A Multivibrational Mode Relaxation Scheme for Two-Temperature Thermochemical State Models

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Contents

Preliminary

Consider compressible Navier-Stokes equations for two-temperature reacting flows:

$$\partial_t \mathbf{u} + \nabla \cdot \mathbf{f}(\mathbf{u}) = \mathbf{S},$$

$$\mathbf{u} = \begin{pmatrix} \rho_s \\ \rho \mathbf{v} \\ \rho E \\ \rho e_V \end{pmatrix}, \quad \mathbf{f} \cdot \mathbf{n} = \begin{pmatrix} \rho U c_s \\ \rho U \mathbf{v} + p \mathbf{n} \\ \rho U H \\ \rho U e_V \end{pmatrix}, \quad \mathbf{U} = \mathbf{v} \cdot \mathbf{n},$$

$$\mathbf{S} = \begin{pmatrix} \dot{\mathbf{w}}_s \\ \dot{\mathbf{w}}_m \\ \dot{w}_E \\ \dot{w}_V := \ldots + \underbrace{\left(Src^{T \leftrightarrow V} \equiv \frac{dE_v}{dt} \right)}_{\text{Translational-vibrational energy exchange source term}} + \ldots \end{pmatrix}$$

: the **Landau-Teller** expression

Consider the Landau-Teller Equation:

$$Src^{T\leftrightarrow V} \equiv \frac{dE_v}{dt} = \sum_{s=mol.} \rho_s \frac{ev_s^0(T) - ev_s(T)}{\tilde{\tau}_s},$$

where

averaged vibrational relaxation time for species s

an averaging function

vibrational relaxation of species s in a medium species r.

$$\tilde{\tau}_s = f(\tau_{sr}).$$

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From Milikan-White [J. Chem. Phys., 1963]:

$$p\tau_{sr}^{\text{MW}} = \exp\left[a_{sr}(T^{-1/3} - b_{sr}) - 18.42\right],$$

where

single characteristic vibrational temperature

reduced mass

$$a_{sr} := g(\mu_{sr}, \theta_{v,s}), \quad b_{sr} := h(\mu_{sr}).$$

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- ◉ Park et al. [JTHT, 1994] suggested a series of **tailored** a_{sr} and b_{sr} values for $CO_2 - N_2$. Camac [Cornell U. Press, 1966] values were used for $CO_2 - CO_2$.

- ◉ **No other values are available for general polyatomic molecules.**

Landau-Teller Expression in CFD

Consider again the Landau-Teller equation:

$$Src^{T\leftrightarrow V} \equiv \frac{dE_v}{dt} = \sum_{s\,=\,mol.} \rho_s \frac{ev_s^0(T) - ev_s(T)}{\tilde{\tau}_s}$$

introducing T_v

$$\simeq \sum_{s\,=\,mol.} \rho_s \frac{ev_s^0(T) - ev_s(T_v)}{\tilde{\tau}_s}$$

$$\simeq \sum_{s\,=\,mol.} \rho_s \frac{C_{vv,s}(T - T_v)}{\tilde{\tau}_s} = \frac{\rho C_{vv}(T - T_v)}{\bar{\tau}}$$

$$\bar{\tau} = \frac{\sum_{s=mol.} \rho_s c_{vv,s}}{\sum_{s=mol.} \frac{\rho_s c_{vv,s}}{\tilde{\tau}_s}} \simeq \frac{\sum_{s=mol.} \frac{\rho_s}{\mathrm{Mw}_s}}{\sum_{s=mol.} \frac{\rho_s}{\mathrm{Mw}_s \tilde{\tau}_s}}.$$

$$\tilde{\tau}_s \Rightarrow : f(\tau_{sr}^{Millikan-White}) + \tilde{\tau}_s^{Park}(T)$$

to account for elastic collisions

Objective

To develop an effective vibrational relaxation time $\bar{\tau}$ for ***generic*** molecules that directly depends on species **vibrational frequencies**.

Multivibrational Mode Approach

Consider again the Landau-Teller equation:

$$Src^{T\leftrightarrow V} \equiv \frac{dE_v}{dt} \simeq \sum_{s=mol.} \rho_s \frac{ev_s^0(T) - ev_s(T_v)}{\tilde{\tau}_s} \simeq \frac{\rho C_{vv}(T - T_v)}{\bar{\tau}}$$

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$$\swarrow$$

$$\sum_{s\,=\,mol.} \rho_s \left(\sum_{m=mode} \frac{ev^0_{s,m}(T) - ev_{s,m}(T_v)}{\tilde{\tau}_s^{(MM)}(T, \theta_{v,m})} \right)$$

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$$\tilde{\tau}_s^{(MM)} = \frac{\sum_{m=mode} | ev^0_{s,m}(T, \theta_{v,m}) - ev_{s,m}(T_v, \theta_{v,m}) |}{\sum_{m=mode} \frac{| ev^0_{s,m}(T, \theta_{v,m}) - ev_{s,m}(T_v, \theta_{v,m}) |}{\tilde{\tau}_s(T, \theta_{v,m})}},$$

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$$\tilde{\tau}_s^{(MM)} = \frac{\sum_{m=mode} \left| ev^0_{s,m}(T,\theta_{v,m}) - ev_{s,m}(T_v,\theta_{v,m}) \right|}{\sum_{m=mode} \frac{\left| ev^0_{s,m}(T,\theta_{v,m}) - ev_{s,m}(T_v,\theta_{v,m}) \right|}{\tilde{\tau}_s(T,\theta_{v,m})}}, \longrightarrow \; : f(\tau_{sr}^{Millikan-White}) + \tilde{\tau}_s^{Park}(T)$$

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$$= g_m \frac{R_s\theta_{v,m}}{e^{\frac{\theta_{v,m}}{T}} - 1}$$

$$\tilde{\tau}_s^{(MM)} = \frac{\sum_{m=mode} \left| ev^0_{s,m}(T,\theta_{v,m}) - ev_{s,m}(T_v,\theta_{v,m}) \right|}{\sum_{m=mode} \frac{\left| ev^0_{s,m}(T,\theta_{v,m}) - ev_{s,m}(T_v,\theta_{v,m}) \right|}{\tilde{\tau}_s(T,\theta_{v,m})}},$$

$$\tilde{\tau}_s(T,\theta_{v,m}) \longrightarrow : f(\tau_{sr}^{Millikan-White}) + \tilde{\tau}_s^{Park}(T)$$

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$$= g_m \frac{R_s \theta_{v,m}}{e^{\frac{\theta_{v,m}}{T}} - 1} \qquad = g_m \frac{R_s \theta_{v,m}}{e^{\frac{\theta_{v,m}}{T_v}} - 1}$$

$$\tilde{\tau}_s^{(MM)} = \frac{\sum_{m=mode} |\, ev^0_{s,m}(T, \theta_{v,m}) - ev_{s,m}(T_v, \theta_{v,m}) \,|}{\sum_{m=mode} \frac{|\, ev^0_{s,m}(T, \theta_{v,m}) - ev_{s,m}(T_v, \theta_{v,m}) \,|}{\tilde{\tau}_s(T, \theta_{v,m})}},$$

$$\tilde{\tau}_s(T, \theta_{v,m}) \xrightarrow{\qquad} : f(\tau_{sr}^{Millikan-White}) + \tilde{\tau}_s^{Park}(T)$$

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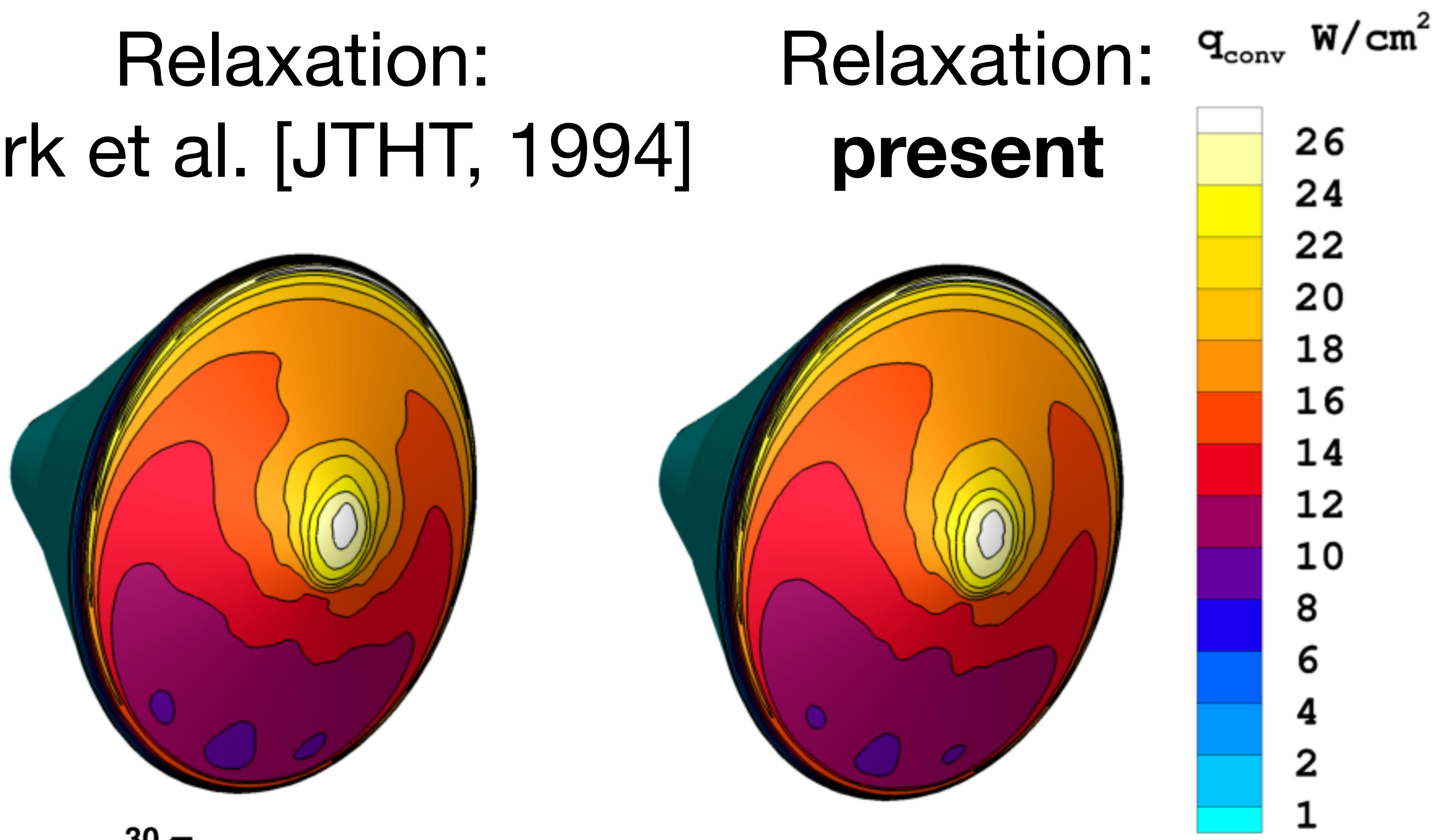
$$= g_m \frac{R_s \theta_{v,m}}{e^{\frac{\theta_{v,m}}{T}} - 1} \qquad\qquad = g_m \frac{R_s \theta_{v,m}}{e^{\frac{\theta_{v,m}}{T_v}} - 1}$$

$$\tilde{\tau}_s^{(MM)} = \frac{\sum_{m=mode} |\, ev^0_{s,m}(T,\theta_{v,m}) - ev_{s,m}(T_v,\theta_{v,m}) \,|}{\sum_{m=mode} \frac{|\, ev^0_{s,m}(T,\theta_{v,m}) - ev_{s,m}(T_v,\theta_{v,m}) \,|}{\tilde{\tau}_s(T,\theta_{v,m})}},$$

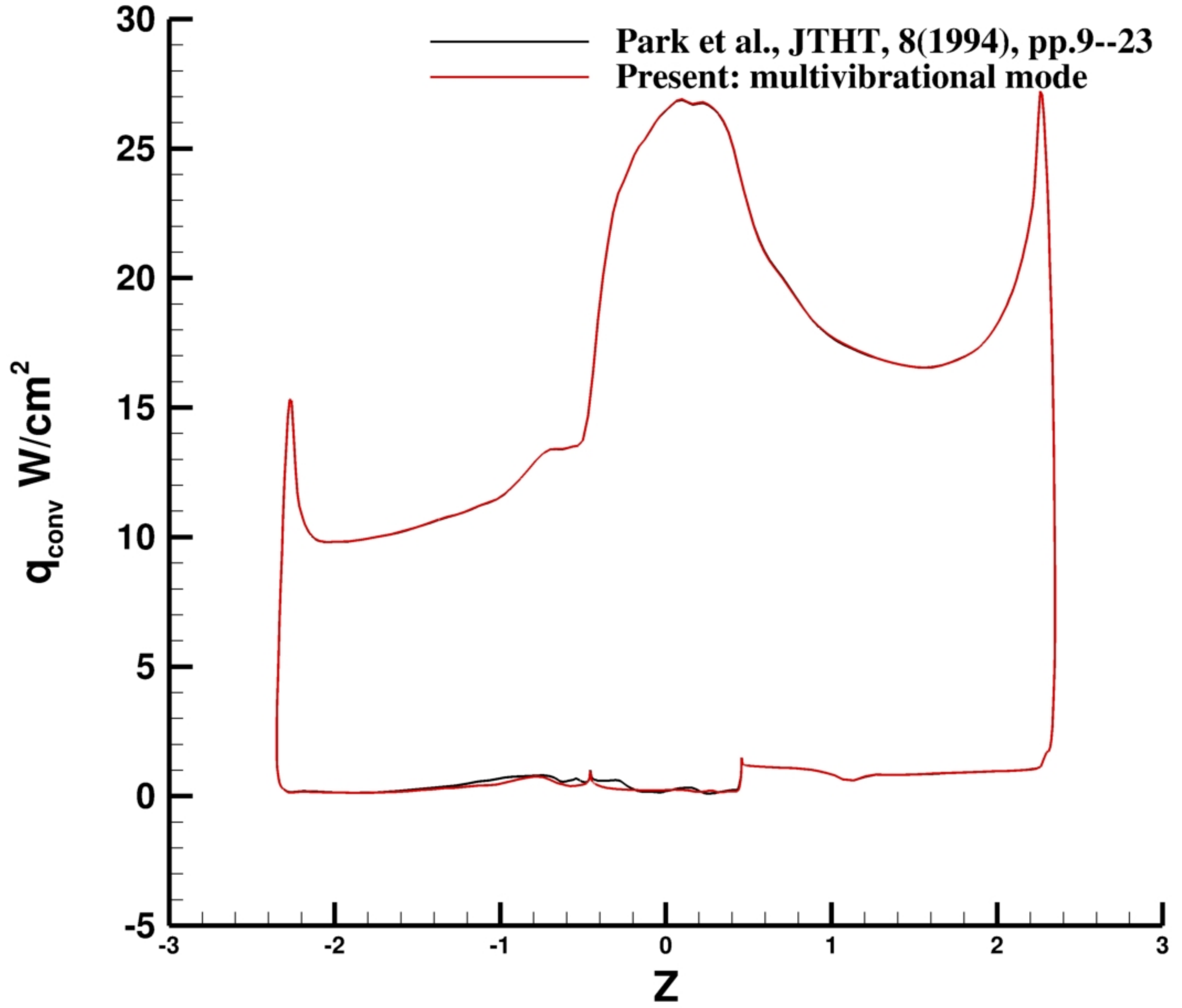
$$\tilde{\tau}_s(T,\theta_{v,m}) \longrightarrow : f(\tau_{sr}^{Millikan-White}) + \tilde{\tau}_s^{Park}(T)$$

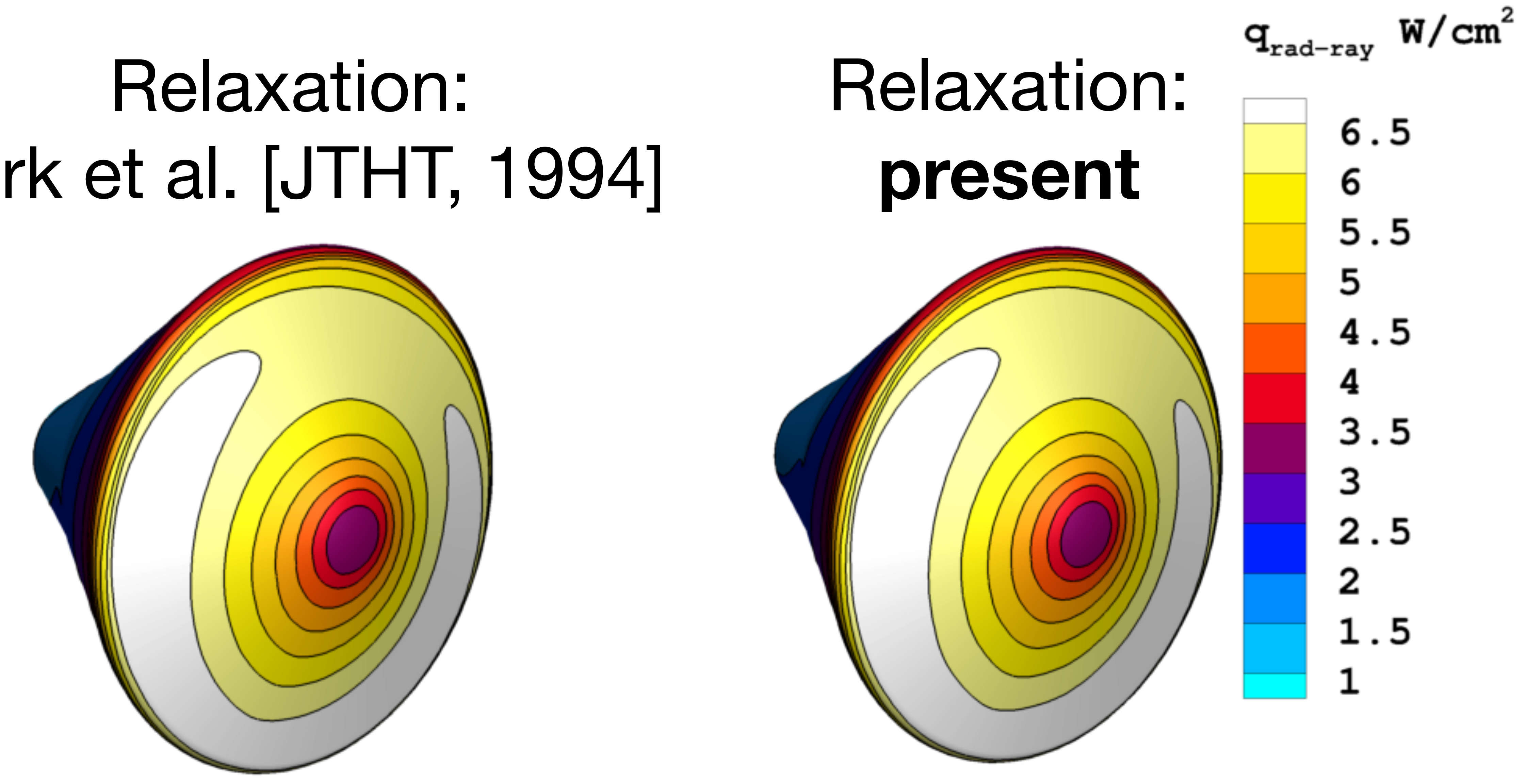
For molecules with single vibrational mode: $\tilde{\tau}_s^{MM} = \tilde{\tau}_s$

Application on CO_2 Mixture


Relaxation:
Park et al. [JTHT, 1994]

Relaxation:
present




Relaxation:
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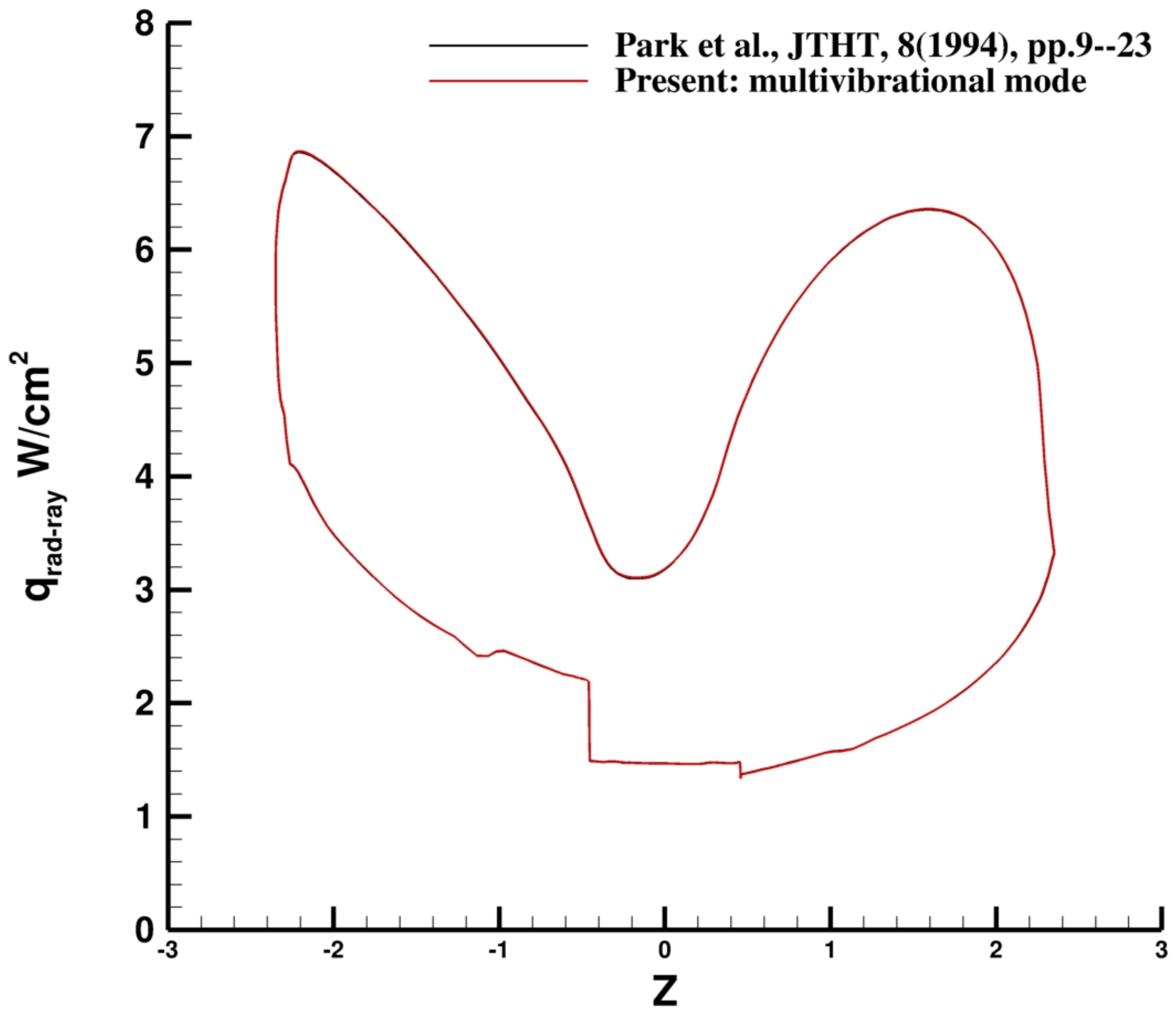
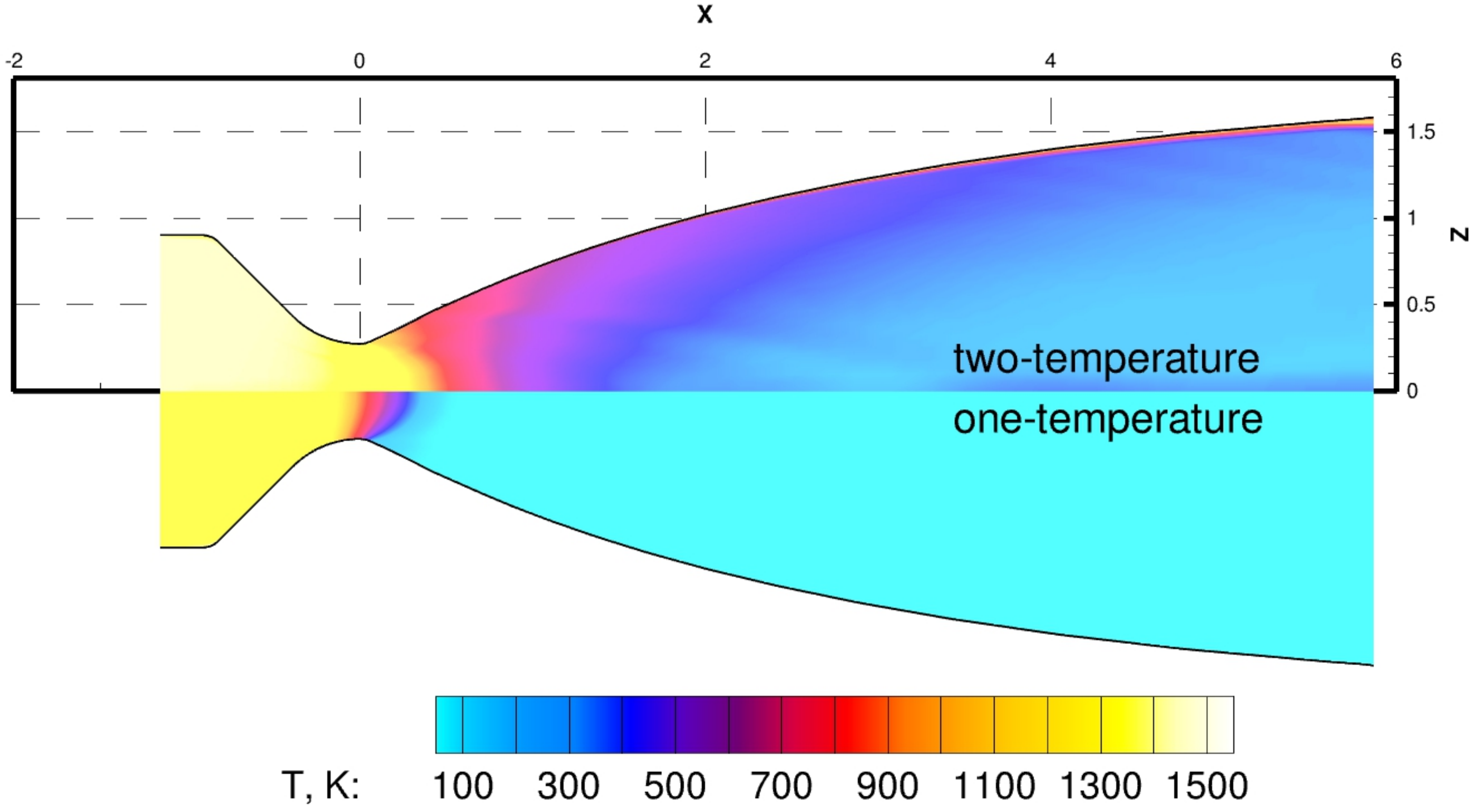
present



Application on non-$\mathrm{CO_2}$ Mixture

$NH_3 - N_2$ gas mixture

Accounting for thermal nonequilibrium could drastically change the temperature profile.



- Relaxation time derived from the Landau-Teller equation is either
  underestimated ($T \ll T_{ve}$) or
  overestimated ($T_{ve} \ll T$).

- Adopting
  Kustova & Oblapenko's work
  [Phys. Rev. E., 2019]:

$$\bar{\tau}_s^{\text{modified}} = \bar{\tau}_s \frac{T_{ve}}{T}\,.$$

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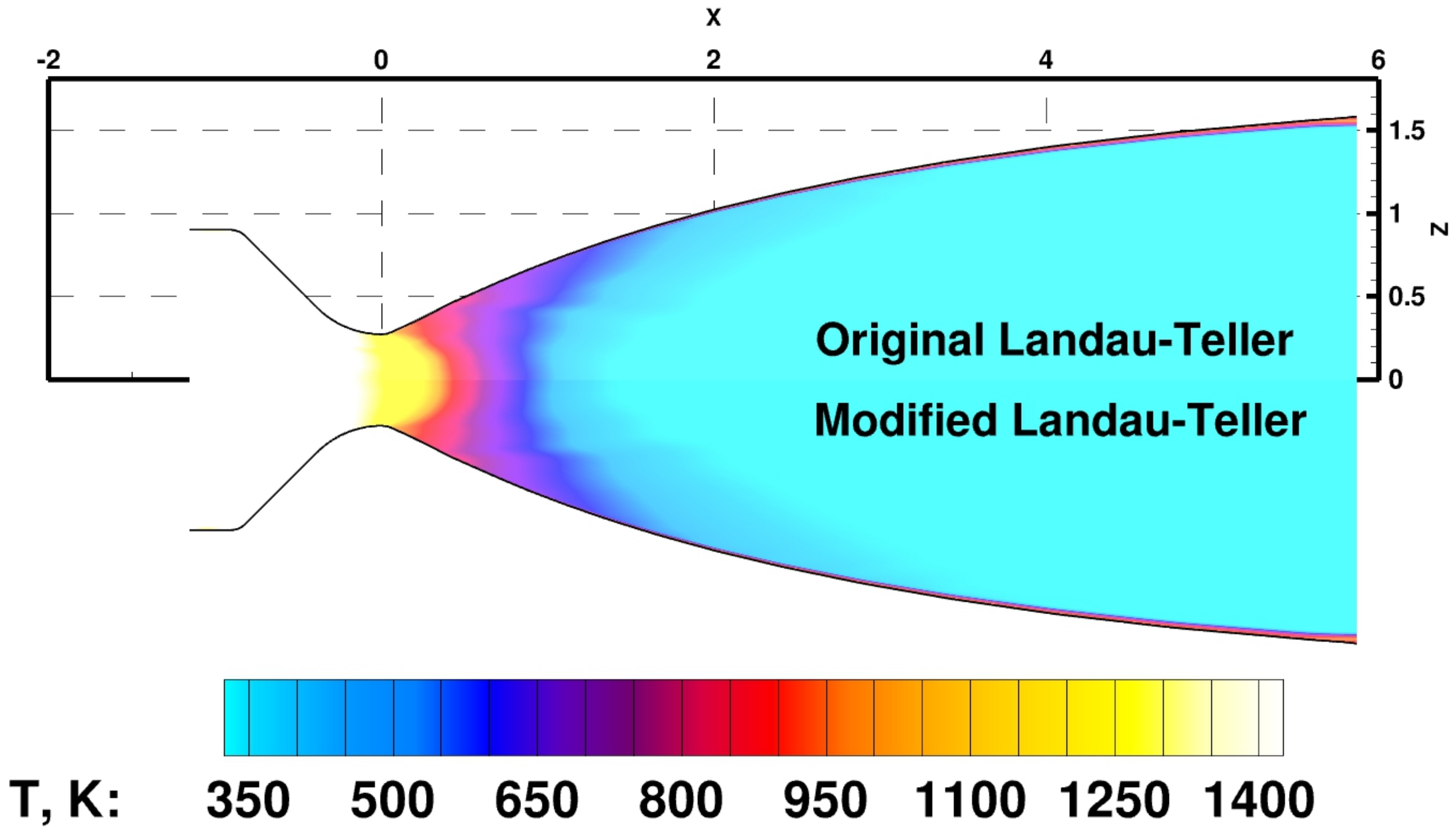

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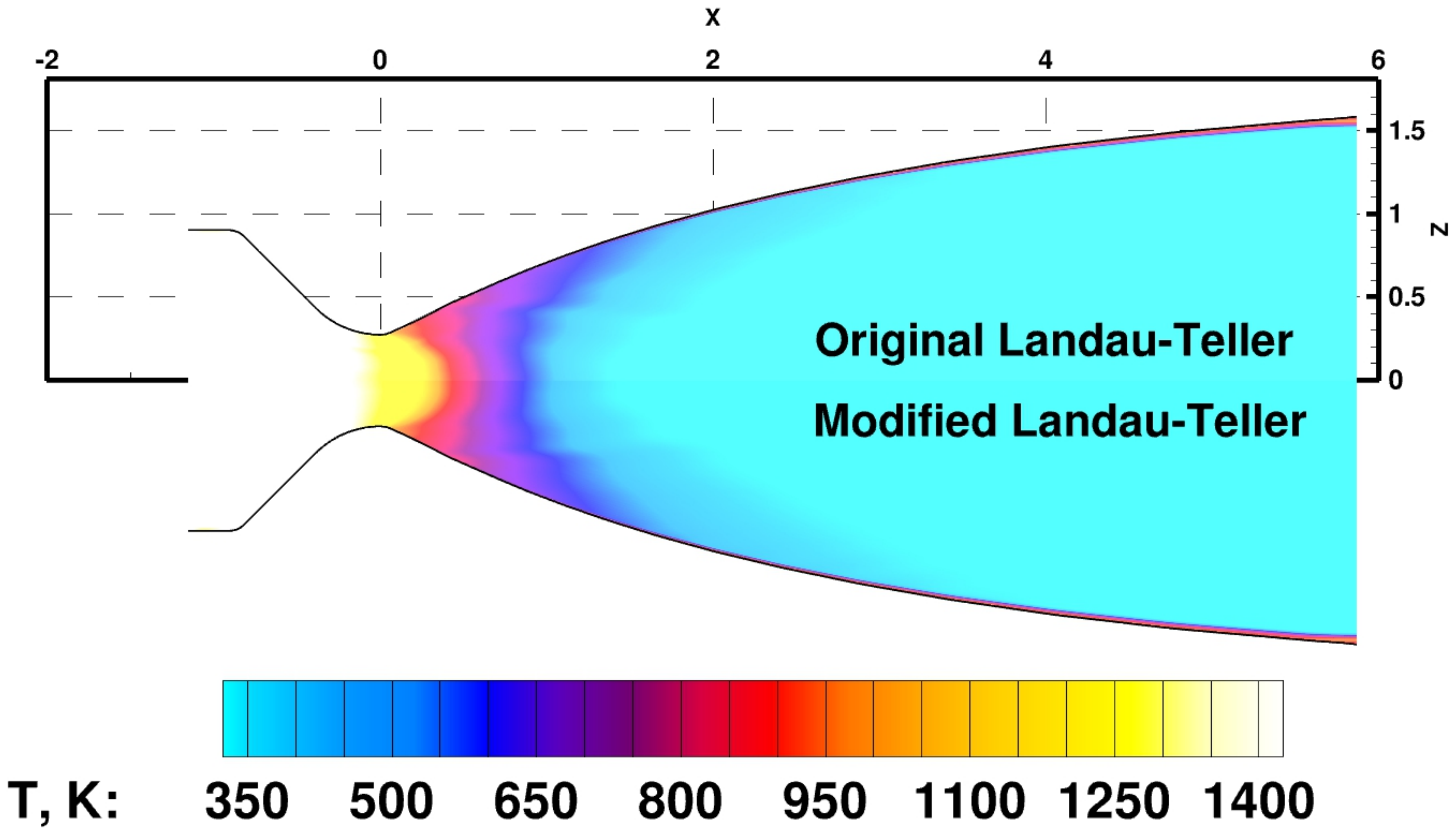
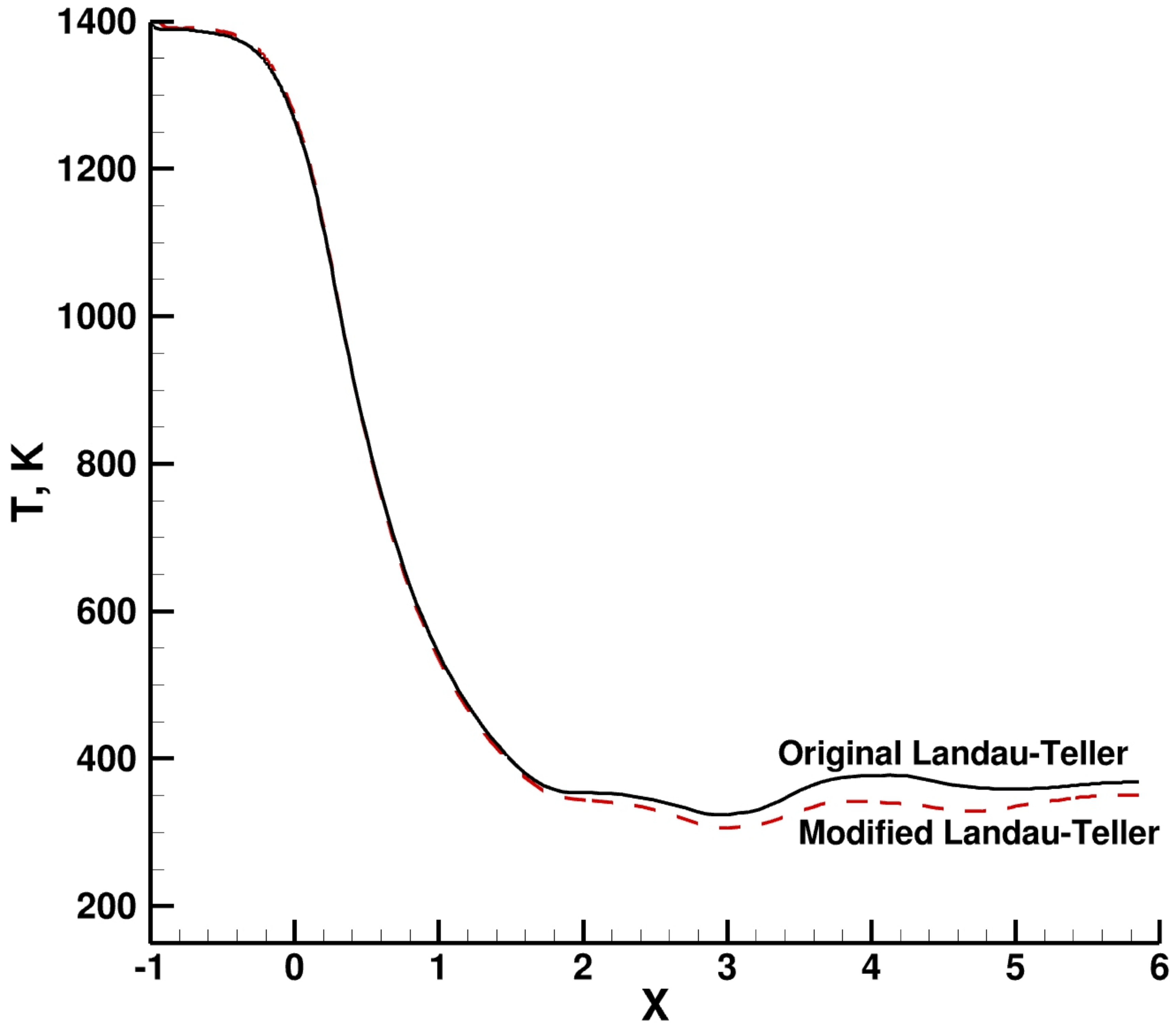
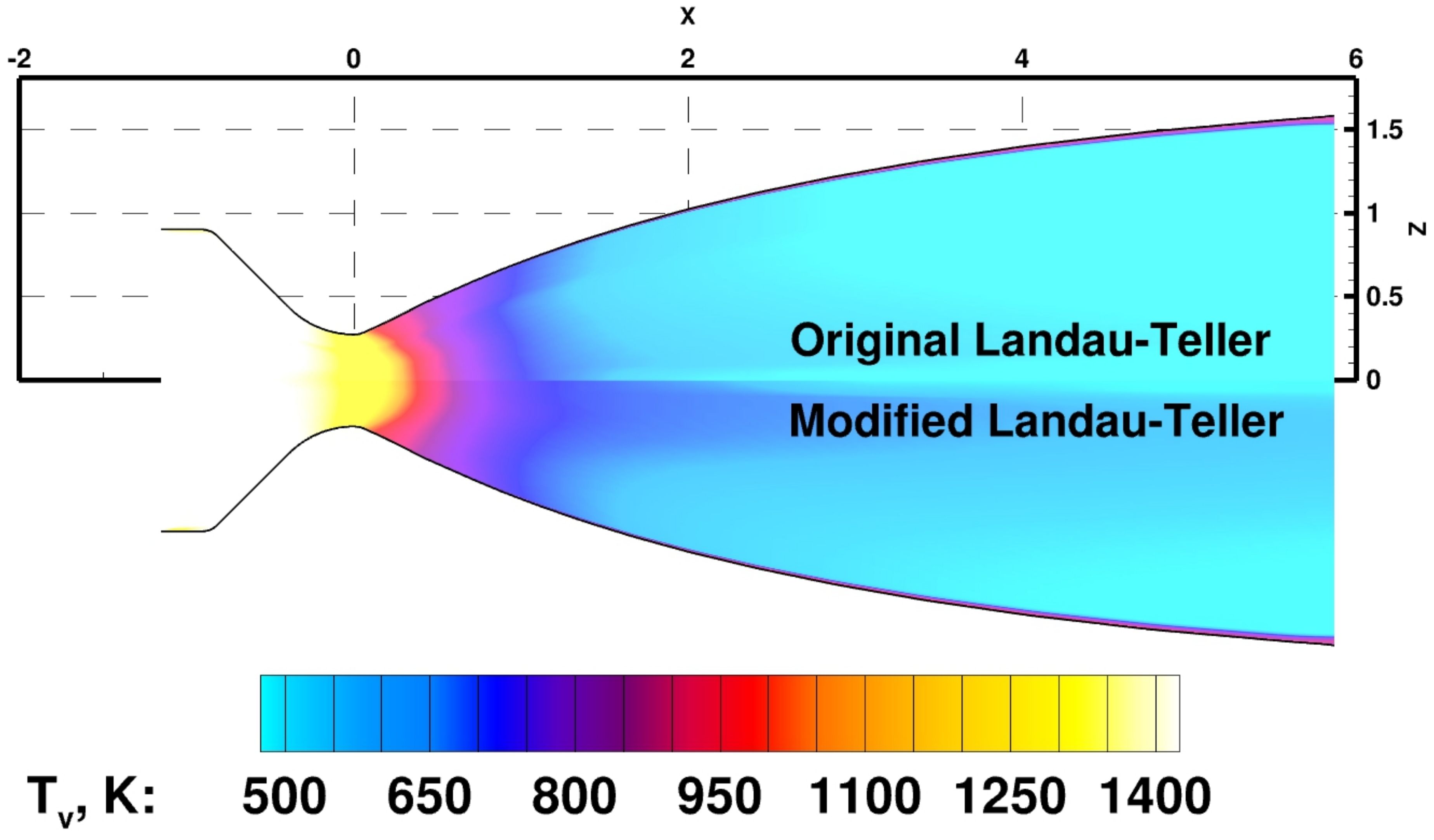


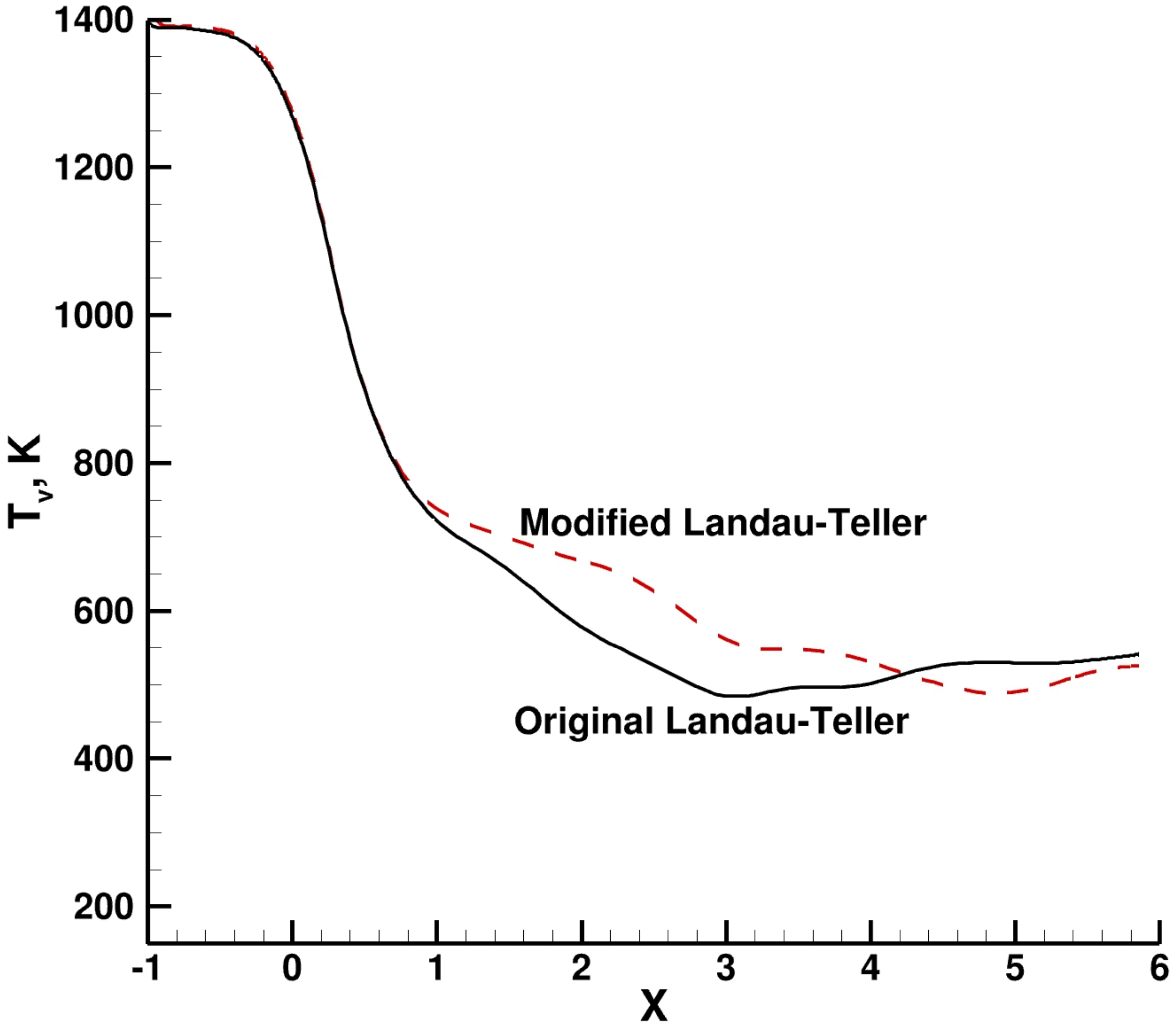


- Relaxation time derived from the Landau-Teller equation is either underestimated ($T \ll T_{ve}$) or overestimated ($T_{ve} \ll T$).

- Adopting Kustova & Oblapenko's work [Phys. Rev. E., 2019]:

$$\bar{\tau}_s^{\text{modified}} = \bar{\tau}_s \frac{T_{ve}}{T} .$$





Contributions

- A new multivibrational relaxation procedure was developed
- The new scheme was shown to be in excellent agreement against the Park's 1994 model for the Martian atmosphere.
- The proposed scheme is applicable to generic molecules that have multiple vibrational frequencies.

Backups

Multivibrational Mode Approach

Consider again the Landau-Teller equation:

$$Src^{T\leftrightarrow V} \equiv \frac{dE_v}{dt} \simeq \sum_{s=mol.} \rho_s \frac{ev_s^0(T) - ev_s(T_v)}{\tilde{\tau}_s} \simeq \frac{\rho C_{vv}(T - T_v)}{\overline{\tau}},$$

$$Src^{T\leftrightarrow V} = \sum_{s=mol.} \rho_s \left(\overbrace{\sum_{m=mode} \frac{ev_{s,m}^0(T) - ev_{s,m}(T_v)}{\tilde{\tau}_s^{(MM)}(T, \theta_{v,m})}} \right) = \frac{\rho C_{vv}(T - T_v)}{\overline{\tau}}.$$

$$\tilde{\tau}_s^{(MM)} = \frac{\sum_{m=mode} \left| \overset{= g_m \frac{R_s \theta_{v,m}}{e^{\frac{\theta_{v,m}}{T}} - 1}}{ev_{s,m}^0(T, \theta_{v,m})} - \overset{= g_m \frac{R_s \theta_{v,m}}{e^{\frac{\theta_{v,m}}{T_v}} - 1}}{ev_{s,m}(T_v, \theta_{v,m})} \right|}{\sum_{m=mode} \frac{\left| ev_{s,m}^0(T, \theta_{v,m}) - ev_{s,m}(T_v, \theta_{v,m}) \right|}{\tilde{\tau}_s(T, \theta_{v,m}) \xrightarrow{\qquad} : f(\tau_{sr}^{MW}) + \tilde{\tau}_s^{Park}(T)}},$$

- Consider now the Landau-Teller Equation:

$$Src^{T\leftrightarrow V} \equiv \frac{dE_v}{dt} = \sum_{s=mol.} \rho_s \frac{ev_s^0(T) - ev_s(T)}{\tilde{\tau}_s},$$

where

averaged vibrational relaxation time for species s

an averaging function

vibrational relaxation of species s in a medium species r.

$$\tilde{\tau}_s = f(\tau_{sr}).$$

The landmark correlation for τ_{sr} is provided by Milikan-White [J. Chem. Phys., 1963]:

$$p\tau_{sr}^{\mathrm{MW}} = \exp\left[a_{sr}(T^{-1/3} - b_{sr}) - 18.42\right],$$

where

single characteristic vibrational temperature

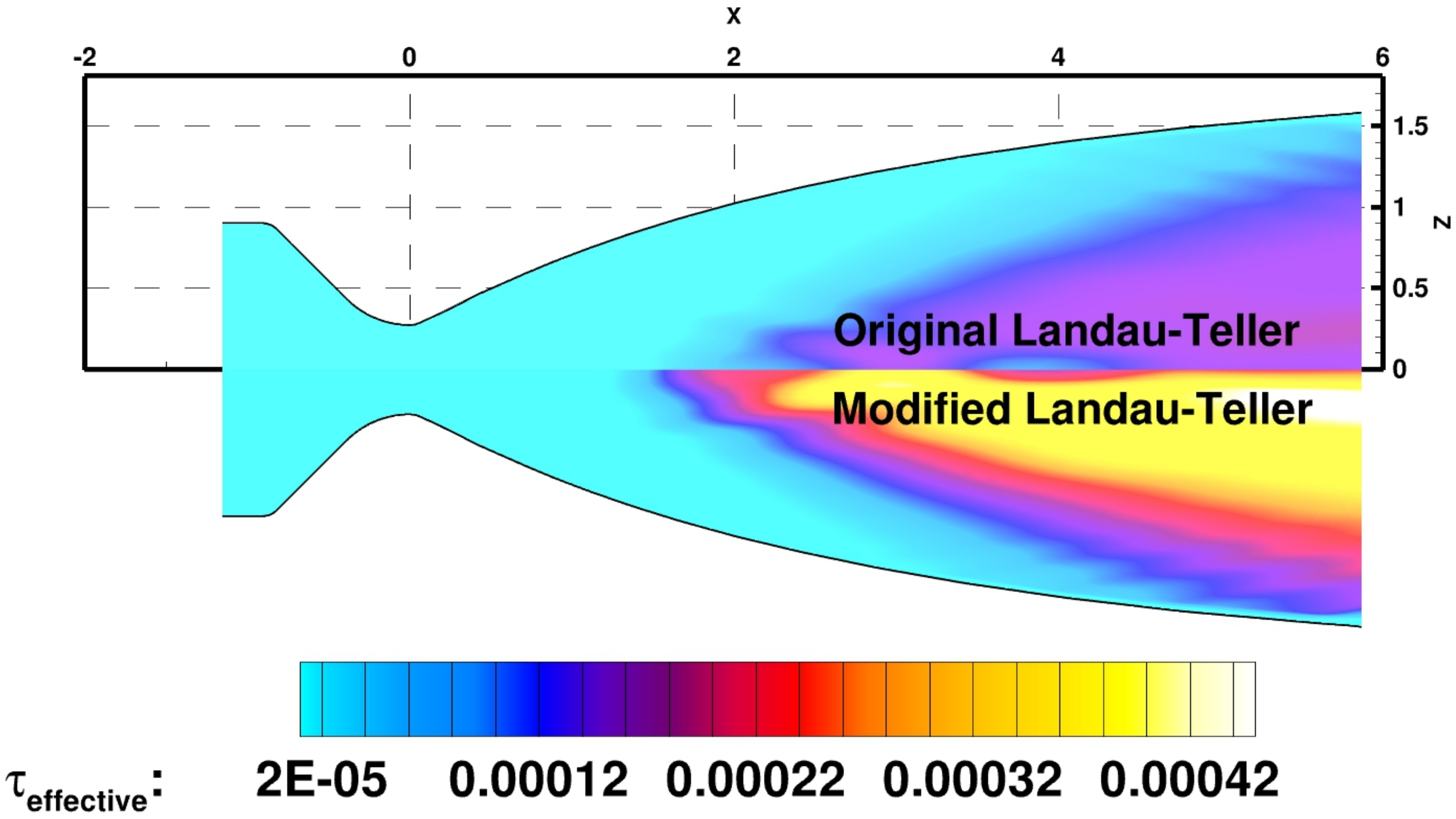
reduced mass

$$a_{sr} := g(\mu_{sr}, \theta_{v,s}), \quad b_{sr} := h(\mu_{sr}).$$

- Some polyatomic molecules, such as CO_2 and NH_3, has **multiple** vibrational frequencies and characteristic vibrational temperatures. **Thus, the above formula is not directly applicable to those molecules.**

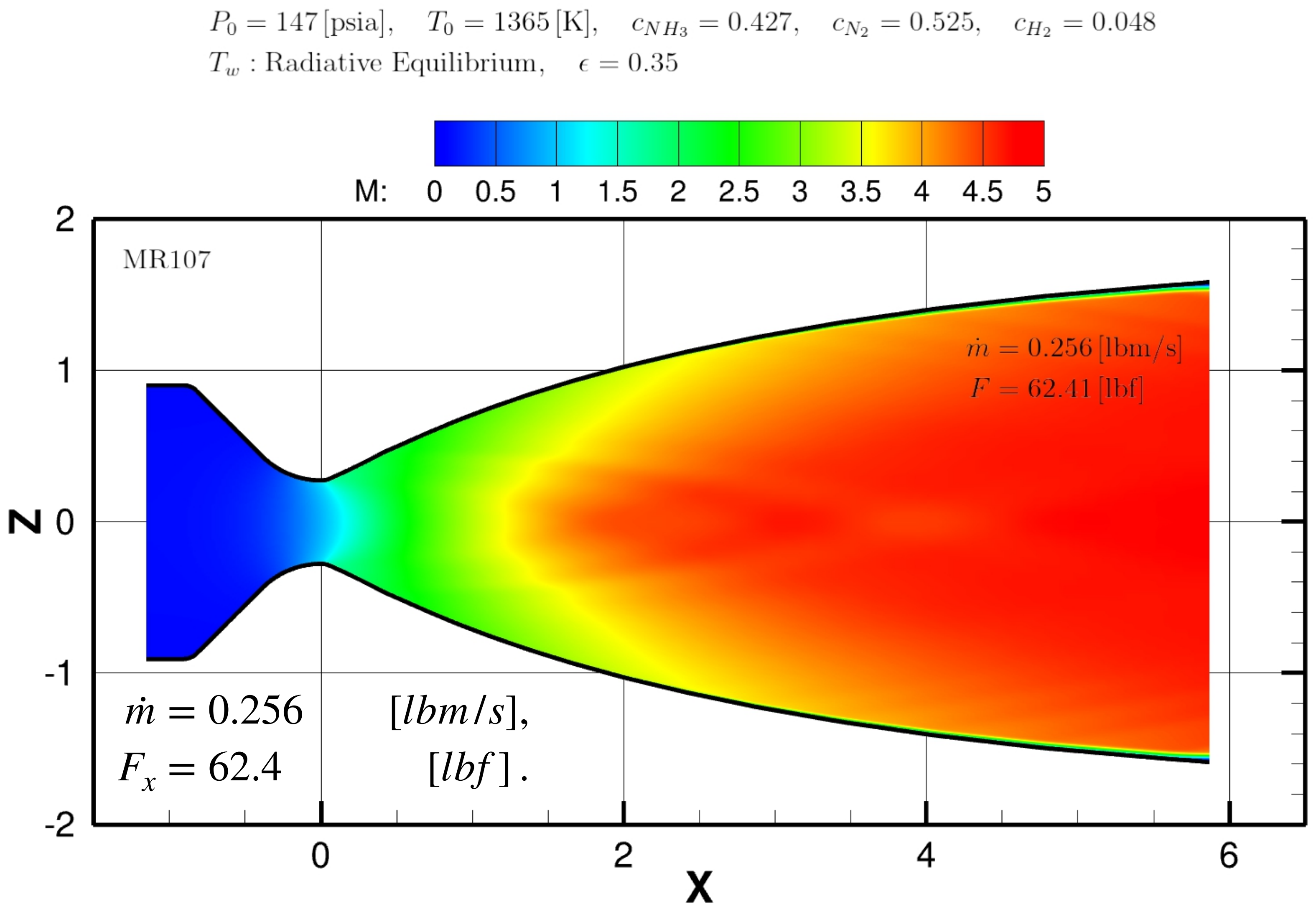
- For $CO_2 - N_2$, Park et al. [JTHT, 1994] suggested a series of **tailored** values for a_{sr} and b_{sr}.

$NH_3 - N_2$ gas mixture



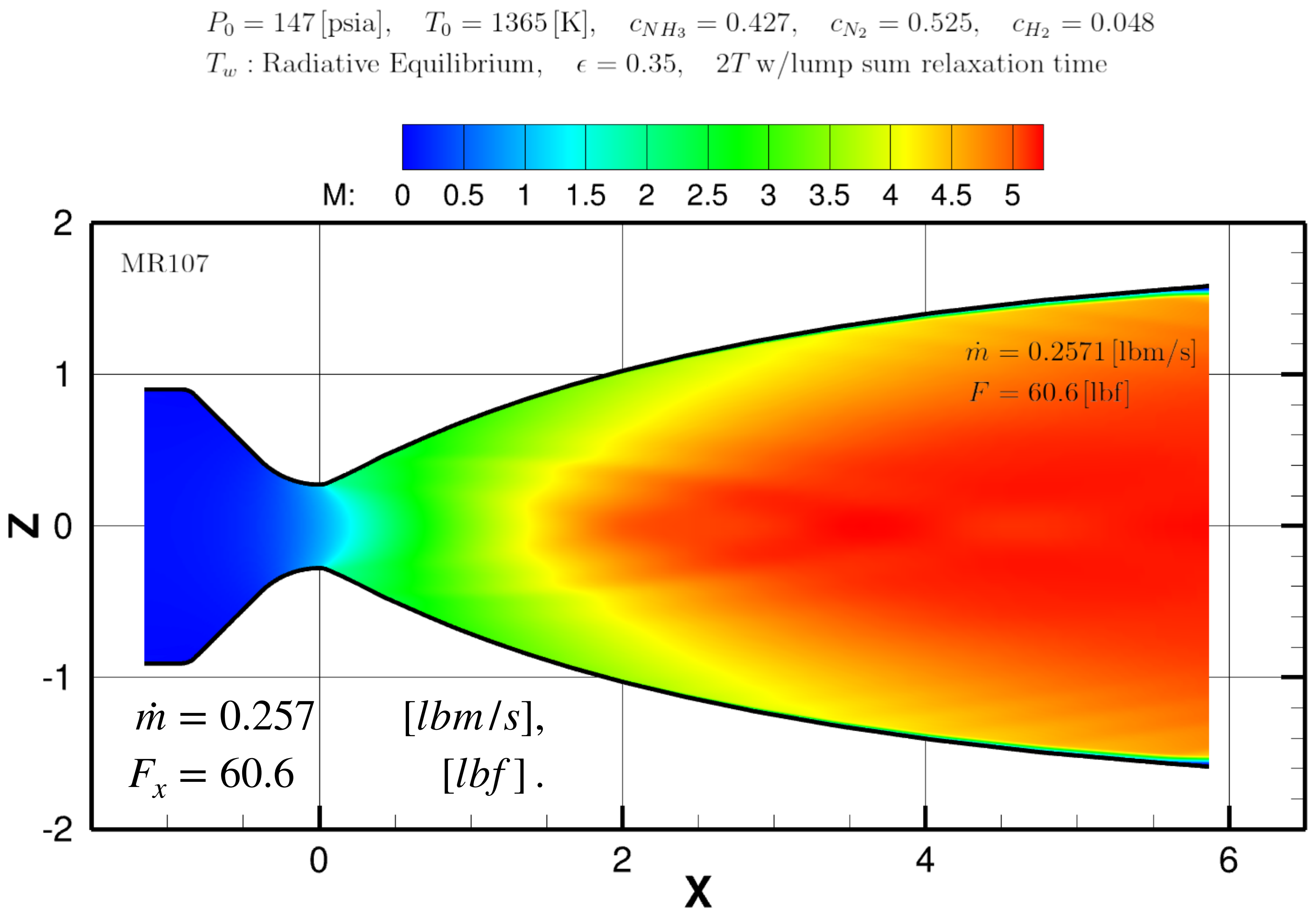
Test Case 1: MR107

One-Temperature

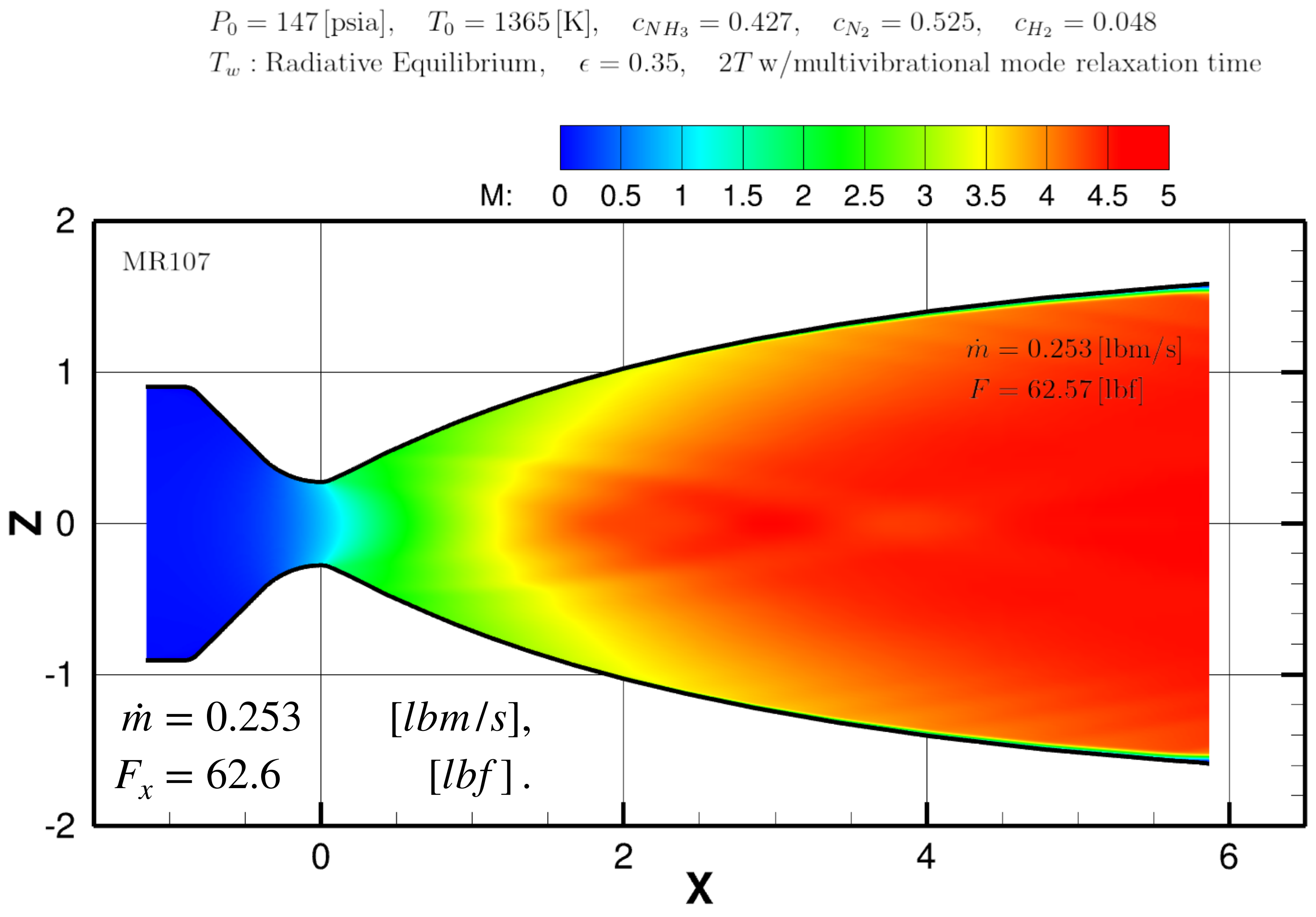


Two-Temperature w/lump sum relaxation time

assuming: $\bar{\theta}_v = 3500\,[K]$



Two-Temperature w/multimode relaxation time

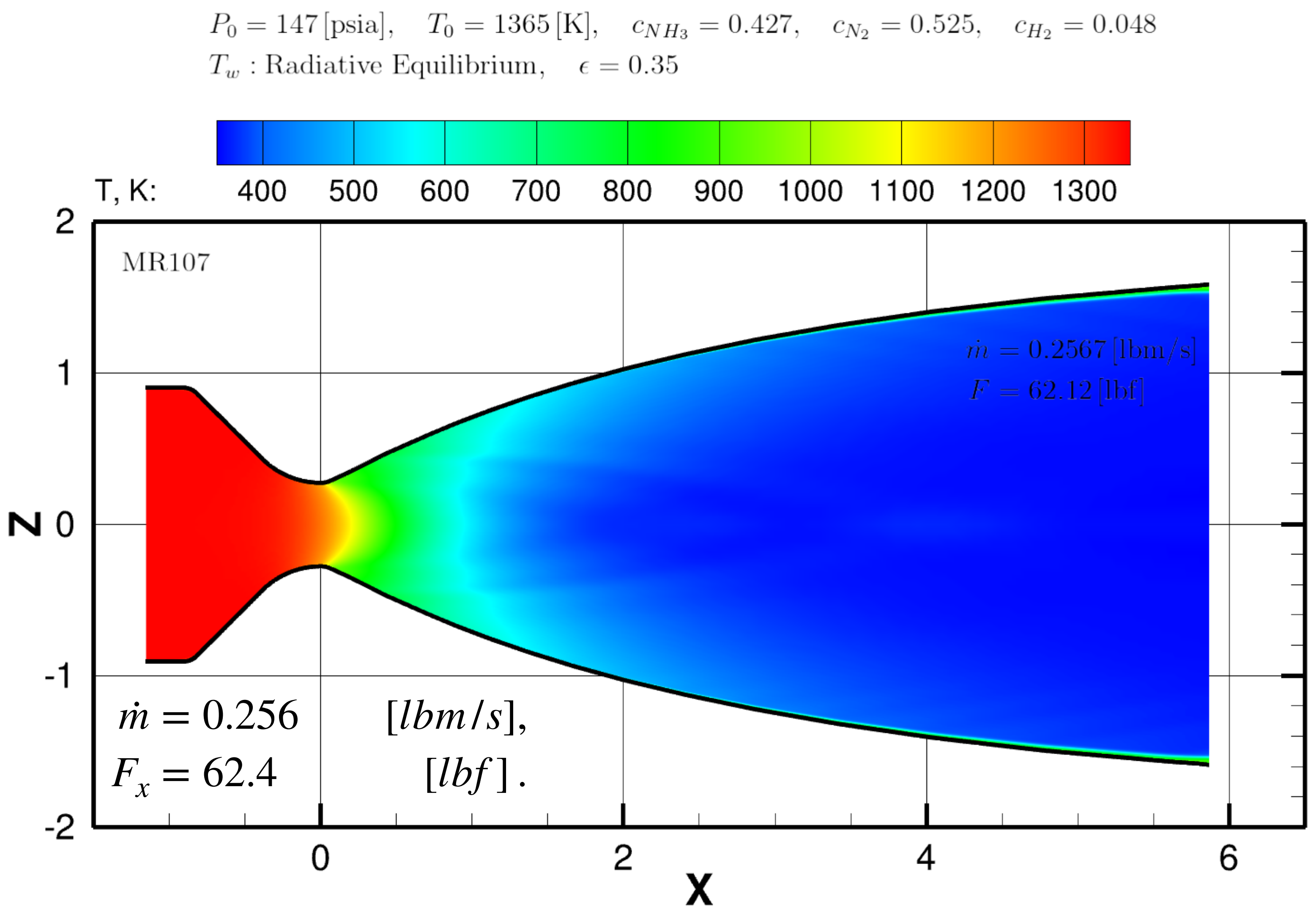


- The lump sum approach with single characteristic temperature of 3500K underpredicts the RCS thrust.

- One-temperature and two-temperature multimode approaches predict comparable RCS thrust.

Test Case 1: MR107

One-Temperature



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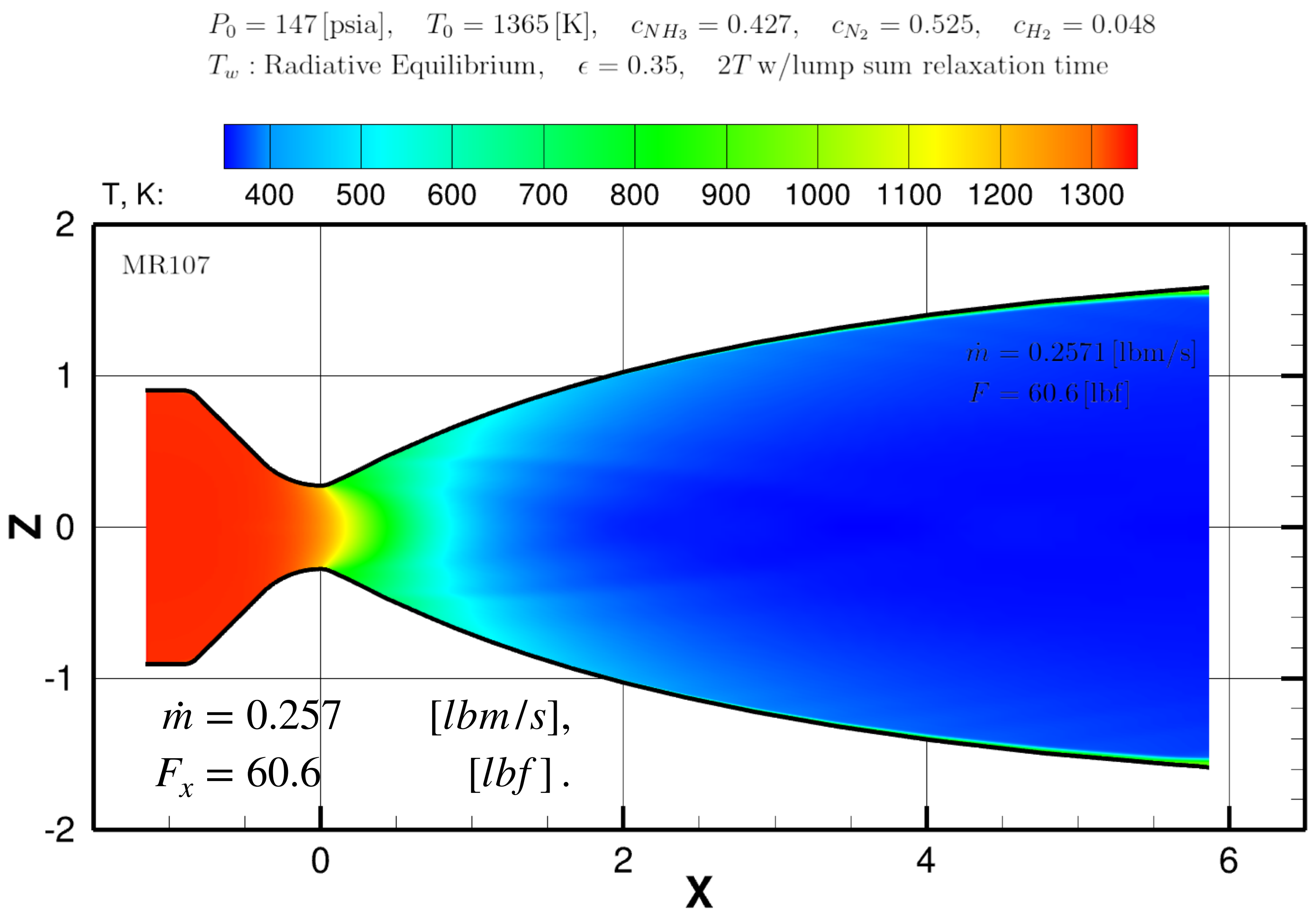
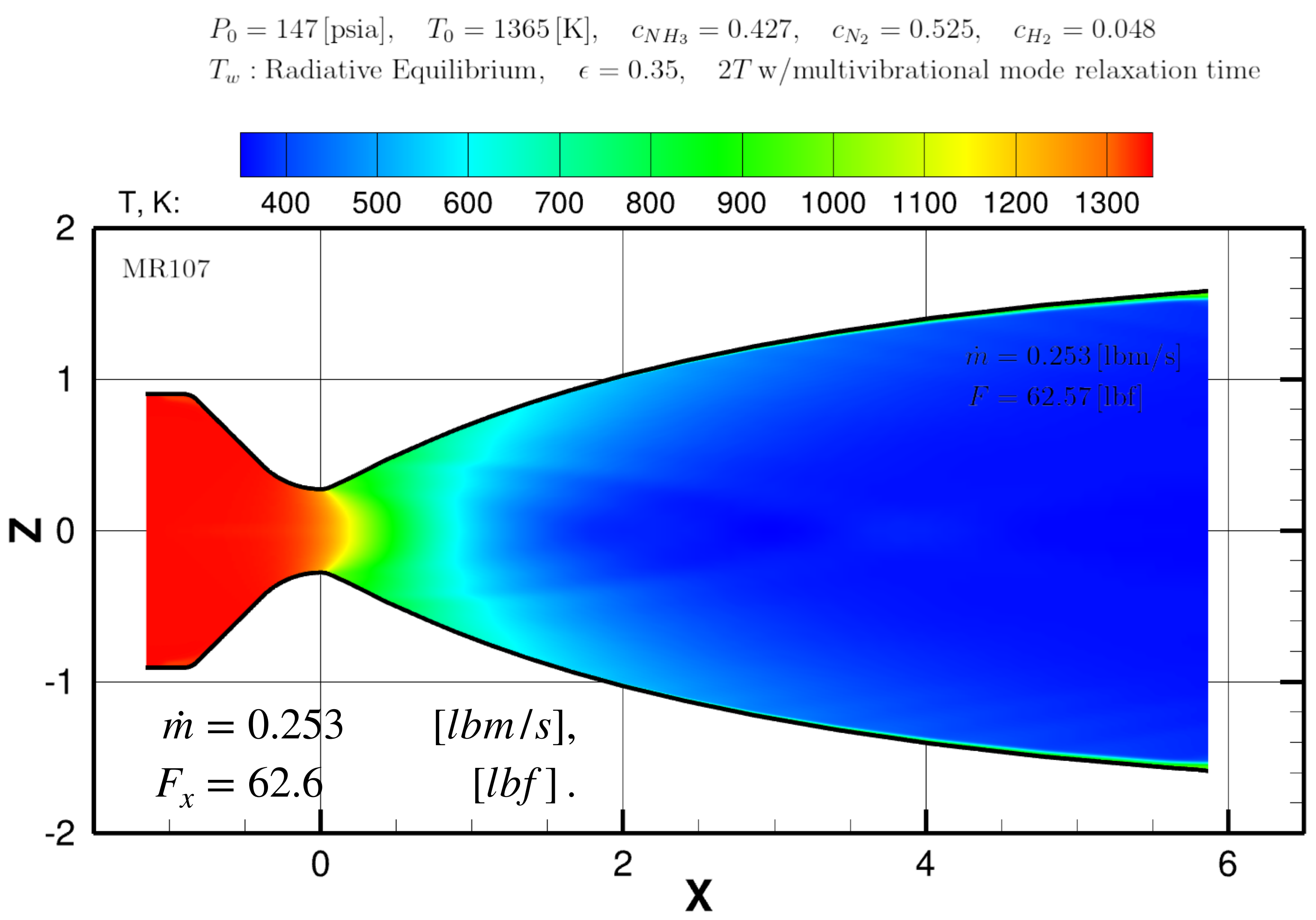
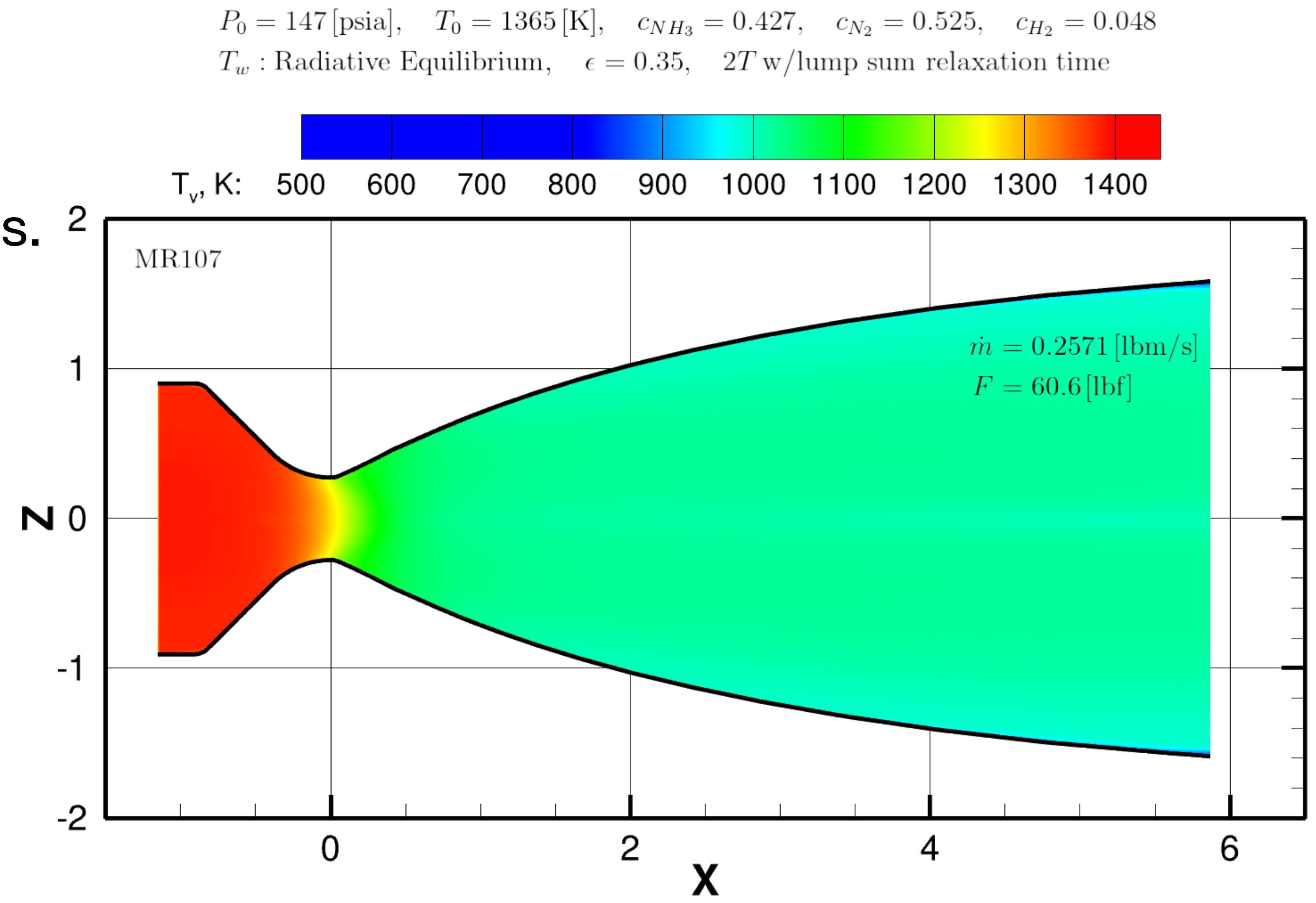
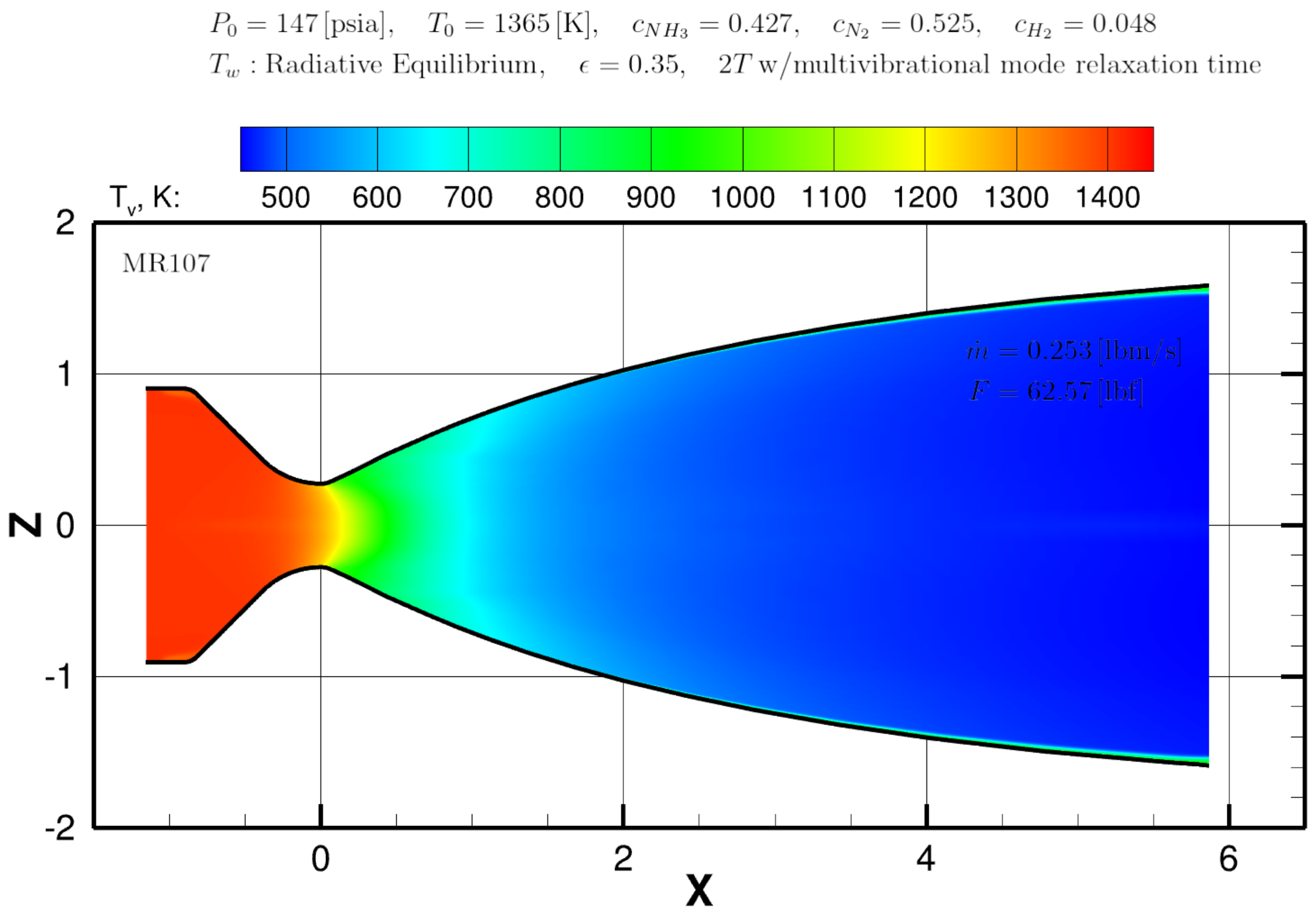


Two-Temperature w/multimode relaxation time



- Comparable nozzle temperature with either approaches.
- Cooler vibrational temperature with the multimode relaxation approach compared with a lump sum approach and single characteristic temperature of 3500K.
- Comparable enthalpy with either of the approaches.





Test Case 1: MR107

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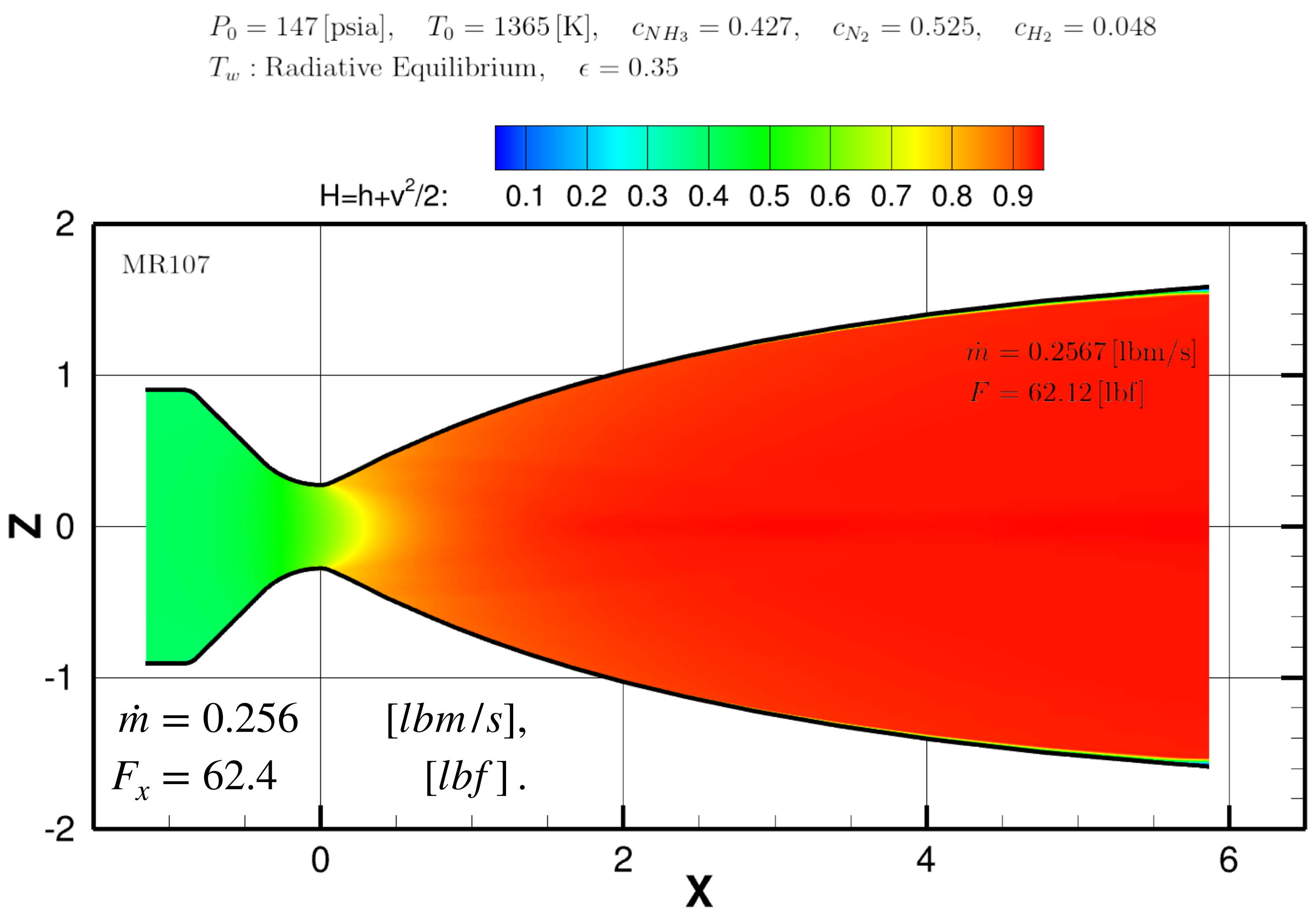

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- Cooler vibrational temperature with the multimode relaxation approach compared with a lump sum approach and single characteristic temperature of 3500K.
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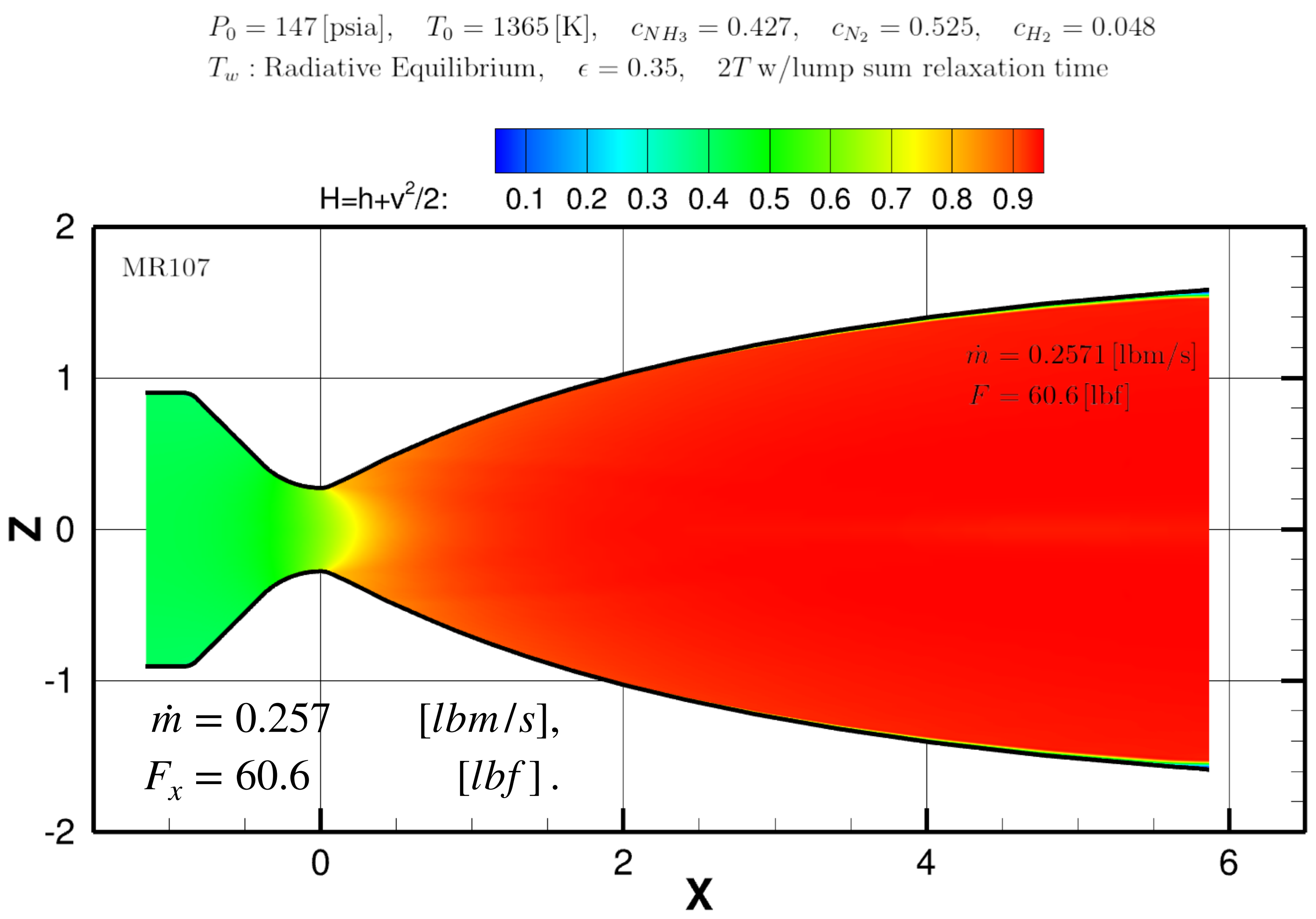
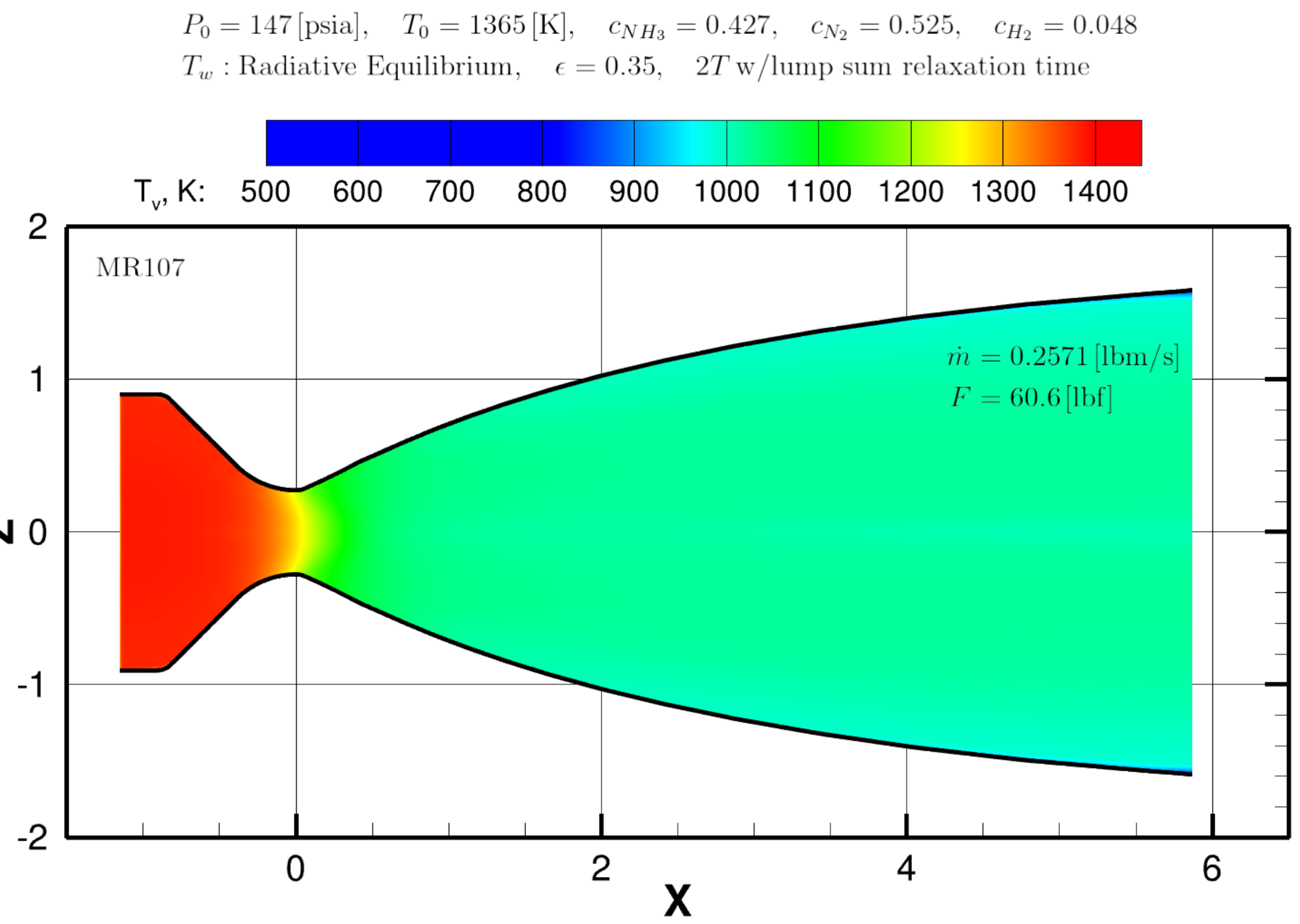
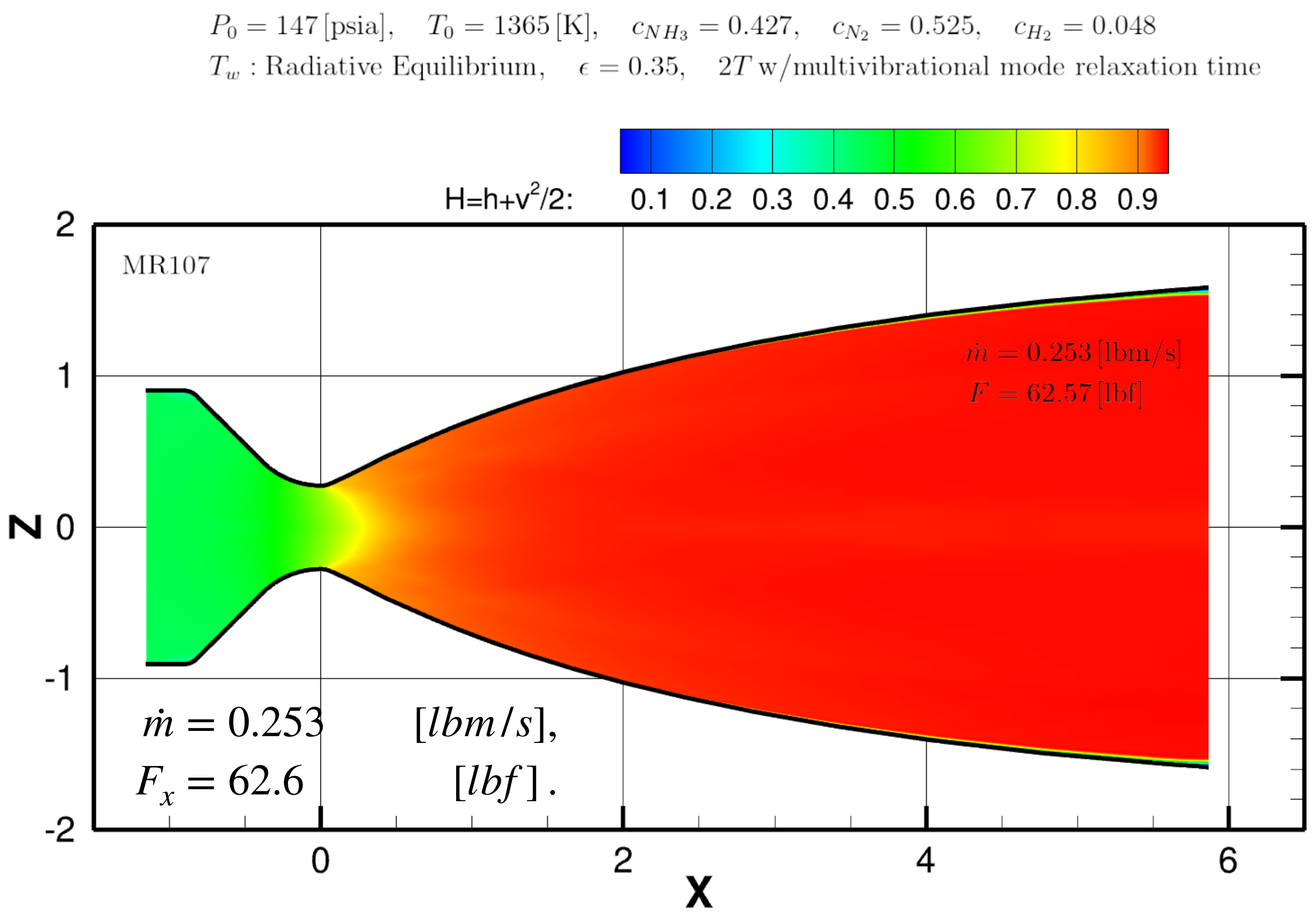
Two-Temperature w/lump sum relaxation time

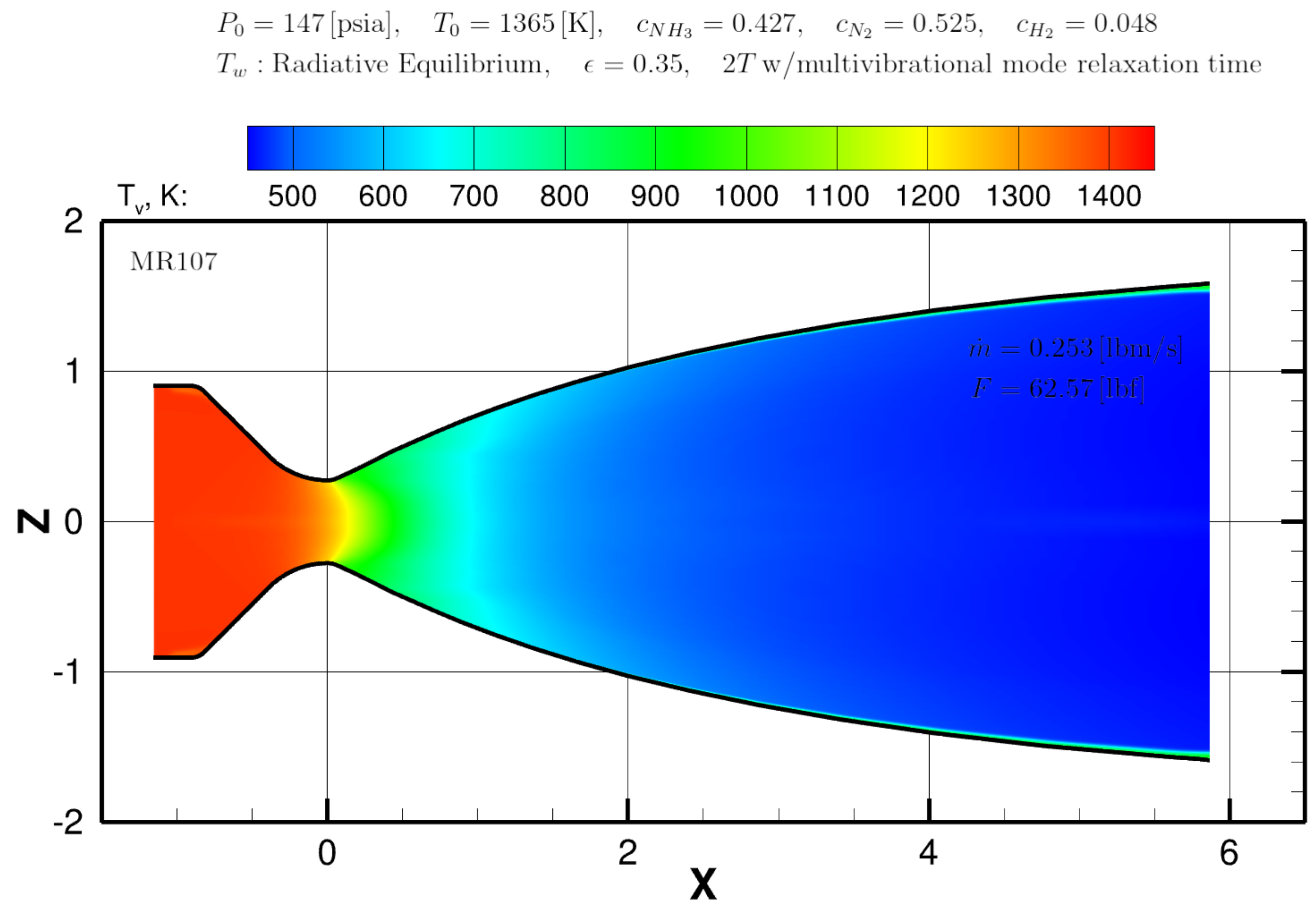
assuming: $\bar{\theta}_v = 3500\,[K]$





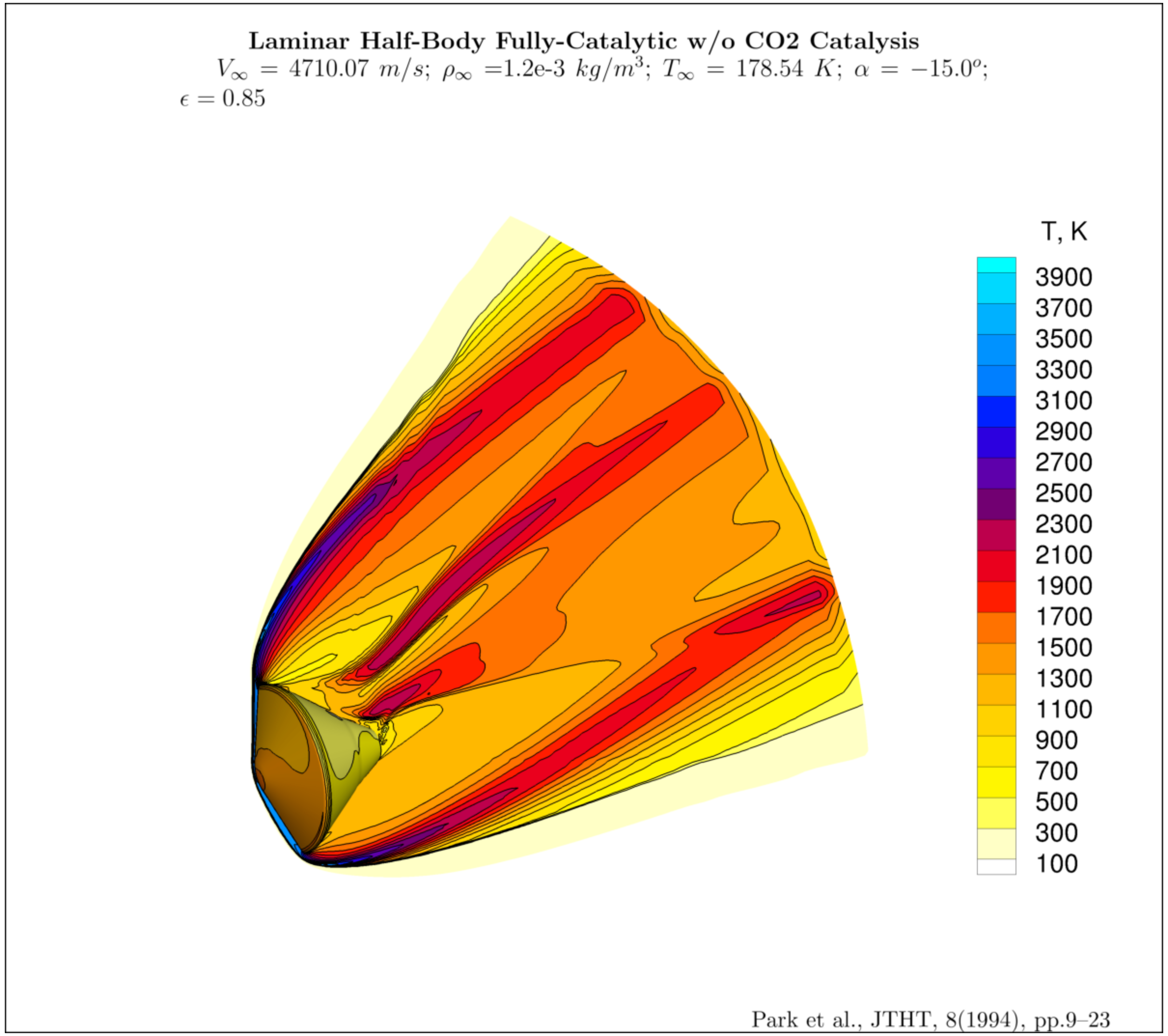
Two-Temperature w/multimode relaxation time





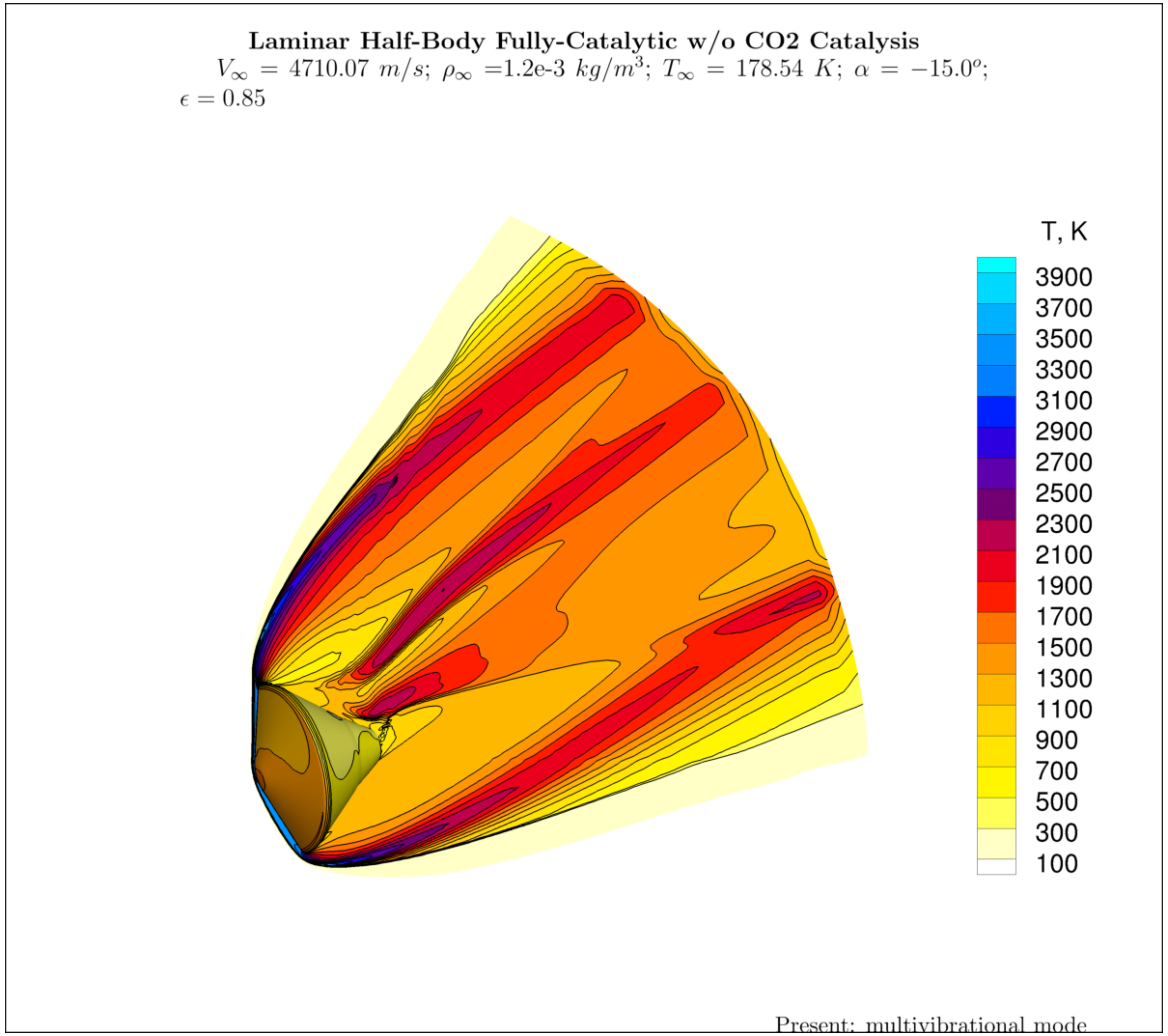
Test Case 2: SRL

Park model



Park et al., JTHT, 8(1994), pp.9–23

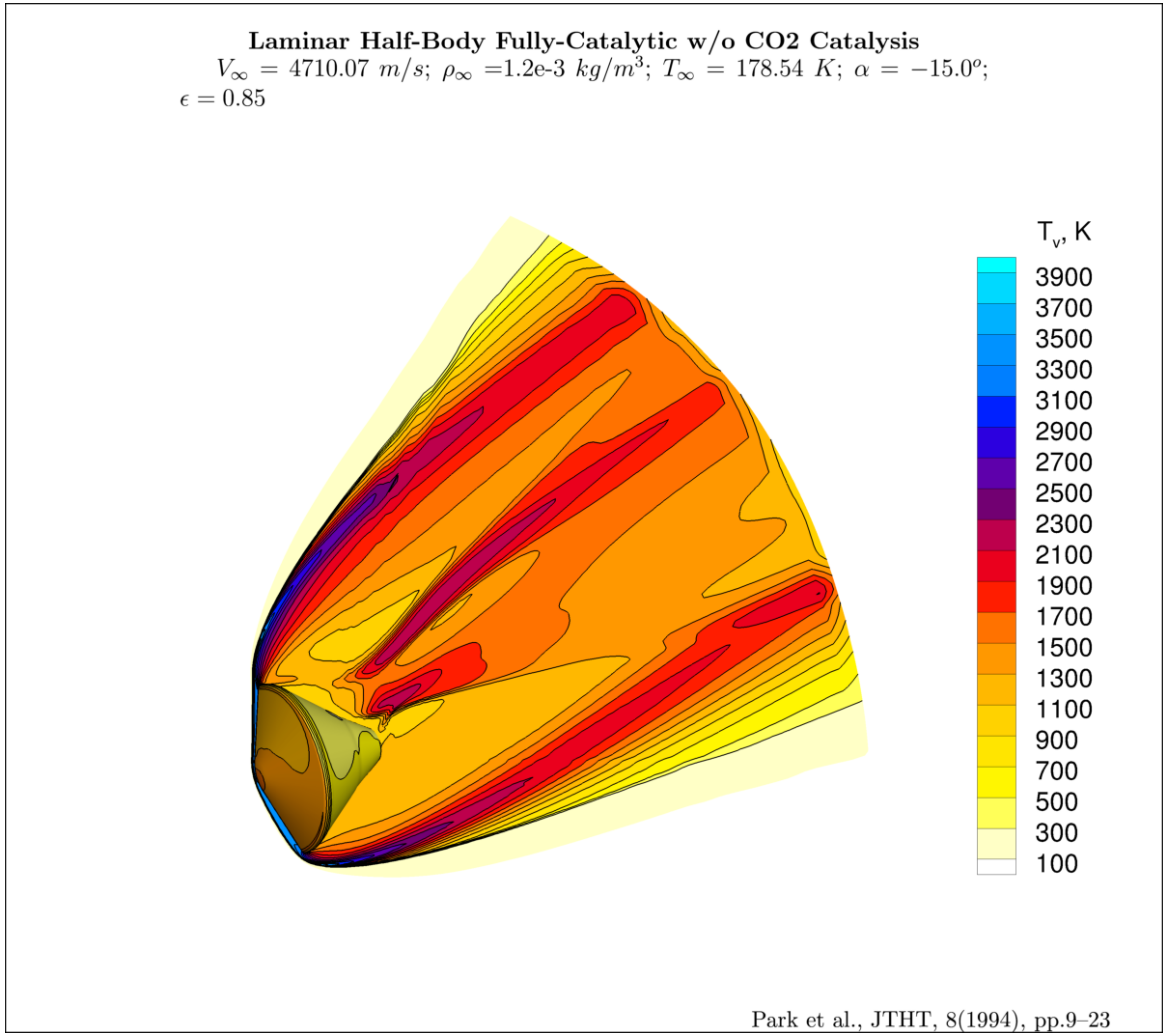
Present



Present: multivibrational mode

Test Case 2: SRL

Park model



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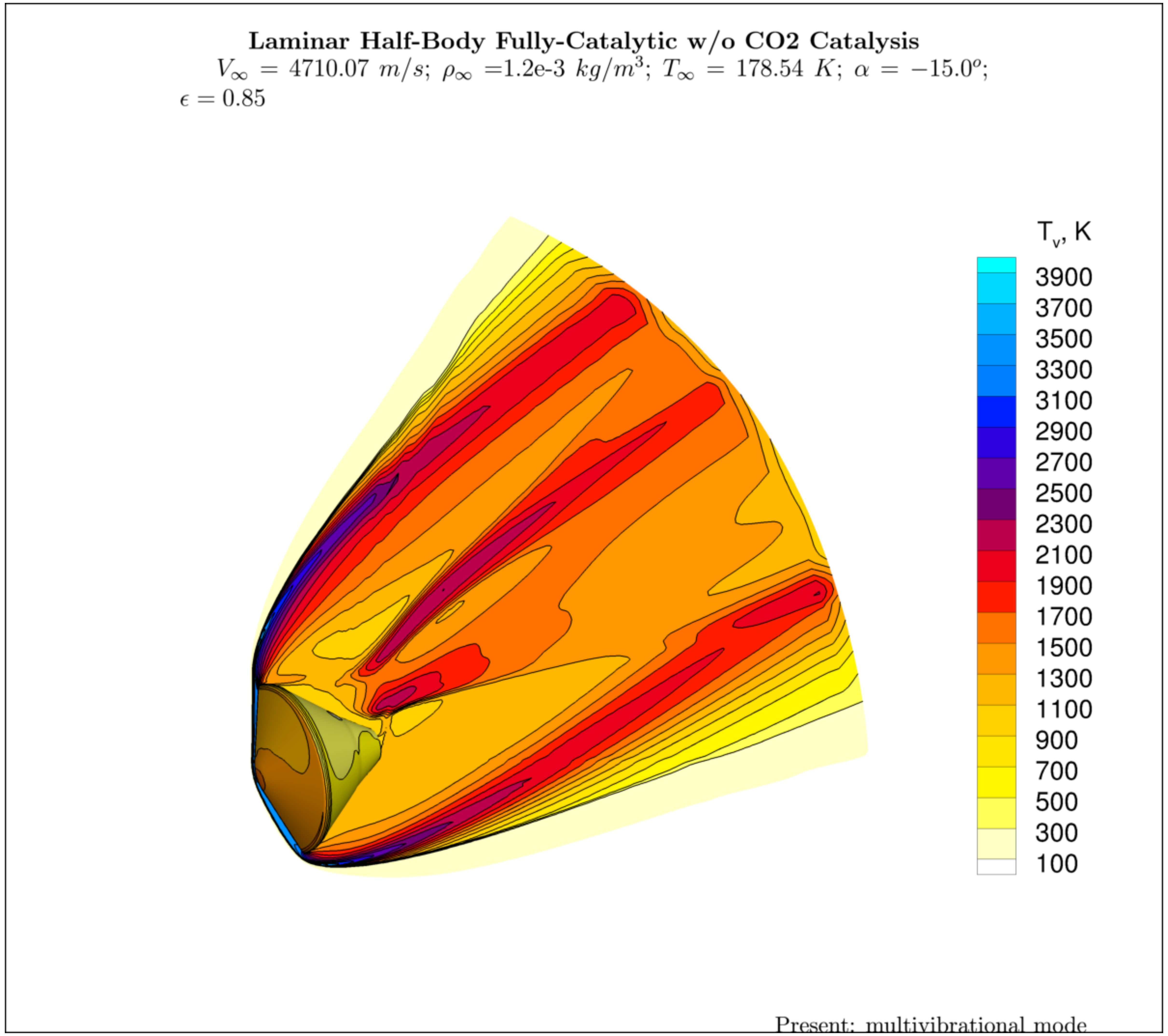
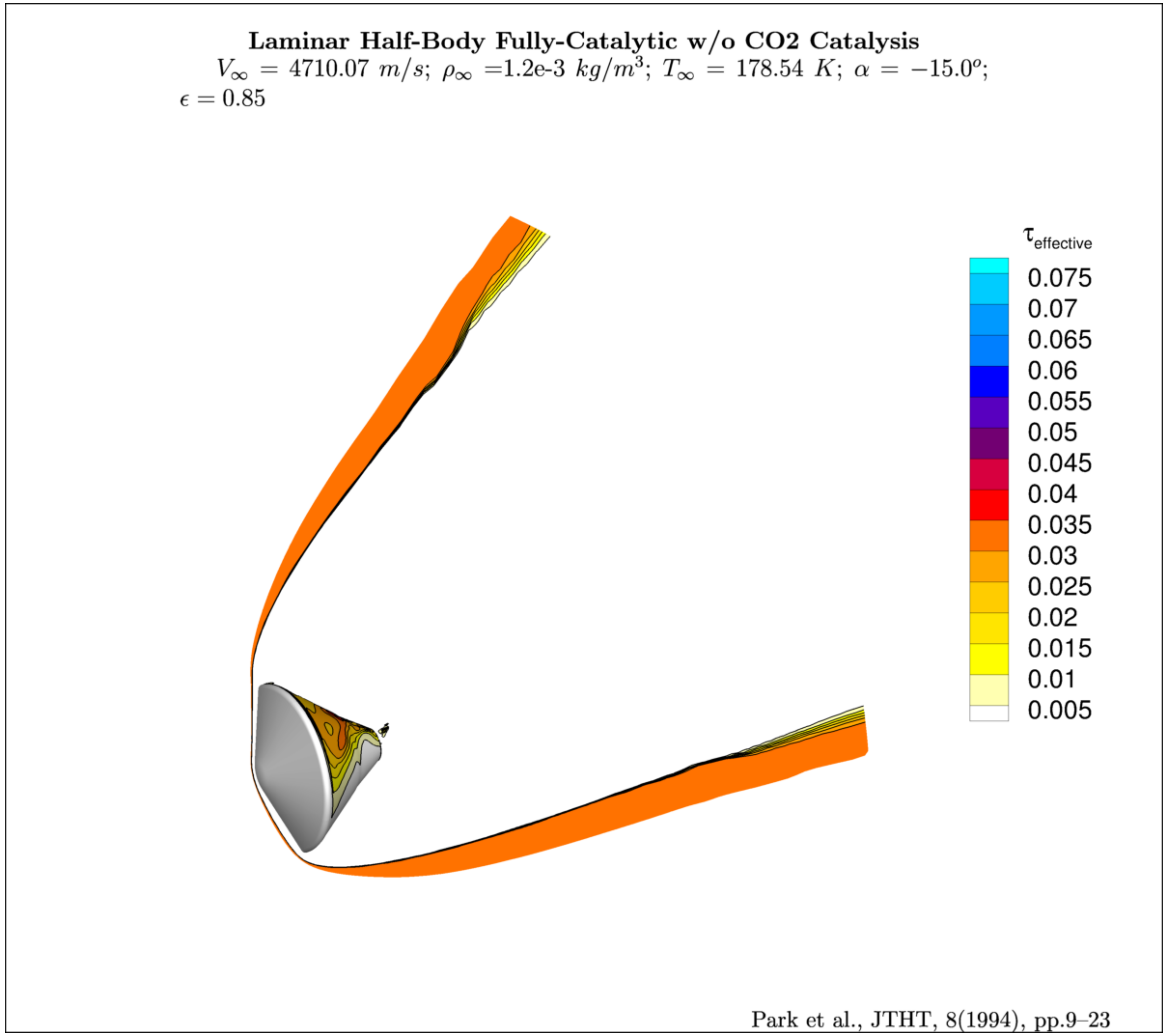
Present



Present: multivibrational mode

Test Case 2: SRL

Park model



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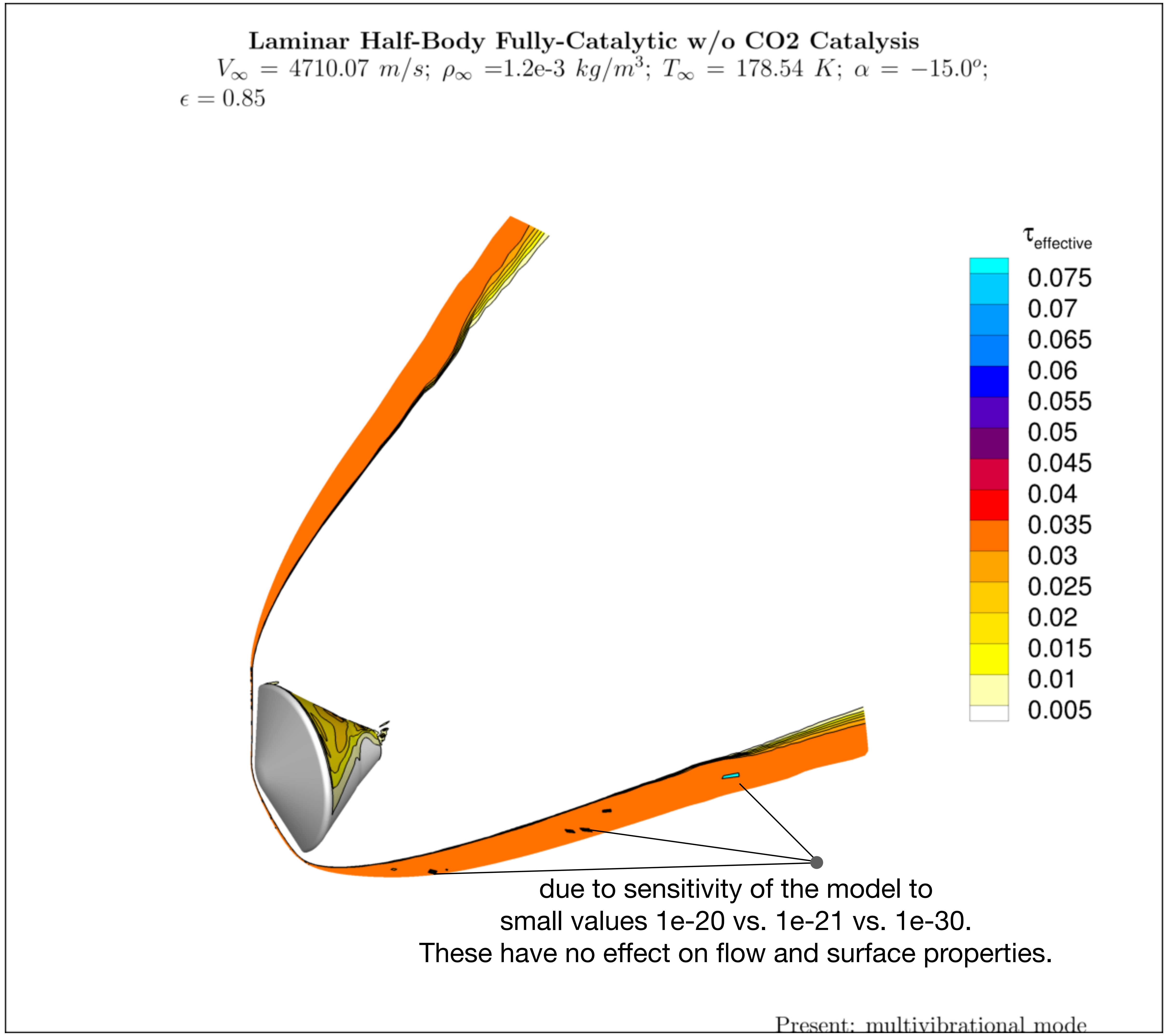
Present

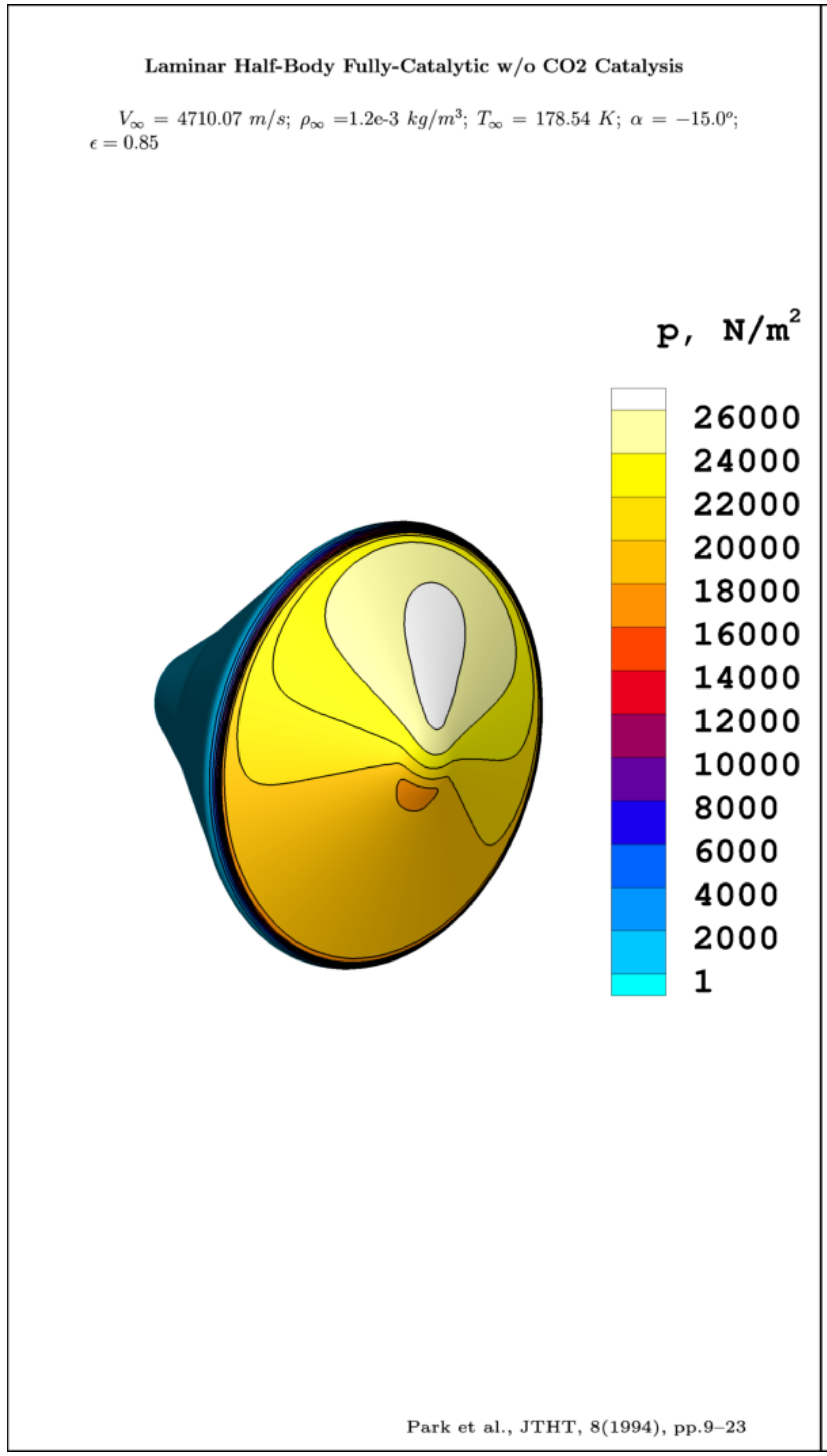


due to sensitivity of the model to
small values 1e-20 vs. 1e-21 vs. 1e-30.
These have no effect on flow and surface properties.

Present: multivibrational mode

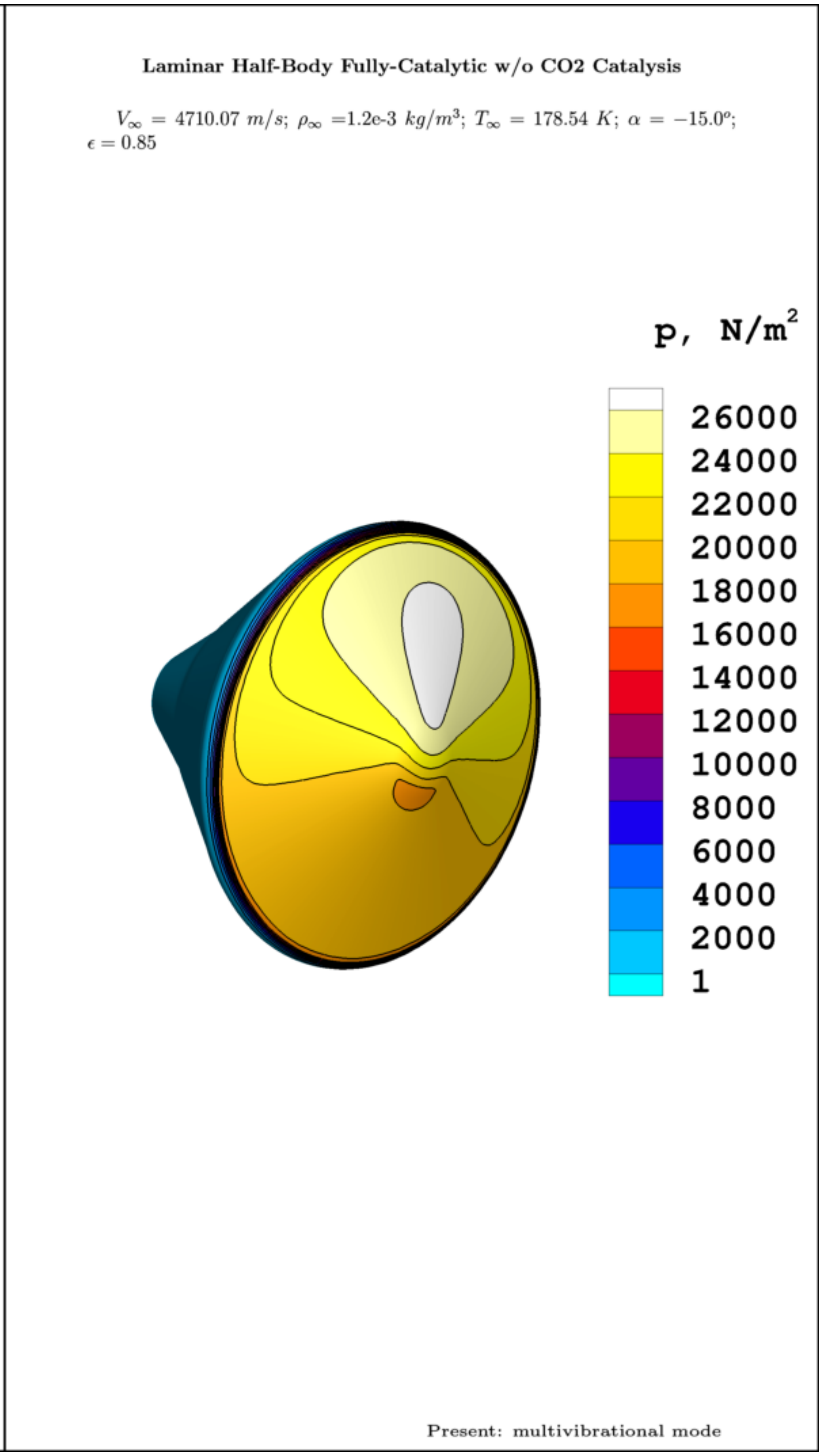
Test Case 2: SRL

Park model



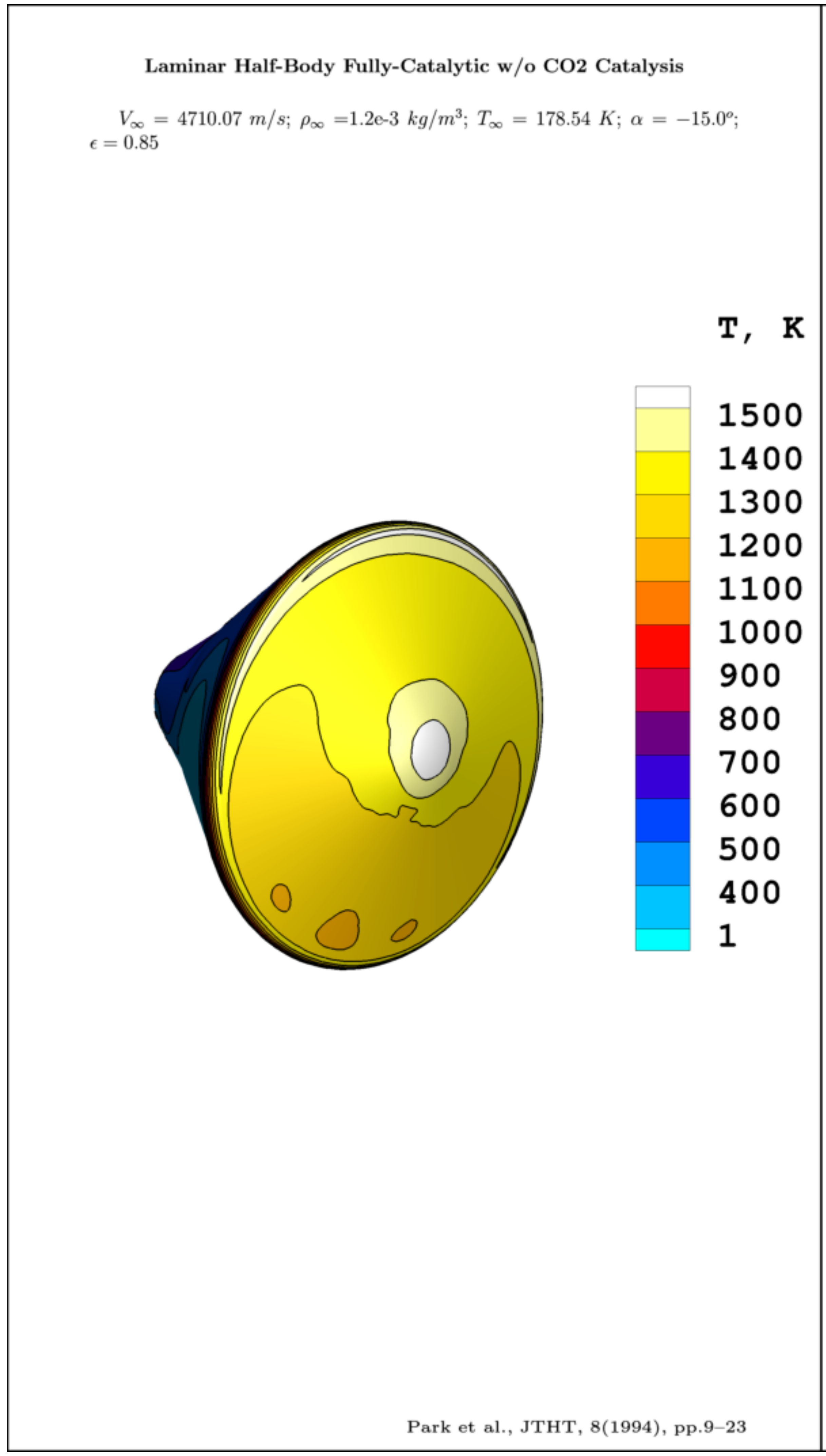
Park et al., JTHT, 8(1994), pp.9–23

Present



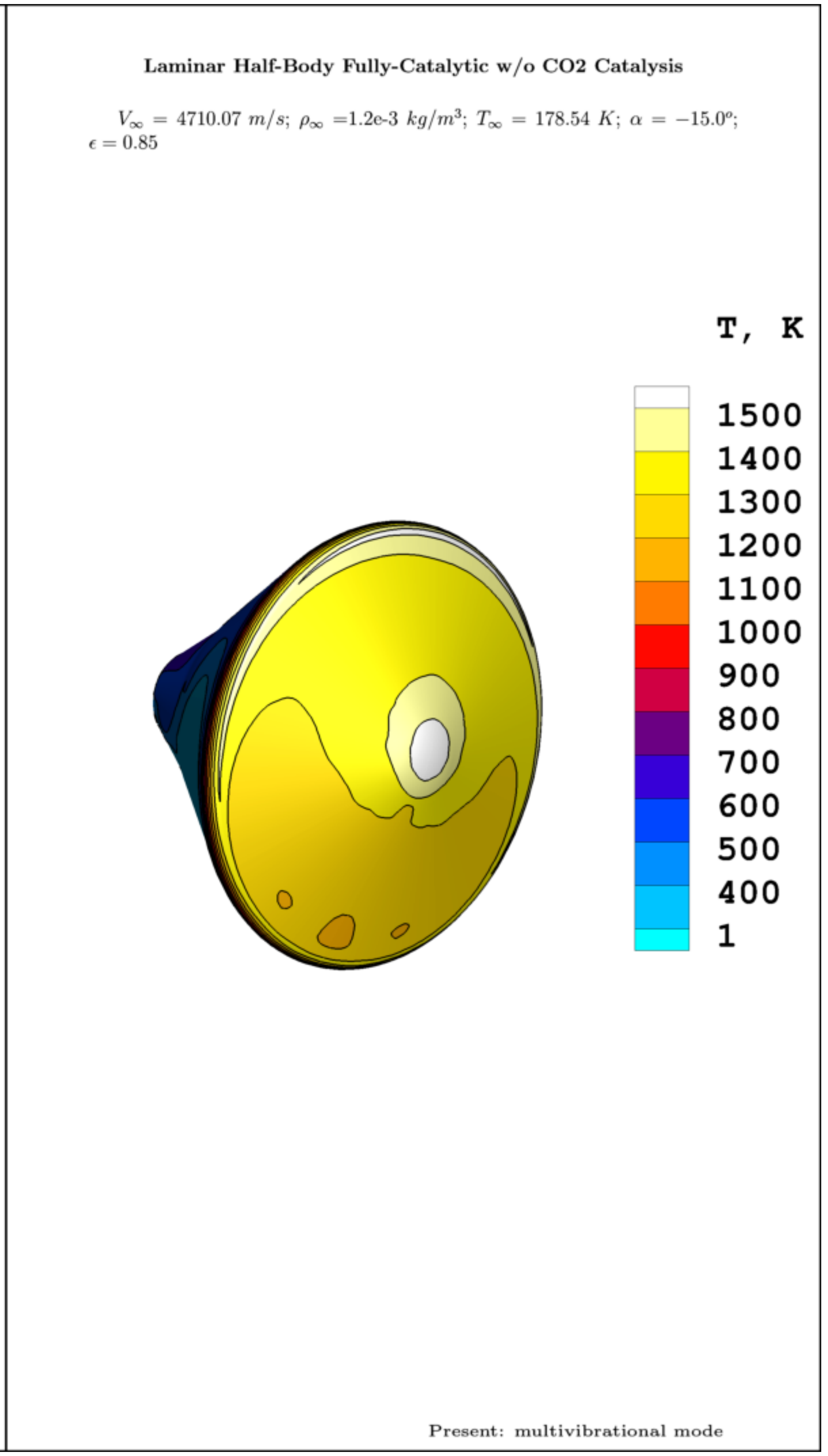
Present: multivibrational mode

Park model



Park et al., JTHT, 8(1994), pp.9–23

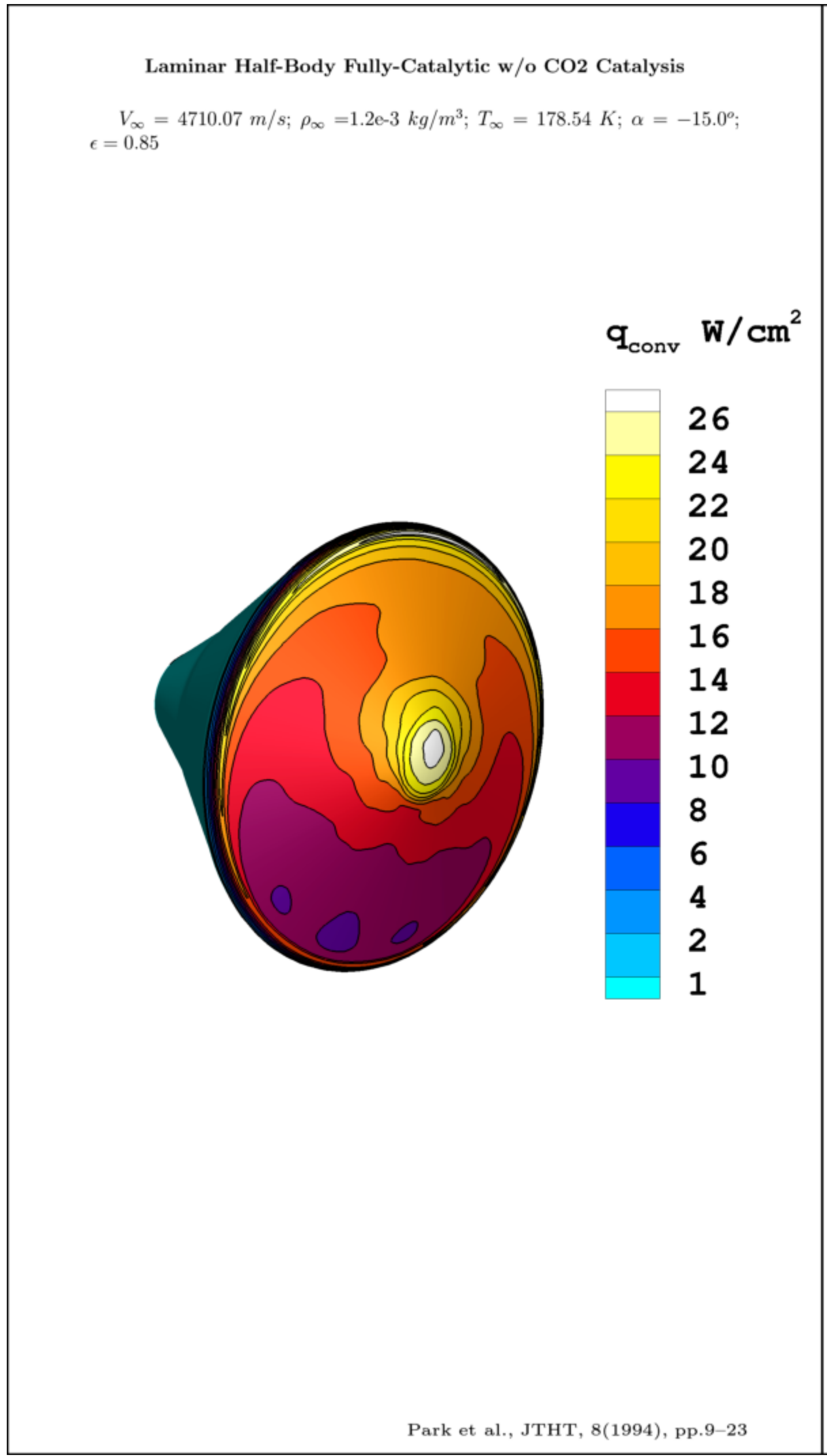
Present



Present: multivibrational mode

Test Case 2: SRL

Park model

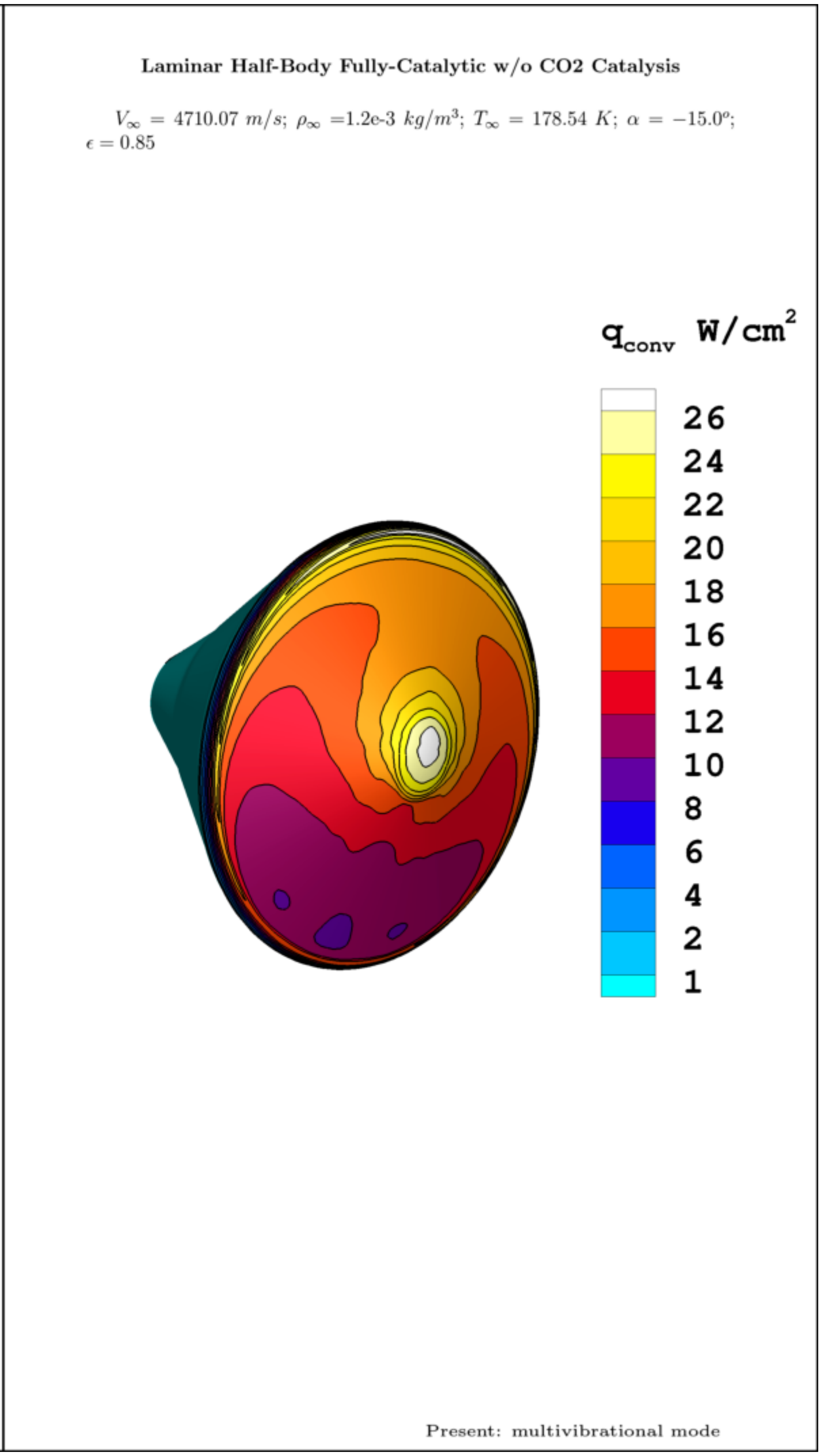


Laminar Half-Body Fully-Catalytic w/o CO2 Catalysis

V_∞ = 4710.07 m/s; ρ_∞ =1.2e-3 kg/m^3; T_∞ = 178.54 K; α = −15.0°; ϵ = 0.85

Park et al., JTHT, 8(1994), pp.9–23

Present



Laminar Half-Body Fully-Catalytic w/o CO2 Catalysis

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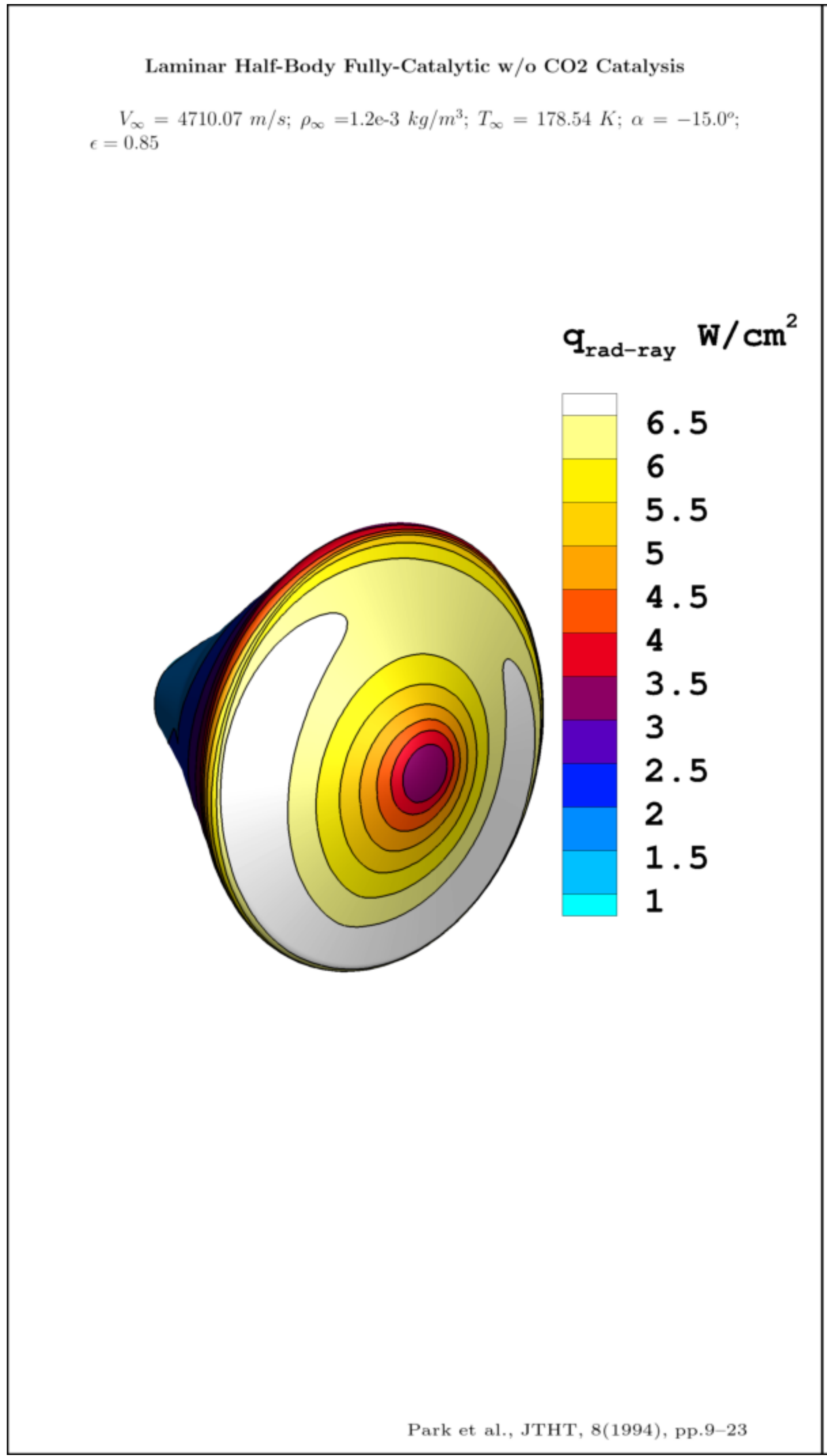
Present: multivibrational mode

Park model



Laminar Half-Body Fully-Catalytic w/o CO2 Catalysis

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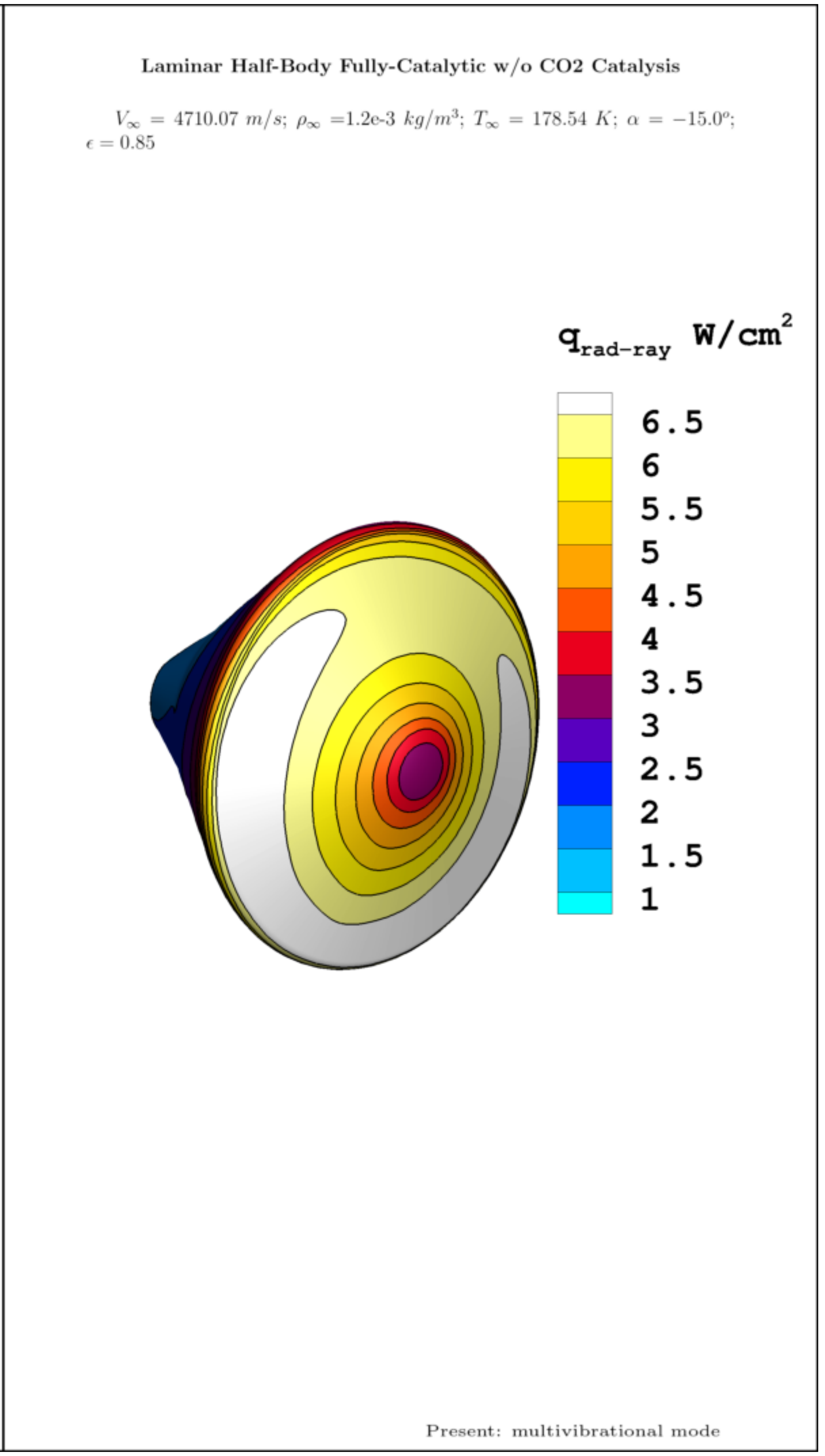
Park et al., JTHT, 8(1994), pp.9–23

Present

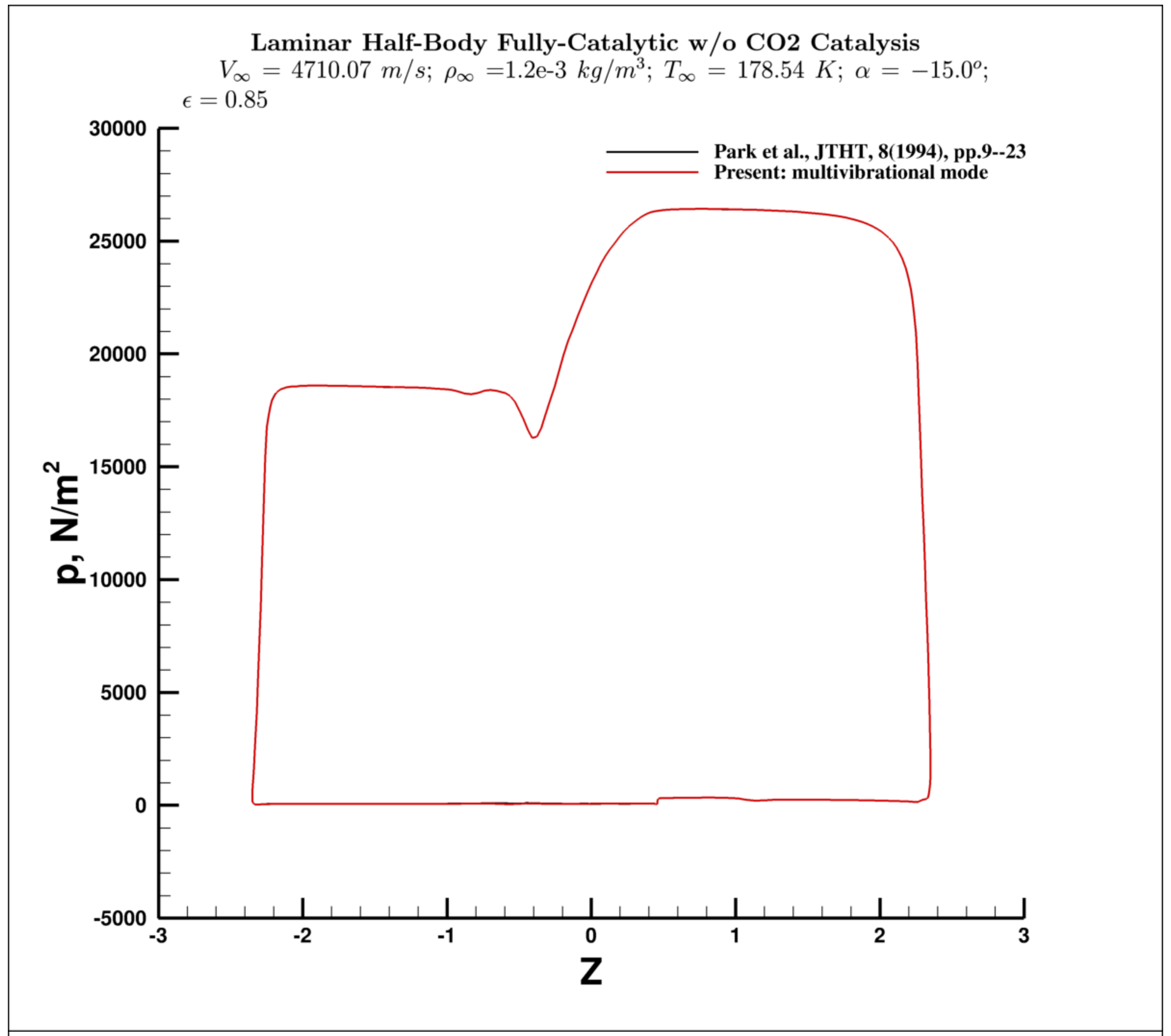


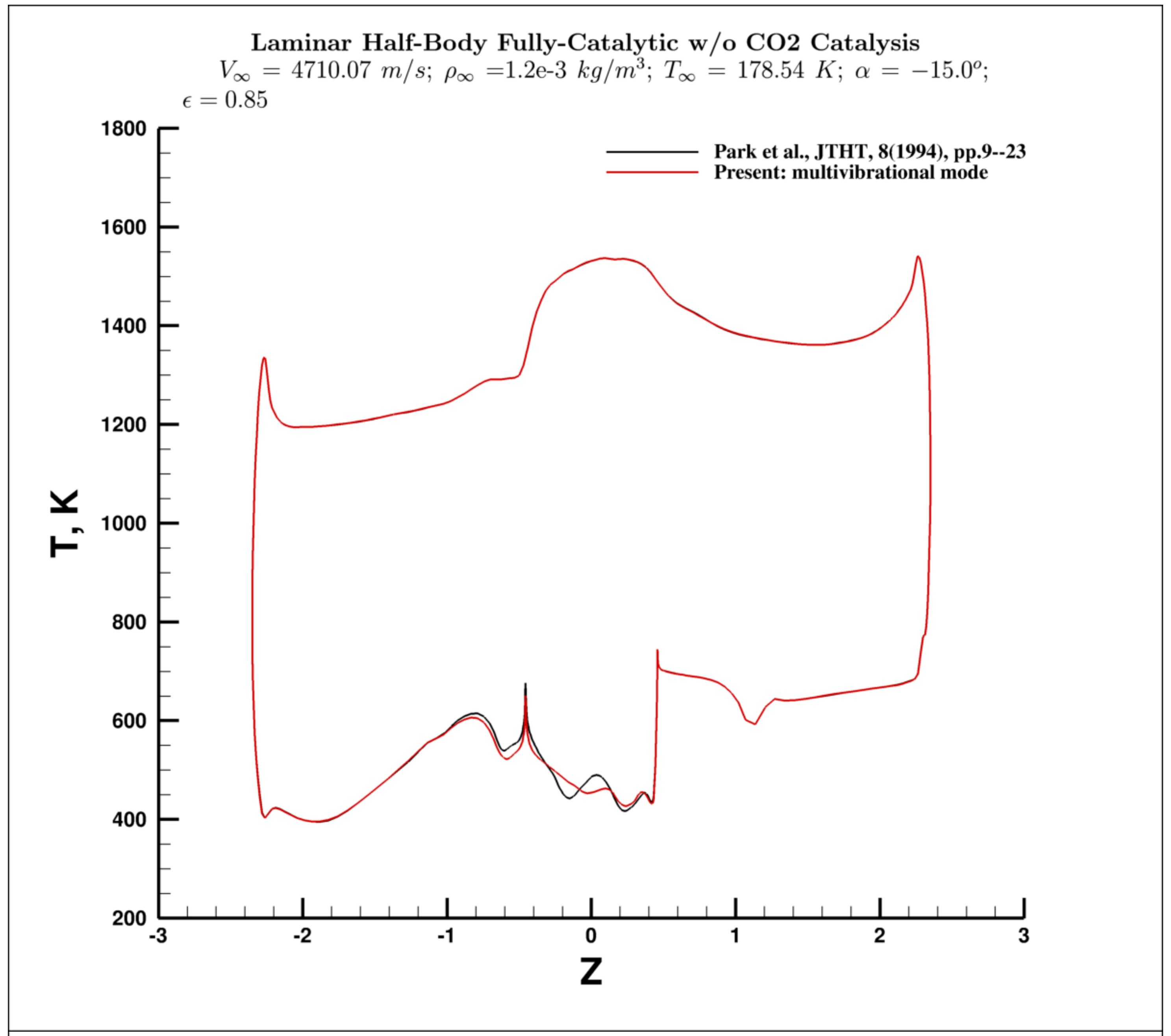
Laminar Half-Body Fully-Catalytic w/o CO2 Catalysis

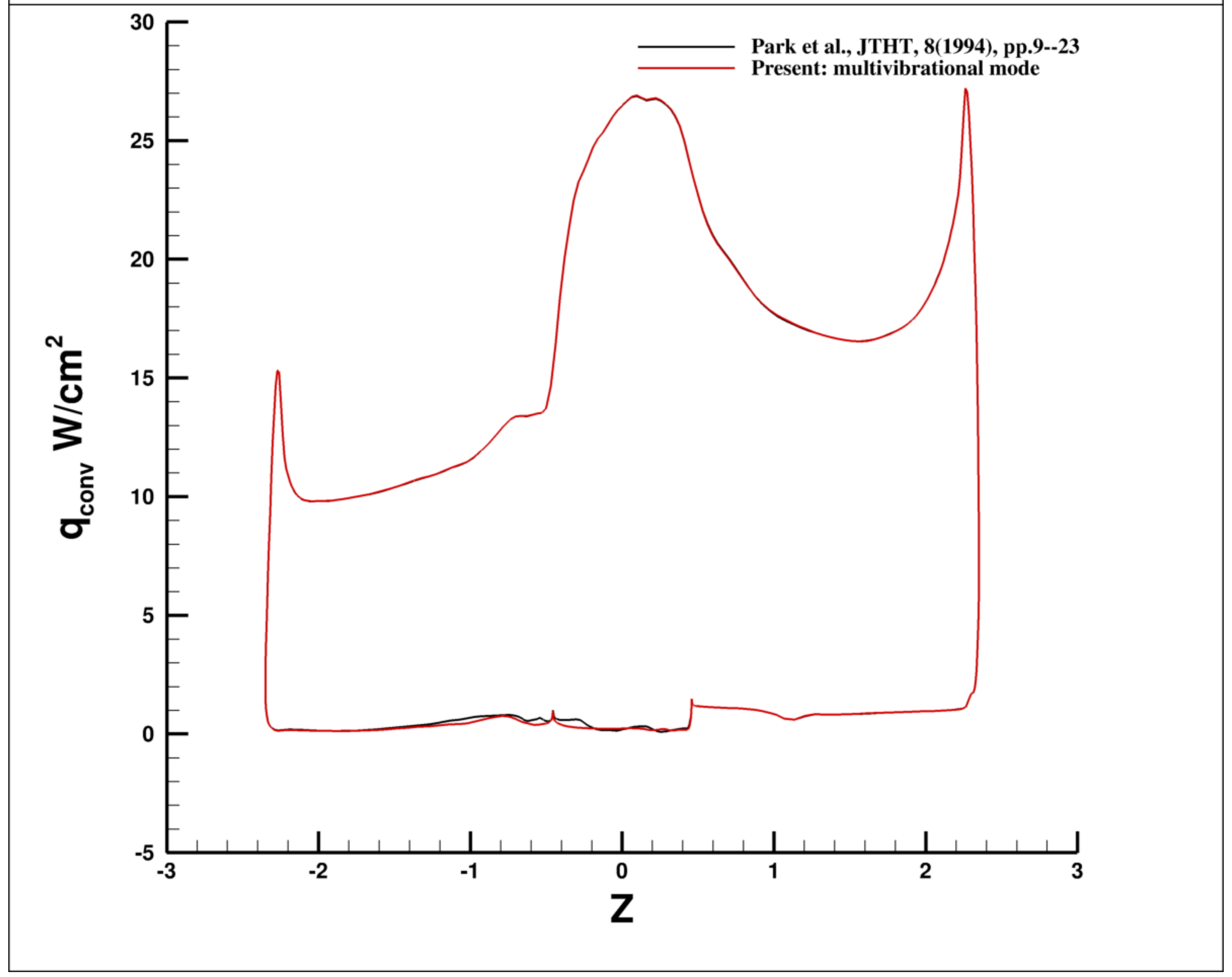
V_∞ = 4710.07 m/s; ρ_∞ =1.2e-3 kg/m^3; T_∞ = 178.54 K; α = −15.0°; ϵ = 0.85

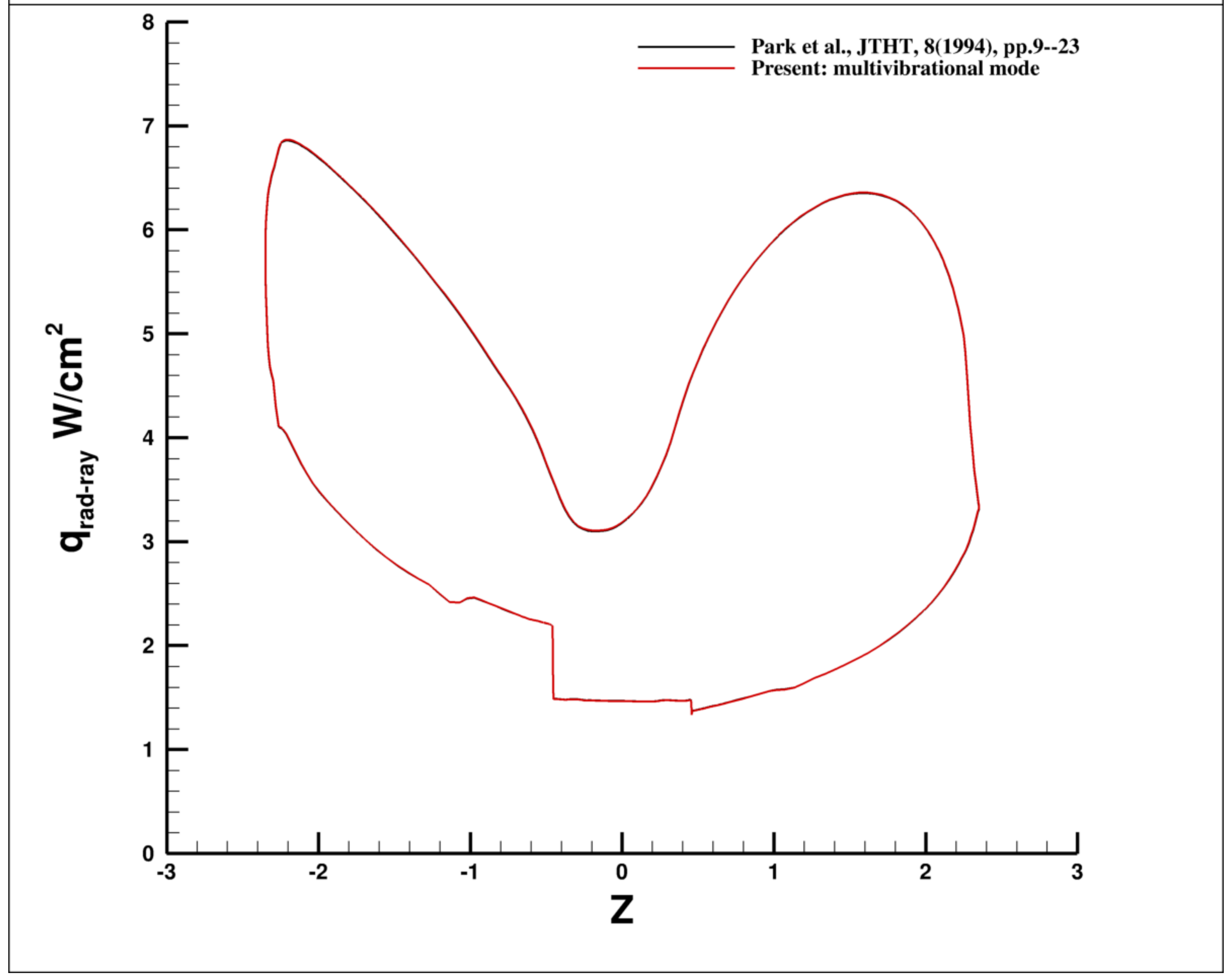
Present: multivibrational mode

Test Case 2: SRL









A (revised) **lump sum approach (not suitable for multimode) — continued**

The τ_s^{MW} relaxation time is a function of colliding species, and therefore must be weighted to arrive at a single valued relaxation time for molecule species s, before being added to τ_s^{Park}. In LAURA v ≥ 5, the weighted harmonic mean is used:

$$\tau_s^{MW} := \frac{\sum_{r\neq e^-} n_r}{\sum_{r\neq e^-} n_r/\tau_{sr}^{MW}} = \frac{\sum_{r\neq e^-} \frac{\rho_r}{\mathrm{Mw}_r}}{\sum_{r\neq e^-} \frac{\rho_r}{\mathrm{Mw}_r\,\tau_{sr}^{MW}}}.$$

This formulation does support a direct derivation from the Boltzmann equation and the Chapman-Enskog framework, which after applying the Landau-Teller's main assumption of weak deviations from the equilibrium, and further assuming that the specific heat is constant gives:

$$\frac{dE_v}{dt} = \sum_s \left(\rho_s (ev_s^0 - ev_s) \sum_r \frac{n_r}{n\tau_{rs}} \right).$$

In LAURA-4, LAURA-A, and at the birth of LAURA-5, a weighted mean, which is suggested by Gnoffo et al. [NASA-TP2867], was used:

$$\tau_s^{MW} := \frac{\sum_{r\neq e^-} n_r \tau_{sr}^{MW}}{n = \sum_{r\neq e^-} n_r} = \frac{\sum_{r\neq e^-} \frac{\rho_r}{\mathrm{Mw}_r} \tau_{sr}^{MW}}{\sum_{r\neq e^-} \frac{\rho_r}{\mathrm{Mw}_r}}.$$

The wighted mean is added to the current LAURA-5 as a user set option for comparison purposes*. The following relation may be devised by comparing the two averaging formulations,

$$(\tau_s^{MW})^{LAURA5} < (\tau_s^{MW})^{LAURA4},$$

which suggests a larger translational-vibrational energy exchange source term with $(\tau_s^{MW})^{LAURA5}$ averaging. The following inequality is used to arrive at the above conclusion:

$$\sum_i A_i B_i < \sum_i A_i \sum_i B_i.$$

---

* : vib_relax_harmonic_mean = .true. (default), which is a more correct way, may also lead to a more stiff numerical discretization.

Corrected Landau-Teller

Using zeroth-order approximation of the Chapman-Enskog, and assuming harmonic-oscillator and weak deviation from equilibrium, the following formulation is derived:

$$Src^{T\leftrightarrow V} \equiv \frac{dE_v}{dt} = \rho C_{vv} \frac{T}{T_v} \frac{(T - T_v)}{\bar{\tau}},$$

where the ratio may be used as a simple correction to the widely implemented translational-vibrational energy exchange source term.

* : corrected_Landau_Teller = .true. ! default = .false.

A proposed multimode approach for LAURA implementation — continued

The Millikan-White (M-W) relaxation time, τ_s, of a molecule species s in a medium of r species gas at a total pressure of p is defined as

$$p\tau_s^{MW} = exp\left[a_{sr}(T^{-1/3} - b_{sr}) - 18.42\right],$$

with the M-W coefficients given as

$$\begin{aligned} a_{sr} &= 0.00116\,\mu_{sr}^{1/2}\theta_{v,s}^{4/3} = \overbrace{0.00116\,\mu_{ss}^{1/2}\theta_{v,s}^{4/3}}^{\text{laura: alantel}}\left(\frac{\mu_{sr}}{\mu_{ss}}\right)^{1/2}, \\ b_{sr} &= 0.015\,\mu_{sr}^{1/4} \end{aligned}$$

unless a more accurate set of coefficients is available; e.g., from Park [1994].

To account for the elastic collision cross section, Park [1994], proposed a correction, τ_s^{Park}, to the M-W vibrational relaxation time as:

$$\begin{aligned} \tau_s^{Park} &= \frac{1}{\left(\sum_{r\neq e^-} n_r\right)\sqrt{8kT/\pi\, m_s}\;\underbrace{\sigma'(50000/T)^2}_{\sigma}} \\ &= \frac{1}{N_A\underbrace{\sqrt{8kN_A/\pi}}_{\sqrt{8\bar{R}/\pi}}\left(\sum_{r\neq e^-}\frac{\rho_r}{\mathrm{Mw}_r}\right)\sqrt{T/\mathrm{Mw}_s}\;\underbrace{\sigma'(50000/T)^2}_{\sigma}}\;. \\ &= \frac{1.1412\times 10^{-29}}{\left(\sum_{r\neq e^-}\frac{\rho_r}{\mathrm{Mw}_r}\right)\sqrt{T/\mathrm{Mw}_s}\;\underbrace{\sigma'(50000/T)^2}_{\sigma}} \end{aligned}$$

A more direct input in the `species_thermo_data`

```
CO2
&species_properties
elec_impct_ion = 4.453 ! ?
disoc_ener = 2.96
alantel = 270.4
siga = 5.e-20,  0.,  0.
mol_wt = 44.0107
cprt0 = 3.50
multivibrational_mode_molecule = .true. !T: read multimode data
use_alantel = .true. !T: ignore multimode; F: ignore alantel
/
3
 0.49436505E+05 -0.62641160E+03  0.53017252E+01  0.25038138E-02
-0.21273087E-06 -0.76899888E-09  0.28496778E-12  0.00000000E+00
-0.45281985E+05 -0.70482794E+01   200.000  1000.000
 0.11769624E+06 -0.17887915E+04  0.82915232E+01 -0.92231568E-04
 0.48636769E-08 -0.18910533E-11  0.63300366E-15  0.00000000E+00
-0.39083506E+05 -0.26526693E+02  1000.000  6000.000
-0.15444233E+10  0.10168471E+07 -0.25614052E+03  0.33694011E-01
-0.21811843E-05  0.69914208E-10 -0.88423515E-15  0.00000000E+00
-0.80432145E+07  0.22541775E+04  6000.000 20000.000
3
2 932.109
1 1914.081
1 3373.804
```

Requires an extra step calculation by user/developer. This is in fact a function of the molecule characteristic temperature.

New: for both single and multimode molecules. Millikan-White coefficients will be directly calculated via characteristic vibrational temperature

New: to be used as legacy version.

New: number of **distinct** vibrational modes [integer]

New: degeneracy [integer] & characteristic-vibrational-temperature [K]

Limiting values in LAURA

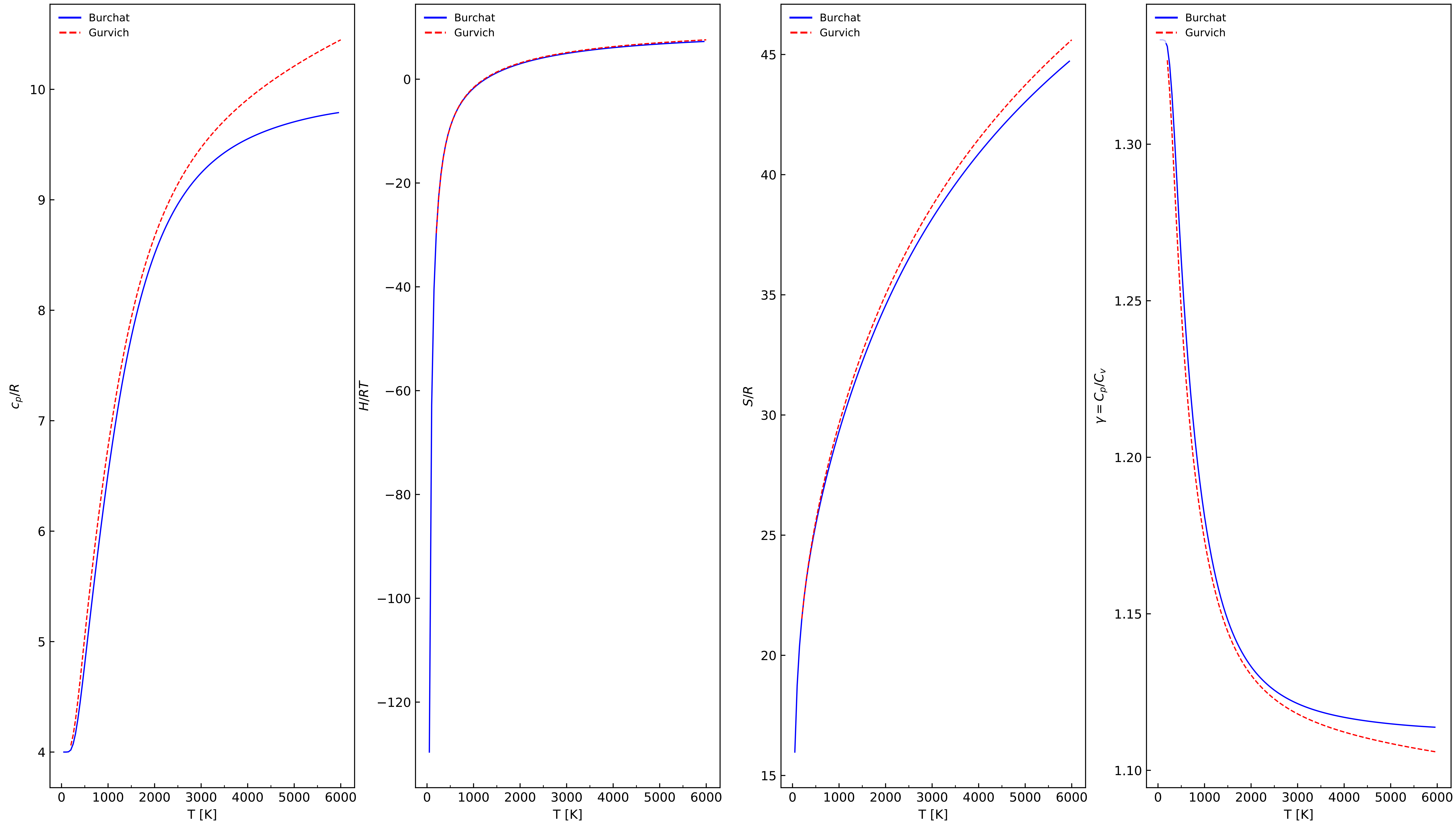
vib_relax_minT $= 200[K]$,

vib_relax_minTv $= 200[K]$,

$$\sigma' = 10^{-21}\,[m^2], \qquad \sigma'^{Park} = \begin{cases} 10^{-20}\,[m^2] & \text{Park 1994 - given arbitrarily;} \\ 10^{-20}\,[m^2] & \text{Park 1989: "the most appropriate value for N2 at T < 19000 [K]";} \\ 10^{-21}\,[m^2] & \text{Park 1989: for T > 19000 [K];} \end{cases}$$

$$\frac{\rho c_{vv}}{\tau} \leq 10^{20}$$

Thermodynamic Properties of NH3



Thermodynamic Properties Effects of NH3

The nozzle performance is nearly the same with NH3 thermodynamic properties suggested by either Gurvich or Burchat.