TFAWS Aerosciences Presentation Session





CFD simulations of the effects of Thermo-Chemical Non-Equilibrium on Two Hypersonic re-entry cases

Neil Castelino, Jason Brian Dsouza, Valerio Viti Song Gao Anup Jain

Presented By Neil Castelino and Jason Brian Dsouza

> Thermal & Fluids Analysis Workshop TFAWS 2023 August 21-25, 2023 NASA Goddard Space Flight Center College Park, MD

CFD simulations of the effects of Thermo-Chemical Non-Equilibrium on Two Hypersonic re-entry cases

Neil Castelino, Jason Brian Dsouza, Valerio Viti Song Gao Anup Jain



© Copyright 2023 ANSYS, Inc.



1. Introduction

- 2. Wind-Tunnel Validation: MacLean Sphere-cylinder case
 - Description, Setup, Results
- 3. Flight Test Validation: JAXA's OREX re-entry capsule
 - Description, Setup, Results
- 4. Conclusion and Future work
- 5. Questions



Selected Test Cases for Validation

MacLean Sphere-cylinder

- Hemispherical nose tip geometry.
- Data from wind-tunnel experiments and results from DPLR code.
- CFD validation against data under controlled conditions.



References

1. Matthew MacLean, Eric Marineau, Ronald Parker, Aaron Dufrene, Michael Holden and Paul Deslardin, Effect of Surface Catalysis on Measured Heat Transfer in Expansion Tunnel Facility, Journal of Spacecraft and Rockets, Volume 50, Number 2 March 2013.

JAXA's OREX Re-entry Capsule

- Blunt body re-entry capsule.
- Rare set of re-entry flight data with ionization effects.
- CFD validation against data with experimental uncertainty.





References

- 2) R. N. Gupta, J. N. Moss, and J. M. Price, Assessment of Thermochemical Nonequilibrium and Slip Effects for Orbital Reentry Experiment (OREX)
- 3) Jung, M., Numerical Study of Plasma Flows and Radio Frequency Blackout for Reentry Vehicle, Ph.D. Thesis, Department of Aeronautics and Astronautics, Kyushu University, Fukuoka, Japan, February, 201
- 4) Wada, Y., Watanabe, Y., Akimoto, T., Yasui, H., Data analysis of electrostatic-probe, Special Publication of the National Aerospace Laboratory SP-24, pp. 227-236, 1994.
- 5) Vu, H., Viti, V., J., Tharp, J, Staggs, E, "Prediction of communication blackout and degradation for a re-entry hypersonic capsule through high-fidelity numerical simulations", AIAA-2023-2561, AIAA SciTech, Jan 19-27, 2023.



MacLean Case Description

- MacLean et al[1] used the new LENS-XX expansion tunnel facility to make surface heat transfer measurements for a planar cylindrical and hemispherical nose tip geometry.
- The DPLR code was also used to predict heat transfer rates for a non-reacting wall and a super catalytic wall conditions.
- It was noted that recombination of disassociated species has a significant impact on surface wall heat transfer rates for hypersonic flows.
- In Ansys Fluent, we use the catalytic wall boundary conditions to simulate these effects.



References

1. Matthew MacLean, Eric Marineau, Ronald Parker, Aaron Dufrene, Michael Holden and Paul DesJardin, Effect of Surface Catalysis on Measured Heat Transfer in Expansion Tunnel Facility, Journal of Spacecraftand Rockets, Volume 50, Number 2 March 2013.



MacLean Case Setup: Computational Domain

- A structured quad mesh was generated for this case.
- Cells are finer closer to the wall in order to predict the surface and stagnation heat transfer rates accurately.
- Cell Reynolds number was used as to quantify the cell resolution near the wall.

$$\operatorname{Re}_{\operatorname{cell}} = \frac{\rho_{\operatorname{wall}} \alpha_{\operatorname{wall}} \Delta y}{\mu_{\operatorname{wall}}}$$



References

1. Matthew MacLean, Eric Marineau, Ronald Parker, Aaron Dufrene, Michael Holden and Paul DesJardin, Effect of Surface Catalysis on Measured Heat Transfer in Expansion Tunnel Facility, Journal of Spacecraftand Rockets, Volume 50, Number 2 March 2013.

Figure 4: Computational domain along with boundary conditions.



MacLean Case Setup: At a glance

Ansys Fluent setup

- Axi-symmetric formulation
- Laminar Flow
- Double-precision
- Steady-state DBNS solver
- 2nd order scheme for convective fluxes
- Green-Gauss Node-Based gradient for viscous fluxes
- Modified Roe scheme.
- Finite-Rate Chemistry solver
- 2T model to capture Thermal Non-Equilibrium
- Gupta model for reacting air mechanism:
 - 11 species: N2, O2, O, N, NO, N+, O+, NO+, N2+, O2+, e-
 - 21 reactions
- Wall Catalytic boundary conditions to model Chemical Non-Equilibrium



Figure 5: Mach number and Vibrational Electronic Temperature contours for axisymmetric case.



MacLean Case Results: Grid Dependence Study

- A grid dependence study was conducted.
- 3 meshes with 250k, 1.04 million, and 4.42 million elements were studied.
- The medium mesh with 1.04 million elements was chosen for further studies.
- A cell Reynolds number of 8 was found to be sufficient to resolve the first cell height.



Figure 6: Grid Dependence Study



MacLean Case Results: Effect of increasing recombination coefficients



ncients with Supta reaction methanism.

Ansys

MacLean Case Results: Comparison of Gupta and Park93 reaction mechanism



Figure 9: Comparison of Heat Transfer Rates on the hemispherical surface for Park93 vs Gupta reaction mechanism at 3 recombination values.



Figure 10: Mass fractions of O and N on the stagnation line at 3 recombination values for Park93 reaction mechanism.



OREX Case Description



- ORbital Re-entry
 EXperiment
- Flight test by JAXA to measure plasma environment during Earth atmospheric re-entry
- Rare set of re-entry flight data with ionization effects
- Geometry is typical blunt-body re-entry capsule with heatshield on windward side
- Large (unquantified) experimental uncertainty due to nature of experiment



Flight time s	Altitude km	Velocity m/s	$\frac{\rm Density}{\rm kg/m^3}$	Temperature K	Wall temperature K
7370.6	101.10	7454.65	5.7100×10^{-7}	195	402
7381.0	96.77	7456.30	1.3810×10^{-6}	192	485
7391.0	92.82	7454.10	3.0090×10^{-6}	189	586
7401.0	88.45	7444.30	4.3060×10^{-6}	187	687
7411.5	84.01	7415.90	1.0953×10^{-5}	189	785
7421.5	79.90	7360.20	1.8455×10^{-5}	199	878
7431.5	75.81	7245.70	3.6576×10^{-5}	207	976
7441.5	71.73	7049.20	6.5184×10^{-5}	215	1091



2) R. N. Gupta, J. N. Moss, and J. M. Price, Assessment of Thermochemical Nonequilibrium and Slip Effects for Orbital Reentry Experiment (OREX)

3) Jung, M., Numerical Study of Plasma Flows and Radio Frequency Blackout for Reentry Vehicle, Ph.D. Thesis, Department of Aeronautics and Astronautics, Kyushu University, Fukuoka, Japan, February, 2018.

4) Wada, Y., Watanabe, y., Akimoto, T., Yasui, H., Data analysis of electrostatic-probe, Special Publication of the National Aerospace Laboratory SP-24, pp. 227-236, 1994.

5) Vu, H., Viti, V., J., Tharp, J, Staggs, E, "Prediction of communication blackout and degradation for a re-entry hypersonic capsule through high-fidelity numerical simulations", AIAA-2023-2561, AIAA SciTech, Jan 19-27, 2



OREX Case Description : Problem definition



Flight	Altitude,	Velocity,	Т	00,	Τw ^a			Mole Fra	ctions		
time,	km	m/s	1	K	К	Xc) 2	X	N ₂	Х	ю
S			OREX	Jacchia		OREX	Jacchia	OREX	Jacchia	OREX	Jacchia
7361.0	105.00	7451.00	218	211.05	332	0.2375	0.1528	0.7625	0.7815	0.0	0.0657
7370.6	101.10	7454.65	195	196.89	402	0.2375	0.1726	0.7625	0.7839	0.0	0.0435
7381.0	96.77	7456.30	192	190.26	485	0.2375	0.1884	0.7625	0.7863	0.0	0.0253
7391.0	92.82	7454.10	189	188.30	586	0.2375	0.2025	0.7625	0.7881	0.0	0.0094
7401.0	88.45	7444.30	187		687	0.2375		0.7625		0.0	
7411.5	84.01	7415.90	189		785	0.2375		0.7625		0.0	
7421.5	79.90	7360.20	199		878	0.2375		0.7625		0.0	
7431.5	75.81	7245.70	207		976	0.2375		0.7625		0.0	
7441.5	71.73	7049.20	215		1091	0.2375		0.7625		0.0	
7451.5	67.66	6720.30	226		1213	0.2375		0.7625		0.0	
7461.5	63.60	6223.40	237		1344	0.2375		0.7625		0.0	
7471.5	59.60	5561.60	248		1458	0.2375		0.7625		0.0	
7481.5	55.74	4759.10	259		1531	0.2375		0.7625		0.0	
7491.5	51.99	3873.40	268		1557	0.2375		0.7625		0.0	
7501.5	48.40	3000.00	271		1388	0.2375		0.7625		0.0	

^aCFD inferred stagnation surface temperatures of Yamamoto (Ref. 5). Also, temperature distributions are specified from the same CFD computations.

				נ נוסט	Table 1. Constraints	oncluded. n Conditior	ıs			
Altitude, km	e, Specific heat ratio, γ_{∞}		Speed of sound, m/s		Mach No., M∞		Mol. wt., kg/k-mole		Density, kg/m ³	
	OREX	Jacchia	OREX	Jacchia	OREX	Jacchia	OREX	Jacchia	OREX	Jacchia
105.0	1.40	1.4108	296.734	298.202	25.11	24.986	28.96	27.838	3.1400x10 ⁻⁷	2.3350x10-7
101.1	1.40	1.4071	280.989	285.819	26.53	26.082	28.96	28.195	5.7100x10 ⁻⁷	4.8341x10 ⁻⁷
96.77	1.40	1.4041	279.053	279.323	26.72	26.694	28.96	28.466	1.3810x10 ⁻⁶	9.3644x10 ⁻⁷
92.82	1.40	1.4015	276.385	276.492	26.97	26.960	28.96	28.701	3.0090x10 ⁻⁶	1.9465x10 ⁻⁶
88.45	1.40		275.002		27.07	28.96			4.3060x10 ⁻⁶	
84.01	1.40		276.506		26.82	28.96			1.0953x10 ⁻⁵	
79.90	1.40		274.430		26.82	28.96			1.8455x10 ⁻⁵	
75.81	1.40		289.365		25.04	28.96			3.6576x10 ⁻⁵	
71.73	1.40		295.069		23.89	28.96			6.5184x10 ⁻⁵	
67.66	1.40		302.444		22.22	28.96			1.2164x10 ⁻⁴	
63.60	1.40		309.776		20.09	28.96			2.0594x10 ⁻⁴	
59.60	1.40		316.900		17.55	28.96			3.3131x10 ⁻⁴	
55.74	1.40		323.528		14.71	28.96			5.3150x10 ⁻⁴	
51 99	1.40		328,254		11.80	28.96			8.2445x10 ⁻⁴	
48.40	1.40		331.126		9.06	28.96			1.2677x10 ⁻³	

References

2-Gupta, R.N., Moss, J.N., Price, J.M., Assessment of Thermochemical Nonequilibrium and Slip Effects for Orbital Reentry Experiment (OREX), 31st AIAA Thermophysics Conference, June 17-20, 1996, New Orleans, LA.
 3-Jung, M., Numerical Study of Plasma Flows and Radio Frequency Blackout for Reentry Vehicle, Ph.D. Thesis, Department of Aeronautics and Astronautics, Kyushu University, Fukuoka, Japan, February, 2018.
 4-Wada, Y., Watanabe, Y., Akimoto, T., Yasui, H., Data analysis of electrostatic-probe, Special Publication of the National Aerospace Laboratory SP-24, pp. 227-236, 1994.



OREX Case Setup: Computational Domain





- Block-structured 2D mesh of 1.27 mil. quad cells
- Gas is air as a mixture of O₂ and N₂, ideal-gas, variable properties
- Assume laminar flow





Ansys Fluent setup

- Axi-symmetric formulation
- Laminar Flow
- Double-precision
- Steady-state DBNS solver
- 2nd order scheme for convective fluxes
- Green-Gauss Node-Based gradient for viscous fluxes
- Modified Roe scheme, CASM = 5
- Finite-Rate Chemistry solver
- 2-temperature model to capture Thermal Non-Equilibrium
- Gupta model for reacting air mechanism:
 - 11 species: N2, O2, O, N, NO, N+, O+, NO+, N2+, O2+, e-
 - 21 reactions
- Wall Catalytic boundary conditions to model Chemical Non-Equilibrium





OREX Case Results: Mesh Independence Study

Refinement	Mesh size
Base mesh	318520
*4	1274080
*8	5096320

Aspect Ratio at Stagnation : 1 Cell Reynolds Number at Stagnation : 1.6

Refinement	Stagnation Heat Flux (KW/m ²)
Base mesh	-117.291
*4	-116.659
*8	-116.410

% difference in Q_{stag} between Base and *4: **0.54%** % difference in Q_{stag} between *4 and *8: **0.21%**



Figure 12: Total Surface Heat Flux on wall Heat Shield



OREX Case Results: Contours



Figure 13: Contour of Mach Number at 88.45 km

Figure 14: Contour of Vibrational Electronic Temperature at 88.45 km

A detached bow shock is formed which causes high temperature and pressure on the surface of the re-entry body



OREX Case Results: Stagnation Heat Flux plot



Figure 15: Stagnation Heat Flux of CFD (using Gupta model) compared to flight test data

References

+ -Gupta, R.N., Moss, J.N., Price, J.M., Assessment of Thermochemical Nonequilibrium and Slip Effects for Orbital Reentry Experiment (OREX), 31st AIAA Thermophysics Conference, June 17-20, 1996, New Orleans, LA.

*Extrapolated data



©2023 ANSYS, Inc.

Conclusion and Future Work

- Two cases were validated against available experimental data. Recombination was found to be a very important component in accurately predicting the heat transfer loads on re-entry objects.
- It is important to validate commercial codes against both wind tunnel data as well as flight data.
- Ansys Fluent provides the ability to model thermal and chemical non-equilibrium using the Two-Temperature Model and Surface Catalysis wall conditions. This is key for hypersonic re-entry applications.
- Further modeling using Park93 reaction mechanism.
- Include thermal radiative effects.
- Use partially catalytic wall conditions for the OREX case.



Thank you for your time!

Do you have any questions?





Additional Slides: OREX Extrapolated Data (Heat Flux)



©2023 ANSYS, Inc.

Additional Slides: OREX Extrapolated Data (Cell Reynolds Number)



71.73 km

88.45 km

