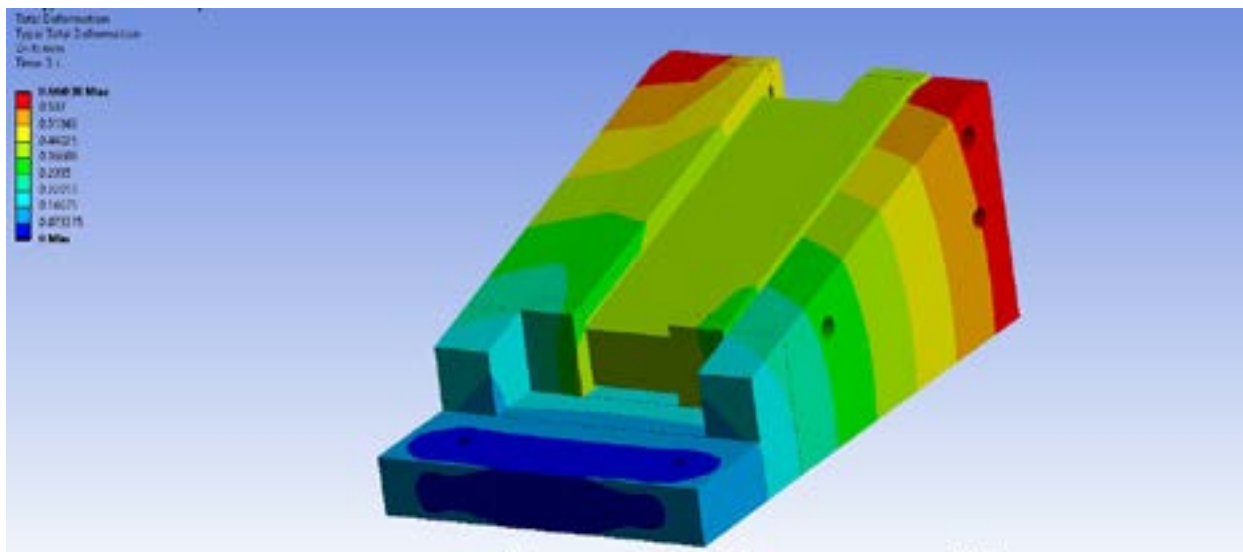
1.3.1 The IGs will be transported within the mount via air or ground without damage or degradation.

1.4.1 The IGs will be able to be stored in the holder without damage or degradation.

The precise size and design of the IG to be loaned by Canon is proprietary. Instead, we show the design of the final hold that addressed the requirements. This design work was led by Ranganathan & Watley, and all credit for the design and analysis must go to them.



The grating is held in place by spring loaded G10 to ensure that cooling of the holder does not present any risk to the IG. Deformation by cooling is shown below, paying careful attention to differential contraction:



The deformation by differential thermal contraction from 200K to 76K was judged to place a minimal load of the IG, and does not present any structural integrity issues to the IG. Thus the most difficult holder requirement was met through this design. We plan to machine and test the holder before receiving the IG and proceeding with the optical testing in due course.

IV. General Guidelines

NASA has recently increased its focus on diversity, equality, and inclusion, and the MUREP program is an exciting and substantive avenue to achieve these important goals. The vision of MUREP is to “enhance the research, academic and technological capabilities at MSIs by providing authentic student learning experiences related to NASA missions that contribute to a Diverse Future STEM Workforce”. As part of this fellowship, we applied for a MUREP award, with the following vision noted in the abstract:

LSIP: Leadership and Science Integration Program for Next Gen URM Leaders

In this proposal, we describe an innovative program for students to obtain formal knowledge and skills in (a) leadership and (b) science case flowdown for astronomical instrumentation construction and management. The focus will be to attract next-generation URM leaders at the undergraduate and graduate student level. We will trial this program at UTSA in year 1 and expand the program nationwide in subsequent years 2 and 3. Our central goal is to increase the skillsets and knowledge base of URM students starting at the core of the science case of NASA current or future missions. This would be a unique course for the USA. We target an often ‘missing-link’ between science and engineering, with a goal of providing a bridge between the two all-too-often disparate disciplines. We will use evidence-based, transformative strategies in astronomy to enable science, technology, engineering, and math (STEM) learning, that is commutable to both science and industry. LSIP is tailored to address national STEM shortage. We plan to archive materials for reuse and hope for continuation of the program using other funds and resources. We have forged strong partnerships with (1) the Hispanic Serving Institute (HSI) at UTSA, (2) NASA Marshall, (3) two star Major General Tony Cucolo of the United States Army, (4) local schools, and (5) local museums, including a Challenger Center. A companion program leverages our connection to local schools to improve school STEM education, making use of NASA EPO and educational resources.

Whilst the proposal was ultimately unsuccessful, we did receive generally positive comments and the PIs (Packham & Gaskin) have committed to update/improve the proposal following the reviewers’ comments and resubmit in an upcoming round.

V. Conclusions & Future Work

During the period of the summer MSFC fellowship, the two main goals were accomplished, namely (1) the design of a holder in which an IG can be mounted and (2) the submission of a MUREP proposal. The main future goals will be the use of the holder during testing of the IG and also the updating and resubmission of the MUREP proposal.

Despite the challenges that remote working during the COVID-19 pandemic, this fellowship was successful in the goals as listed above, and also in the overarching goals of introducing NASA scientists/engineers to potential collaborators outside of the center.

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An Explicit Time Stepping Scheme for Generalized Flow Simulation System Program

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An explicit time stepping scheme has been developed for transient thermo-fluid dynamic analysis of fluid systems and components. The scheme decouples the conservation of mass, momentum and energy equations into three separate equations and solve them efficiently. Proposed solvers have been integrated into a network flow simulation software GFSSP (Generalized Fluid System Simulation Program) based on the unstructured finite volume method. In order to access the performance and convergence of the algorithms, they are used to predict blowdown of a pressurized tank. Numerical predictions are compared with simulations using the implicit scheme and are found to be in qualitative agreement.

I. Introduction

In the present study, an explicit time stepping based finite volume procedure for the prediction of complex coupled transients in fluid network is presented. In the past, most of the developments in network solver were in implicit time stepping based finite volume procedures for flow network with branching. In this network modeling approach, the fluid region is partitioned into a series of discrete nodes connected by branches and solid region is partitioned into a series of solid nodes connected by solid-to-solid conductors. In coupled fluid-structure problems, the solid nodes are connected by fluid-to-solid conductors, which model convection from the fluid to the pipe wall, see Figure 1. Conservation equations are expressed in conservative unsteady finite volume form for fluid network. The conservation equations for scalar fields such as pressure, temperature and concentration of species are solved at the internal fluid nodes in conjunction with the thermodynamic equation of state, whereas momentum conservation is solved for mass flow rates at the branches. The conservation of energy for solid nodes is solved at the solid nodes for solid node temperature simultaneously with all the other fluid flow conservation equations. This way the reduced-order fluid network modeling provides a feasible approach to aerospace system modeling and analysis [11], [12], [14] and [13]. Yet there are practical aerospace configurations for which predicting complex transients such as thermo-fluid and fast-slow-fast transients in long-time simulations require very accurate predictions with these network models. Despite this, there has been little attempt at developing an efficient explicit time stepping capability for simulations in fluid network. It is important to note here that there has been a growing interest in efficient explicit time-stepping approaches for computational fluid dynamic analysis of fluid flow components. For simulation of unsteady compressible flows, techniques based on explicit discretizations of the governing equations of fluid mechanics have proven to be quite useful [15], [16], [1], [10], [17], [4], [5] [3], [6], [18]. To guarantee numerical stability of explicit schemes, the time step needs to satisfy the CFL condition which is determined by the spatial mesh size and wave speed. However, as the CFL condition needs to hold globally, the time step size would be controlled by the smallest spatial step size or by the highest wave speed which increases the computational cost [3, 6, 7, 18]. Thus, to improve computational efficiency, explicit local time-stepping algorithm have been studied in [2, 4, 5, 15–17] However, their usage in network fluid flow computation is limited. Generalized Fluid System Simulation Program (GFSSP) [12] is a network simulation software based on unstructured upwind finite volume spatial discretization of conservation of mass, energy and species, and the momentum equation. GFSSP currently uses implicit time stepping schemes for time accurate simulations. This method is based on backward difference formula in conjunction with a Newton-iterative scheme for solving conservation equations. Implicit, unconditionally stable time stepping methods allow to use larger time steps, which reduces the computational time as compared to explicit methods. Note that the time step can not be too large in order to keep a good accuracy of the solution. For a Large Eddy Simulation of turbulent flows, the ratio between the time step and each cell characteristic length can not exceed 2-3 [8]. Moreover, implicit methods seem to have two drawbacks. First, an efficient parallel implementation of these methods may be difficult, especially if a strong scalability is required. In addition, implicit methods can be less accurate than

explicit methods due to a residual numerical noise.

The goal of this paper is to investigate a first order in time explicit time stepping scheme for network flow simulations. In order to carry out a systematic comparative study, we use the blowdown of a pressurized tanks as the benchmark problem.

II. Explicit Time Stepping Based Finite Volume Formulation of Fluid Network

The prediction of network flow dynamics involves numerically solving unsteady mass, momentum, and energy conservation equations along with the equation of state. The conservation equations are written in conservative finite volume form for a flow network of internal nodes, boundary nodes and branches. Fluid enters the network through a inlet boundary node and exits through a outlet boundary node and at the boundary nodes pressure and temperature are prescribed. A control volume is defined at each internal node and the boundaries of which are assumed to have inflow and outflow of mass and energy. Assuming that the flow is driven by the pressure differential between the upstream and downstream nodes the scheme computes pressure from the mass conservation equation and temperature from the energy conservation equation at the internal nodes in conjunction with the equation of state. Details of the governing equations, explicit time stepping and finite volume discretization are explained below.

A. Mass Conservation Equation

Figure 1 displays a schematic showing adjacent nodes, their connecting branches, and the indexing system used in this paper. In order to solve for the unknown variables, mass and entropy conservation equations and the equation of thermodynamic state are written for each internal node and flow rate equations are written for each branch. Figure 1 is a

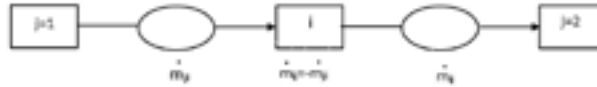


Fig. 1 Typical flow network consisting of fluid nodes, solid nodes, flow branches and conductors

schematic showing adjacent nodes, their connectivity, and the indexing convention. The mass conservation equation at the i th node can be expressed as follows, and each term has the unit of pounds of mass per second:

$$(m_i)_{t+\Delta t} = (m_i)_t - \Delta t \sum_{j=1}^n (\dot{m}_{ij})_t \quad (1)$$

B. Energy Conservation Equation

The energy conservation equation for node i can be expressed following the first law of thermodynamics and using enthalpy as the dependent variable. It can be written as

$$(h_i)_{t+\Delta t} = \frac{(m_i)_t (h_i)_t / \Delta t + \{ \sum_{j=1}^n \max(-(\dot{m}_{ij})_t, 0) (h_j)_t - \sum_{j=1}^n \max((\dot{m}_{ij})_t, 0) (h_i)_t \} + \{ (m_i)_{t+\Delta t} (p_i)_{t+\Delta t} / (\rho_i)_{t+\Delta t} J - (m_i)_t (p_i)_t / (\rho_i)_t J \} / \Delta t + \dot{Q}_i}{(m_i)_t / \Delta t} \quad (2)$$

The max operator used in (2) is known as an upwind differencing scheme and has been extensively employed in the numerical solution of Navier-Stokes equations in convective heat transfer and fluid flow applications. When the flow direction is not known, this operator allows the transport of energy only from its upstream neighbor. In other words, the upstream neighbor influences its downstream neighbor but not vice versa.

C. Momentum Conservation Equation

The momentum conservation equation (2) represents the balance of fluid forces acting on a given branch. The flow rate in a branch is calculated from this equation. It should also be noted that the flow rate, $\dot{m}_{ij}$, is a vector quantity. A negative value of $\dot{m}_{ij}$ signifies that the flow is directed from the j^{th} node to the i^{th} node:

$$(\dot{m}_{ij})_{t+\Delta t} = (\dot{m}_{ij})_t / V_{t+\Delta t} + g_c A_{ij} [(p_i - p_j) A_{ij} - K_f \dot{m}_{ij} |\dot{m}_{ij}| A_{ij}] / V_{t+\Delta t} \quad (3)$$

The first term inside the parentheses on the right side of the momentum equation represents the pressure gradient in the branch. The pressures are located at the upstream and downstream faces of a branch. The second term represents the frictional effect. Friction is modeled as a product of K_f , the square of the flow rate, and area. K_f is a function of the fluid density in the branch and the nature of flow passage being modeled by the branch.

D. Equation of State for Real Fluid

Transient flow calculations require the knowledge of resident mass in a control volume. The resident mass in the i th control volume is calculated from the equation of state for real fluids:

$$(p_i)_{t+\Delta t} = (m_i)_t R(T_i)_t Z/V \quad (4)$$

The compressibility factor Z and temperature T_i in Eq. (4) are calculated from the thermodynamic property program [9] for a given pressure and enthalpy.

III. Simulation of the Blowdown of a Pressurized Tank

In this Section, the capabilities of the explicit scheme based flow formulation of GFSSP to simulate the process of blowing down a pressurized tank will be demonstrated. Consider a tank with an internal volume of 10 ft^3 , containing air at a pressure and temperature of 100 psia and 80°F, respectively. Air is discharged into the atmosphere through an orifice of 0.1-in diameter for a period of 200 s. GFSSP will be used to determine the pressure, mass flow rate, and temperature history of the isentropic blowdown process. These predicted values are then compared with the implicit scheme based GFSSP solution. The physical schematic for the problem is shown in Figure 2 and a schematic of the

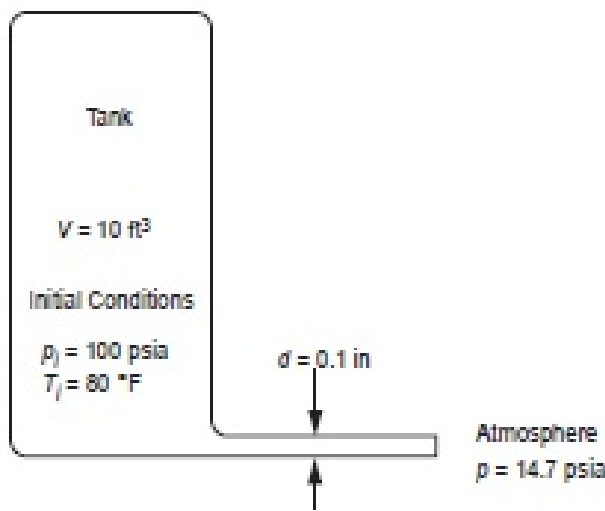


Fig. 2 Venting air tank schematics: Physical schematic



Fig. 3 Venting air tank schematics: MIG schematic.

corresponding GFSSP model is shown in Figure 3. The venting process is modeled with six nodes and five branches. Node 1 is an internal node that represents the tank. For the unsteady formulation, the node volume and the initial conditions must be supplied for each internal node and a history file must be supplied for each boundary node. The history file contains the pressures, temperatures, and concentrations at discrete times. At a minimum, this file should

include values at the process start time and at some time corresponding to the expected process stop time. Additional times can be included to account for nonlinear variation in the values if required. The initial pressure within the tank (node 1) was 100 psia. Resistance option 22 was used for branch 12 with a flow coefficient of 1. Air is modeled using the ideal gas option that is available in MIG.

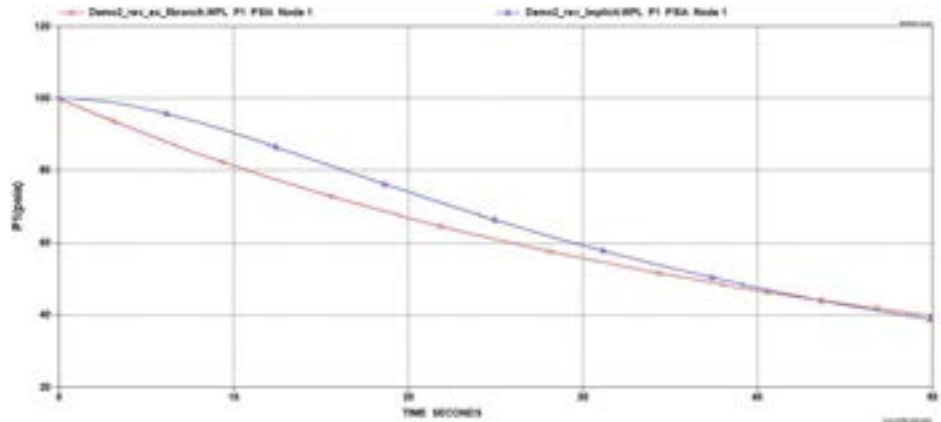


Fig. 4 Comparison of the predicted pressure history by implicit scheme and explicit scheme.

The numerical solutions using both implicit and explicit schemes are shown in Figures 4-5. The Figure 4 shows a comparison between the implicit GFSSP solution and the explicit GFSSP solution of pressures. The Figure 5 shows a comparison between the implicit GFSSP solution and the explicit GFSSP solution of temperatures. Overall, our results show that the proposed explicit scheme performs comparably to the implicit scheme in the blowdown problem we tested.

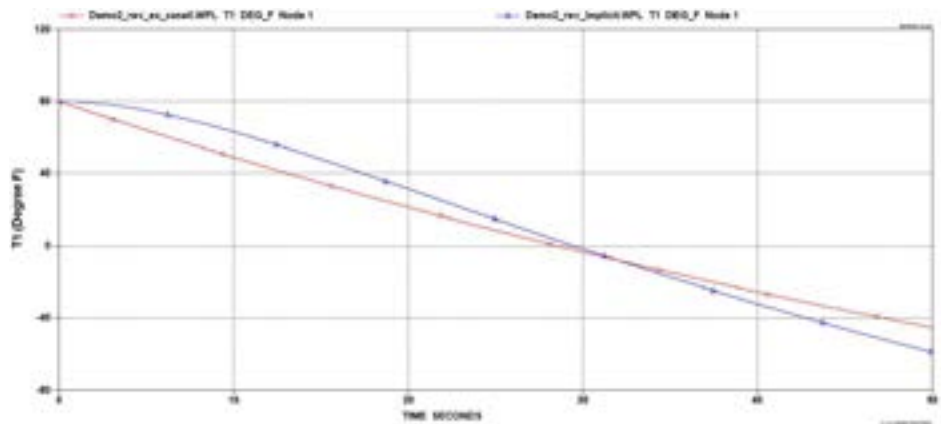


Fig. 5 Comparison of the predicted temperature history by implicit scheme and explicit scheme.

IV. Conclusions

In this paper, we have developed an explicit time stepping for transient simulations. Proposed solvers have been integrated into a network flow simulation software GFSSP (Generalized Fluid System Simulation Program) based on the unstructured finite volume method. Proposed explicit scheme's performance has been compared with the implicit scheme used currently in GFSSP. Overall, our results show that the proposed explicit scheme performs comparably in the blowdown problem we tested. For future work, there are several topics that could be considered such as higher order multistep time stepping method and multistage Runge-Kutta time stepping methods.

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**APPENDIX A—NASA MARSHALL SPACE FLIGHT CENTER
FACULTY FELLOWSHIP PROGRAM ANNOUNCEMENT**

MARSHALL AEROSPACE FELLOWSHIP PROGRAM

MAY 31, 2021 – AUGUST 6, 2021



Application Deadline February 17, 2021

- The Marshall Space Flight Center is offering Aerospace Fellowships for qualified researchers and graduate students at U.S. colleges and universities to conduct research with NASA colleagues during a ten-week residential program in Huntsville, Alabama.
- Aerospace Fellows will receive stipends of \$15,000 (Assistant Professor, Research Faculty), \$17,000 (Associate Professor), \$19,000 (Professor), and/or \$13,000 (Graduate Student).
- A relocation allowance of \$1,500 will be provided to those fellows who live more than fifty miles from MSFC and a \$500 travel supplement for one round-trip.
- Applicants must be U.S. citizens who hold full-time teaching, research appointments, or are graduate students at accredited U.S. universities or colleges.
- During the ten-week program, fellows are required to conduct their research on-site at the Marshall Space Flight Center.

Women and under-represented minorities, and persons with disabilities are encouraged to apply.

APPENDIX B—NASA MARSHALL SPACE FLIGHT CENTER FACULTY FELLOWSHIP PROGRAM DESCRIPTION

Program Description

- The Marshall Aerospace Fellowship program is a residential research experience. Fellows are required to conduct their research, during the ten-week program, on-site at the Marshall Space Flight Center.
- Participants cannot receive remuneration from other entities or other programs or other university or government sources during the Aerospace Fellowship 10-week period.
- An oral presentation by the Fellow to the Marshall group with which s/he has been affiliated is required, near the end of the fellowship period.
- A written final report is required at the end of the Fellowship.
- A written evaluation of the program by the Fellow is expected at the end of the Fellowship.

Eligibility

- US citizen
- Full time teaching or research appointment, or graduate student appointment at an accredited US university or college.
- Fellowship is awarded for one summer period, but Fellow may apply again for a second year.
- Women, under-represented minorities, and persons with disabilities are encouraged to apply.
- Graduate student applicants must be chosen by the Faculty Researcher who is applying, and both must be matriculated at the same university. Each must submit a completed application. If selected by Marshall, the faculty member and the graduate student would be a team engaged in the same research project at Marshall. To be selected, the graduate student must remain enrolled at the same university for a minimum period of two years following the summer research, teaming with the faculty researcher.

Selection

The applicants selected to be Aerospace Fellows will be chosen by the Marshall group which has been assigned the area of investigation (concentration) chosen by the applicant.

Marshall Collaborator

A Marshall Collaborator will be identified to serve as the co-investigator and day-to-day contact. At the end of the ten-week period, the Aerospace Fellow and the Marshall Collaborator will prepare a white paper summarizing the summer effort, including results and recommending follow-up work.

Compensation

Stipends for Aerospace Fellows are set as follows for the 10-week period:

Graduate Students	\$13,000
Assistant Professors and Research Faculty	\$15,000
Associate Professors	\$17,000
Professors	\$19,000

A relocation allowance of \$1,500 will be provided to fellows who live more than fifty miles from the Marshall Center.

A travel supplement of \$500 will be provided to those fellows receiving the relocation allowance.

National Aeronautics and

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George C. Marshall Space Flight Center

Huntsville, Alabama 35812
