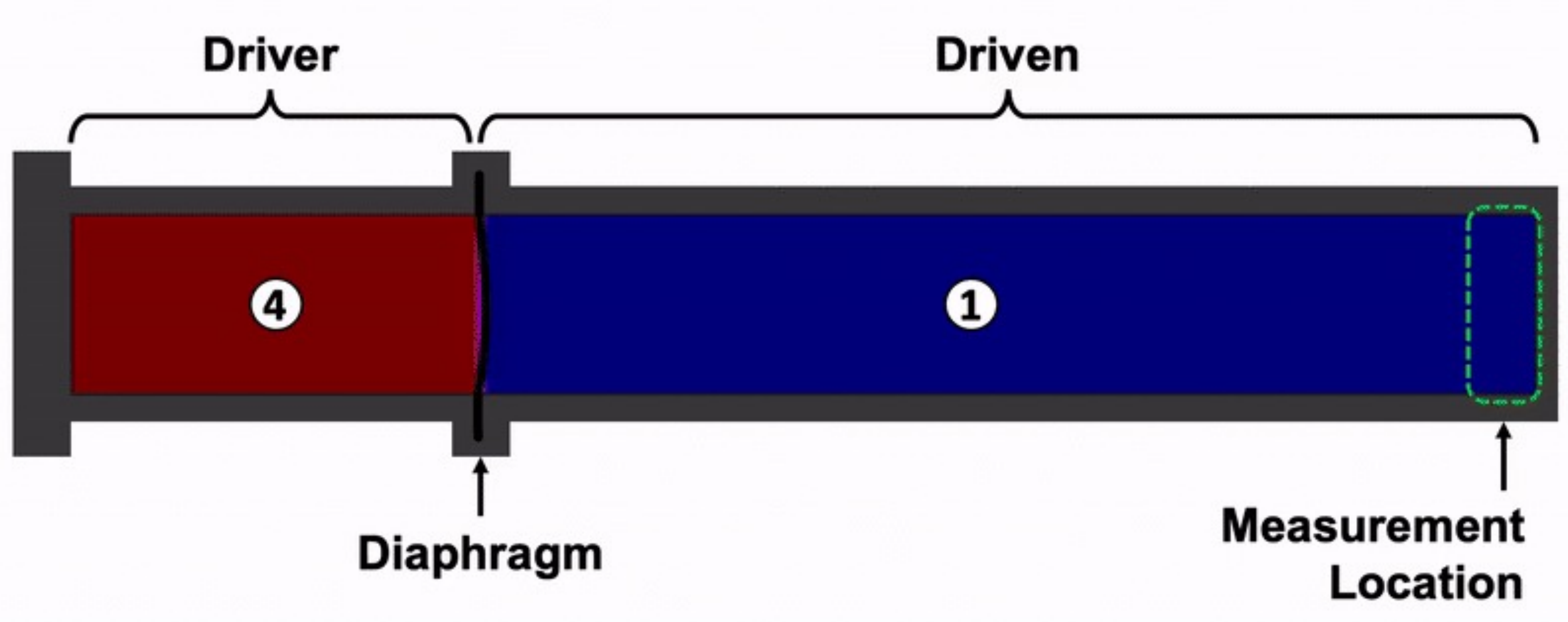
THEORY AND SIMULATION OF HIGH-TEMPERATURE GAS IN SHOCK TUBES

Aaron Larsen
Ozgur Tumuklu (now at RPI)
Kyle Hanquist



Movie from Hanson Research Group
Stanford University

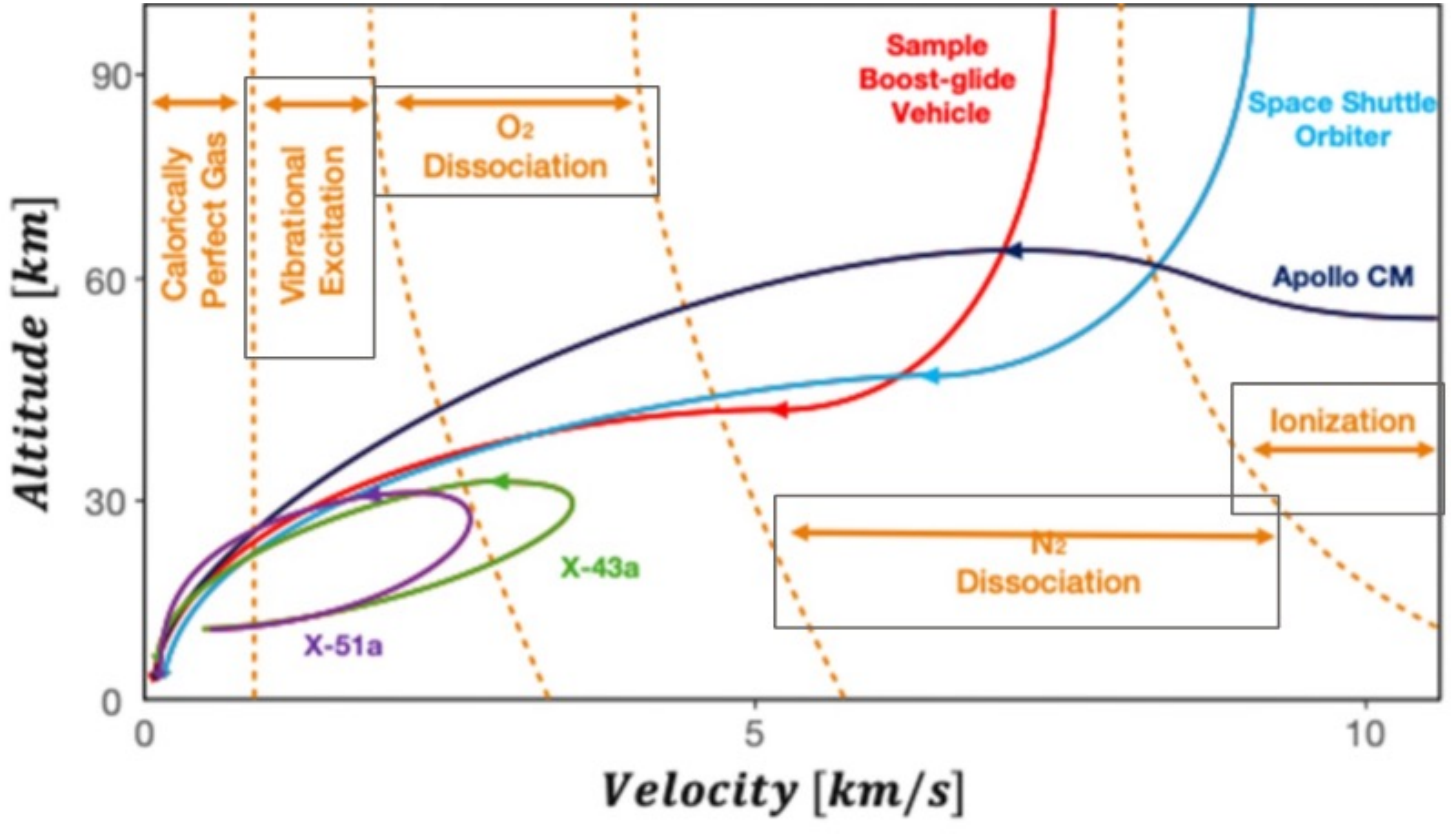
ARIZONA RESEARCH CENTER FOR HYPERSONICS

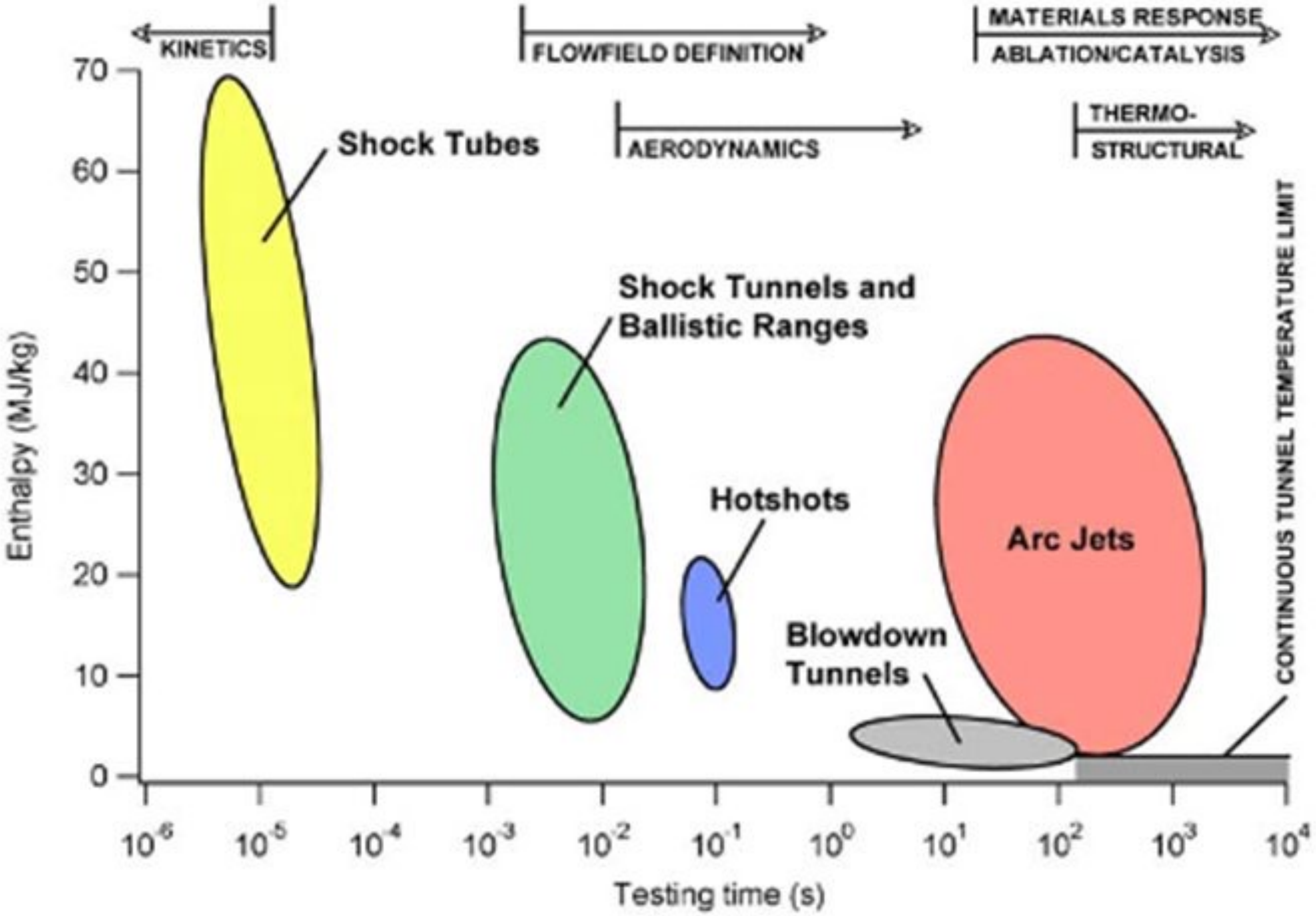
ARCH

Outline

- Motivation
- Background
- Approaches
  - Analytical
  - NASA CEA (Chemical Equilibrium with Applications)
  - Computational Fluid Dynamics
    - brODErs
    - SU2
- Results
  - Comparison between post-shock conditions
- Conclusions and Future Work

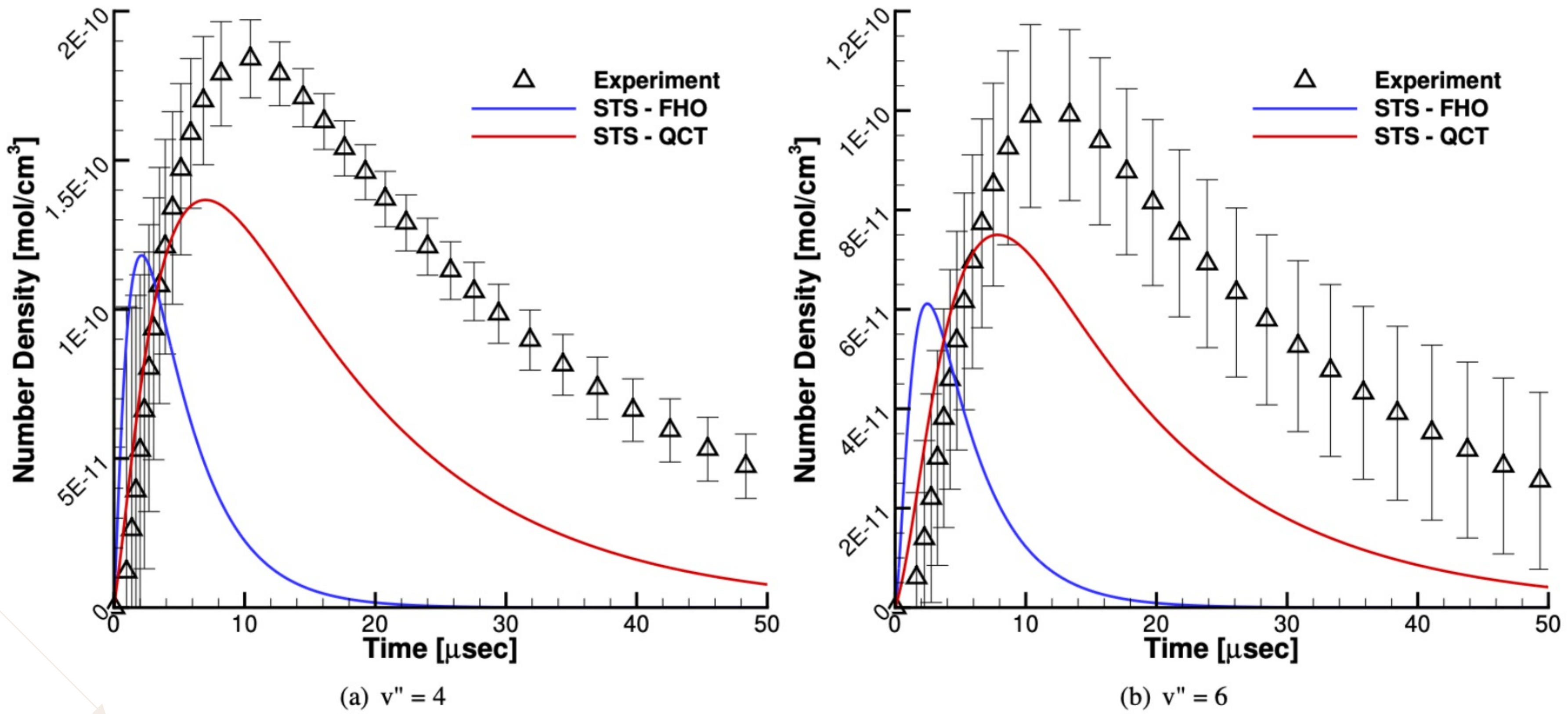
Motivation


Calorically Perfect Gas
Vibrational Excitation
O_2 Dissociation
Sample Boost-glide Vehicle
Space Shuttle Orbiter
Apollo CM
Ionization
N_2 Dissociation
X-43a
X-51a
90
60
30
0
0
5
10
Altitude [km]
Velocity [km/s]


KINETICS
FLOWFIELD DEFINITION
MATERIALS RESPONSE
ABLATION/CATALYSIS
AERODYNAMICS
THERMO-STRUCTURAL
Shock Tubes
Shock Tunnels and Ballistic Ranges
Hotshots
Arc Jets
Blowdown Tunnels
CONTINUOUS TUNNEL TEMPERATURE LIMIT
70
60
50
40
30
20
10
0
Enthalpy (MJ/kg)
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
Testing time (s)

Motivation

- Shock tubes and especially reflected shock tubes are used to assess high-fidelity chemical kinetic approaches
- Assumptions are made when **modeling** the shock tube (e.g., heat bath) = *uncertainty*
  - Are discrepancies due to assumptions or chemical kinetic data/approaches?
- **Experimentalists** also make assumptions when extracting shock tube data = *uncertainty*
- Goal: reduce this *uncertainty*



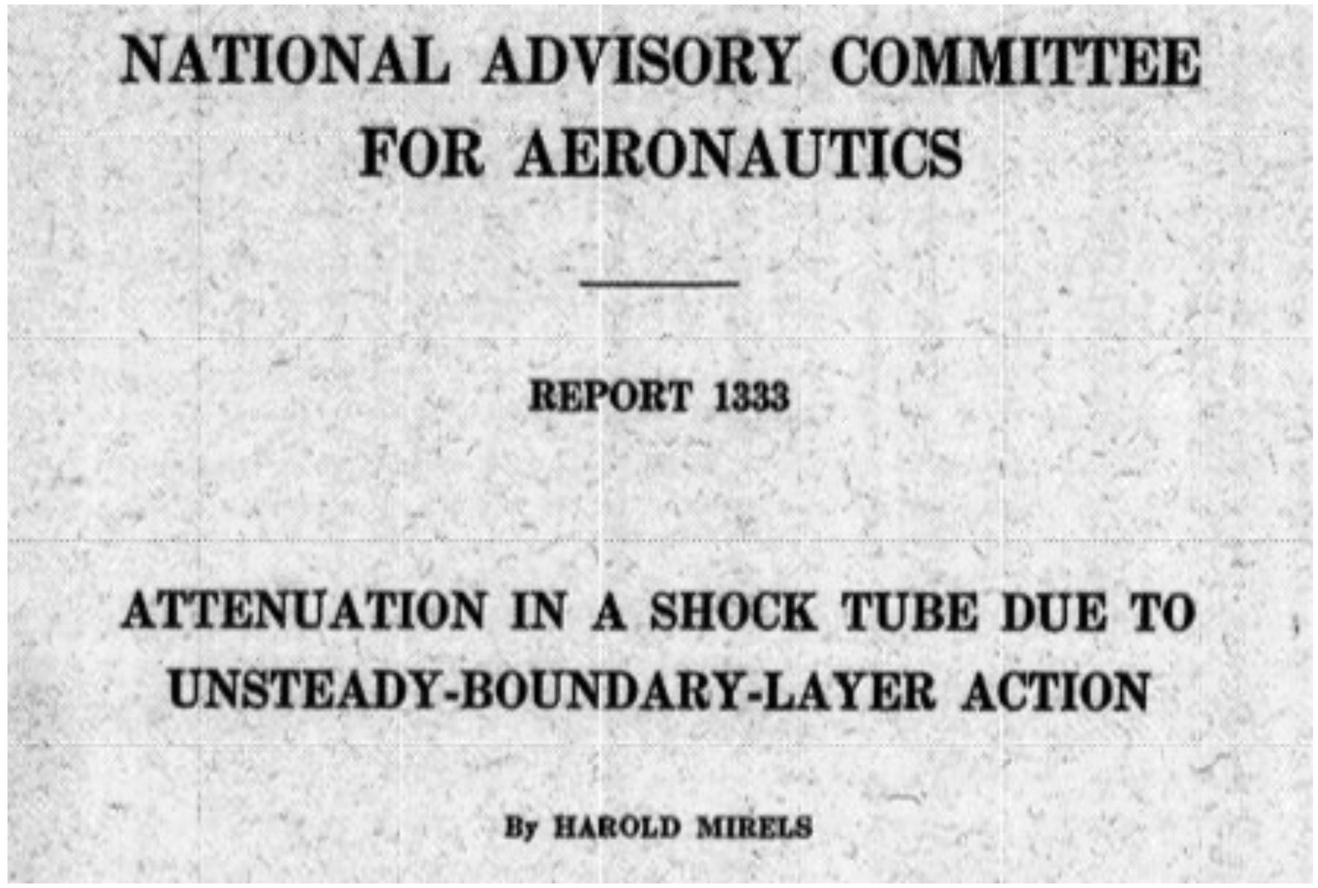
(a) v'' = 4

(b) v'' = 6

Vibrational state populations in a reflected shock tube flow (10,700 K) – modeling vs. Experiment

Hanquist, et al., AIAA Paper 2020-3275

Background

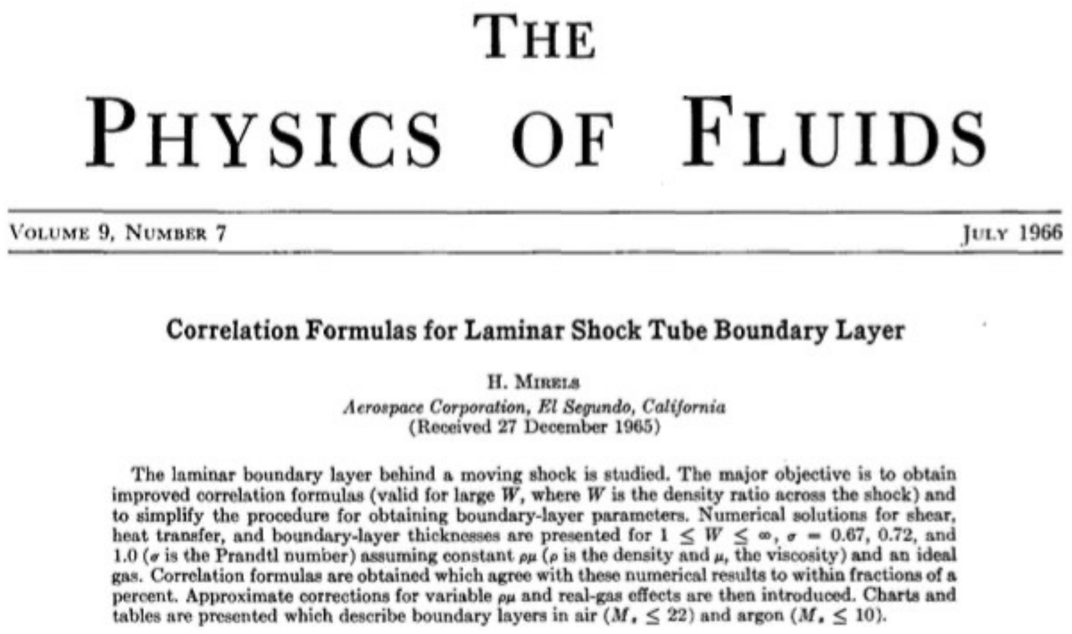


NATIONAL ADVISORY COMMITTEE
FOR AERONAUTICS

REPORT 1333

ATTENUATION IN A SHOCK TUBE DUE TO
UNSTEADY-BOUNDARY-LAYER ACTION

By HAROLD MIRELS



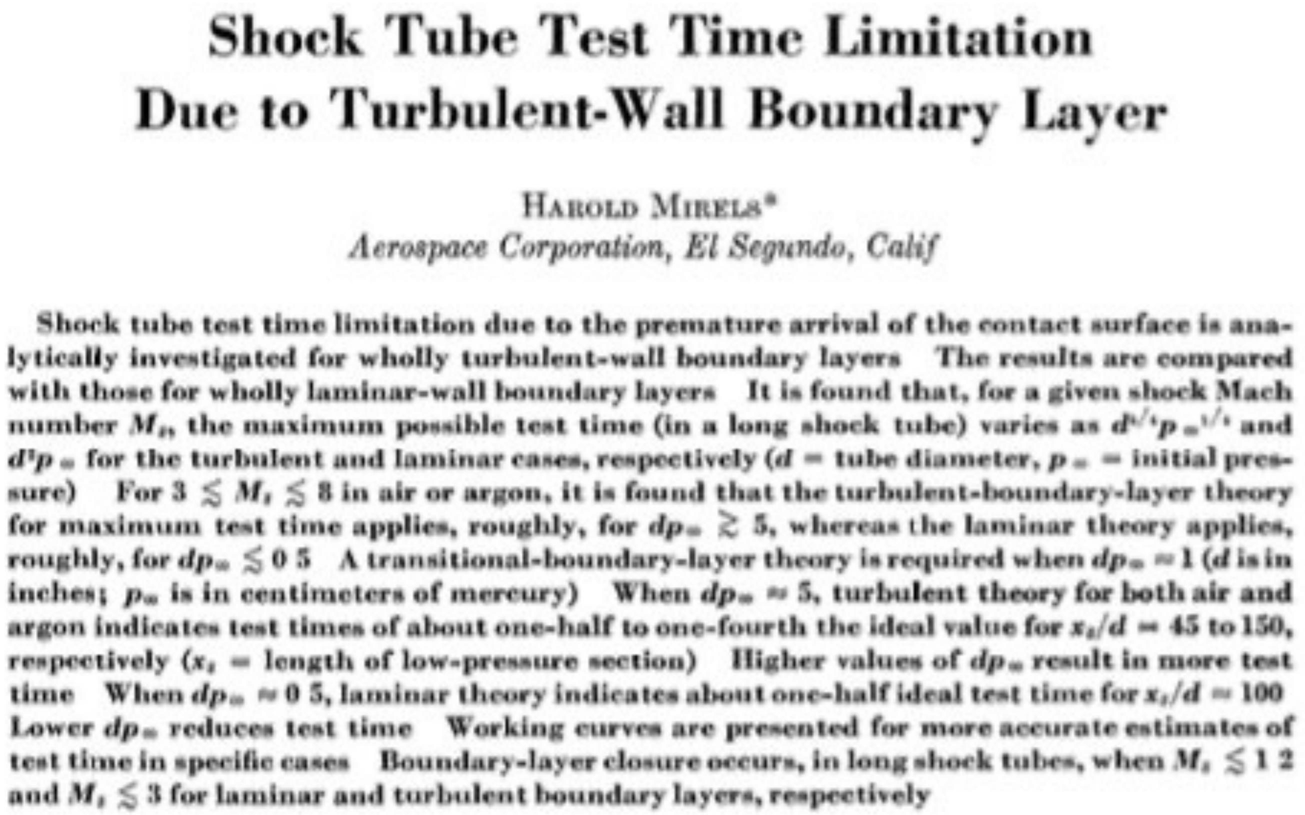
THE
PHYSICS OF FLUIDS

VOLUME 9, NUMBER 7 JULY 1966

Correlation Formulas for Laminar Shock Tube Boundary Layer

H. MIRELS
Aerospace Corporation, El Segundo, California
(Received 27 December 1965)

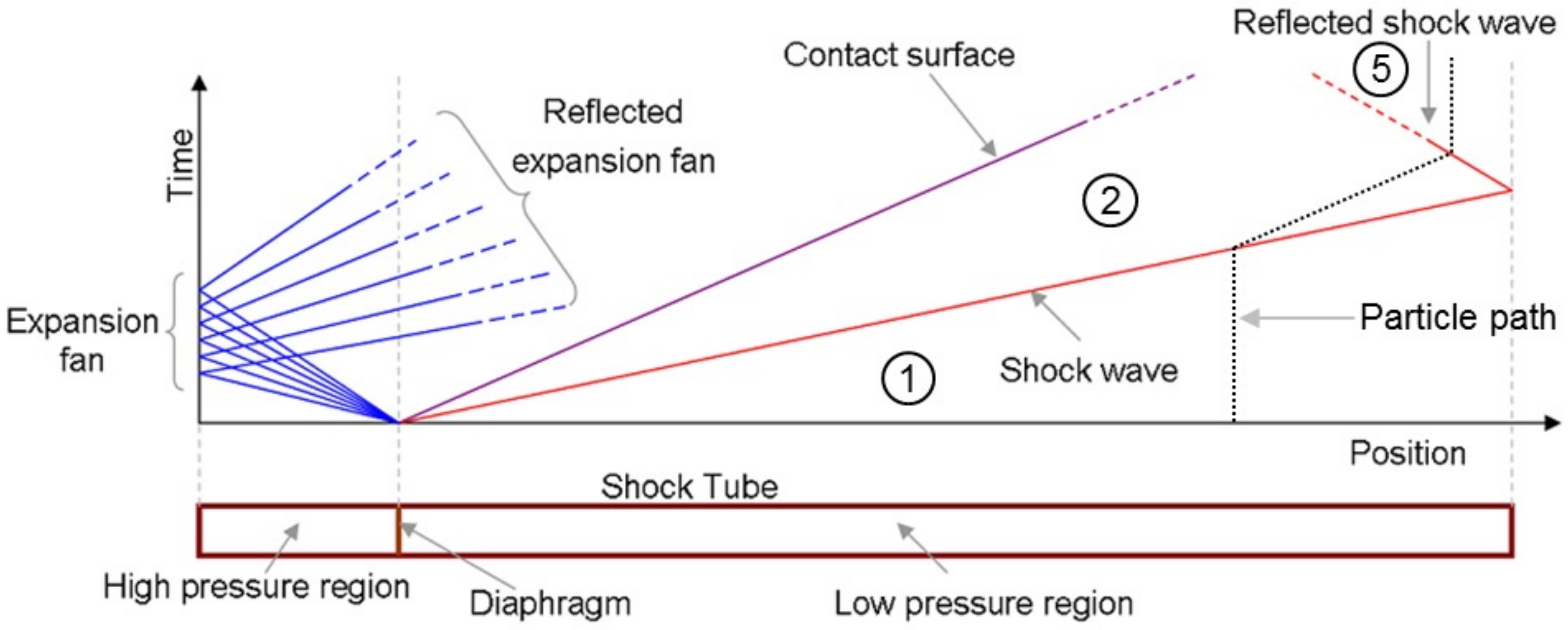
The laminar boundary layer behind a moving shock is studied. The major objective is to obtain improved correlation formulas (valid for large W, where W is the density ratio across the shock) and to simplify the procedure for obtaining boundary-layer parameters. Numerical solutions for shear, heat transfer, and boundary-layer thicknesses are presented for $1 \leq W \leq \infty$, $\sigma = 0.67, 0.72$, and 1.0 (σ is the Prandtl number) assuming constant $\rho\mu$ (ρ is the density and μ, the viscosity) and an ideal gas. Correlation formulas are obtained which agree with these numerical results to within fractions of a percent. Approximate corrections for variable $\rho\mu$ and real-gas effects are then introduced. Charts and tables are presented which describe boundary layers in air ($M_s \leq 22$) and argon ($M_s \leq 10$).



Shock Tube Test Time Limitation
Due to Turbulent-Wall Boundary Layer

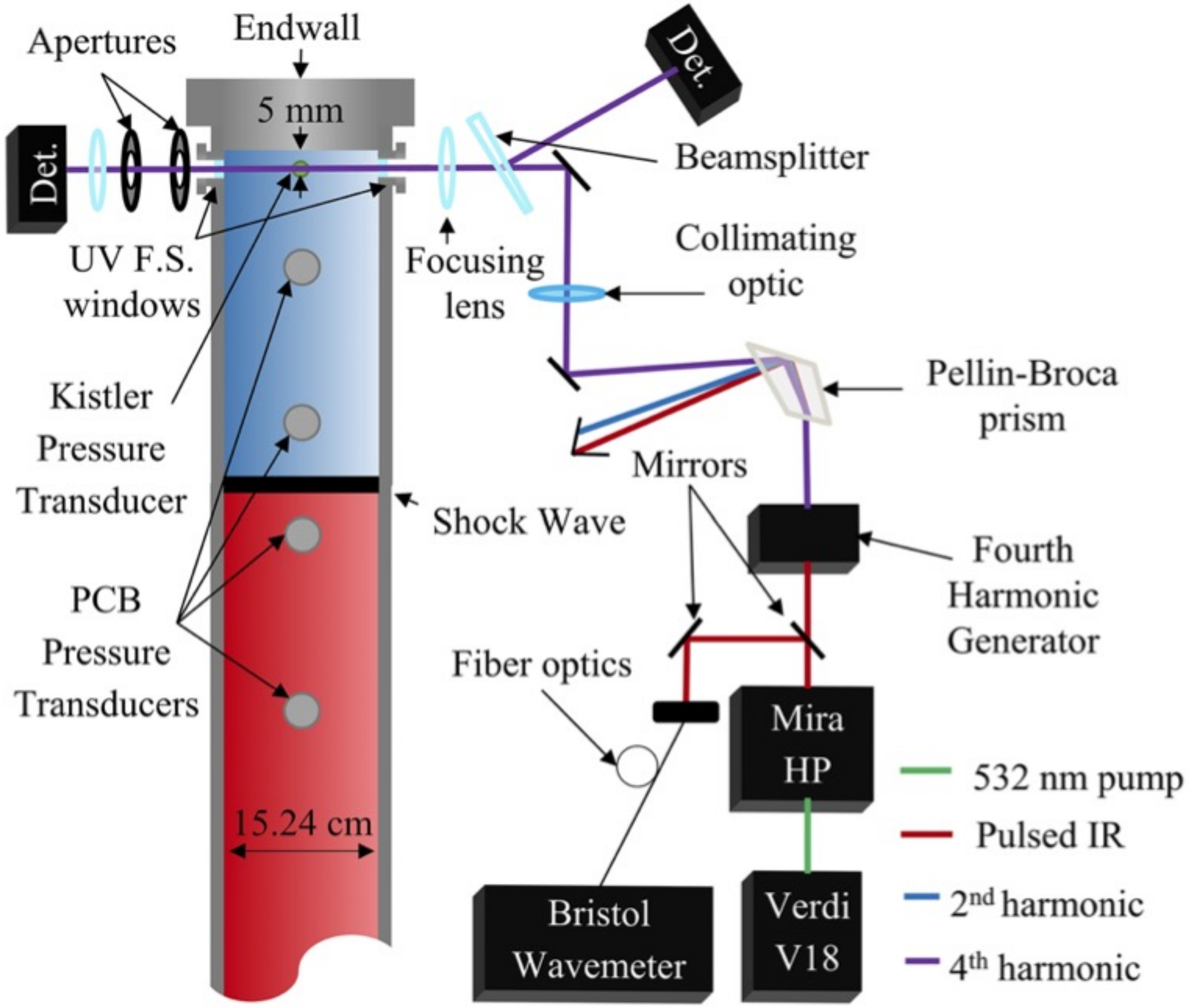
HAROLD MIRELS*
Aerospace Corporation, El Segundo, Calif

Shock tube test time limitation due to the premature arrival of the contact surface is analytically investigated for wholly turbulent-wall boundary layers The results are compared with those for wholly laminar-wall boundary layers It is found that, for a given shock Mach number M_s, the maximum possible test time (in a long shock tube) varies as $d^{5/4}p_\infty^{1/4}$ and d^2p_∞ for the turbulent and laminar cases, respectively (d = tube diameter, p_∞ = initial pressure) For $3 \lesssim M_s \lesssim 8$ in air or argon, it is found that the turbulent-boundary-layer theory for maximum test time applies, roughly, for $dp_\infty \gtrsim 5$, whereas the laminar theory applies, roughly, for $dp_\infty \lesssim 0\ 5$ A transitional-boundary-layer theory is required when $dp_\infty \approx 1$ (d is in inches; p_∞ is in centimeters of mercury) When $dp_\infty \approx 5$, turbulent theory for both air and argon indicates test times of about one-half to one-fourth the ideal value for x_s/d = 45 to 150, respectively (x_s = length of low-pressure section) Higher values of dp_∞ result in more test time When $dp_\infty \approx 0\ 5$, laminar theory indicates about one-half ideal test time for x_s/d = 100 Lower dp_∞ reduces test time Working curves are presented for more accurate estimates of test time in specific cases Boundary-layer closure occurs, in long shock tubes, when $M_s \lesssim 1\ 2$ and $M_s \lesssim 3$ for laminar and turbulent boundary layers, respectively



Experimental setup

- Experimental design setup by Streicher et al. using shock tubes with nondilute O_2
- Pressure transducers and lasers near the wall assist with collection of pressure and velocity data
- Attempt to assess different modeling approaches



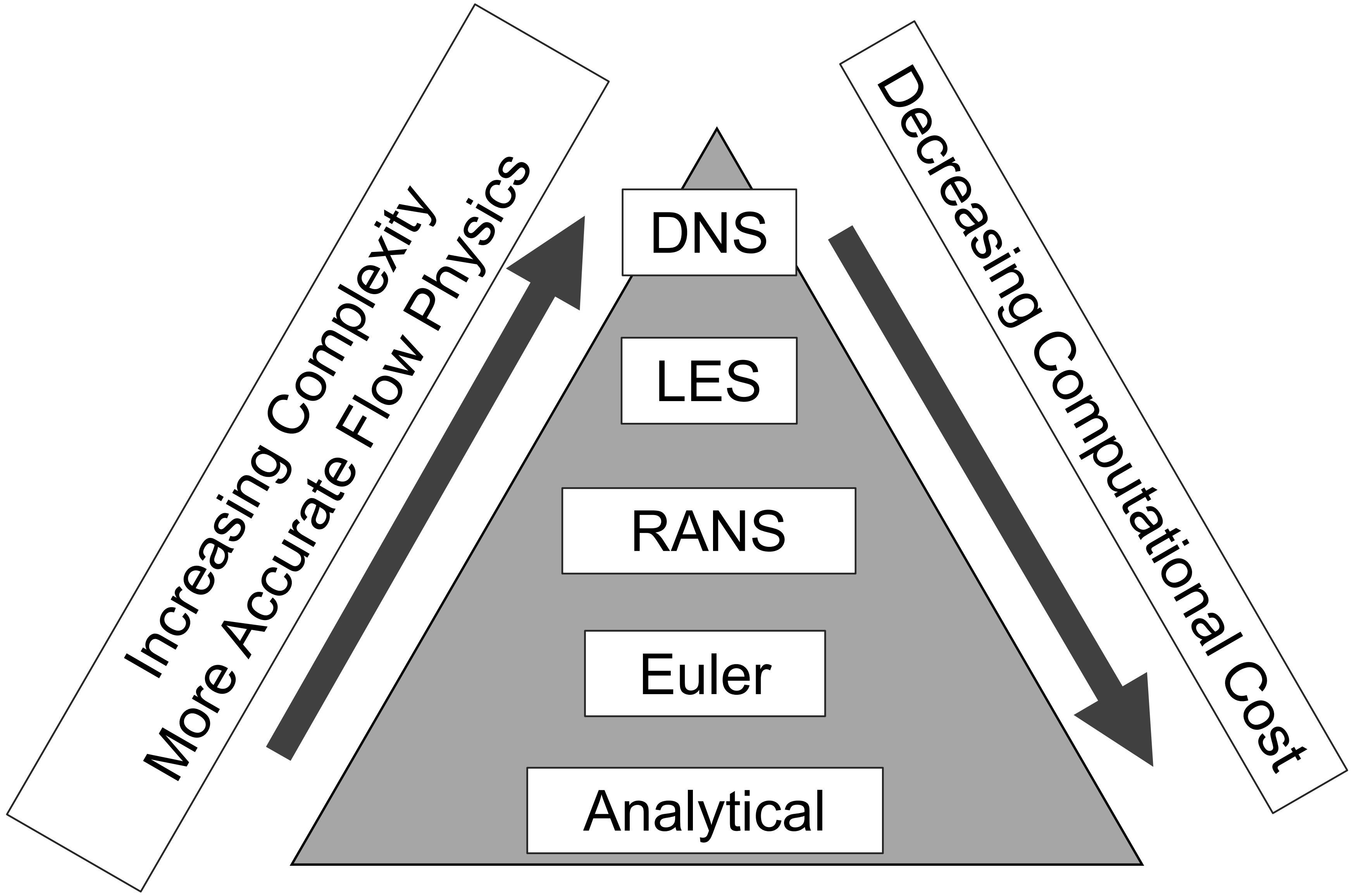
Streicher, et al, Physics of Fluids, 2020.

Objectives

- Compare computational tools to model shock tubes
- Validate against experimental data
- Model reflected shock tubes
- Apply vibrational state-to-state modeling within shock tubes

Approaches

- Analytical
- NASA CEA (Chemical Equilibrium with Applications)
- brODErs
- CFD



Analogy to CFD

Analytical

We assume the gas is calorically perfect. Using the experimental setup by Streicher et al, we have the following conditions in section 1 of the shock tube: $p_1 = 0.07$ Torr $= 9.33$ Pa and $u_p = 2.51$ mm/μs=2510 m/s. We further set the entire shock tube at $T = 295$ K. The speed of sound in section 1 is

$$a_1 = \sqrt{(1.4)\left(259.84\frac{\text{J}}{\text{kg K}}\right)(295\text{ K})} = 327.59\ \frac{\text{m}}{\text{s}}$$

Using the following relation, we are able to calculate the pressure in section 2 of the shock tube:

$$u_p = \frac{a_1}{\gamma}\left(\frac{p_2}{p_1} - 1\right)\left(\frac{\frac{2\gamma}{\gamma+1}}{\frac{p_2}{p_2} + \frac{\gamma-1}{\gamma+1}}\right)^{\frac{1}{2}} \implies \frac{p_2}{p_1} = 100.781$$

$$p_2 = \frac{p_2}{p_1}p_1 = 940.289\text{ Pa}$$

Analytical

To calculate the wave speed, the density ratio across the shock is needed

$$\frac{\rho_2}{\rho_1} = \frac{1 + \frac{\gamma+1}{\gamma_1}\left(\frac{p_2}{p_1}\right)}{\frac{\gamma+1}{\gamma-1} + \frac{p_2}{p_1}} = 5.67$$

$$w = \frac{u_p}{1 - \frac{\rho_1}{\rho_2}} = 3047.22\ \frac{\mathrm{m}}{\mathrm{s}} \implies M_s = \frac{w}{a_1} = 9.30198$$

Computing the velocity behind the shock, relative to the wave, u_2

$$u_2 = w - u_p = 3047.22 - 2510 = 537.22\ \frac{\mathrm{m}}{\mathrm{s}}$$

Additionally, the temperature behind the shock wave is

$$T_2 = T_1 \frac{p_2}{p_1}\left(\frac{\frac{\gamma+1}{\gamma-1} + \frac{p_2}{p_1}}{1 + \left(\frac{\gamma+1}{\gamma-1}\right)\left(\frac{p_2}{p_1}\right)}\right) = 5241.41\ \mathrm{K}$$

Analytical

We now can solve for the properties behind the reflected wave. Due to the nature of the reflected wave $u_5 = 0$. We can find the Mach number of the reflected wave using the relation

$$\frac{M_R}{M_R^2 - 1} = \frac{M_s}{M_s^2 - 1}\sqrt{1 + \frac{2(\gamma - 1)}{(\gamma + 1)^2}(M_s^2 - 1)\left(\gamma + \frac{1}{M_s^2}\right)} \implies M_R = 2.57$$

To find the pressure behind the reflected shock

$$p_5 = p_2\left(1 + \frac{2\gamma}{\gamma + 1}(M_R^2 - 1)\right) = 7088.89 \text{ Pa}$$

and to find the temperature post-reflected shock, we have

$$T_5 = T_2\left(\left[1 + \frac{2\gamma}{\gamma + 1}(M_R^2 - 1)\right]\left[\frac{2 + (\gamma - 1)M_R^2}{(\gamma + 1)M_R^2}\right]\right) = 11571.5 \text{ K}$$

NASA CEA

- NASA's Chemical Equilibrium with Applications program calculates chemical equilibrium compositions and properties
- For shock related problems, the conservation equations are solved for
- Shock-tube parameters are input and the incident and reflected fluid conditions are output for frozen and equilibrium mixtures
- Databases with transport and thermodynamic properties of individual species are used

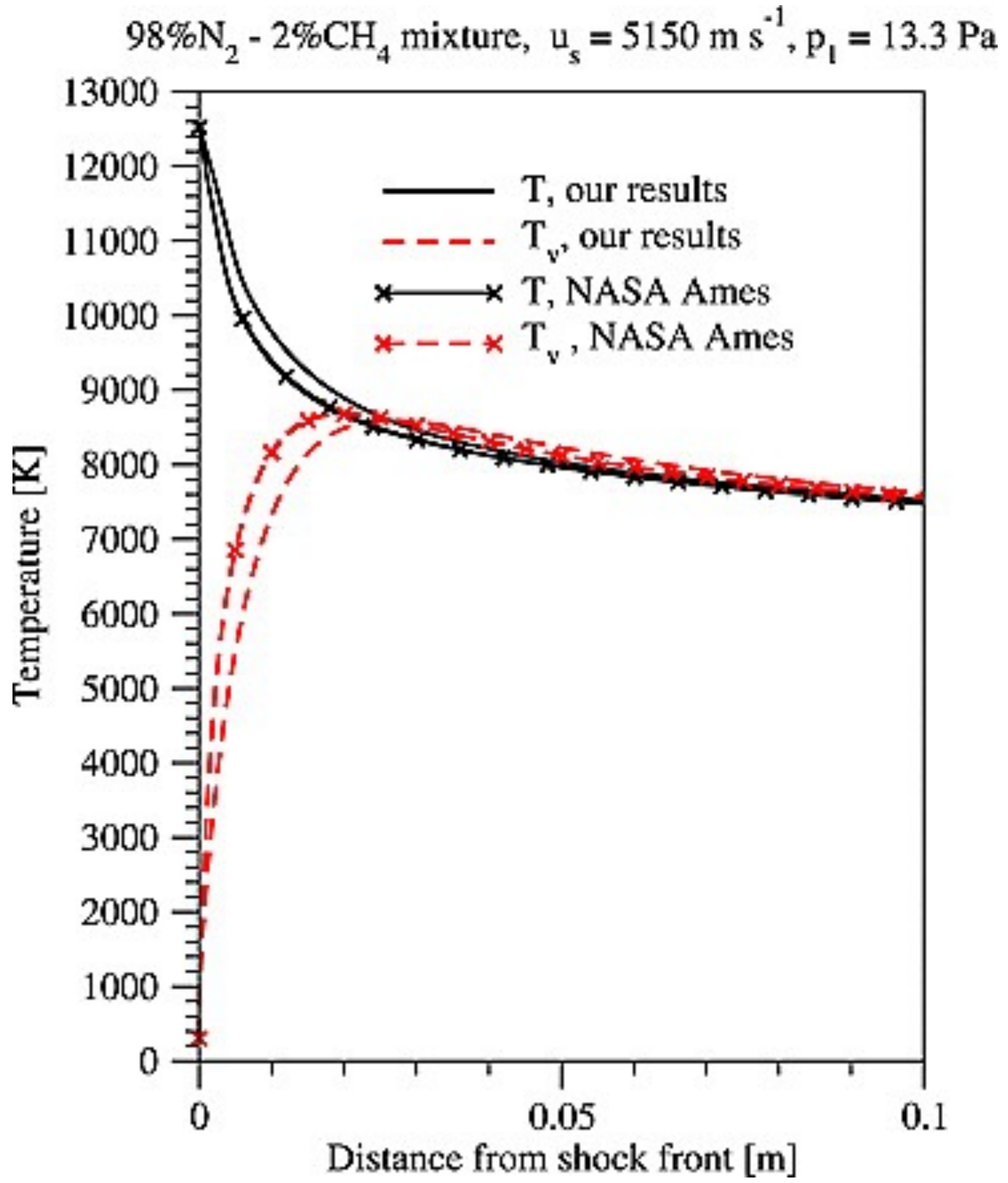
NASA CEA

- Using NASA CEA with u = 3047.22 m/s, p = 0.07 Torr, and T = 295

Chemistry	Shock Type	Velocity [m/s]	Pressure [Pa]	Temperature [K]
Frozen	Incident	405.68	989	4163.44
Frozen	Reflected	558.18	9080	8074.64
Equilibrium	Incident	273.90	1038	2621.99
Equilibrium	Incident	344.18	12932	3307.21

brODErs

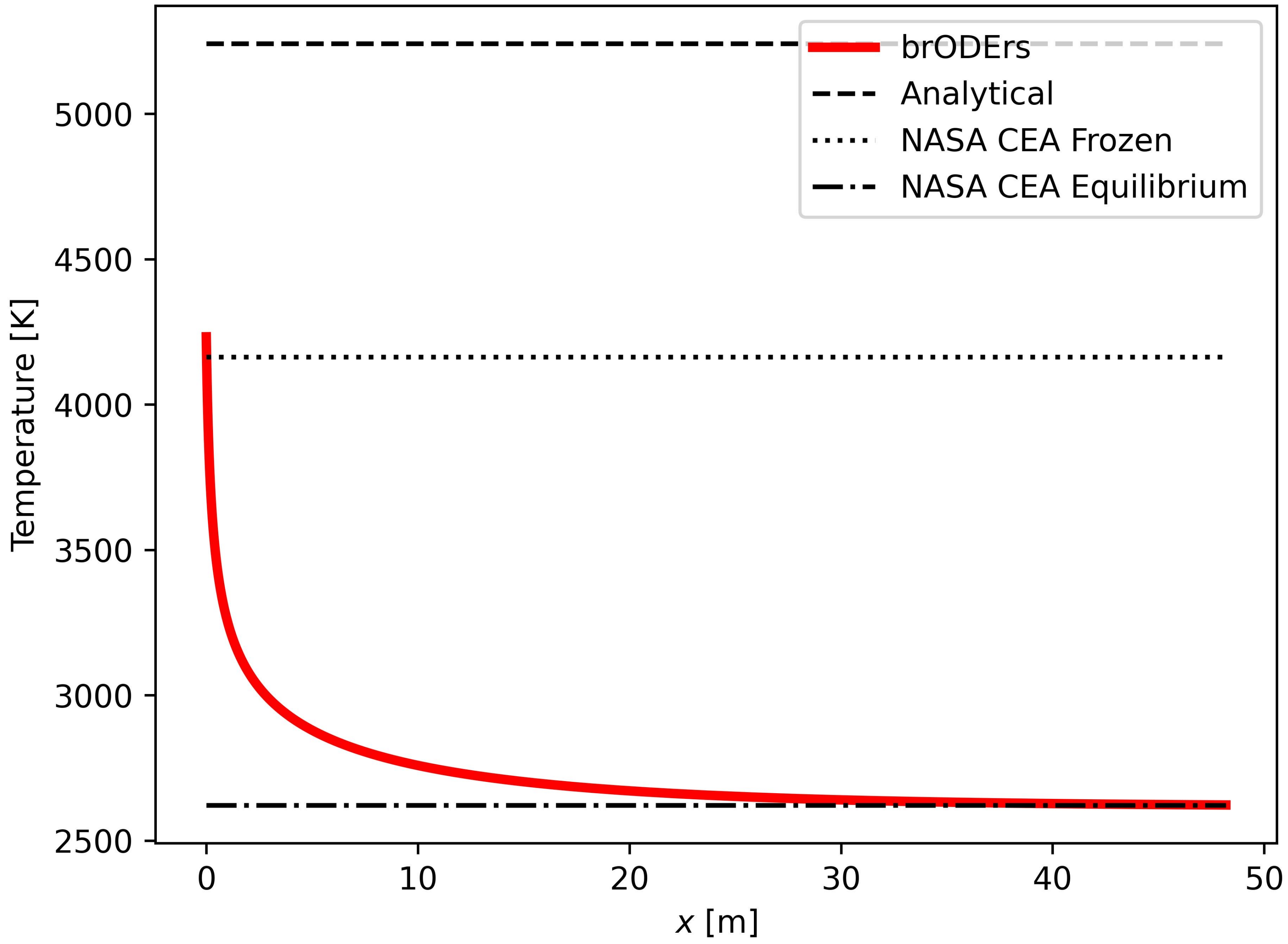
- brODErs is a collection of ODE solvers for chemically reacting hypersonic flows developed at the von Karman Institute for Fluid Dynamics
- The downstream flow field is computed by solving one-dimensional conservation equations of mass, momentum, global energy, as well as conservation of vibrational energy of the
- Problem Setup:
    - Freestream Pressure = 9.33 Pa
    - Freestream Temperature = 295 K
    - Freestream Velocity = 3047.22 m/s



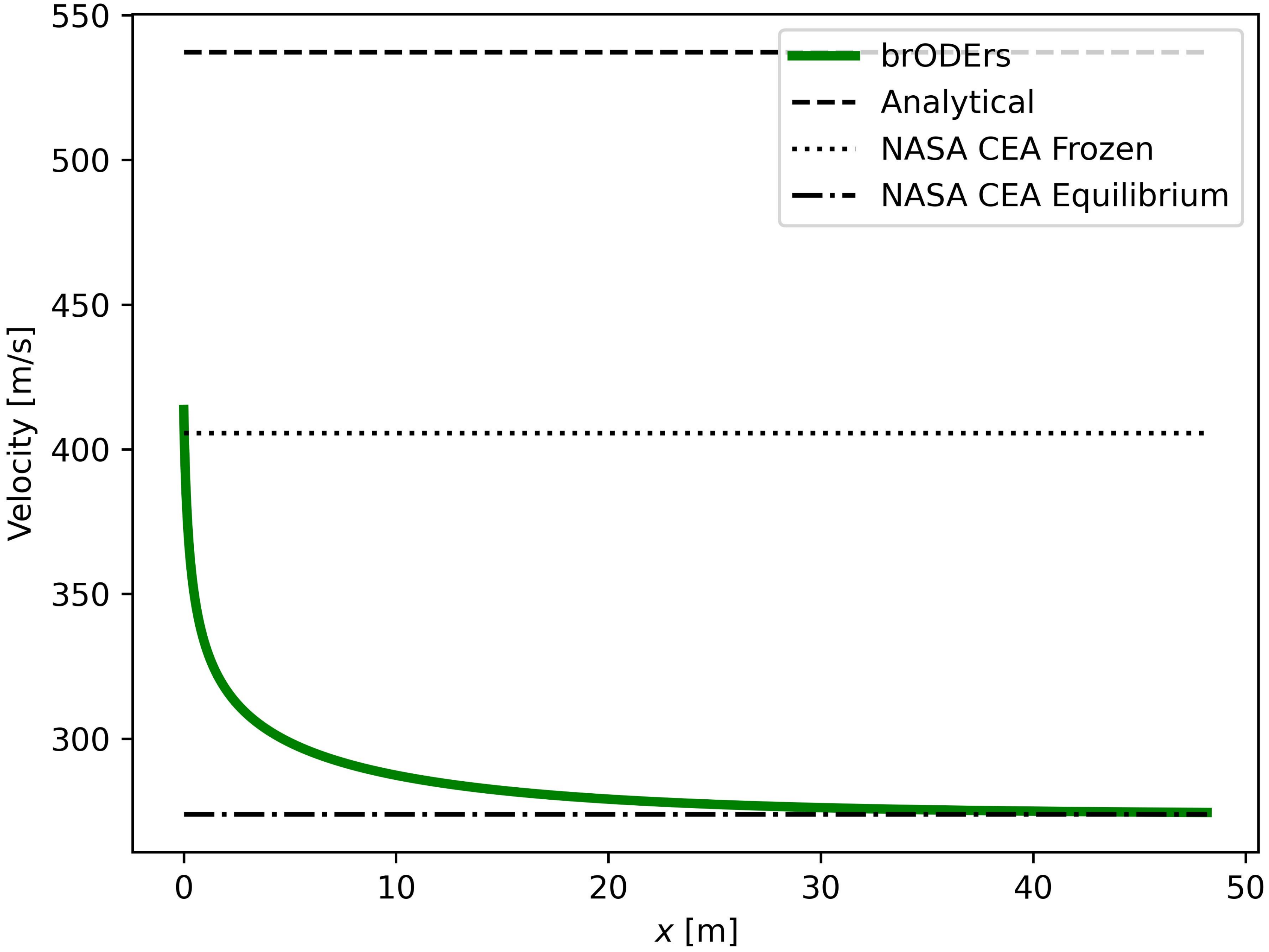
Magin, T. E., Caillault, L., Bourdon, A., & Laux, C. O. (2006). Nonequilibrium radiative heat flux modeling for the Huygens entry probe. Journal of Geophysical Research: Planets, 111(E7).

brODErs – 1T

Translational Temperature

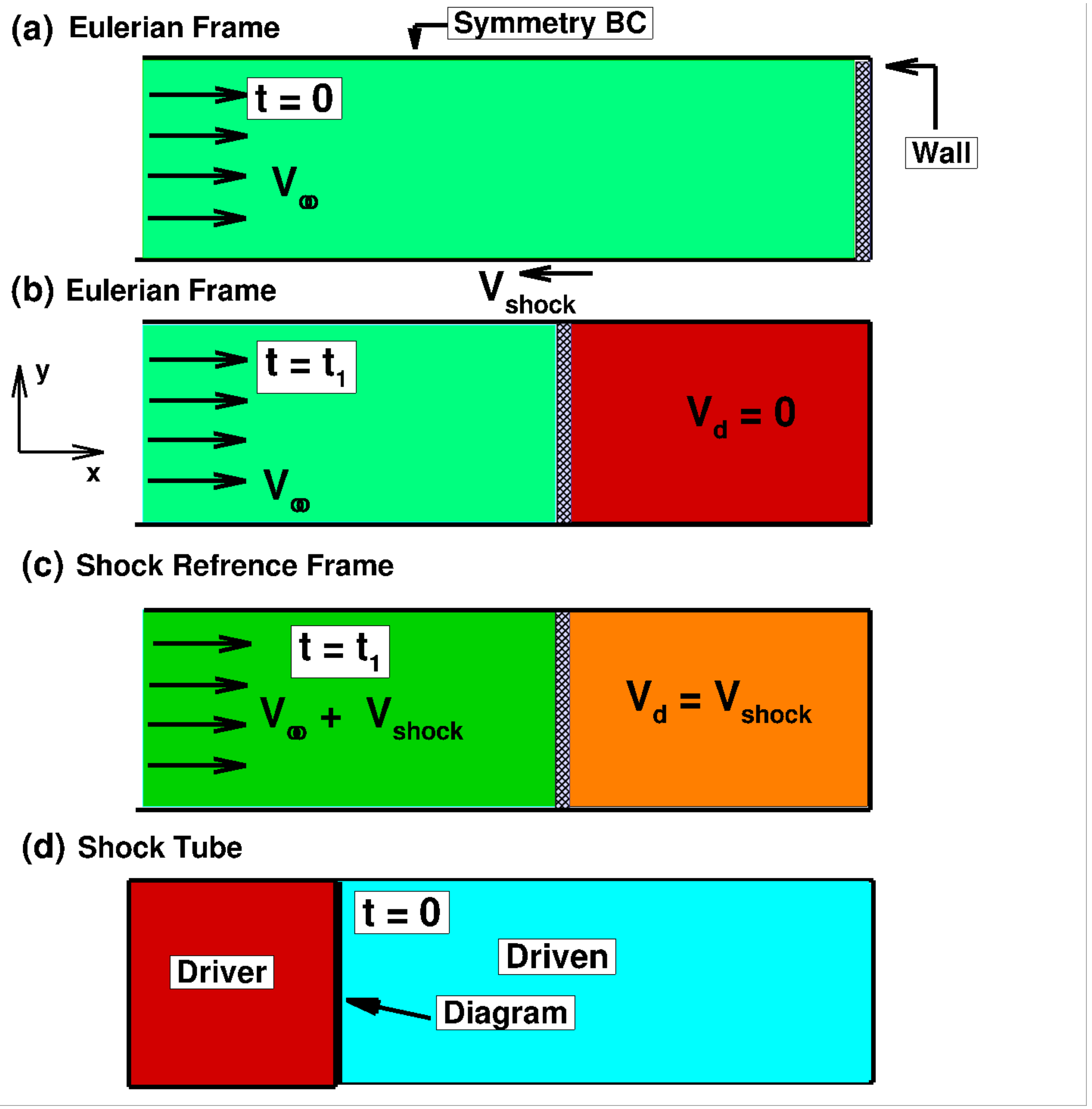


Particle Velocity



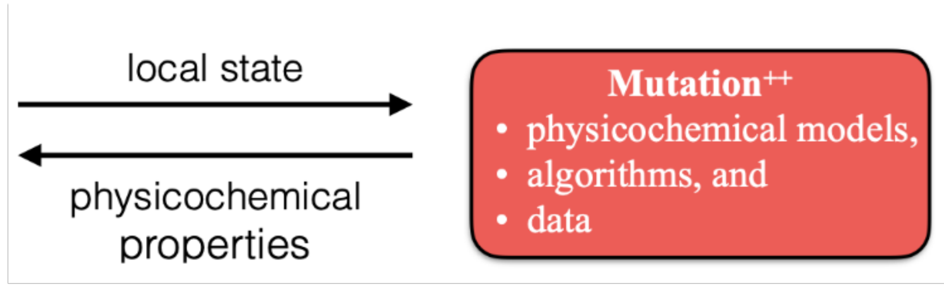
CFD – Unsteady

- 1D simulation of shock-tube
- Focusing on what occurs after the diaphragm is ruptured (figure a)
- Mixture: O_2
- Chemical reaction rates determined by Park (1993)
- Approaches
  - 2T – Translational and Vibrational effects
  - 1T – Forces thermal equilibrium
  - Frozen – No chemical reactions occurring



CFD – Unsteady

- Navier-Stokes Solver
- Mesh: 1D with 10000 cells; 1 m long
- Boundary Conditions
    - Symmetry walls (no boundary layer effects)
    - Euler condition on the far wall (no gradients across the wall)
- SU2-NEMO CFD Code

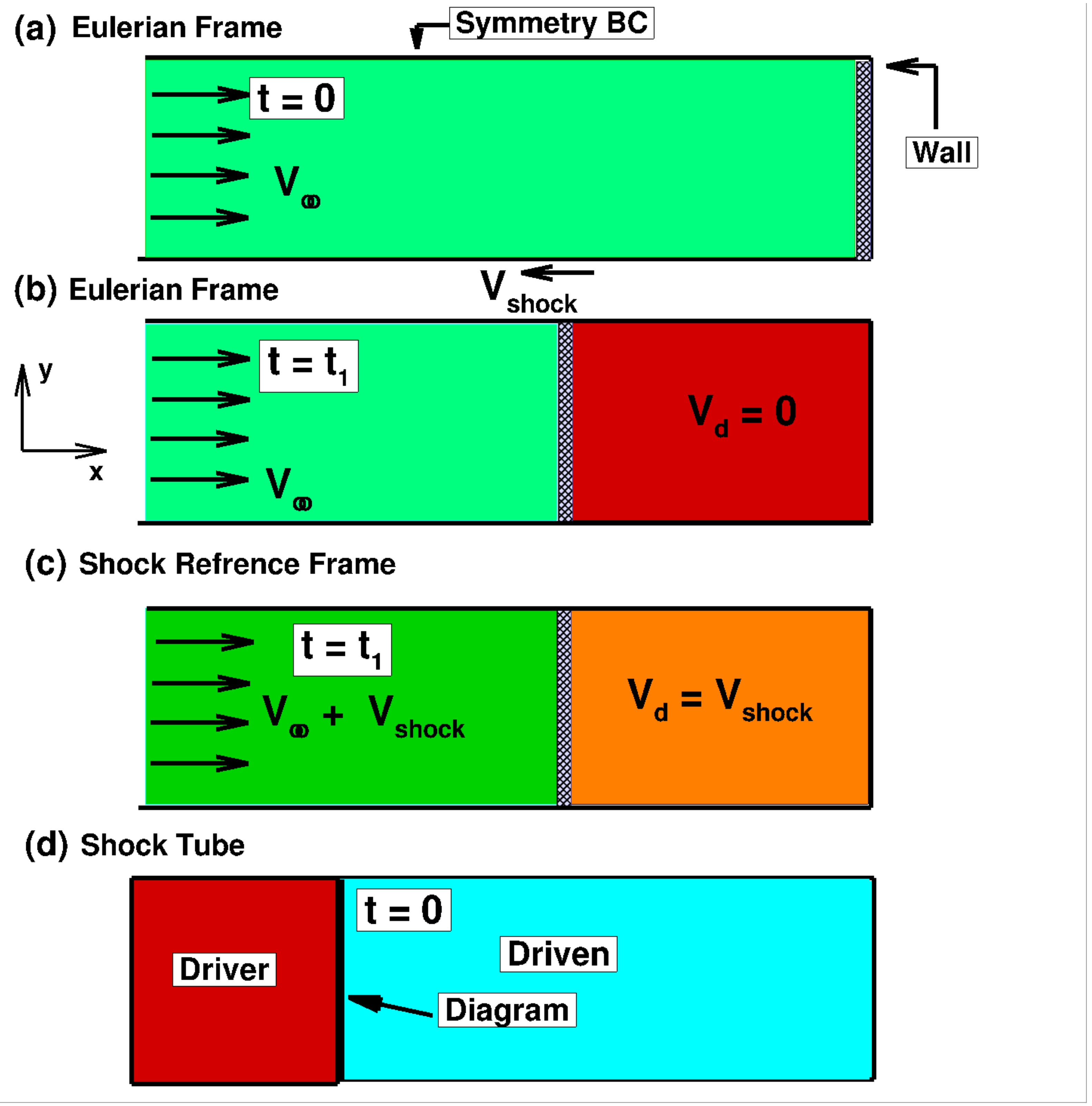


local state

physicochemical properties

Mutation^{++}

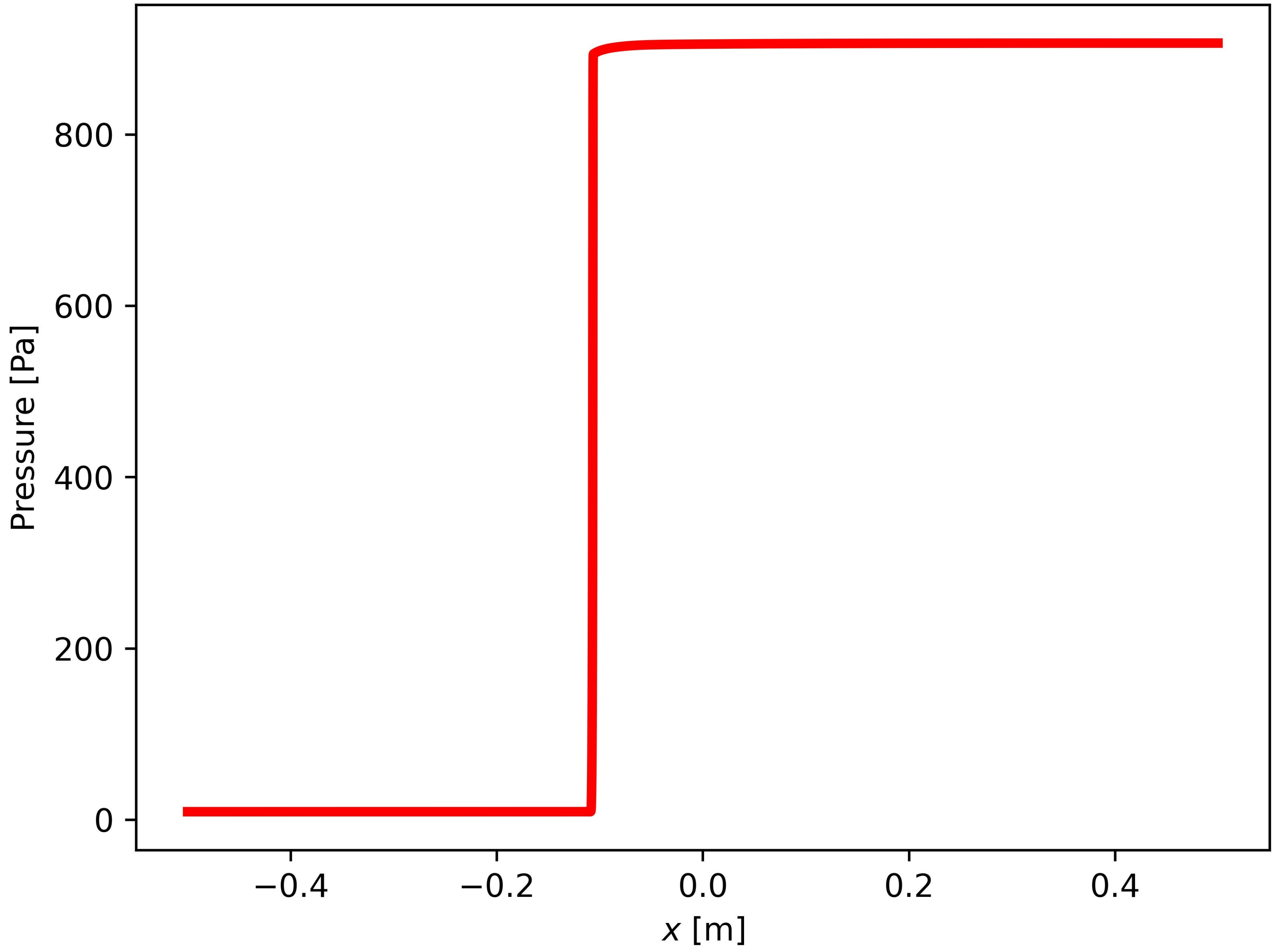
- physicochemical models,
- algorithms, and
- data



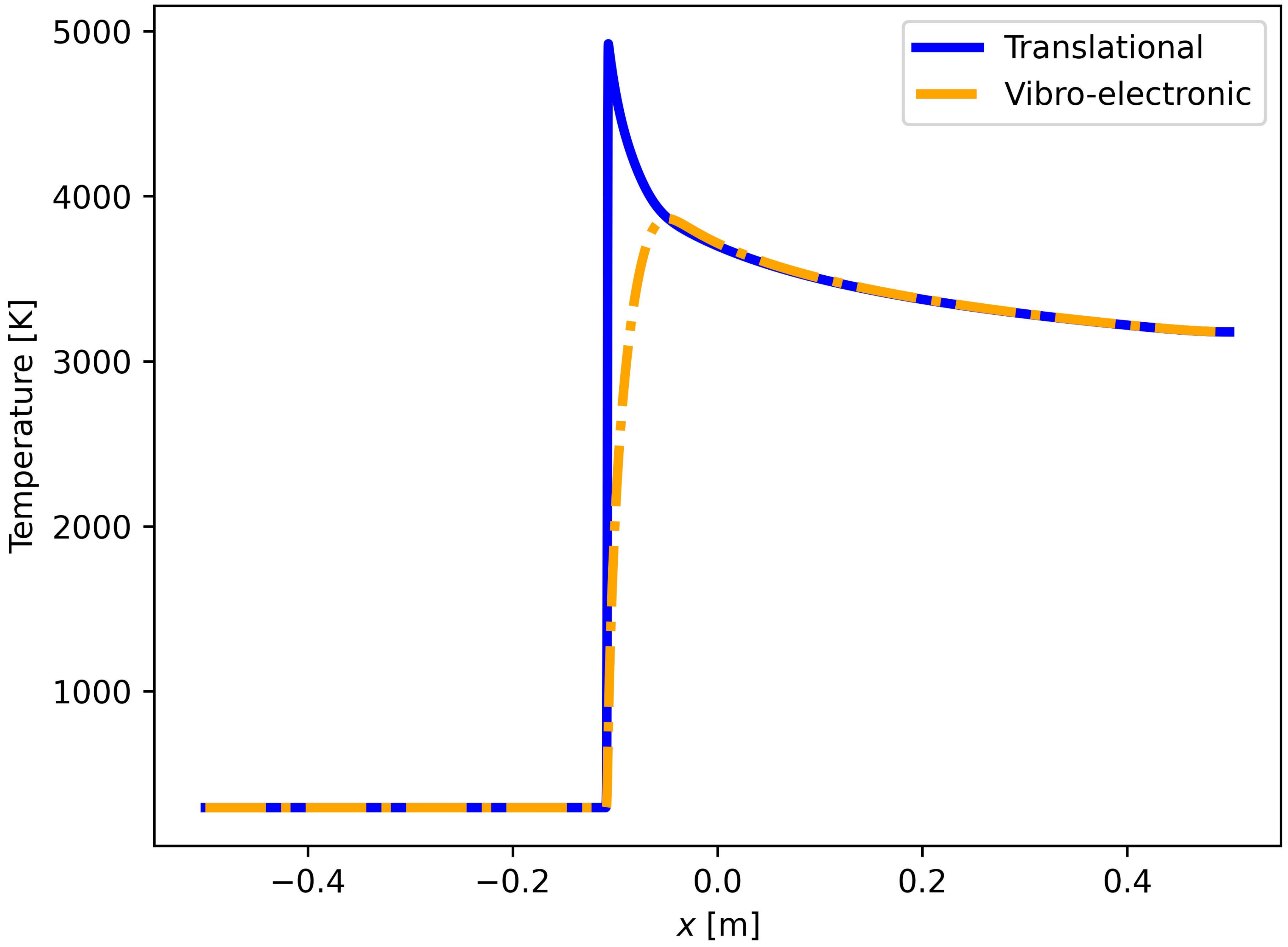
Maier, et al., AIAA Paper 2023-3488

CFD – Unsteady

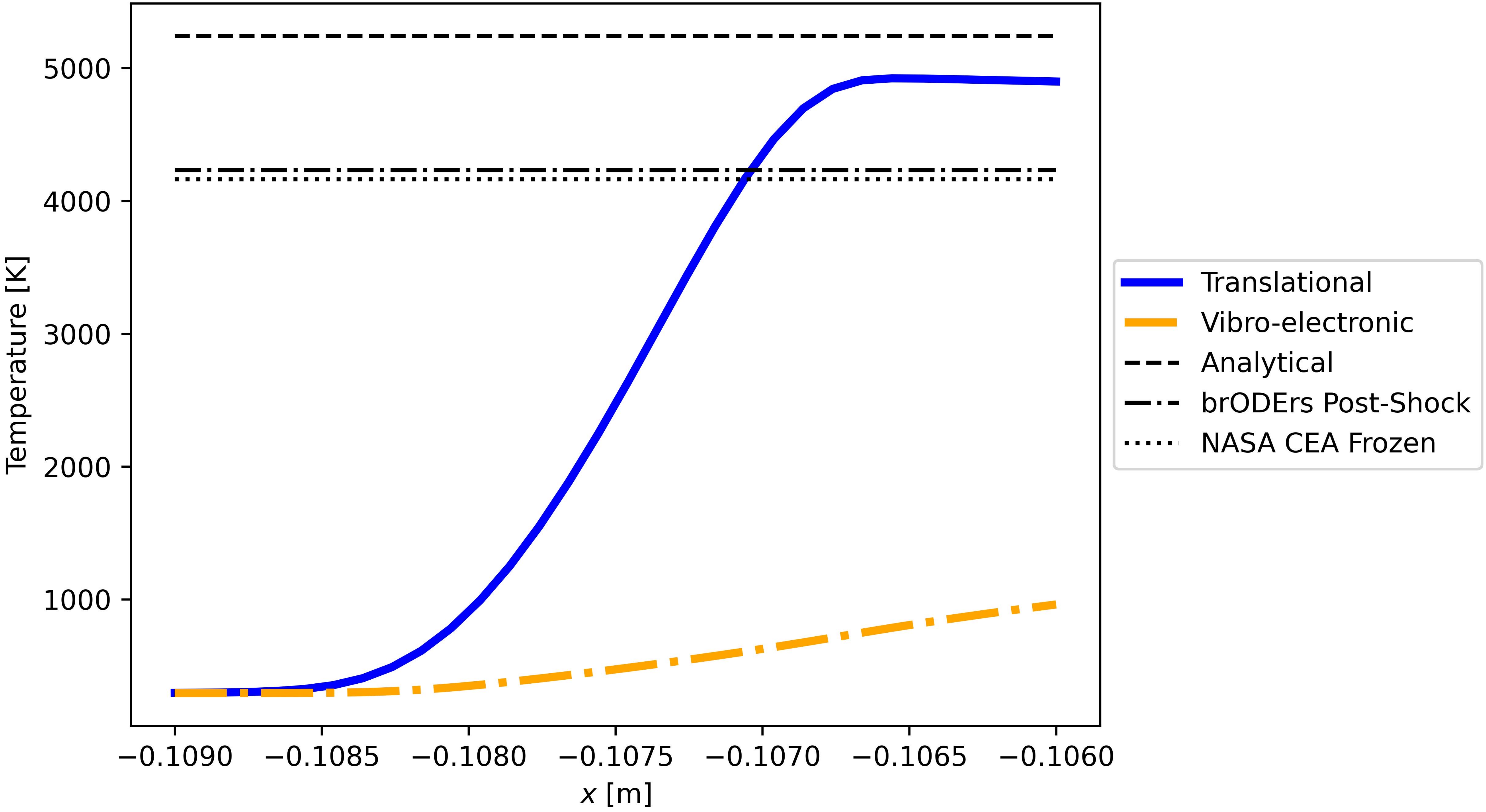
Pressure



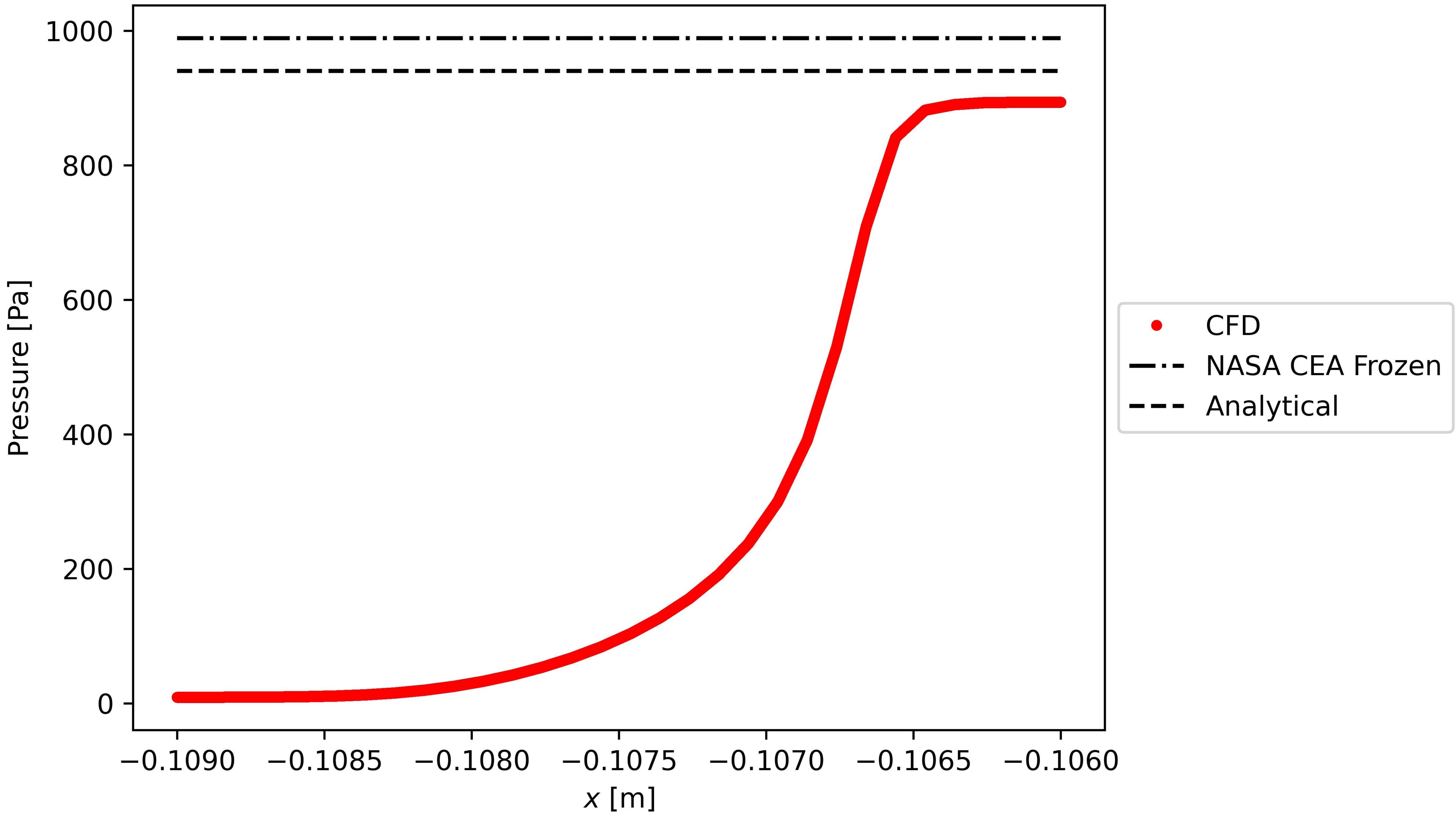
Temperature



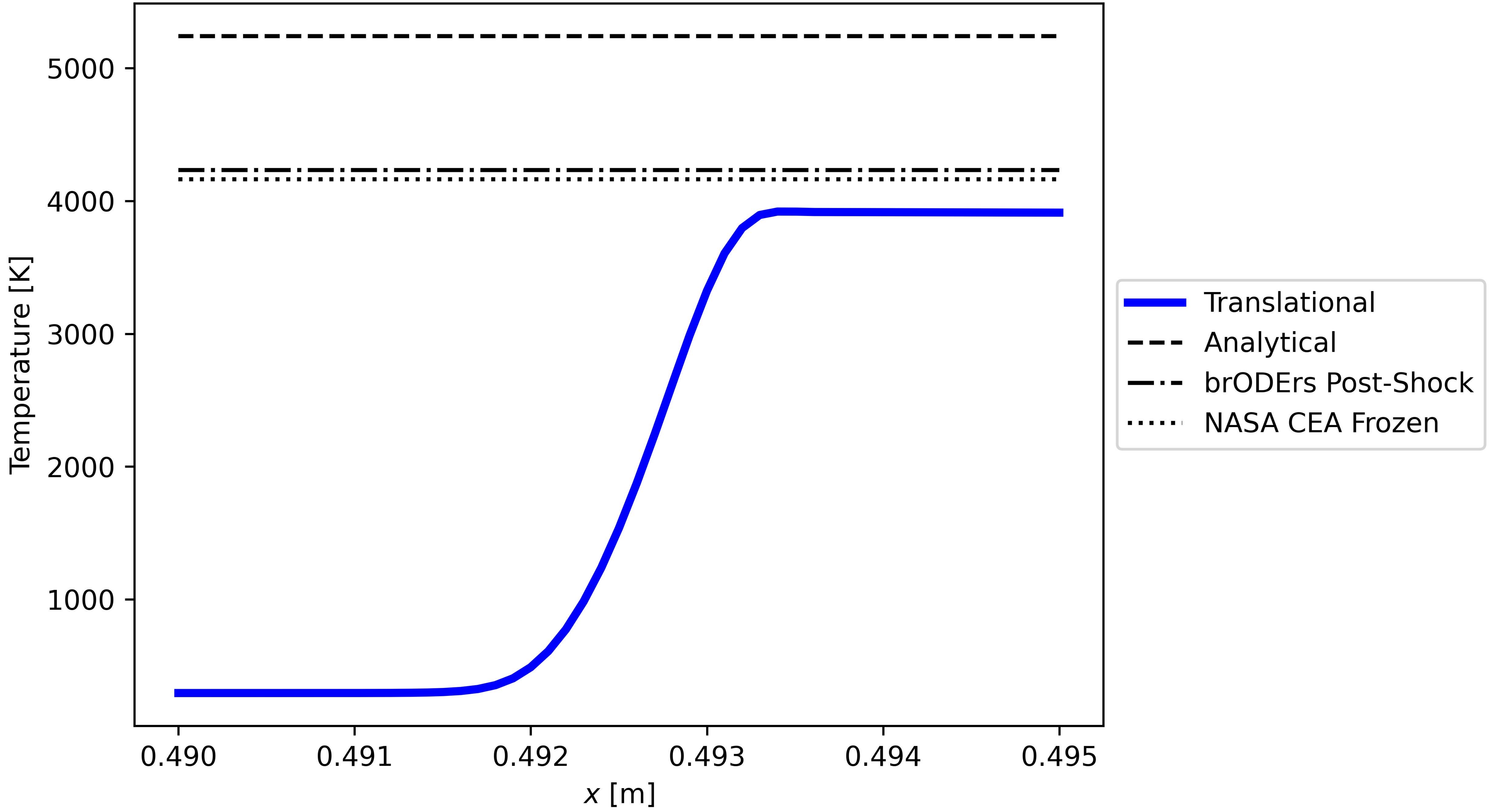
CFD – Unsteady



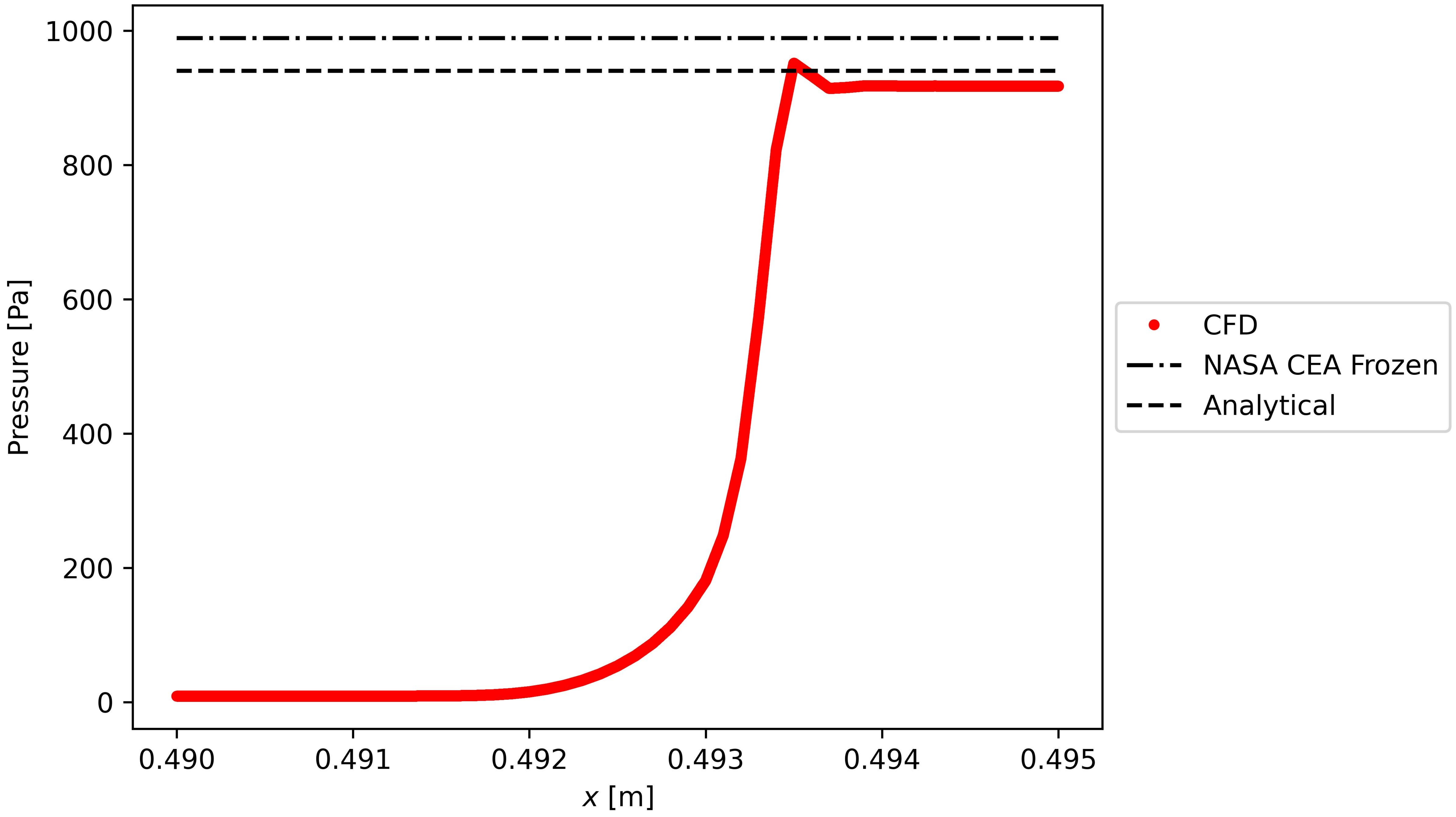
CFD – Unsteady



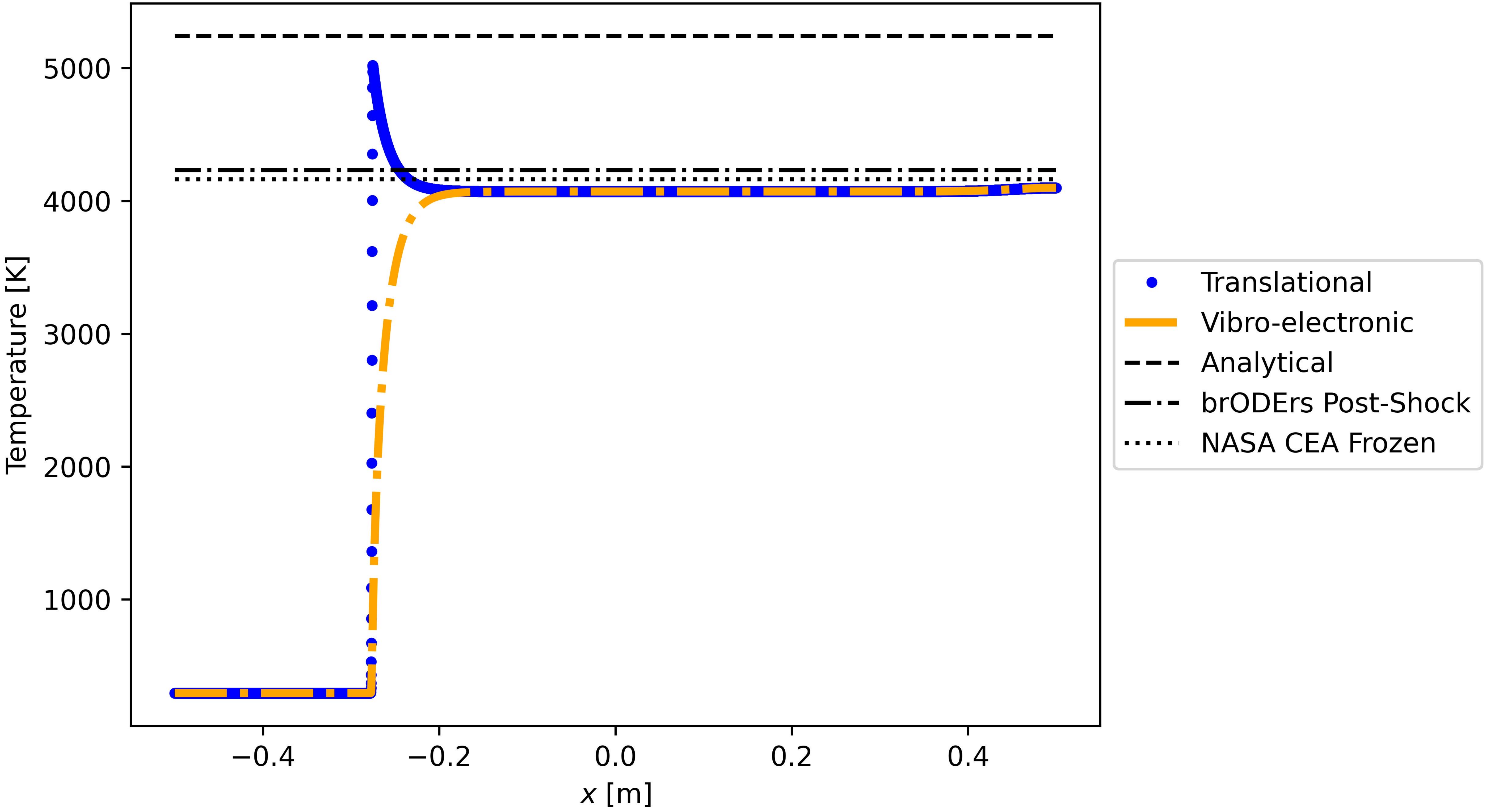
CFD – Unsteady – 1T



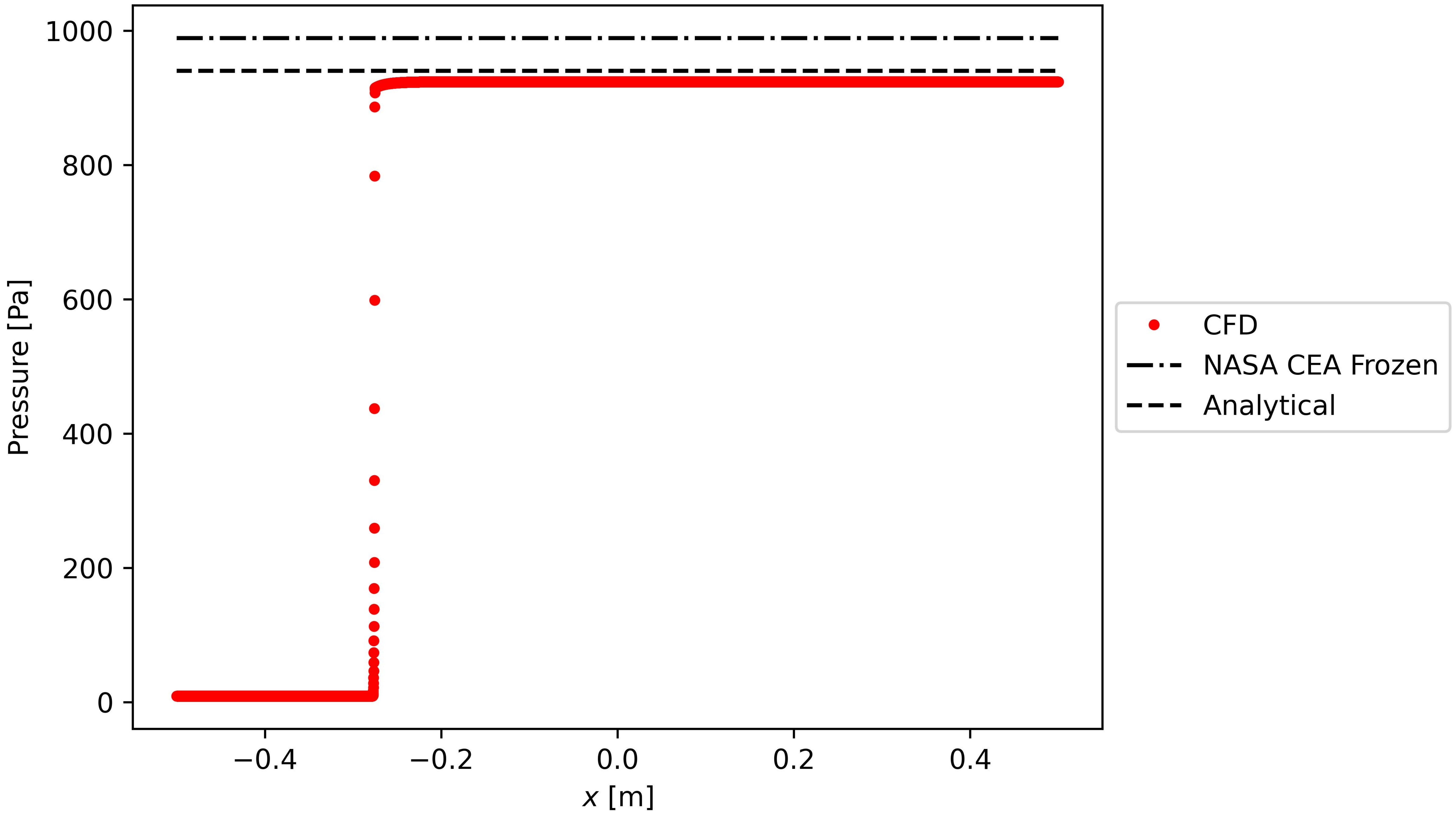
CFD – Unsteady – 1T



CFD – Unsteady – Frozen



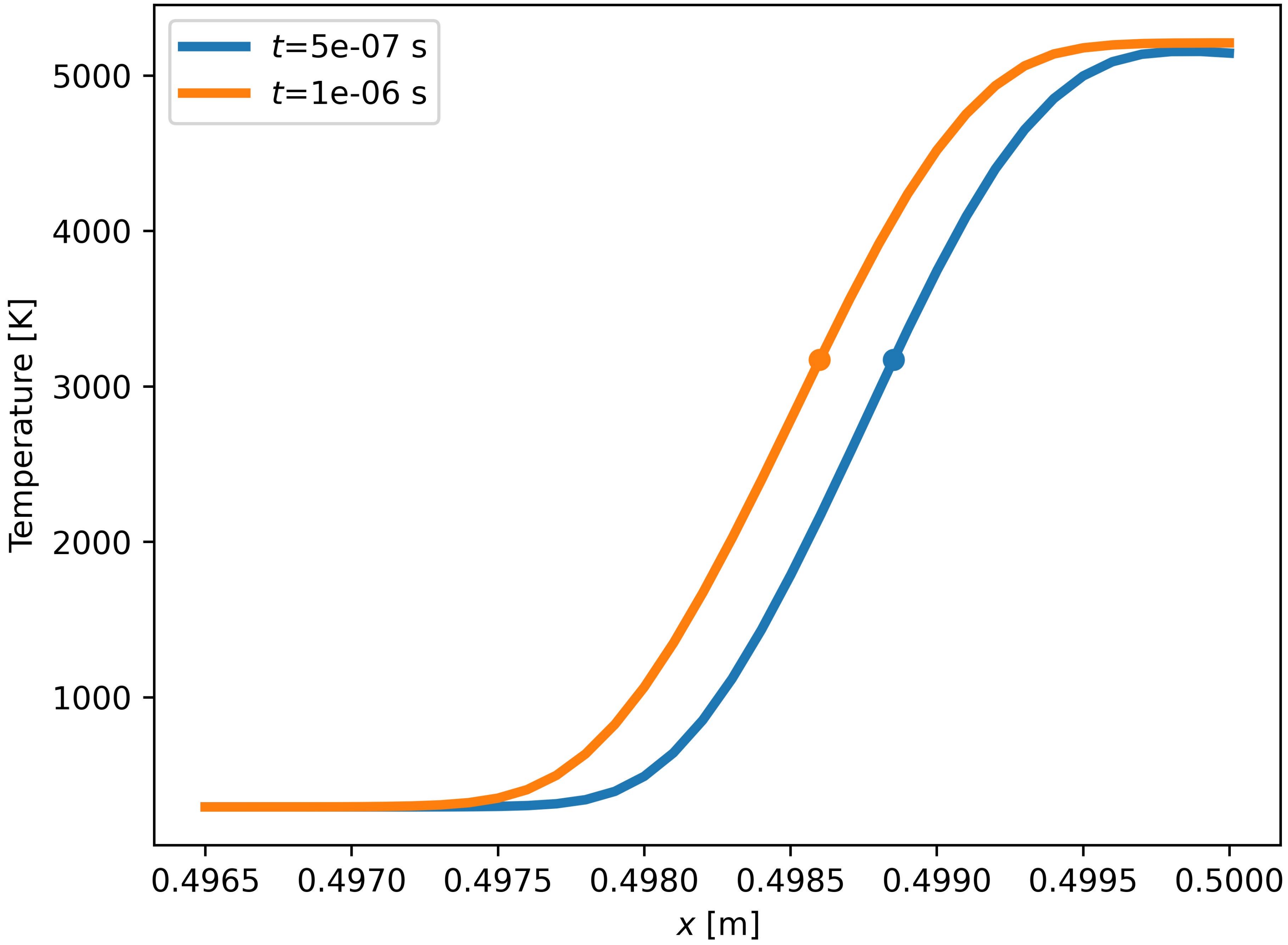
CFD – Unsteady – Frozen



CFD – Unsteady

- We are able to calculate the speed of the shock wave
    - dx = physical distance of shock between two snapshots
    - dt = 1e-10 set within the simulation
    - Simulation snapshot every 5000 iterations

$$u_2 = \frac{dx}{5000 \cdot dt} = 504.75\ \frac{\text{m}}{\text{s}}$$



Summary of Results

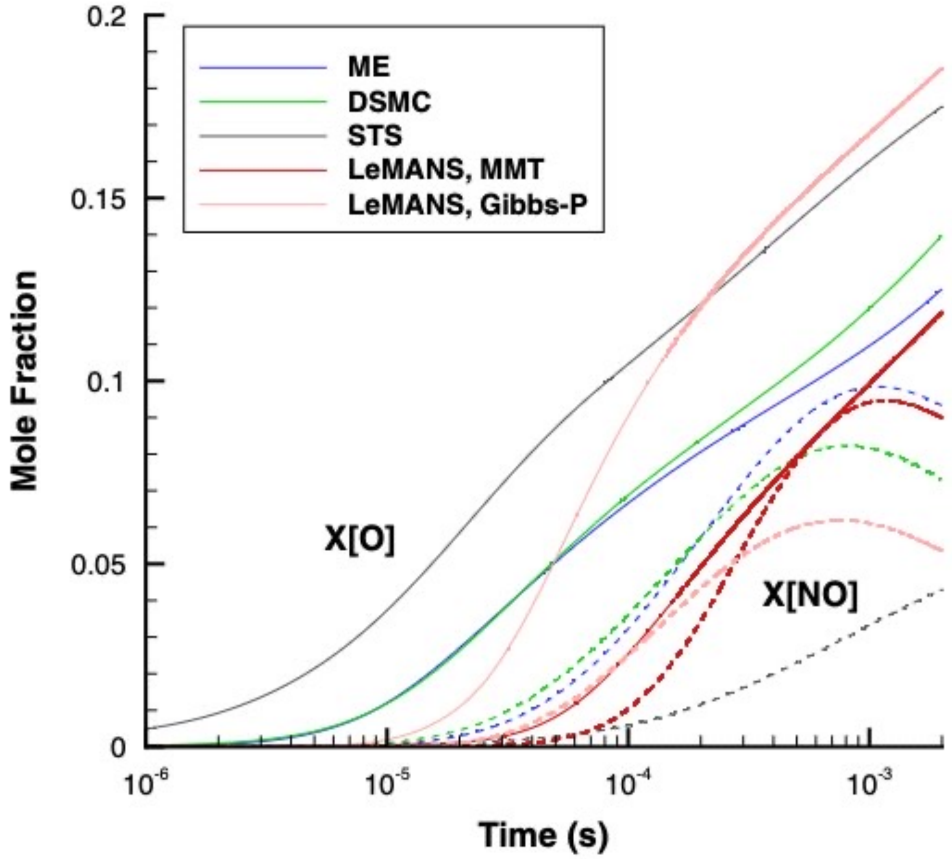
Post-Shock Property	Analytical	NASA CEA	brODErs (Post-Shock)	CFD (Frozen)	CFD	CFD (1T)
Pressure [Pa]	940.29	989	986.11	924.1	894.03	951.98
Temperature [K]	5241.41	4163.44	4233.08	5020.5	4923.67	3920.4
Velocity [m/s]	537.22	405.68	413.70	504.75		

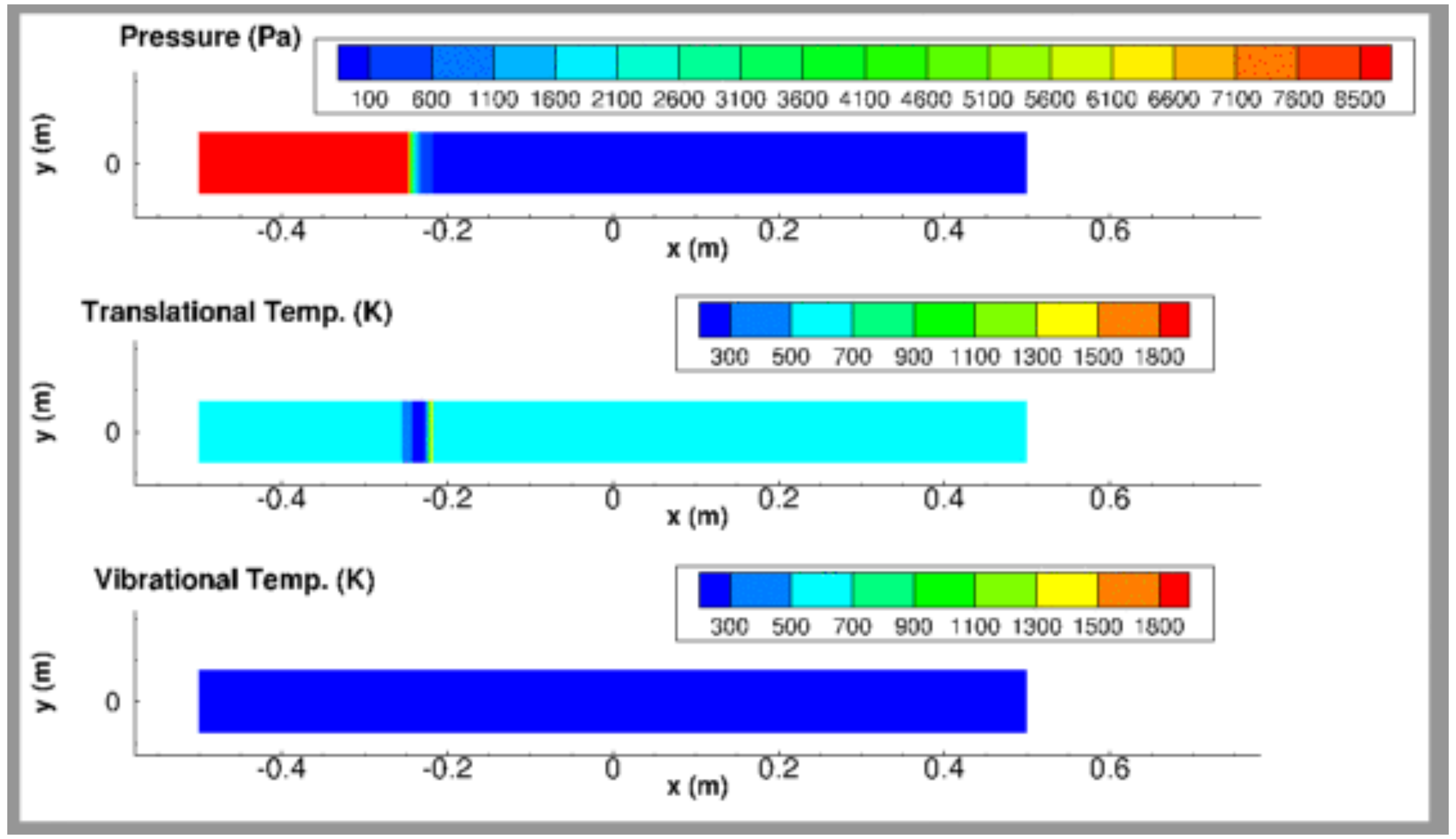
Conclusions

- Shock tubes are:
  - A simple experiment (diagnostics not simple!)
  - Simple to model with analytical theory but this theory misses out on some relevant physics
  - Challenging to perform CFD on
- CFD simulations with frozen chemistry match closest with the analytical calculations, due to the frozen assumption
- Computational Cost
  - CFD is the most expensive, takes into account the most chemistry and kinetics
  - NASA CEA is fastest
  - brODErs fast but can include more

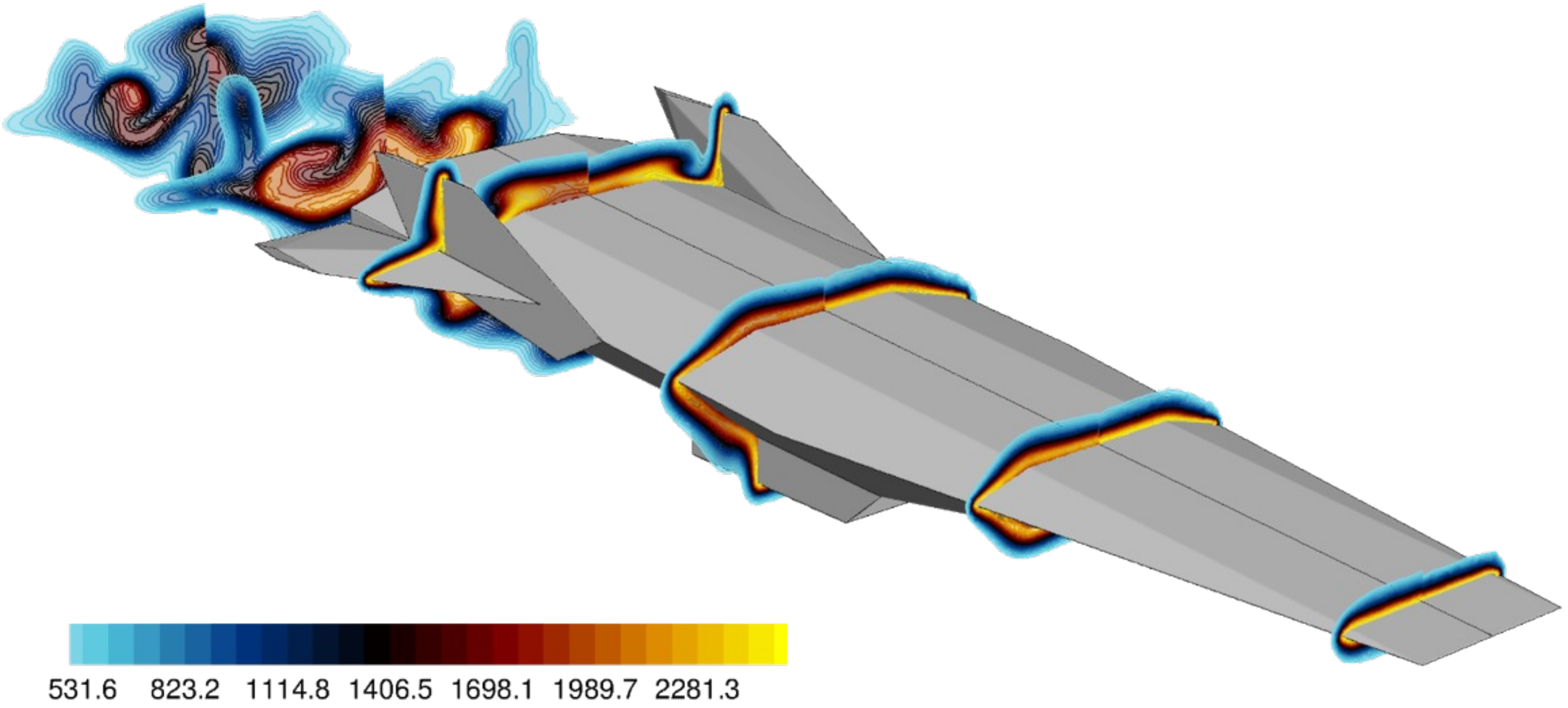
Future Work

- Model a full shock tube with expansion and reflected waves
- Model boundary layer effects
- Apply state-to-state transitions to the shock-tube environment
  - Presentation on Vibrational State-to-State Thermochemical Modeling of High Temperature Oxygen Flows on Friday





Gimelshein, et al, JTHT, 2022.



QUESTIONS/DISCUSSION

aaronml@arizona.edu
chanl.arizona.edu