VIBRATIONAL STATE-TO-STATE THERMOCHEMICAL MODELING OF HIGH-TEMPERATURE OXYGEN FLOWS

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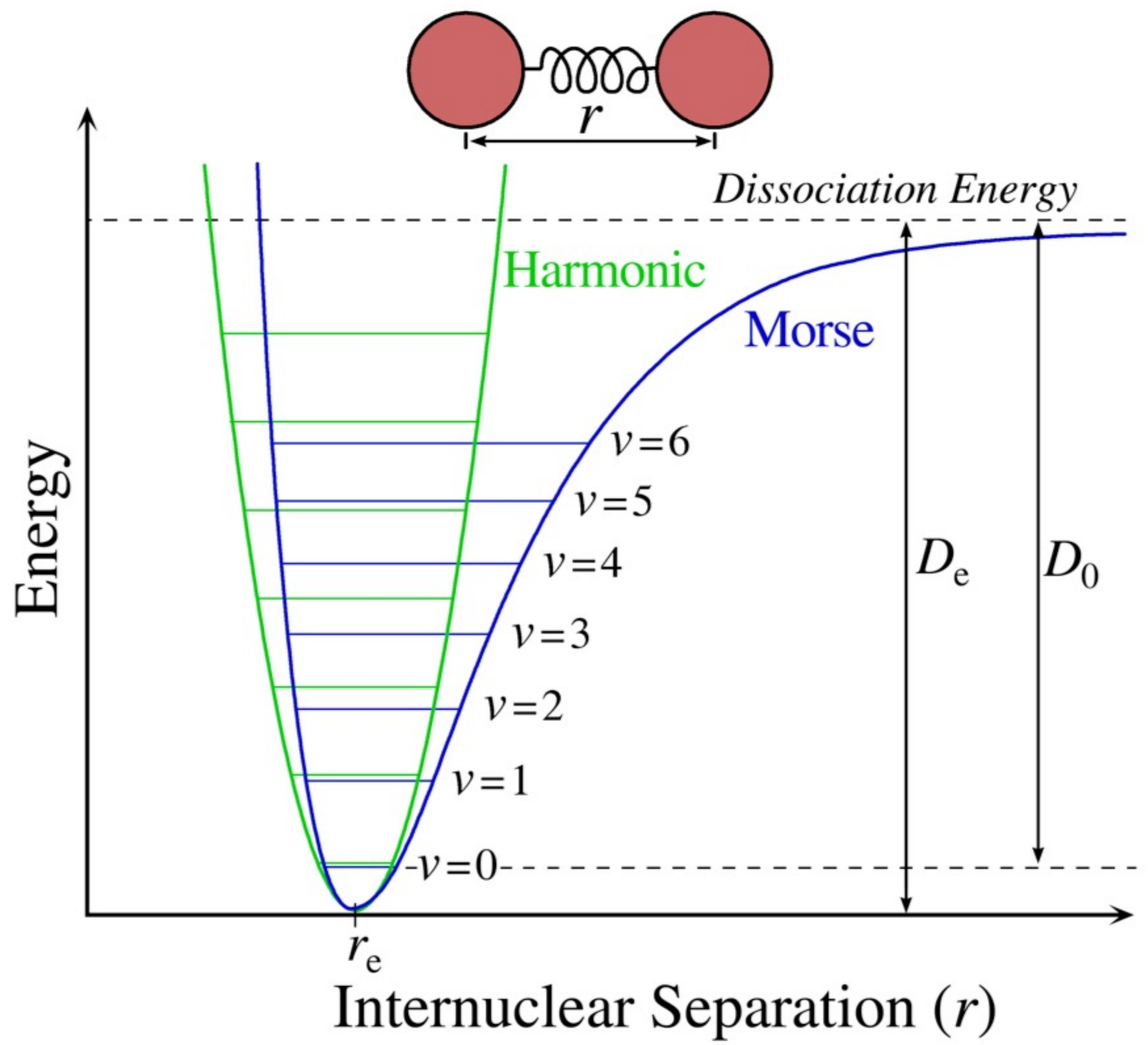
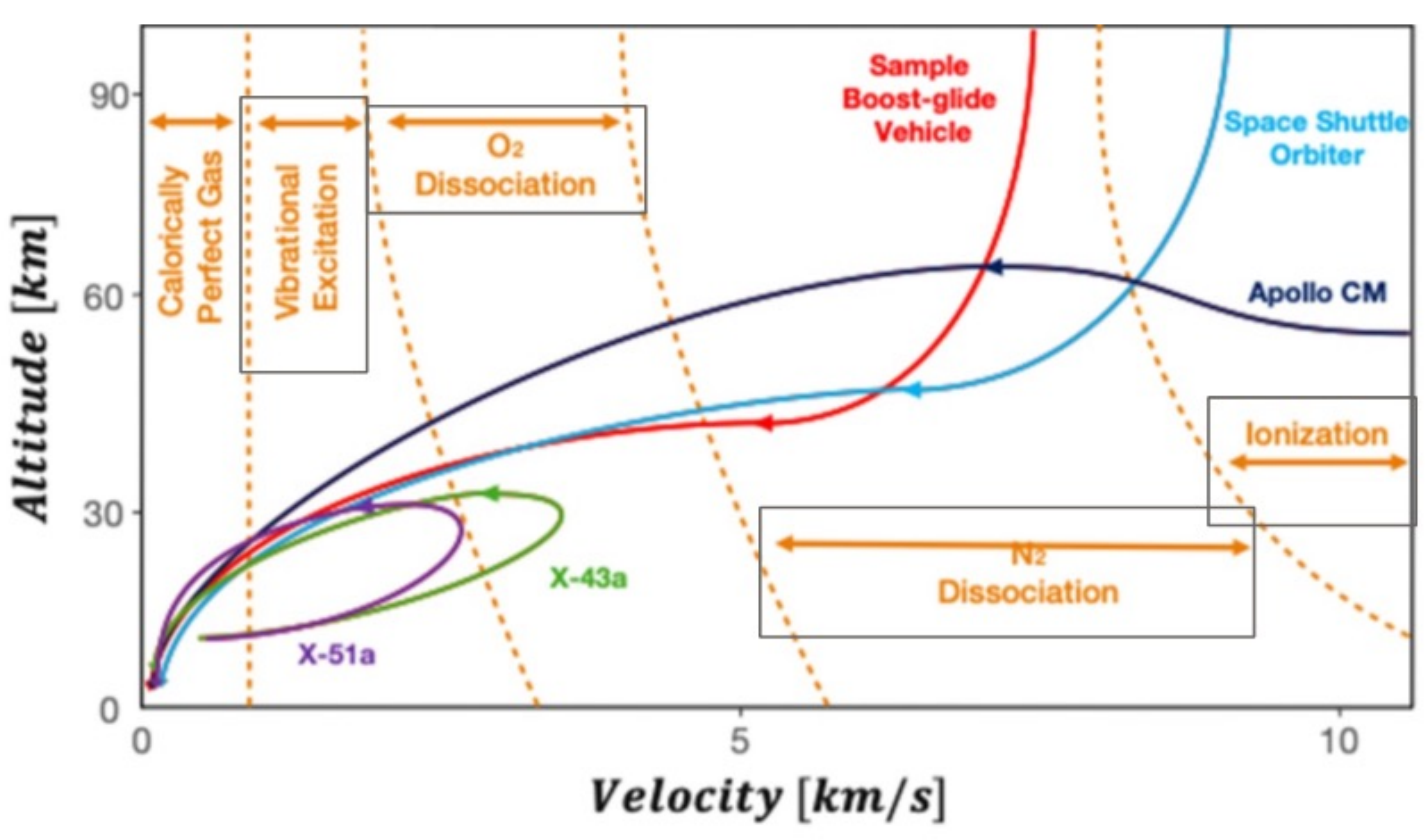


ARCH

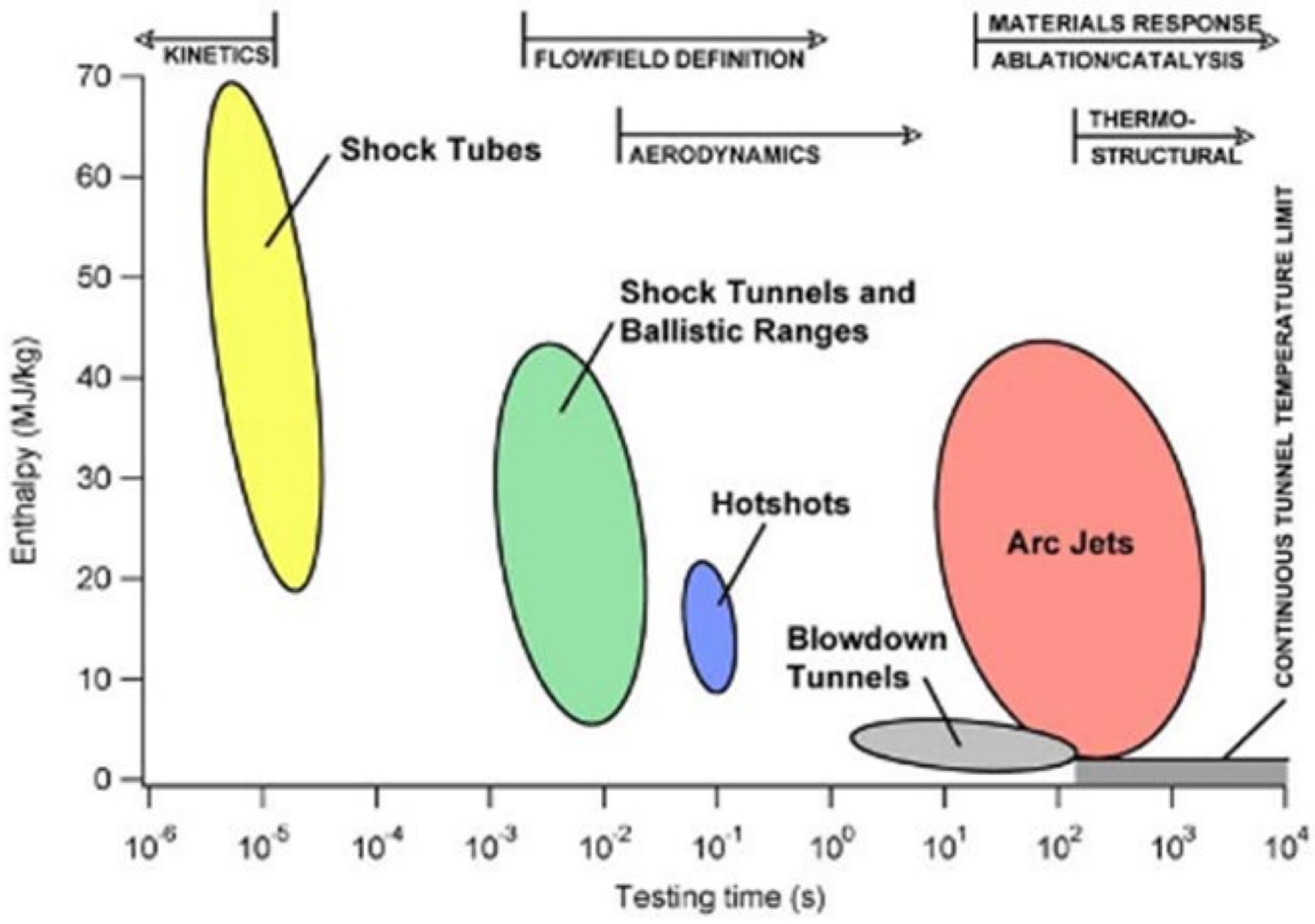
Outline

- Motivation
- Background
- Approaches
  - Mapping approaches
  - State-to-State / Mutation++
  - Multi-Temperature
- Results
  - Mapping
    - Contours
  - State-to-State simulations of oxygen and oxygen diluted in argon
- Conclusions and Future Work

Motivation

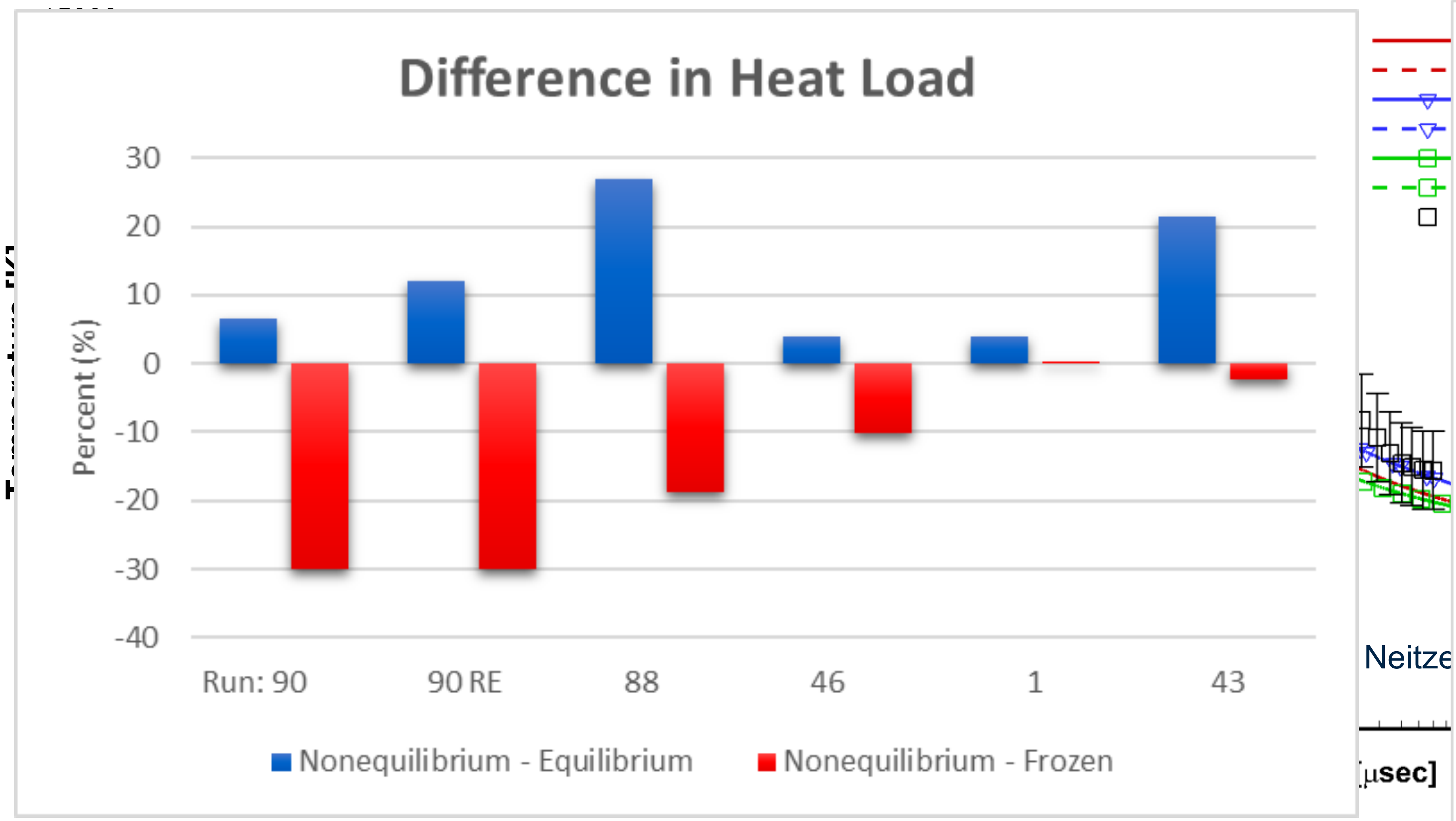


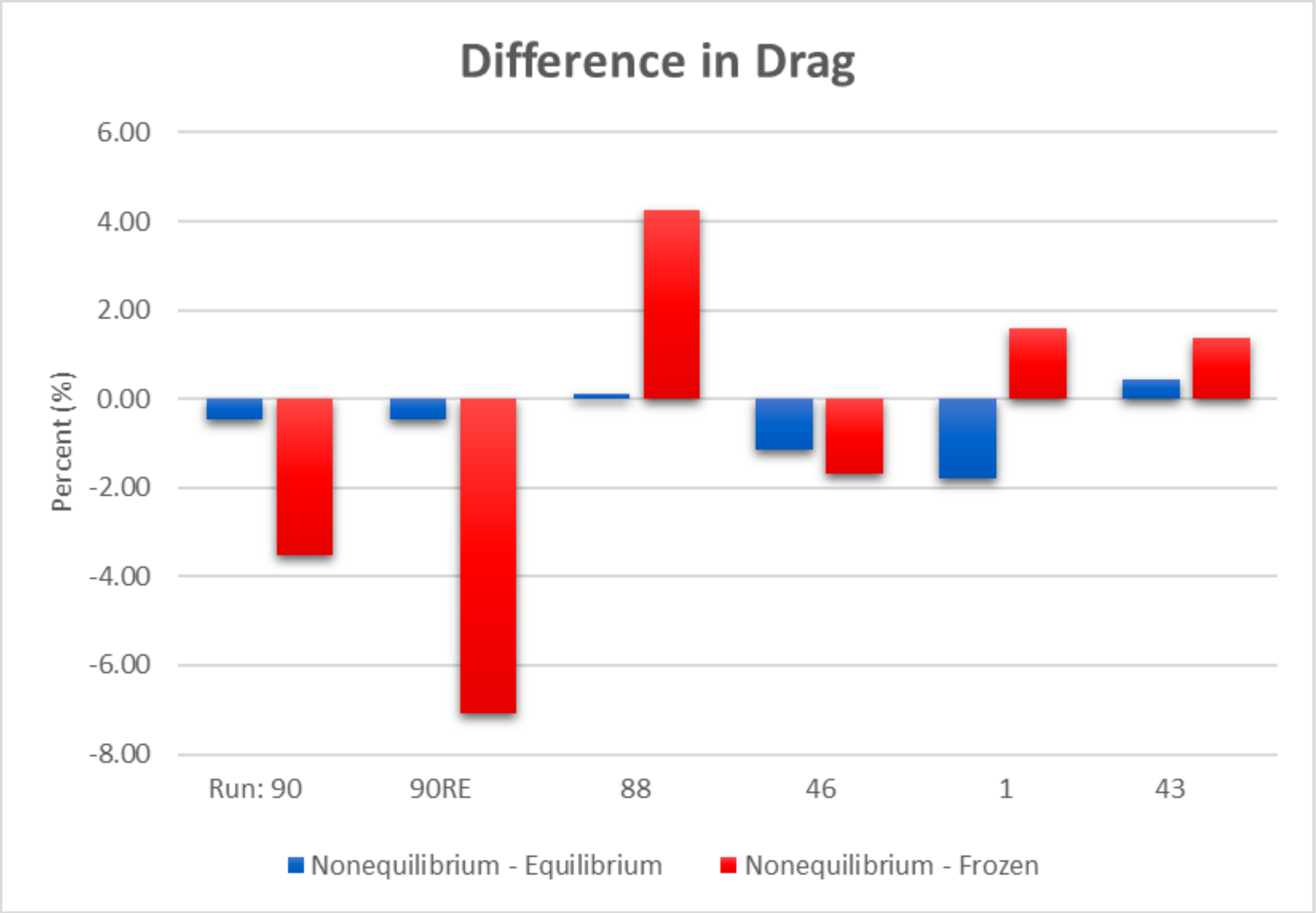
Calorically Perfect Gas
Vibrational Excitation
O2 Dissociation
Sample Boost-glide Vehicle
Space Shuttle Orbiter
Apollo CM
Ionization
N2 Dissociation
X-43a
X-51a
Altitude [km]
Velocity [km/s]



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
Enthalpy (MJ/kg)
Testing time (s)

Background - Nonequilibrium Flows

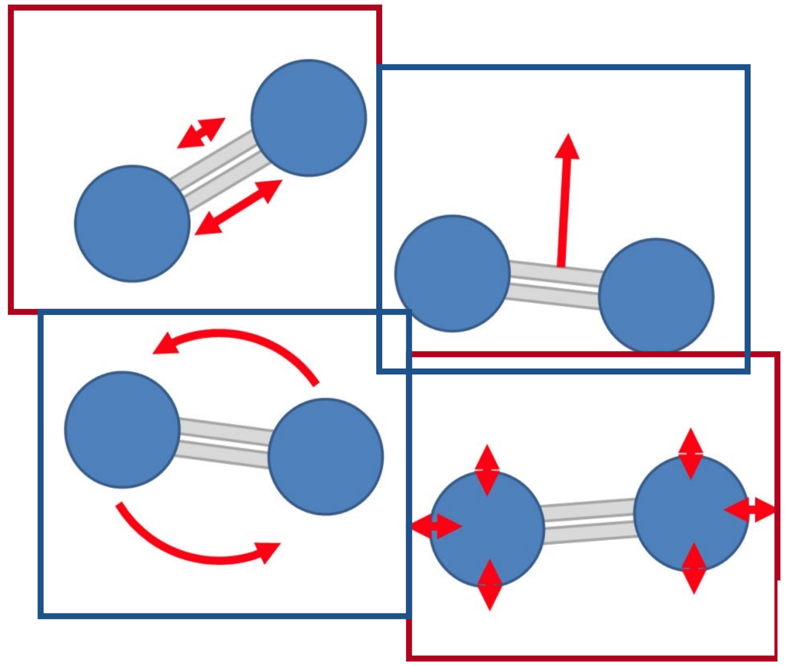




Neitzel, Andrienko, and Boyd, "Aerothermochemical Nonequilibrium Modeling for Oxygen Flows," JTHT, 2017.

Holloway, Hanquist, and Boyd, "Assessment of Thermochemistry Modeling for Hypersonic Flow over a Double Cone," JTHT, 2020.

Background - Nonequilibrium Flows – Multi-Temperature



Two-temperature (2T)

Energy Transfer

$T_{tr} = T_{rot} \rightleftarrows T_{vib} = T_{ee}$

$$\frac{\partial(\rho e_{vib})}{\partial x} = \rho_{O_2} \frac{e_{vib}^{*} - e_{vib}}{\tau_{vib}}$$

Millikan-White (MW)

$$p\tau_{vib} = \exp\left(A\left(T^{-1/3} - B\right) - 18.42\right) \quad [atm - sec]$$

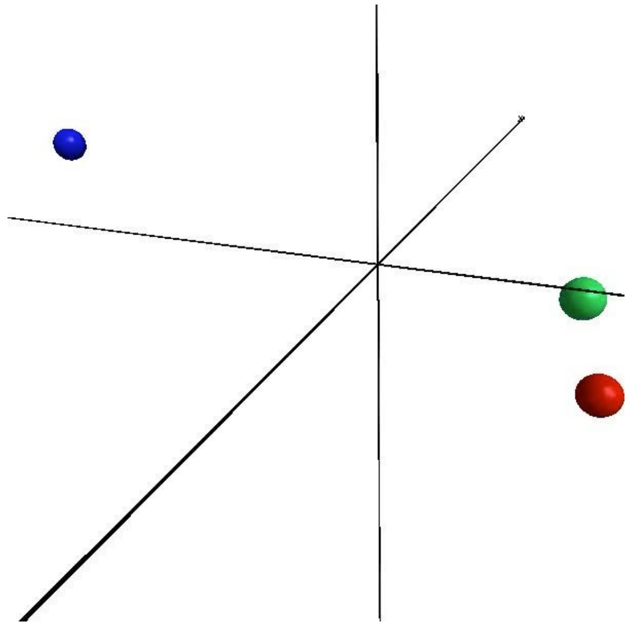
Park's High Temperature Correction (HTC)

$$p\tau_{Park} = \frac{1}{n\sigma_{vib}c} \quad [atm - sec]$$

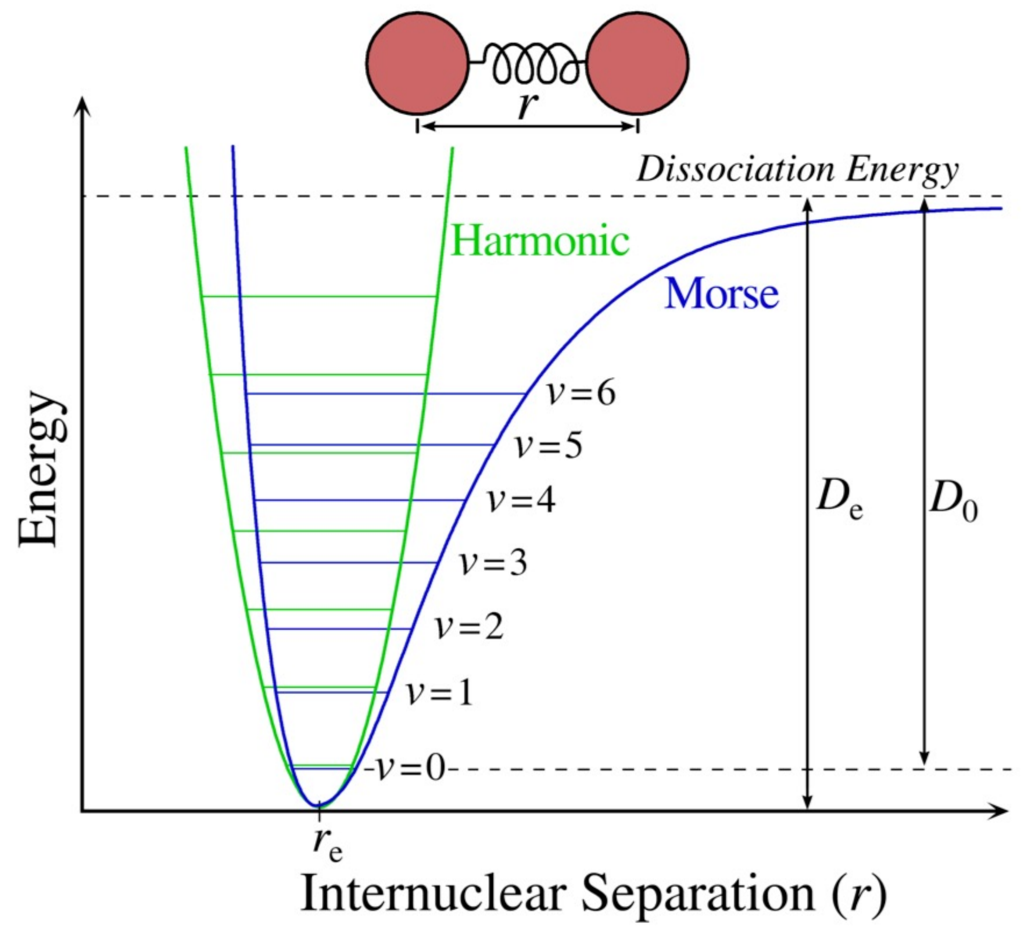
Chemistry

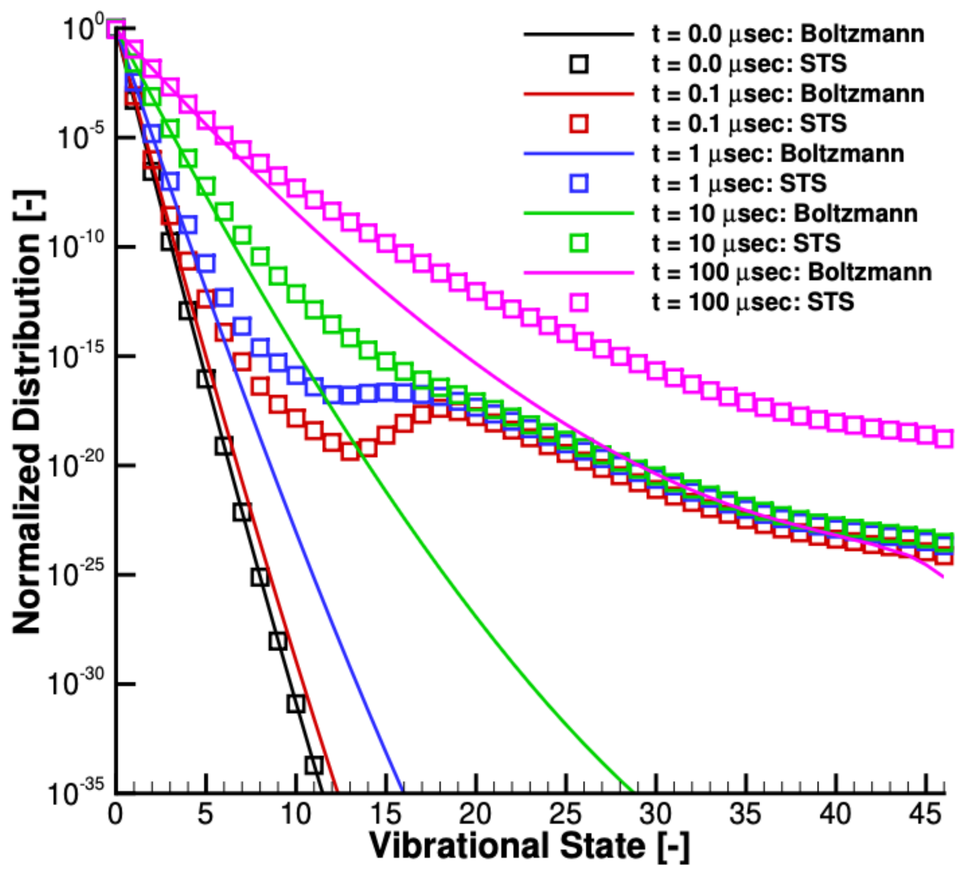
$O_2 + O \longleftrightarrow O + O + O$

$$k_f = A \cdot T^{\alpha} \exp(-E/T)$$

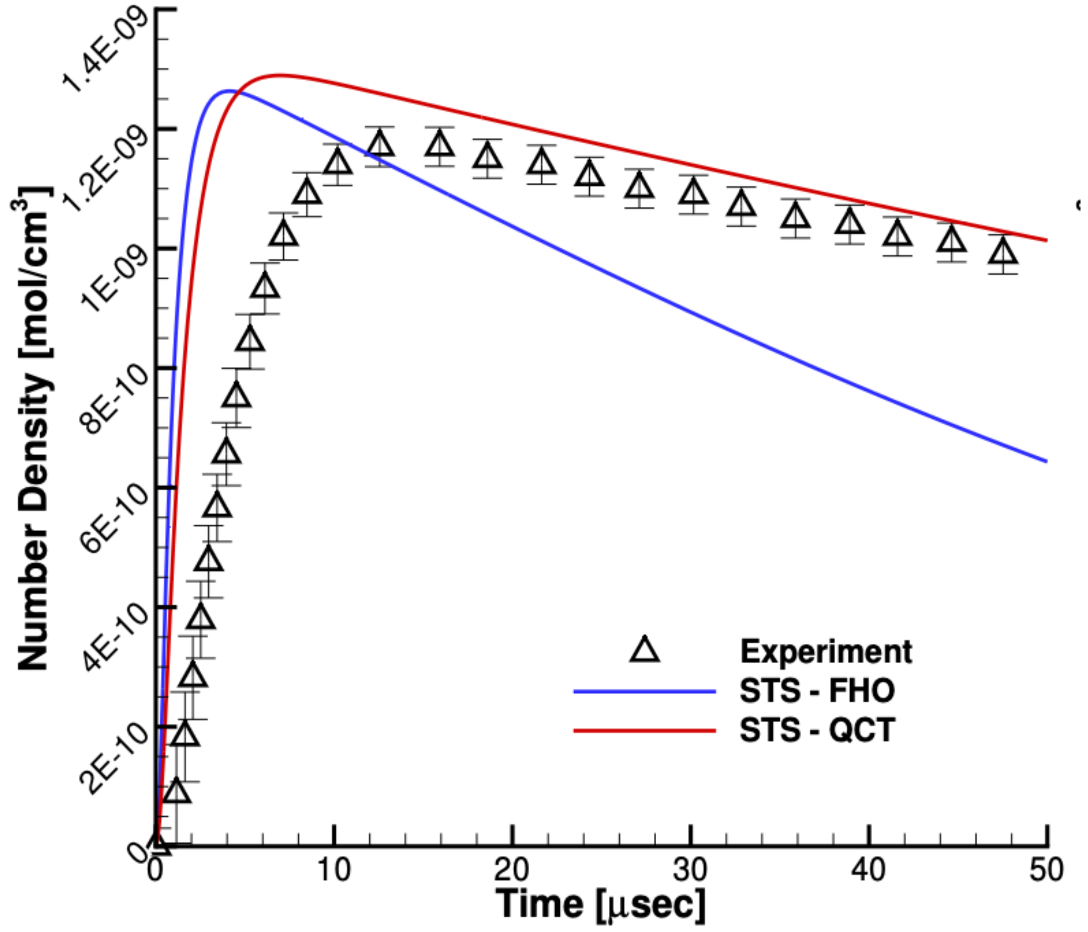


Background – Nonequilibrium Flows – State Resolved





Non-Boltzmann distribution in Mach 5 flow



4th vibrational state of O_2

Bound-Bound Transitions (rates)
Bound-Free Transitions (rates)

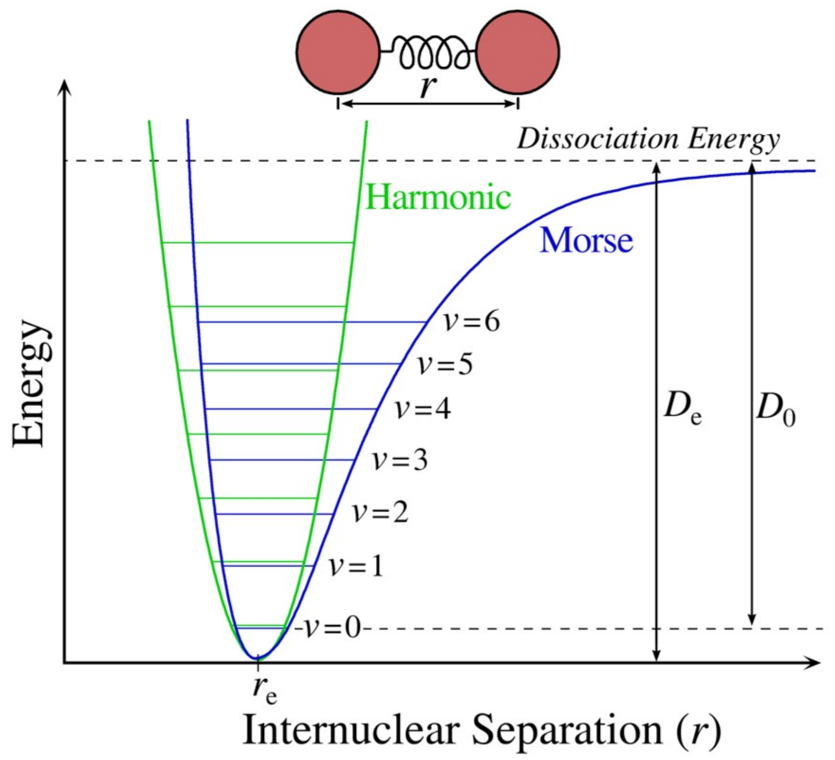
Analytical theory (e.g., Forced Harmonic Oscillator (FHO))
Quantum chemistry (e.g., Quasi-classical Trajectory (QCT))

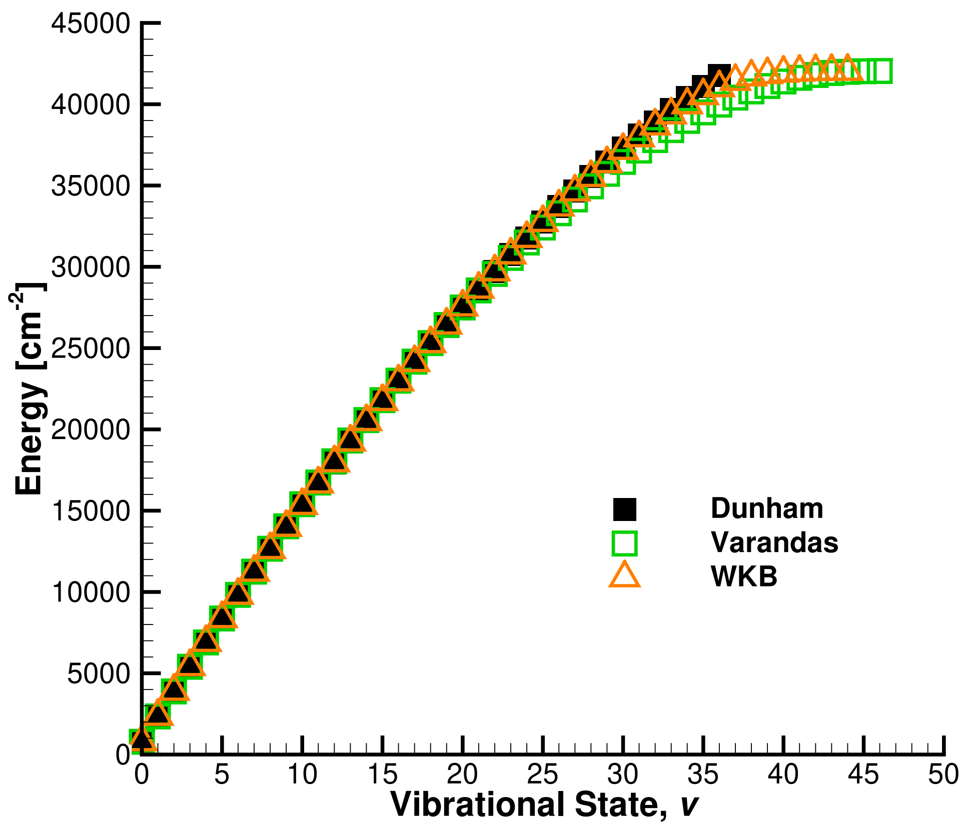
$$\frac{dn_v}{dx} = \sum_s \left(R_{v,s} n_O^2 n_s - D_{v,s} n_v n_s\right) + \sum_s \left(K_{v',v} n'_v n_s - K_{v,v'} n_v n_s\right), \qquad v = 0, \ldots, v_{max}$$

Motivation

Bound-Bound Transitions (rates) → Analytical theory (e.g., Forced Harmonic Oscillator (FHO))
Bound-Free Transitions (rates) → Quantum chemistry (e.g., Quasi-classical Trajectory (QCT))

- Rates from quantum chemistry are <u>expensive</u> and often done on <u>different</u> vibrational energy ladders
- This creates a modeling challenge for complex mixtures
- Goal: develop a consistent mapping between vibrational ladders





Motivation - Example

Assess chemical kinetics with shock tube data

Shock-tube measurements of coupled vibration–dissociation time-histories and rate parameters in oxygen and argon mixtures from 5000 K to 10 000 K

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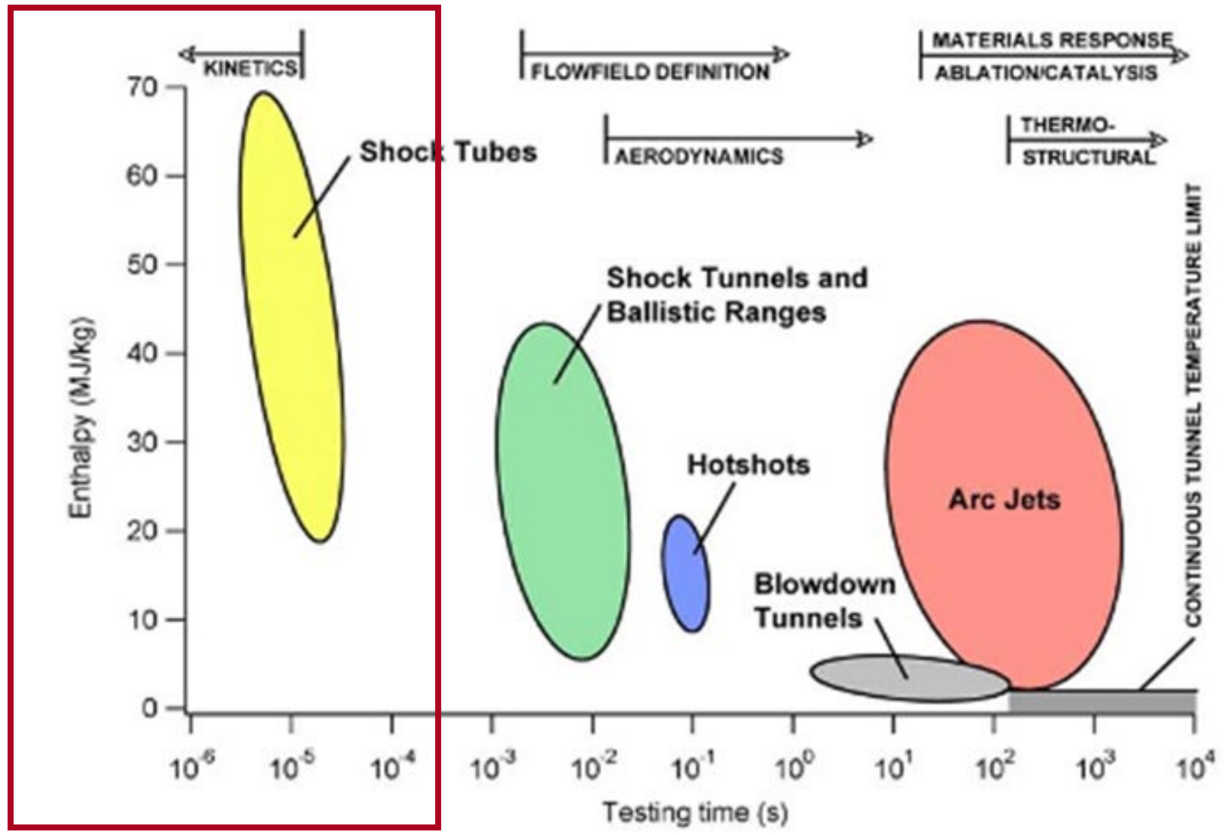
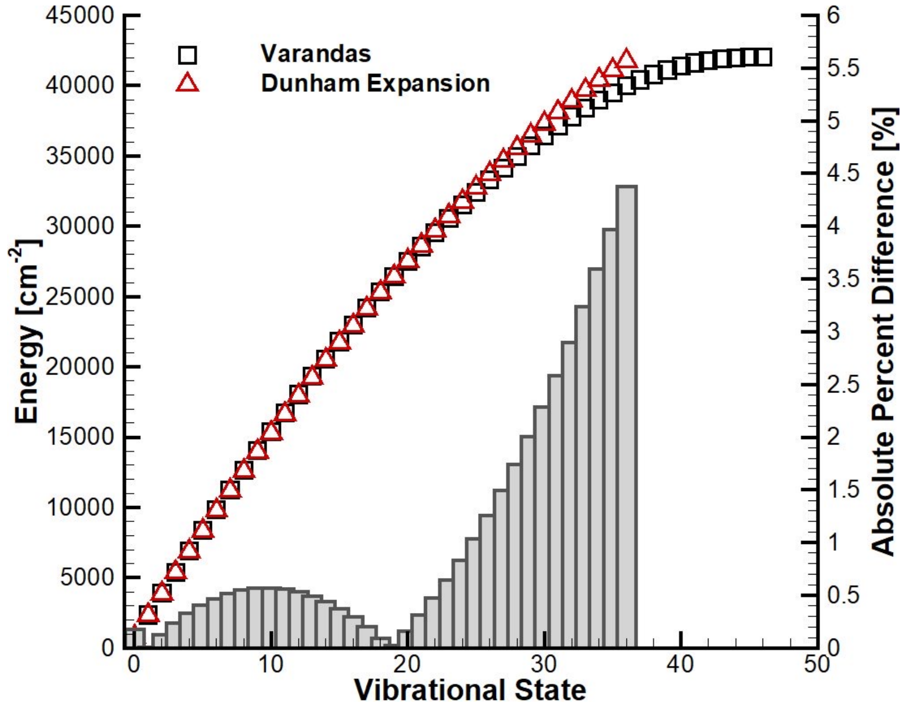


- O_2-O (Varandas – 0 -> 46 vibrational energy levels)
- O_2-O_2 (Varandas – 0 -> 46 vibrational energy levels)
- O_2-Ar (Dunham – 0 -> 36 vibrational energy levels)

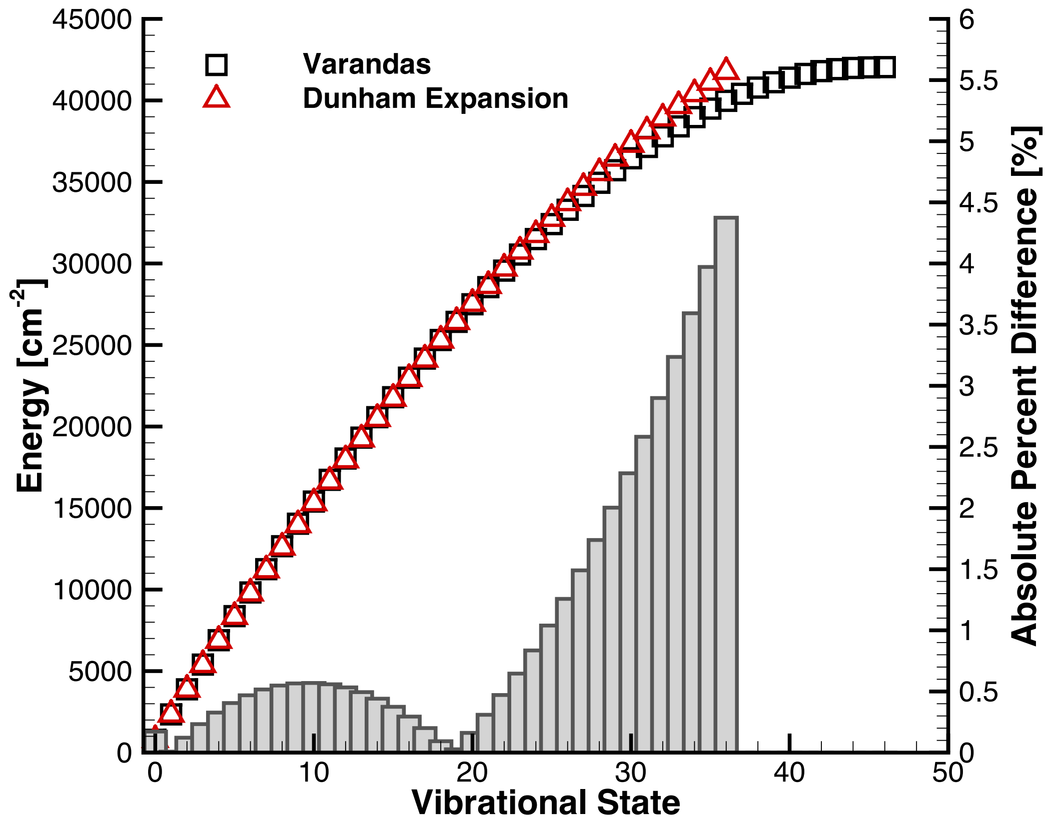


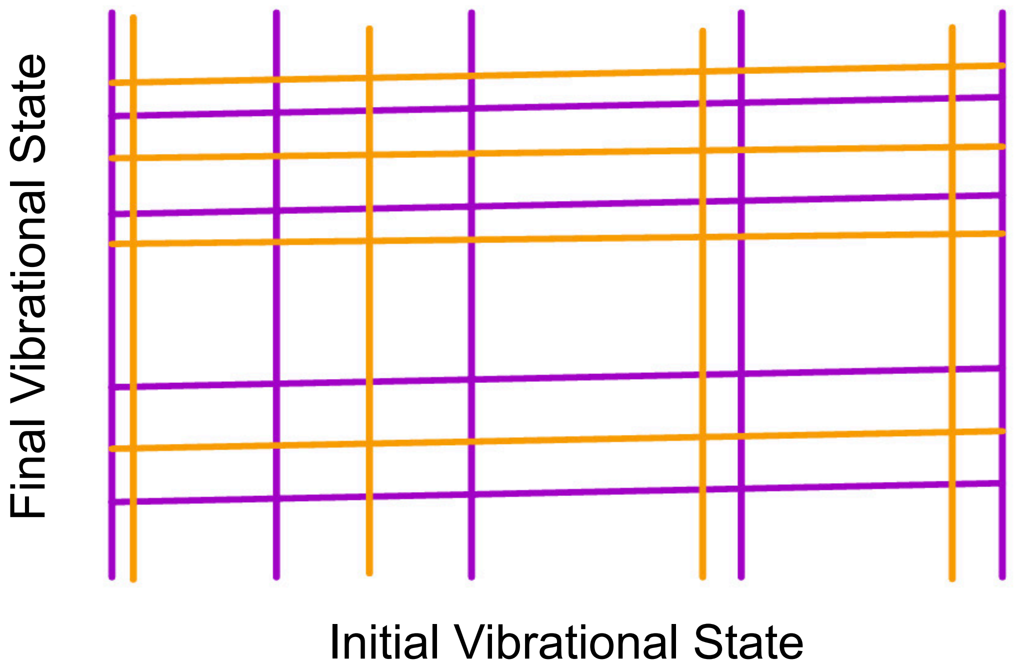
OBJECTIVE 1: MAP RATES FROM ONE VIBRATIONAL LADDER TO ANOTHER

Approach – Mapping – Taylor Series Expansion

$$\begin{bmatrix} \sum \xi_k & \sum (x_k - x_0)\xi_k & \sum (y_k - y_0)\xi_k \\ \sum (x_k - x_0)\xi_k & \sum (x_k - x_0)^2\xi_k & \sum (x_k - x_0)(y_k - y_0)\xi_i \\ \sum (y_k - y_0)\xi_k & \sum (x_k - x_0)(y_k - y_0)\xi_k & \sum (y_k - y_0)^2\xi_i \end{bmatrix} \begin{bmatrix} K|_0 \\ \partial K/\partial x|_0 \\ \partial K/\partial y|_0 \end{bmatrix} = \begin{bmatrix} \sum K_k\xi_k \\ \sum (x_k - x_0)K_k\xi_k \\ \sum (y_k - y_0)K_k\xi_k \end{bmatrix}$$

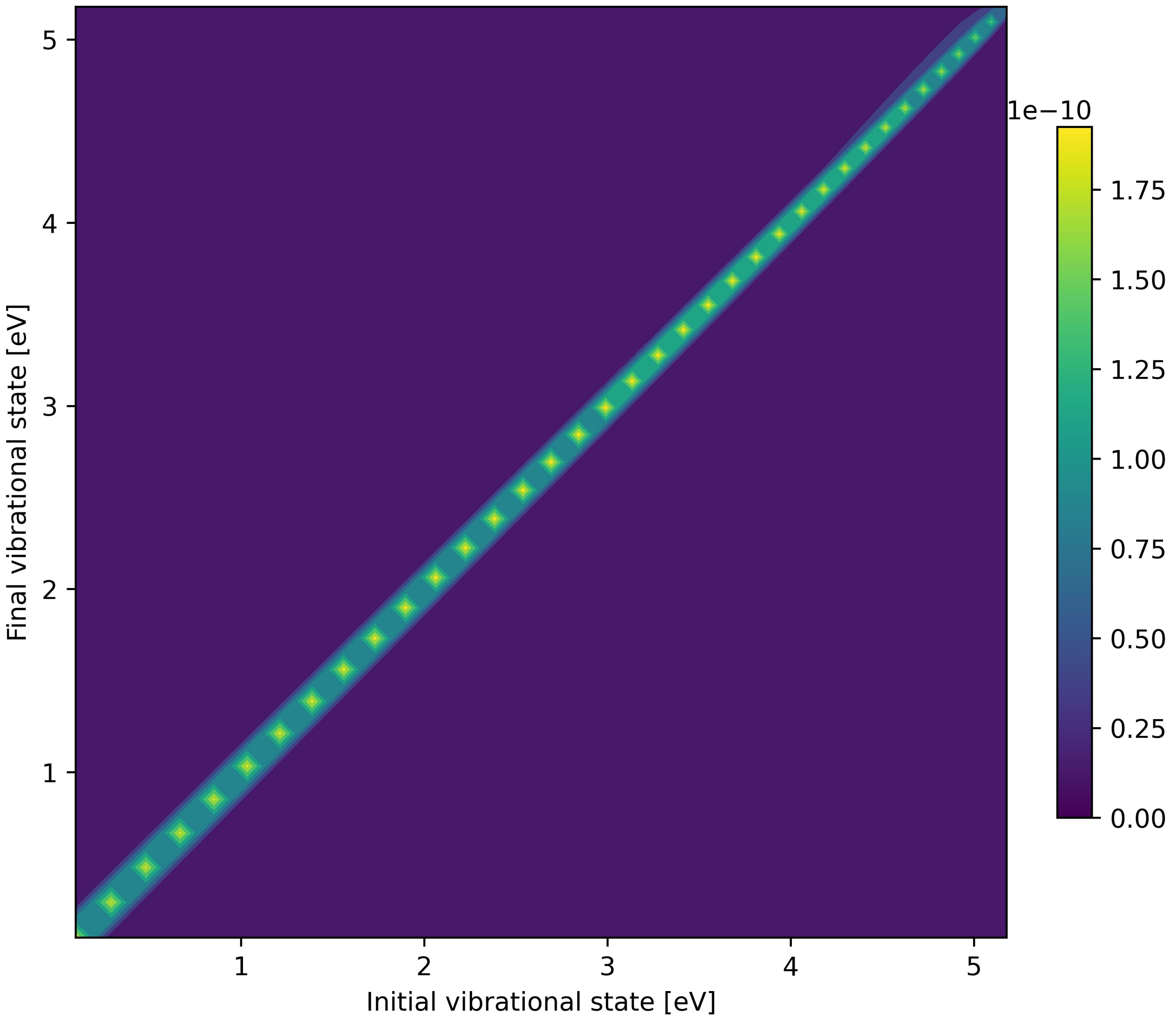
$$\xi_k = \frac{1}{(x_k - x_0)^4 + (y_k - y_0)^4}$$



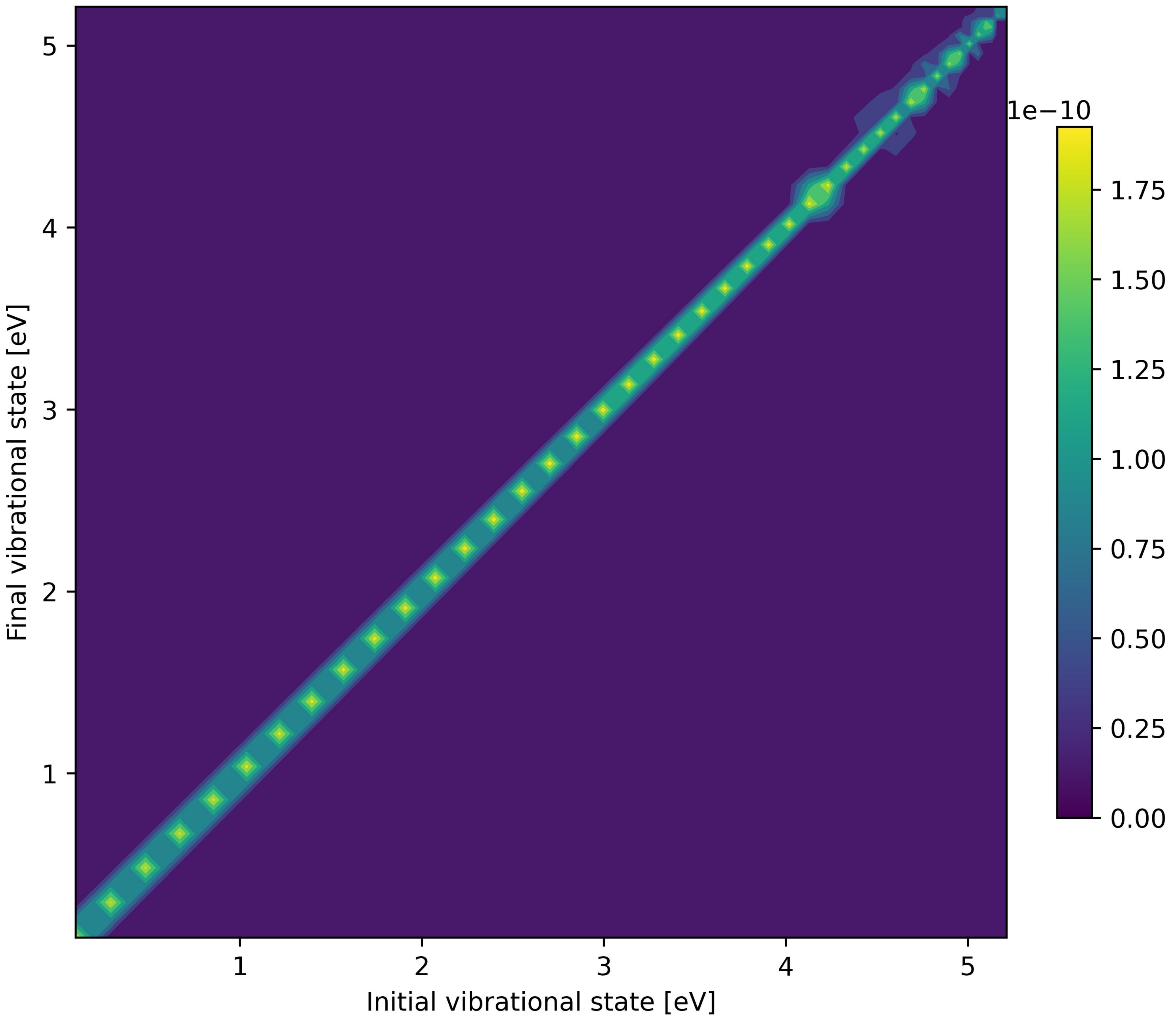


*Andrienko and Boyd, “Kinetics of O2-N2 collisions at hypersonic temperatures,” AIAA Paper 2018-3438.
**Mavriplis, “Revisiting the least-squares procedure for gradient reconstruction on unstructured meshes,” AIAA Paper 2003-3986.

Results – Mapping – Taylor Series Expansion



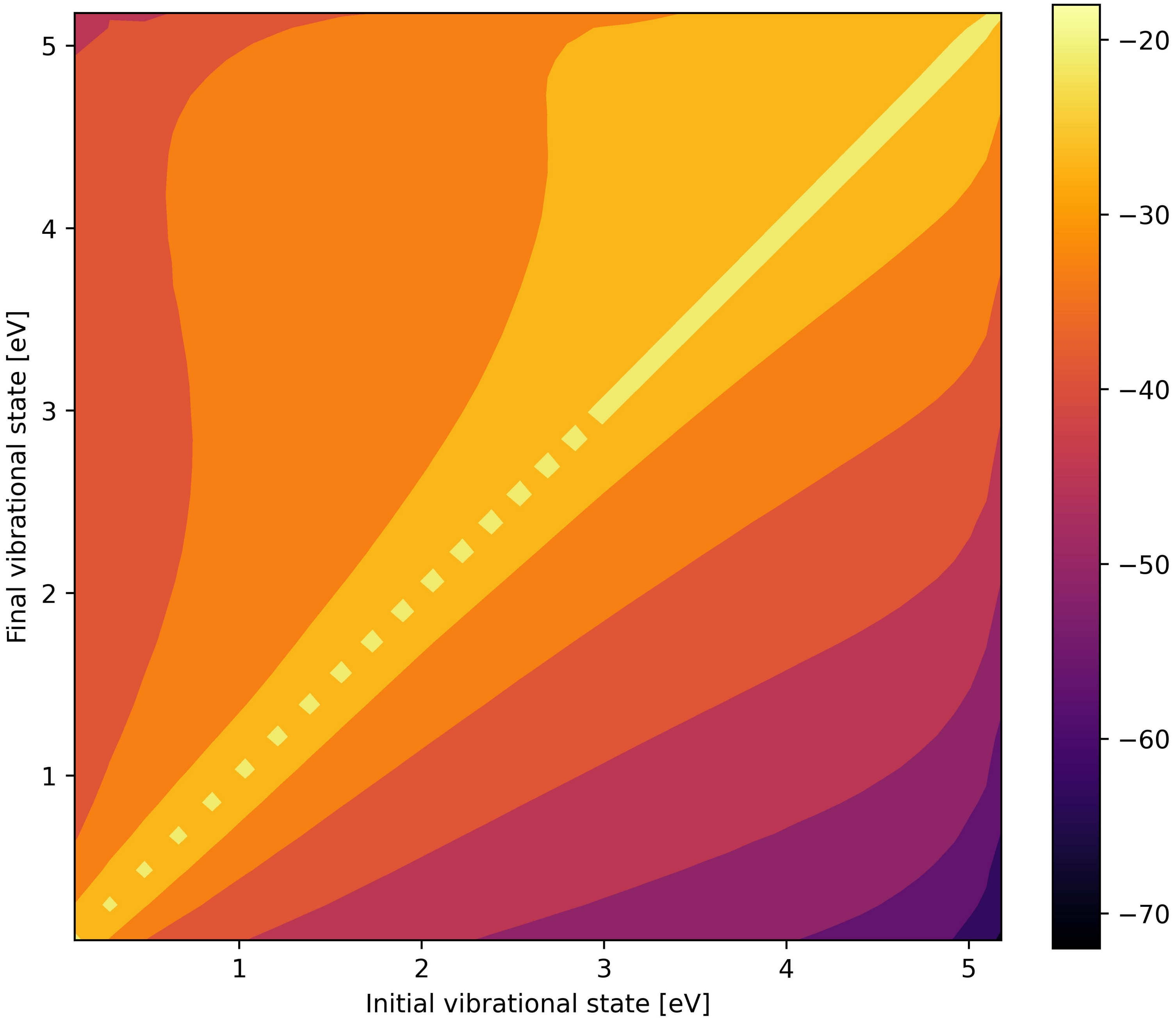
Original/Known - Dunham (36 state ladder)



Mapped/Unknown - Varandas (46 state ladder)

O_2-Ar bound-bound rates at 3000 K

Results – Mapping – Taylor Series Expansion



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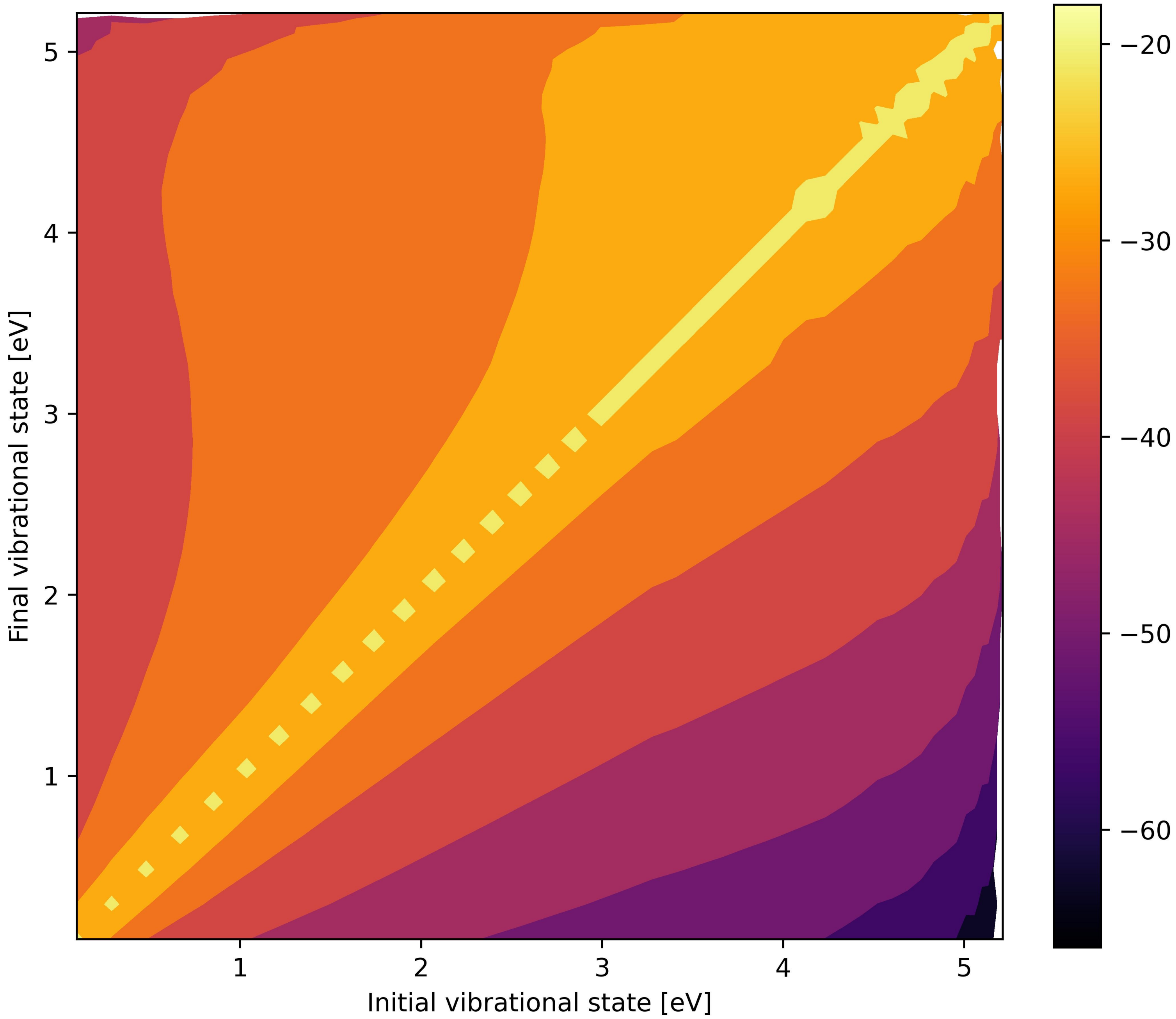
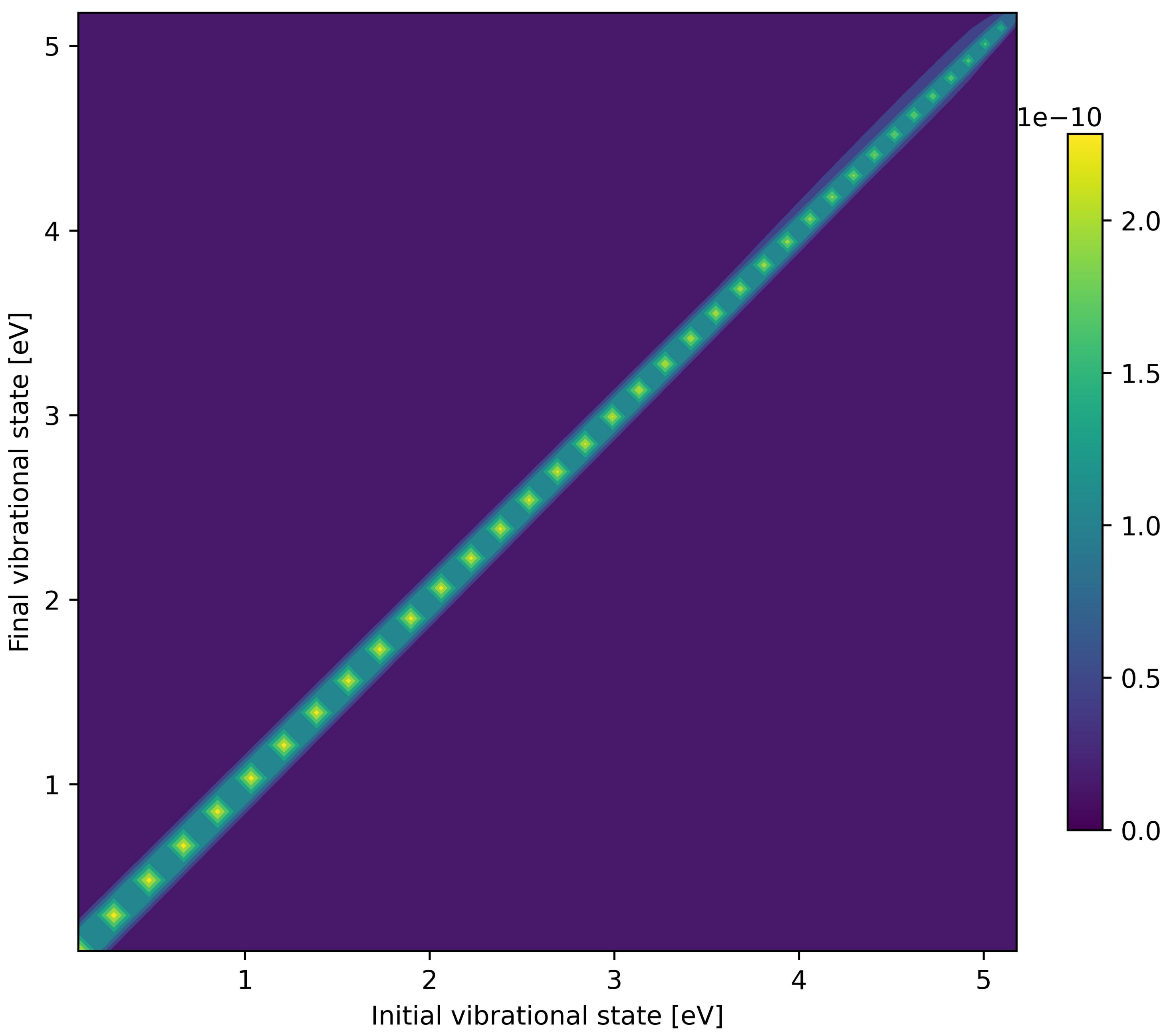


Mapped/Unknown - Varandas (46 state ladder)

O_2-Ar bound-bound **log**(rates) at 3000 K

Results – Mapping – Taylor Series Expansion



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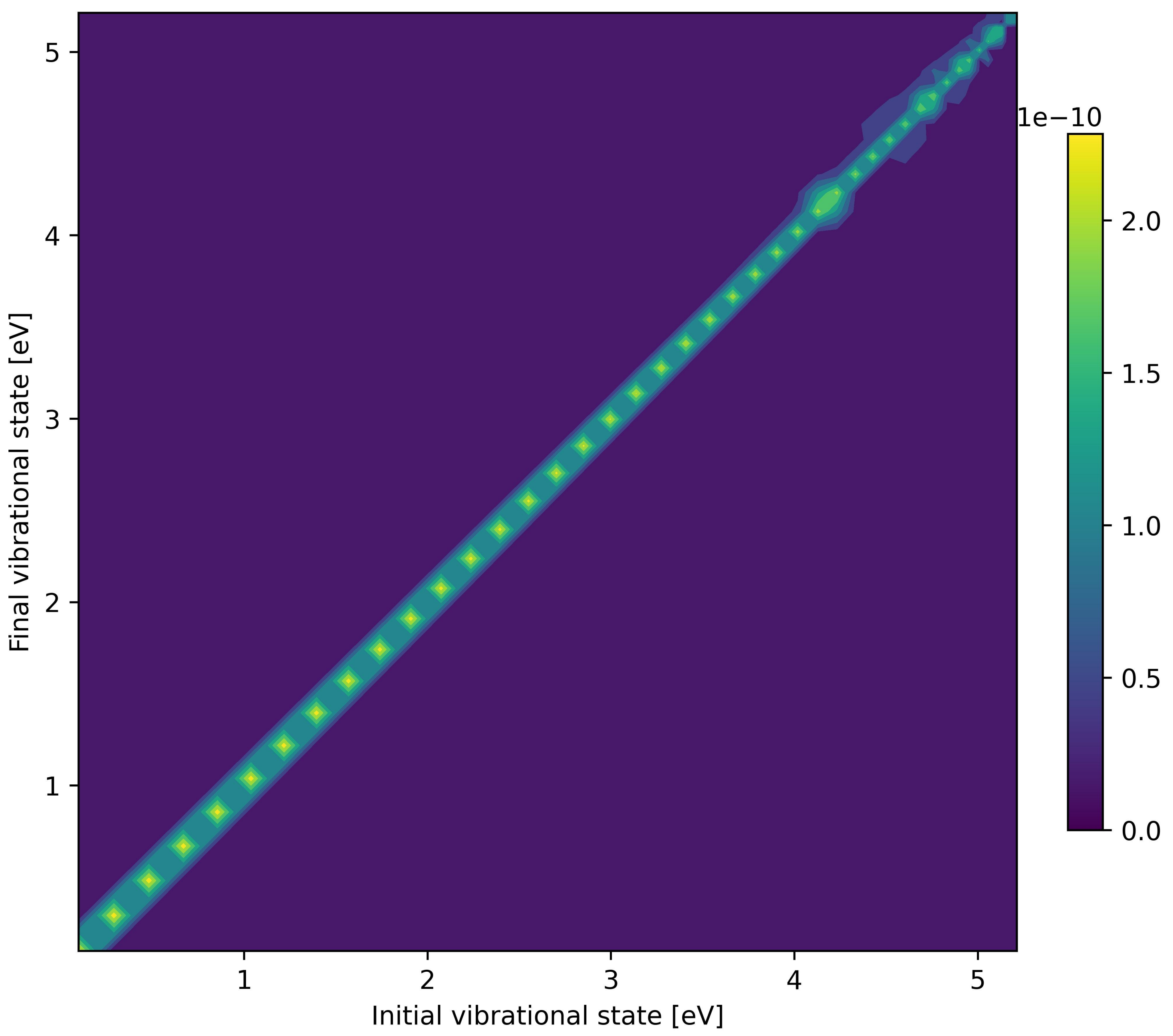

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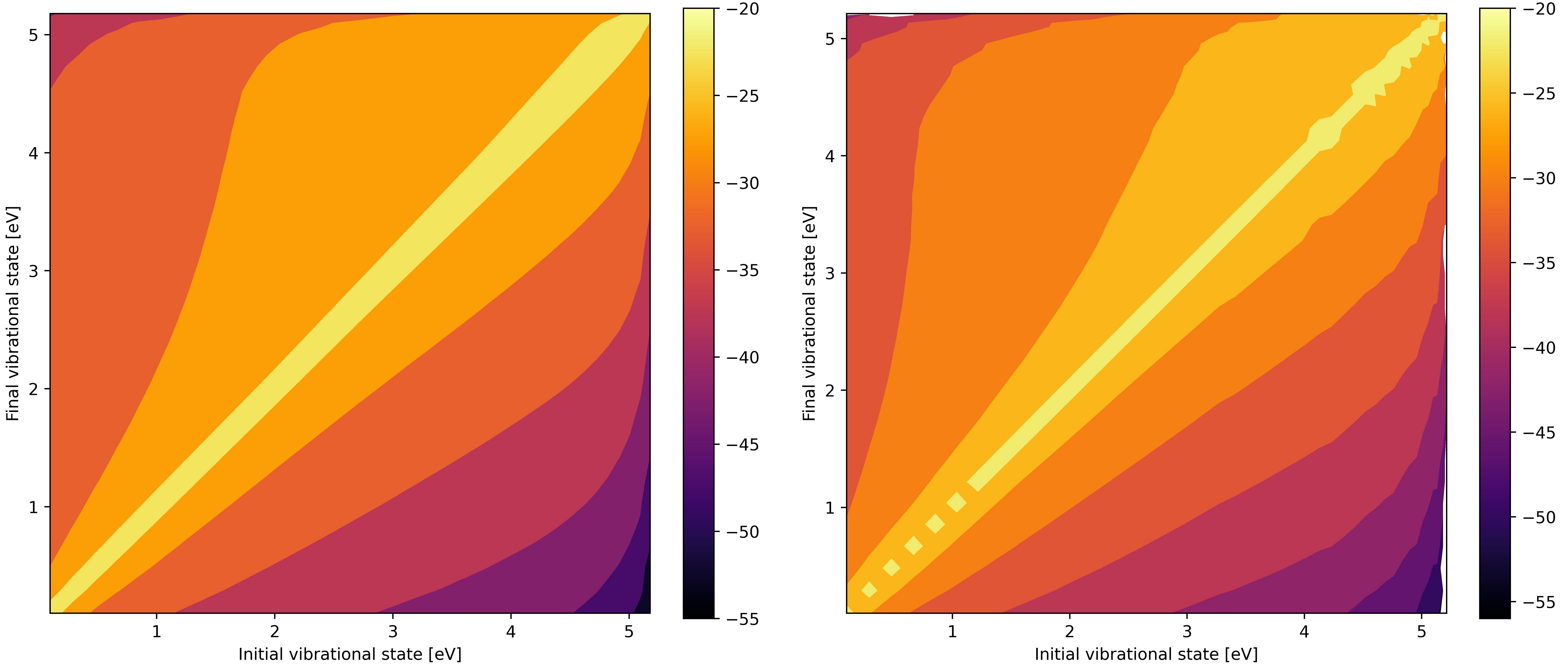
O_2-Ar bound-bound rates at 5000 K

Results – Mapping – Taylor Series Expansion



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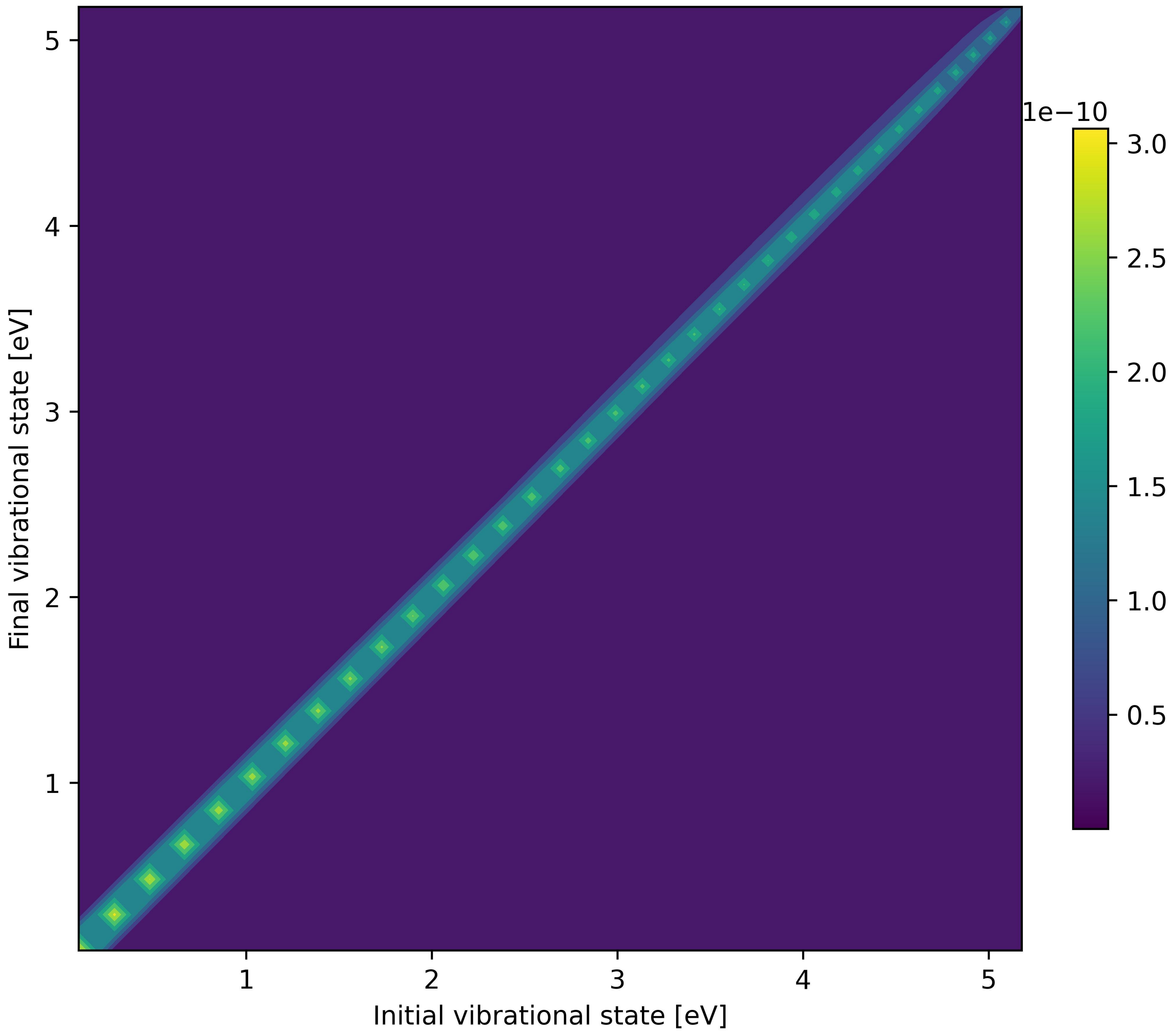

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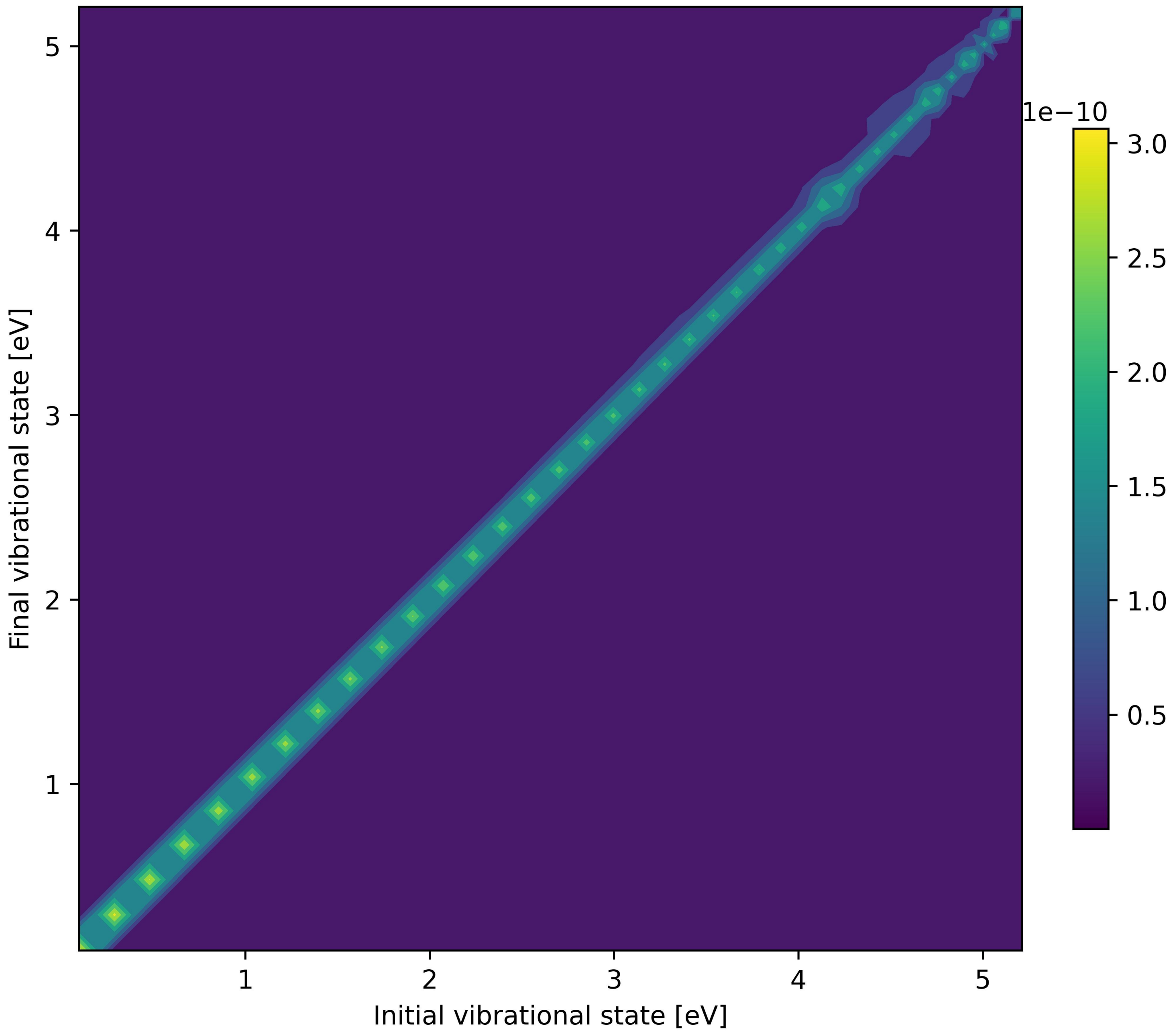
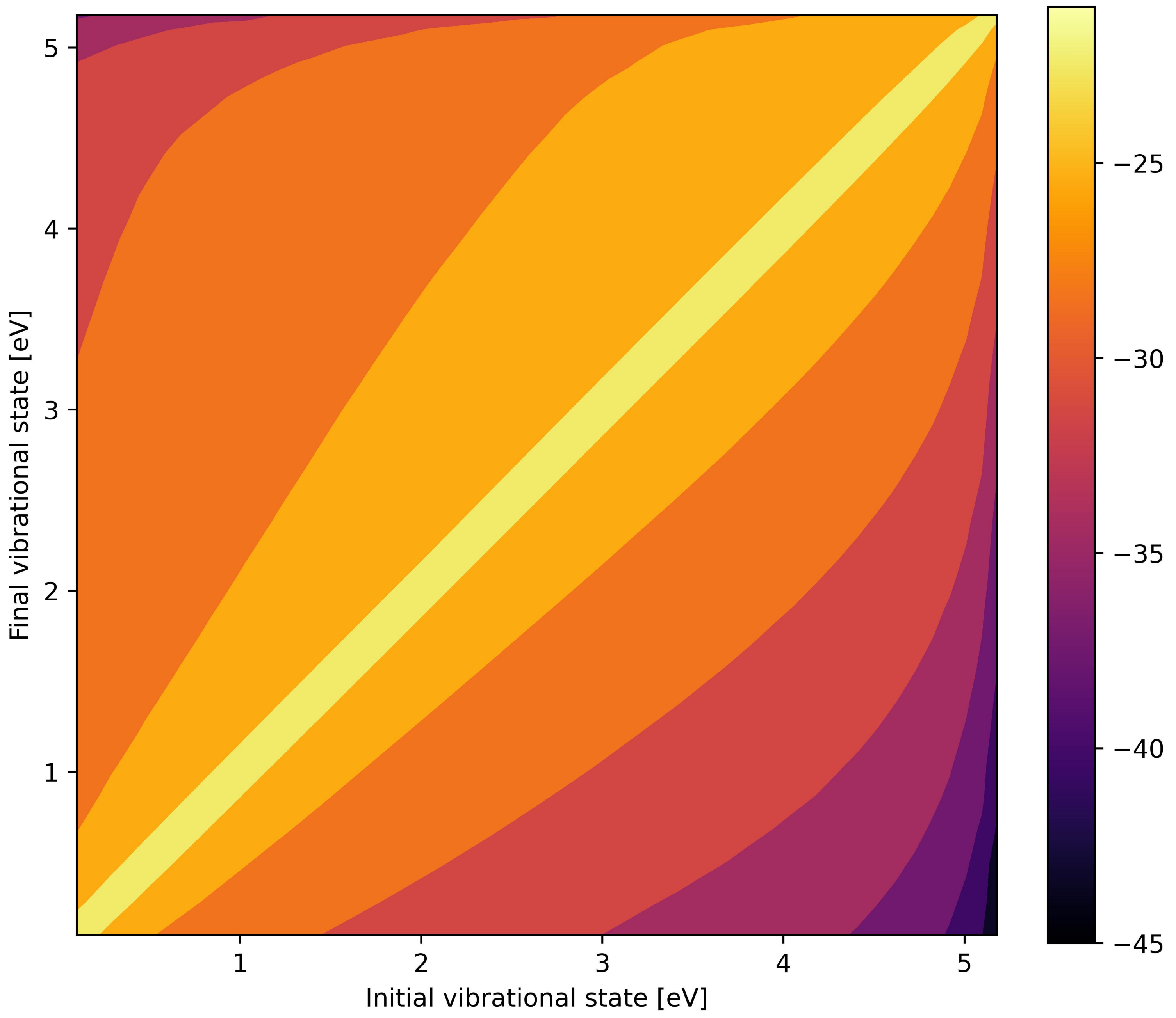


Mapped/Unknown - Varandas (46 state ladder)

O_2-Ar bound-bound rates at 10000 K

Results – Mapping – Taylor Series Expansion



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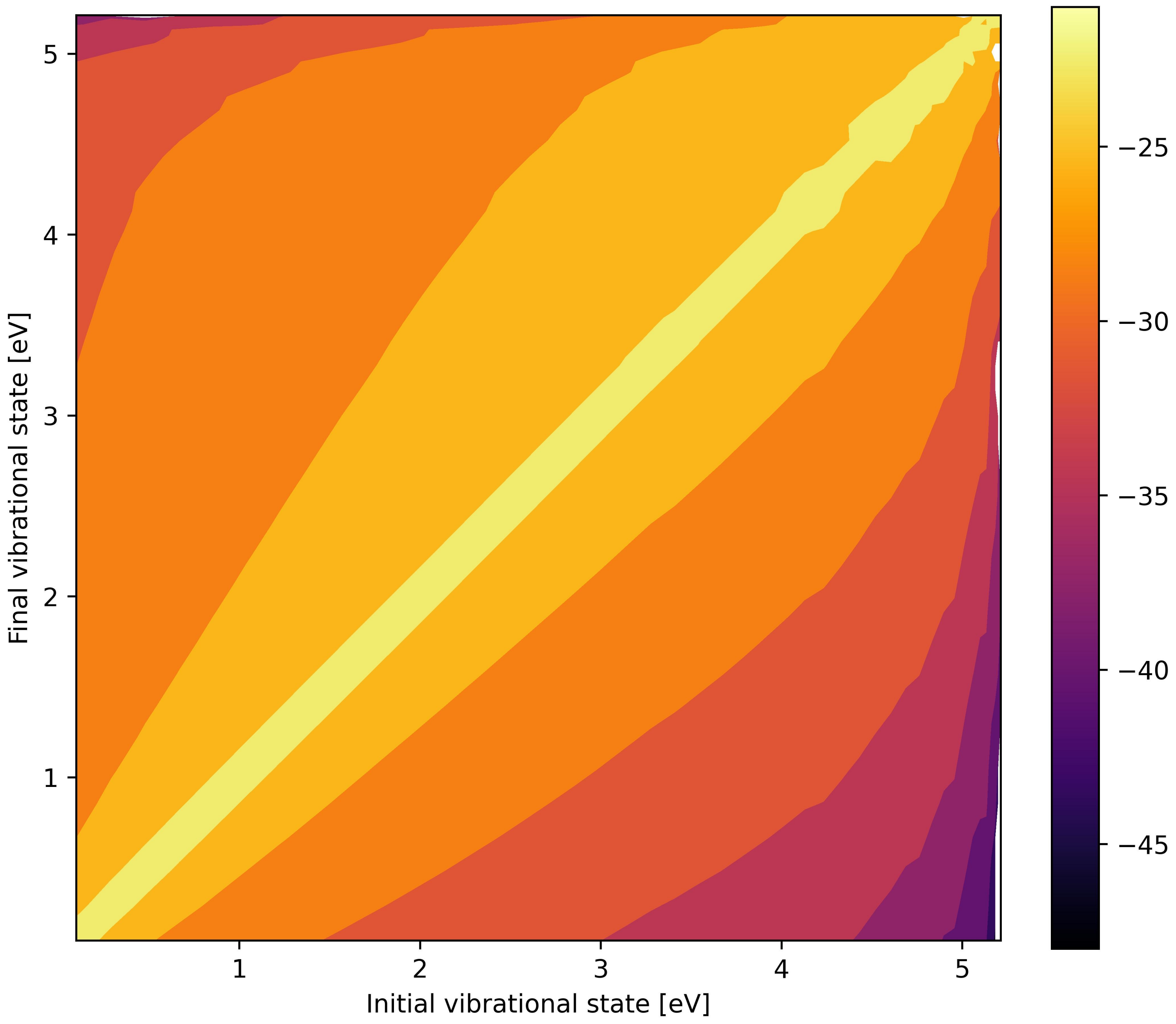

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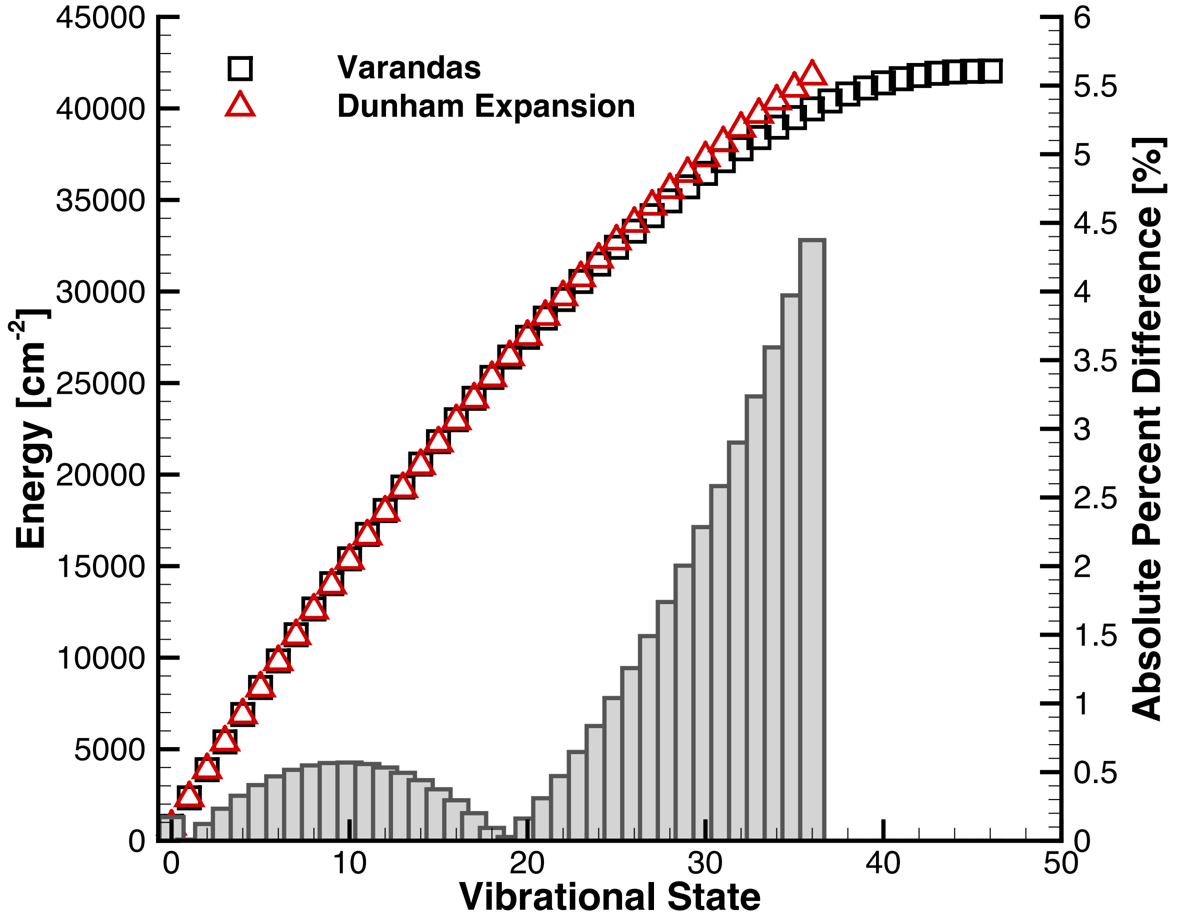
O_2-Ar bound-bound **log**(rates) at 10000 K

Mapping Approaches – Radial Basis Functions (RBF)

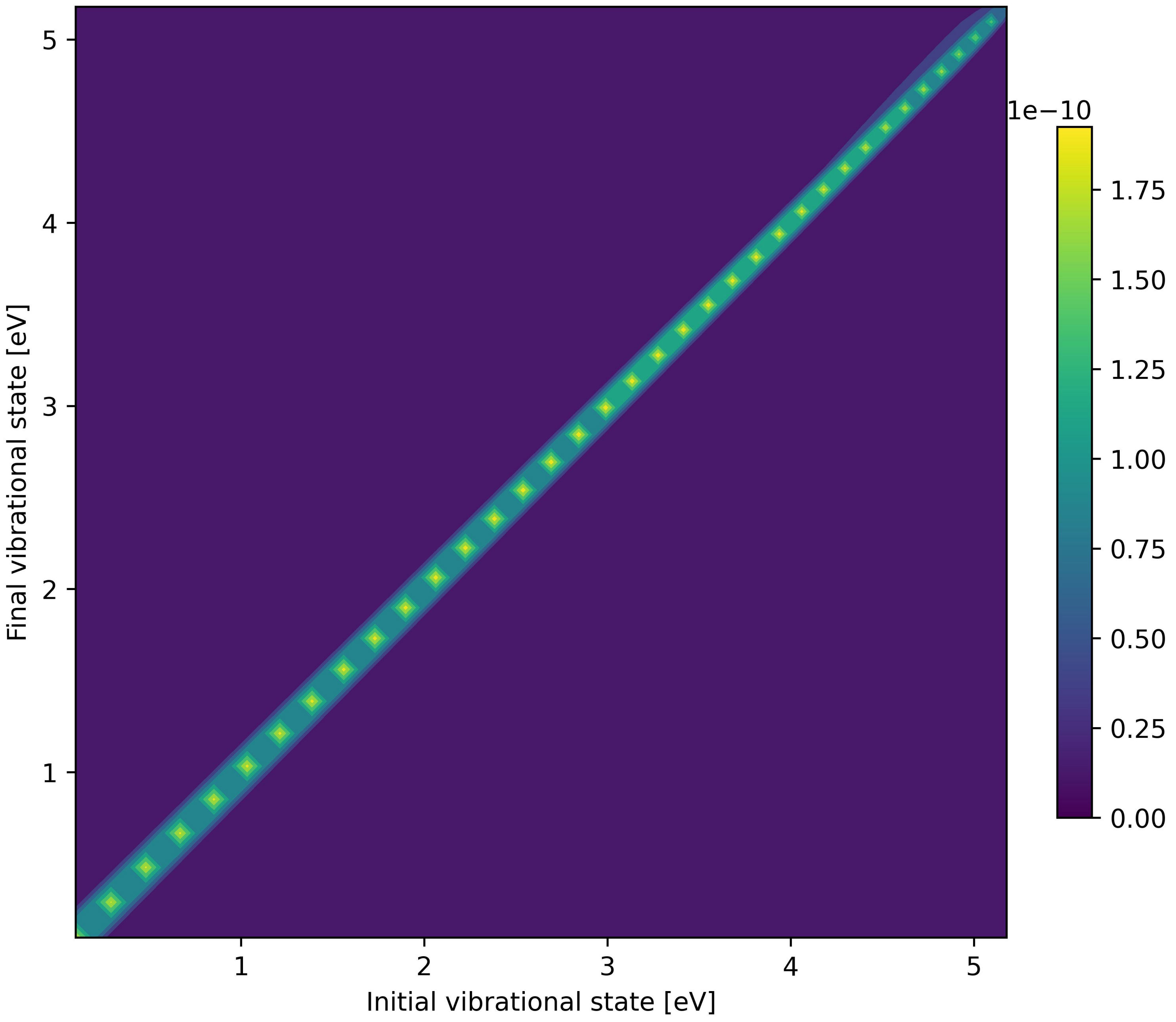
$$\phi(r) = r^2 \log(r) \qquad r = \|\mathbf{v} - \mathbf{d}_i\|$$

$$f(\mathbf{v}) = \sum_{i=1}^{N} w_i \phi\left(\|\mathbf{v} - \mathbf{d}_i\|\right)$$

$$\begin{bmatrix} \phi\left(\|\mathbf{d}_1 - \mathbf{d}_1\|\right) & \cdots & \phi\left(\|\mathbf{d}_1 - \mathbf{d}_n\|\right) \\ \phi\left(\|\mathbf{d}_2 - \mathbf{d}_1\|\right) & \cdots & \phi\left(\|\mathbf{d}_2 - \mathbf{d}_n\|\right) \\ \vdots & \ddots & \vdots \\ \phi\left(\|\mathbf{d}_n - \mathbf{d}_1\|\right) & \cdots & \phi\left(\|\mathbf{d}_n - \mathbf{d}_n\|\right) \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$



Results – Mapping – Radial Basis Functions



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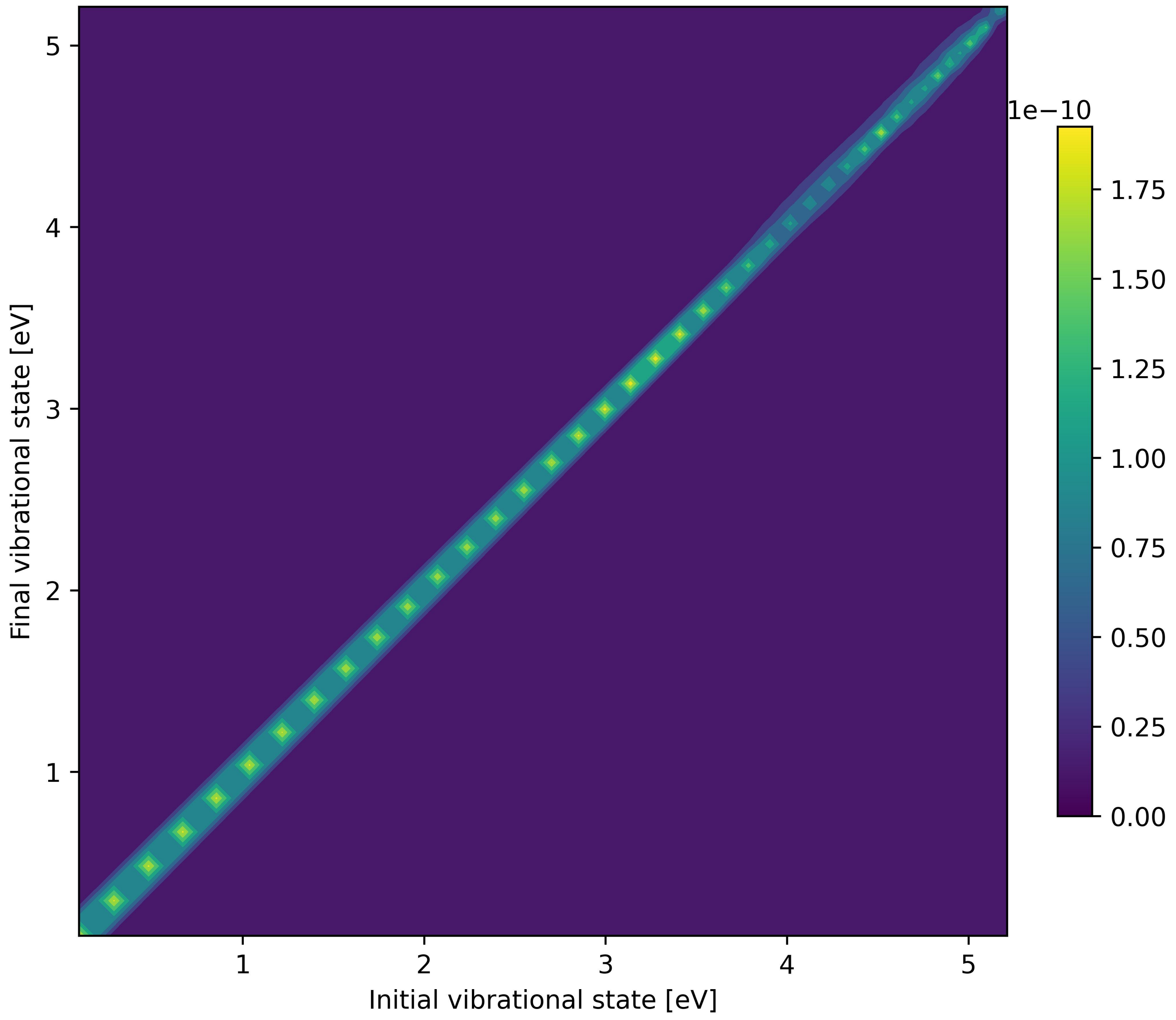

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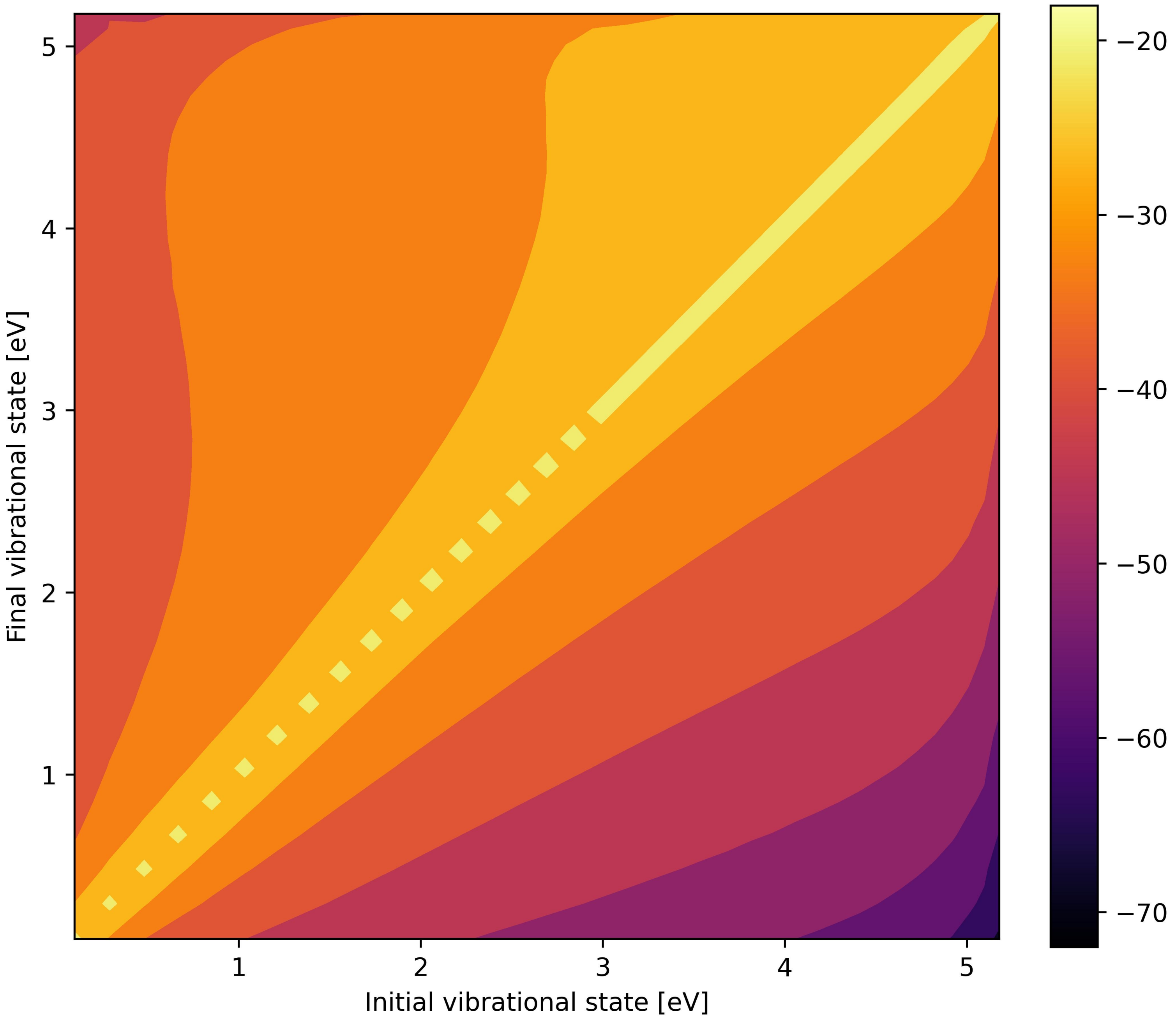
O_2-Ar bound-bound rates at 3000 K

Results – Mapping – Radial Basis Functions



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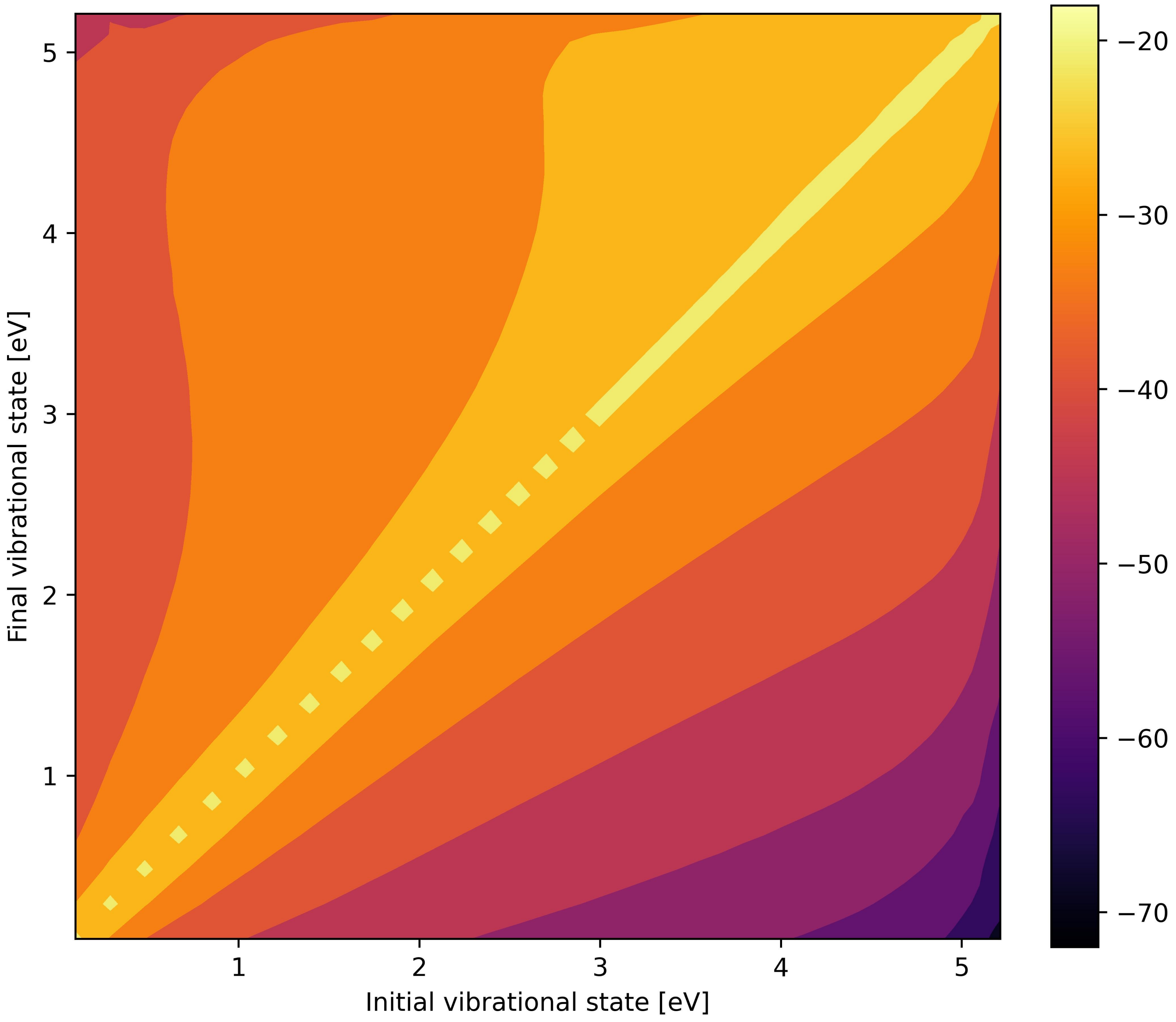
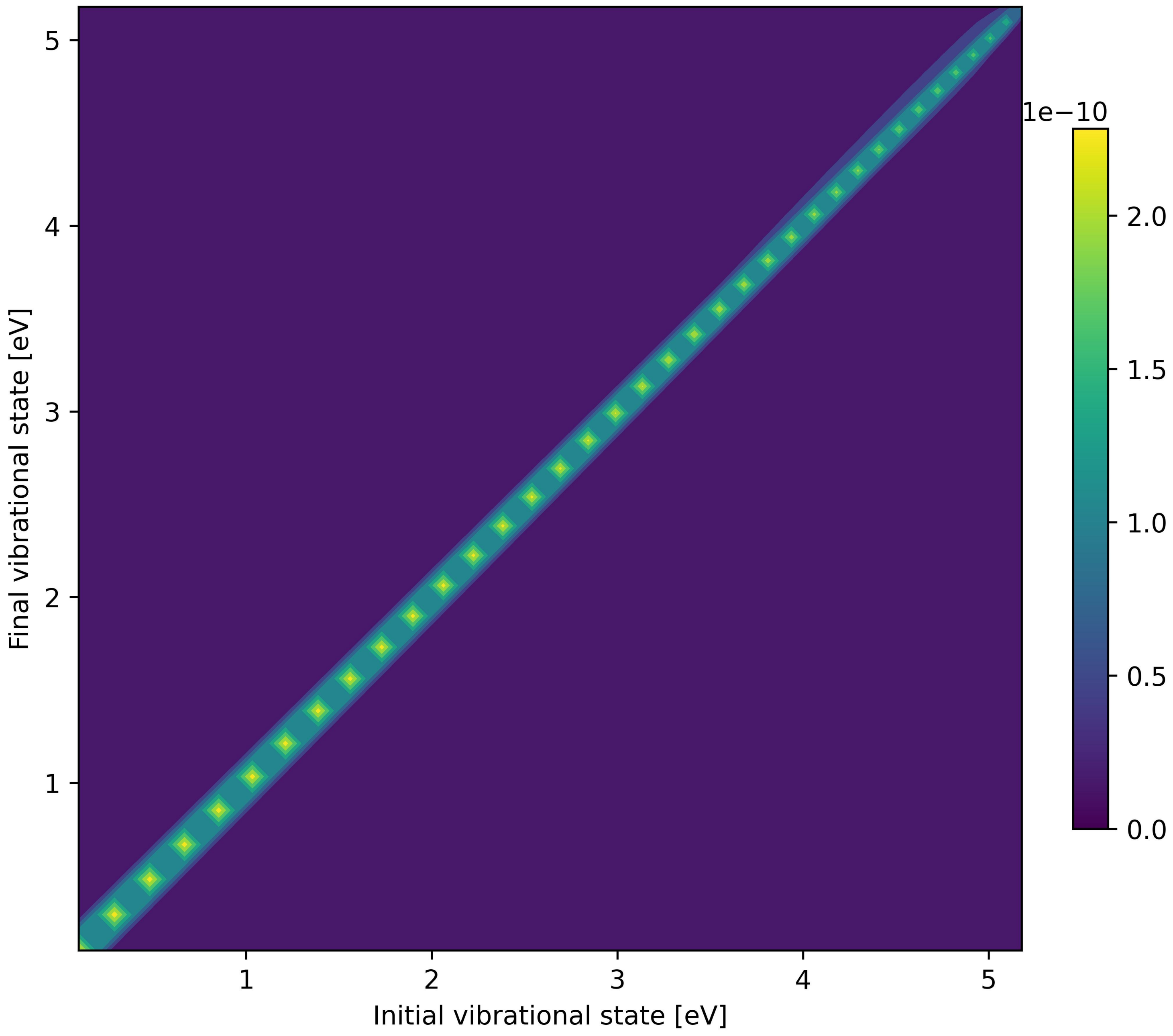


Mapped/Unknown - Varandas (46 state ladder)

O_2-Ar bound-bound **log**(rates) at 3000 K

Results – Mapping – Radial Basis Functions



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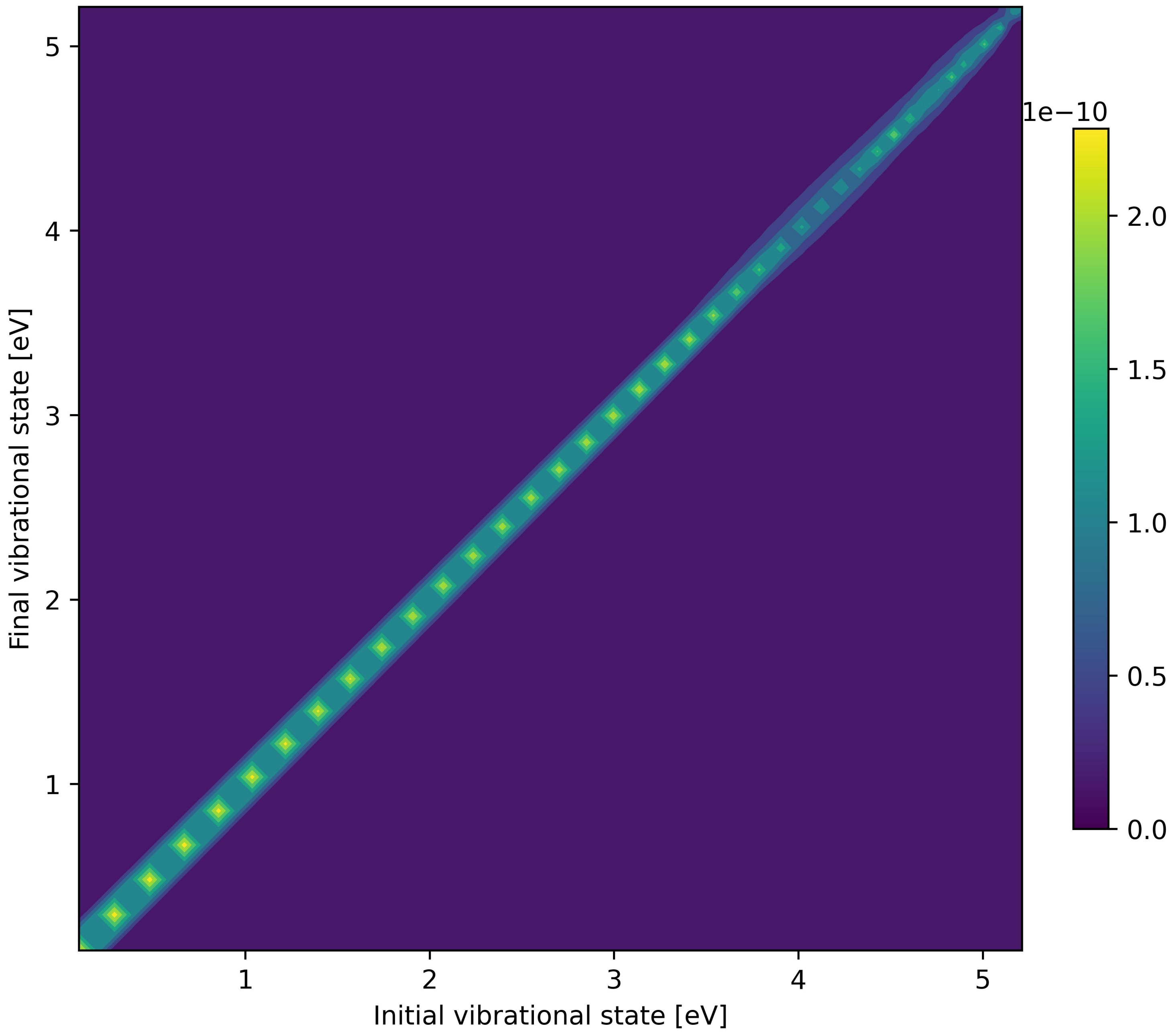
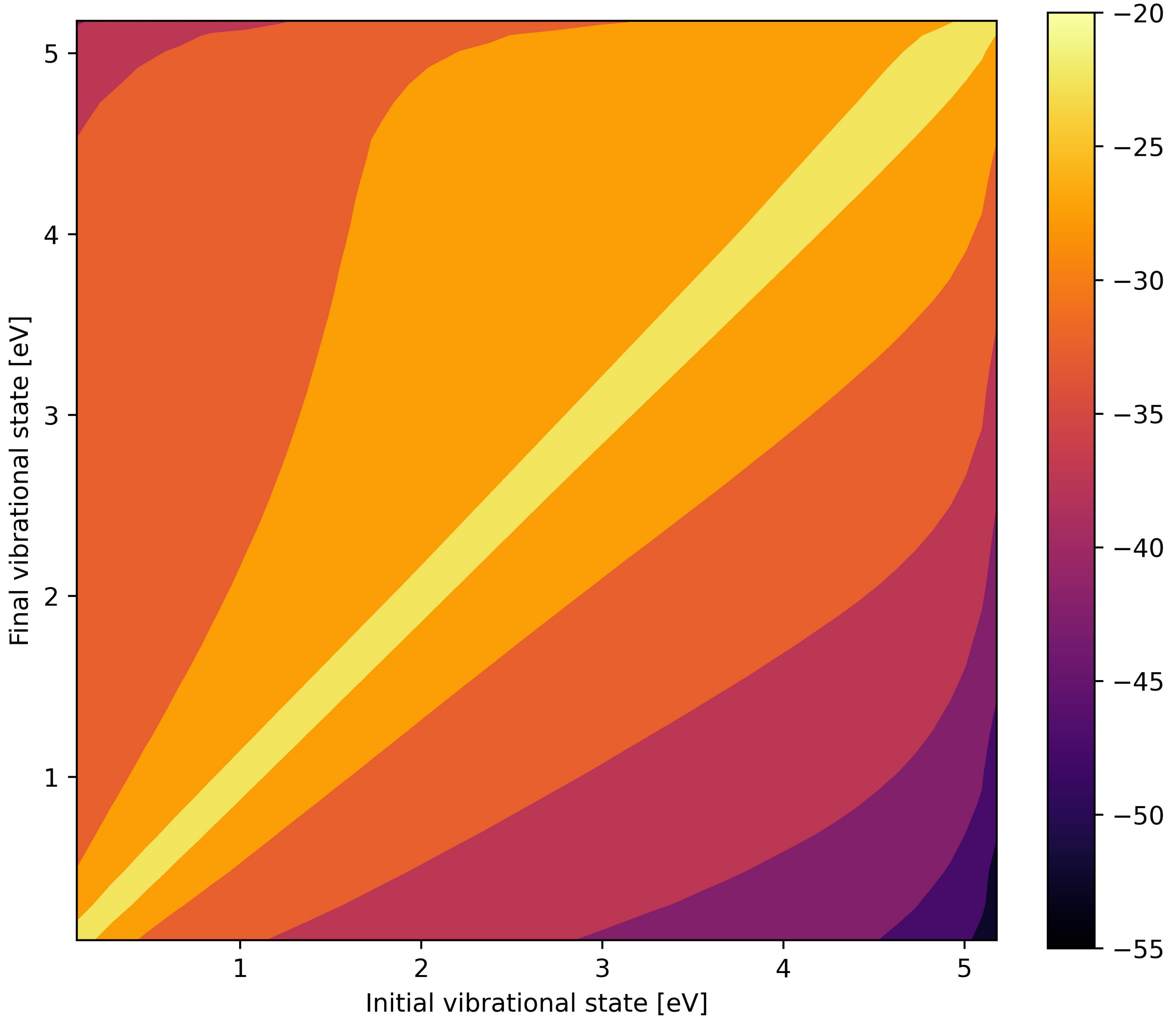


Mapped/Unknown - Varandas (46 state ladder)

O_2-Ar bound-bound rates at 5000 K

Results – Mapping – Radial Basis Functions



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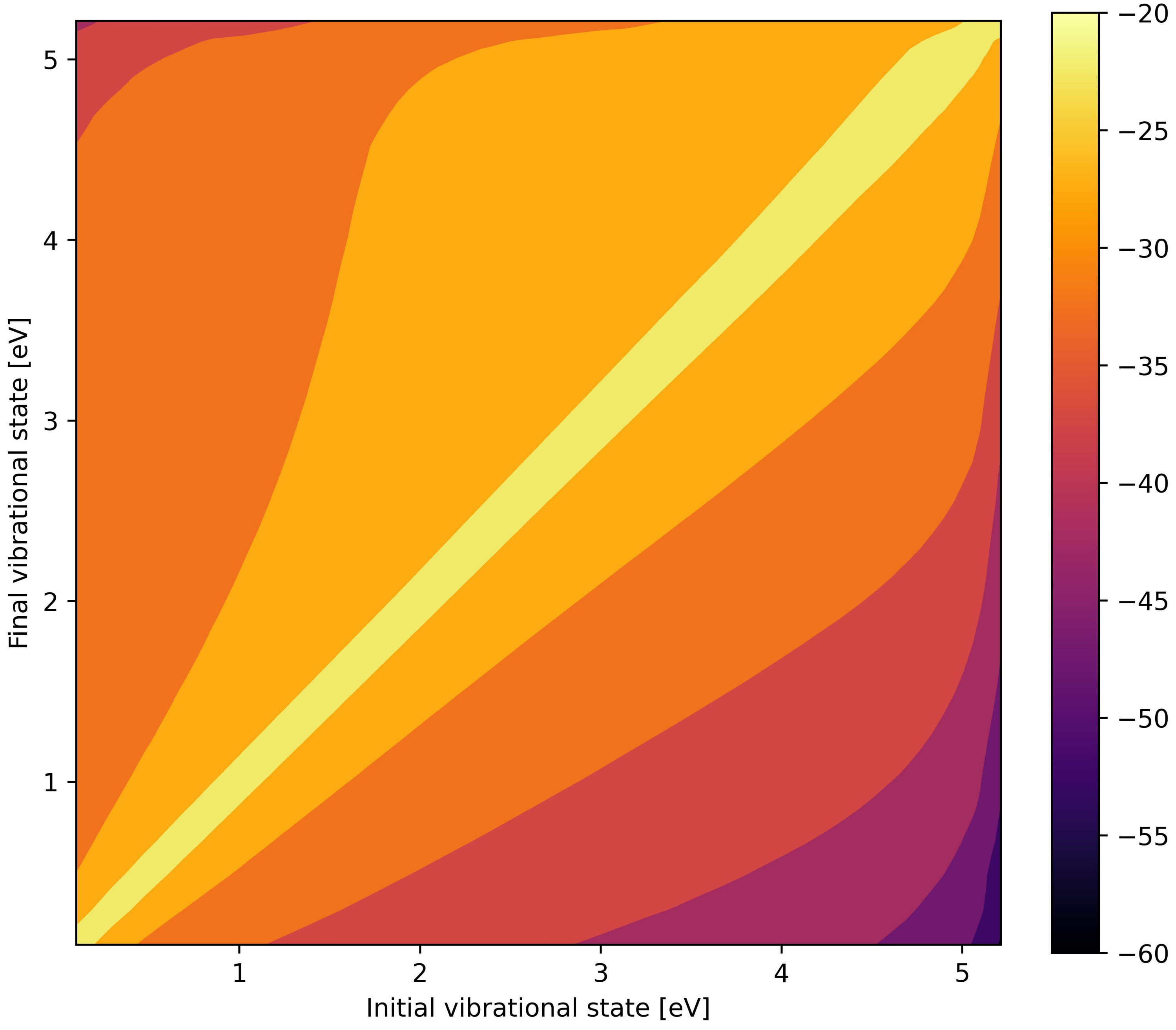

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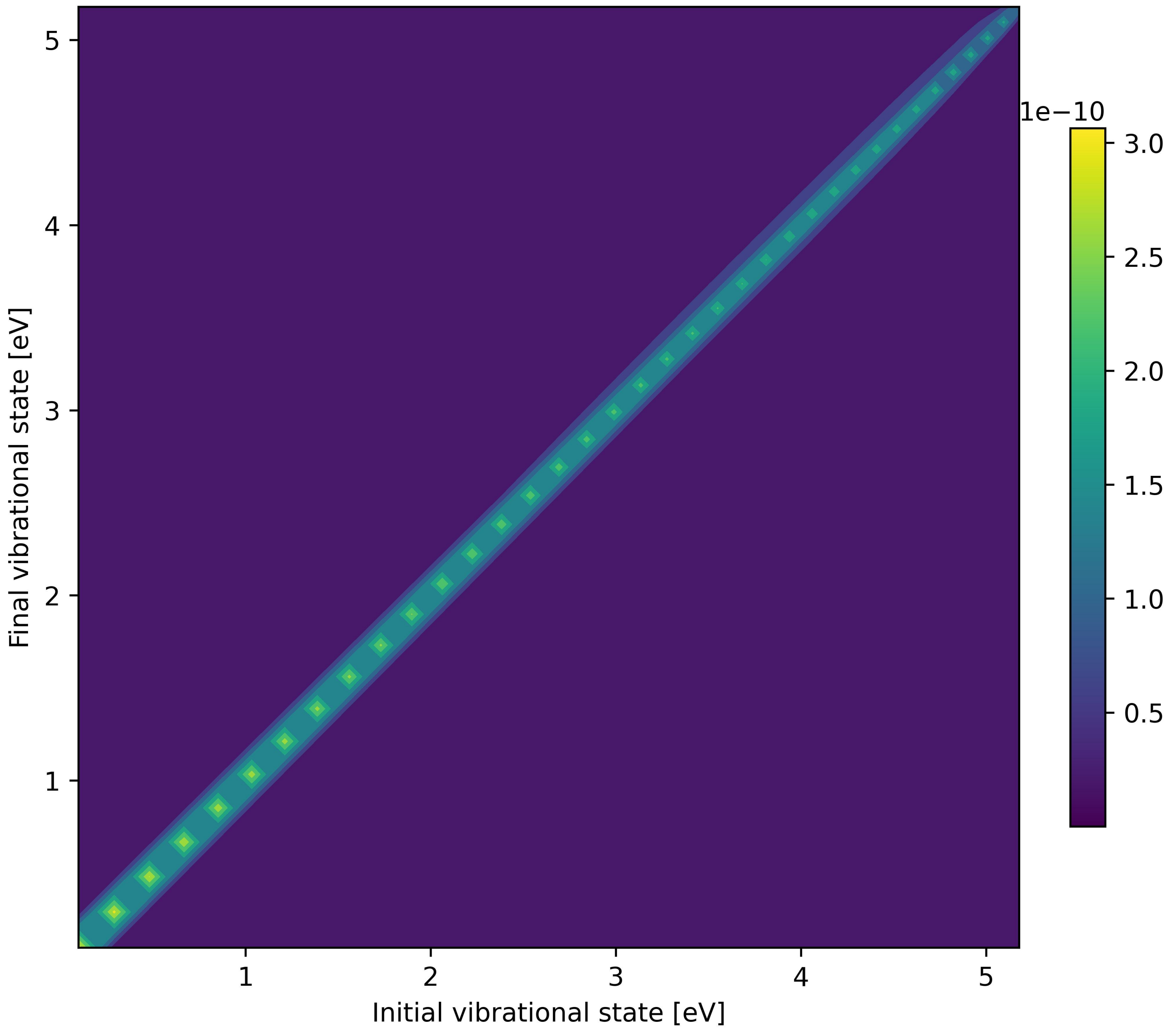

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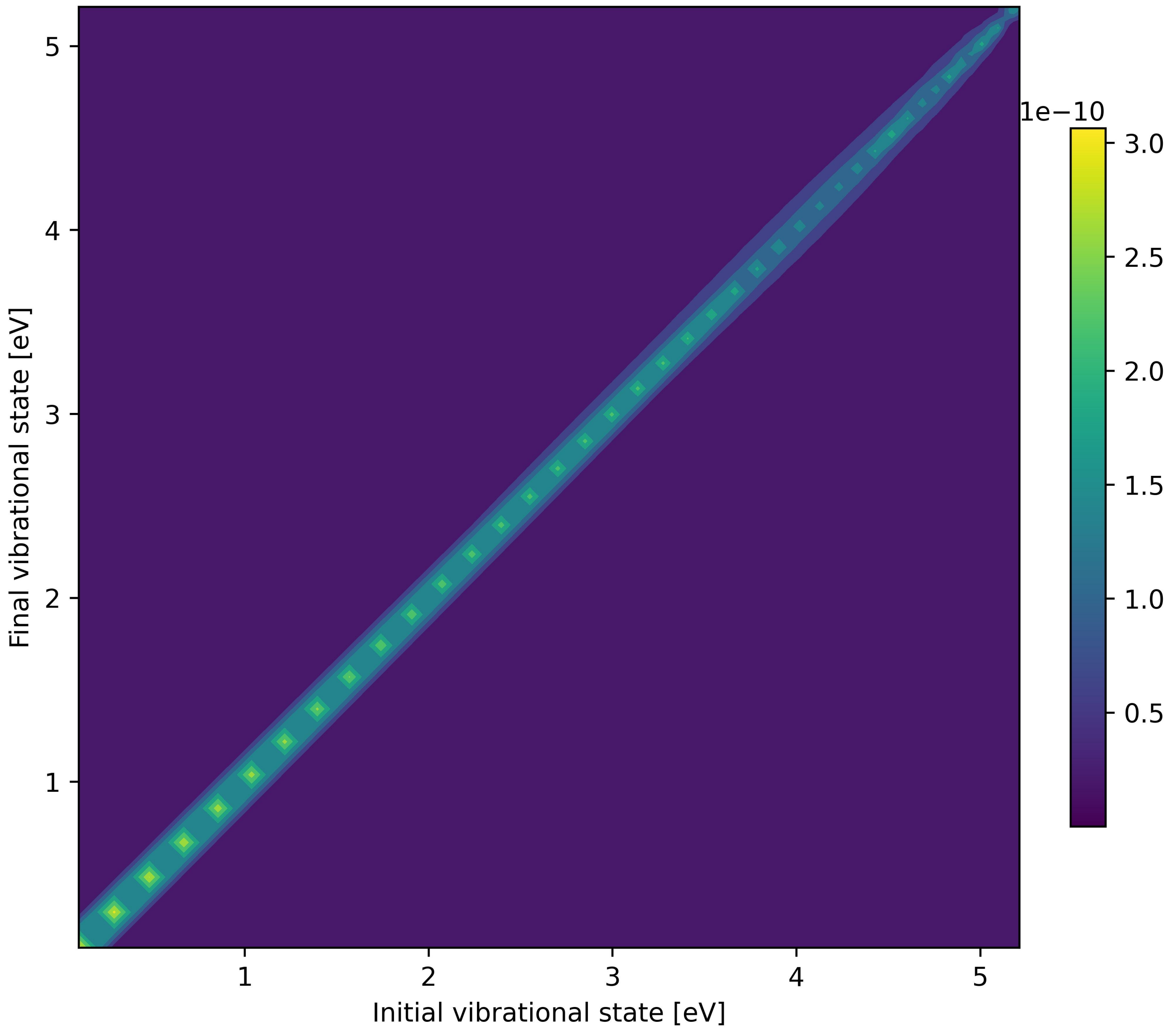
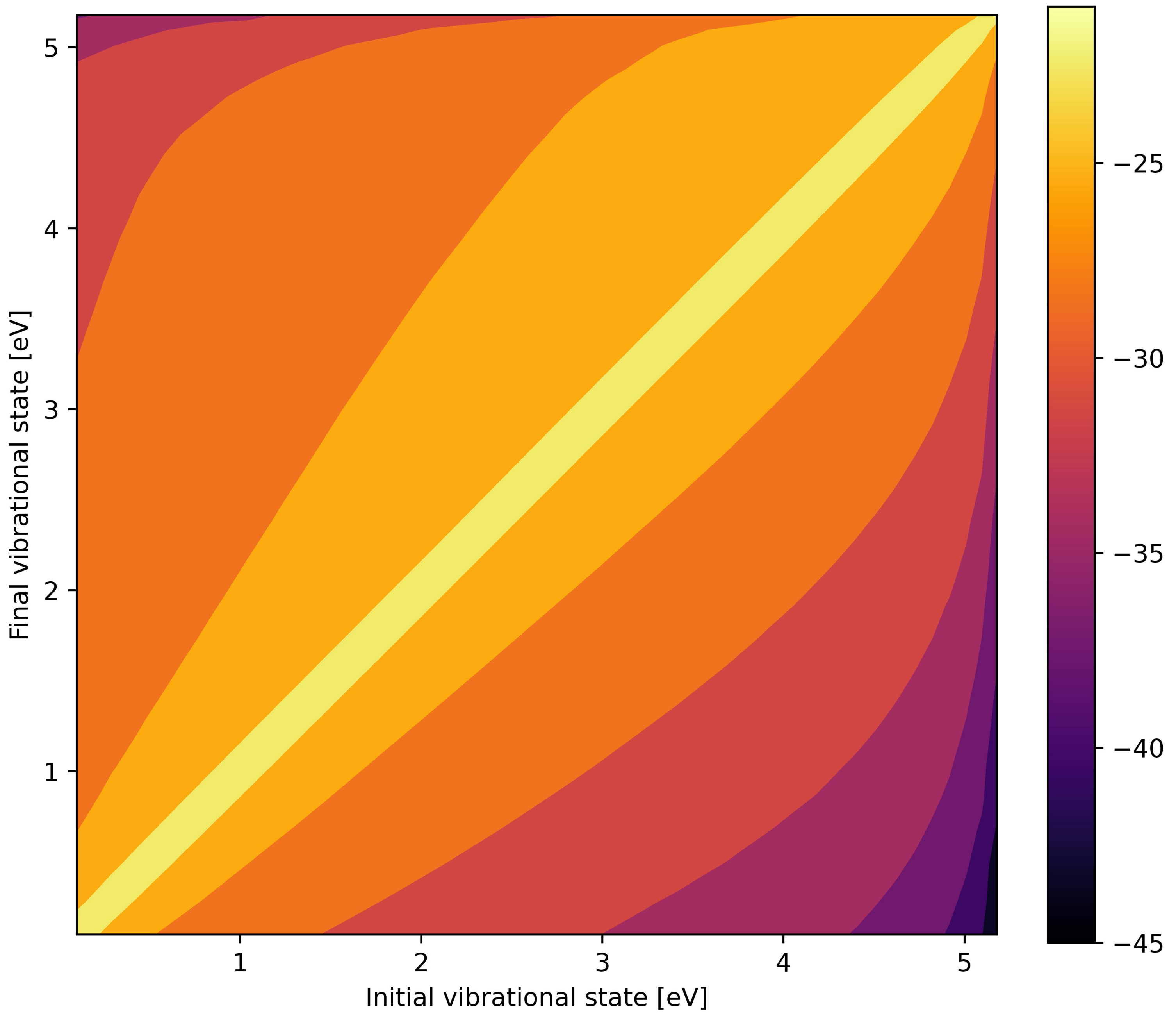


Mapped/Unknown - Varandas (46 state ladder)

O_2-Ar bound-bound rates at 10000 K

Results – Mapping – Radial Basis Functions



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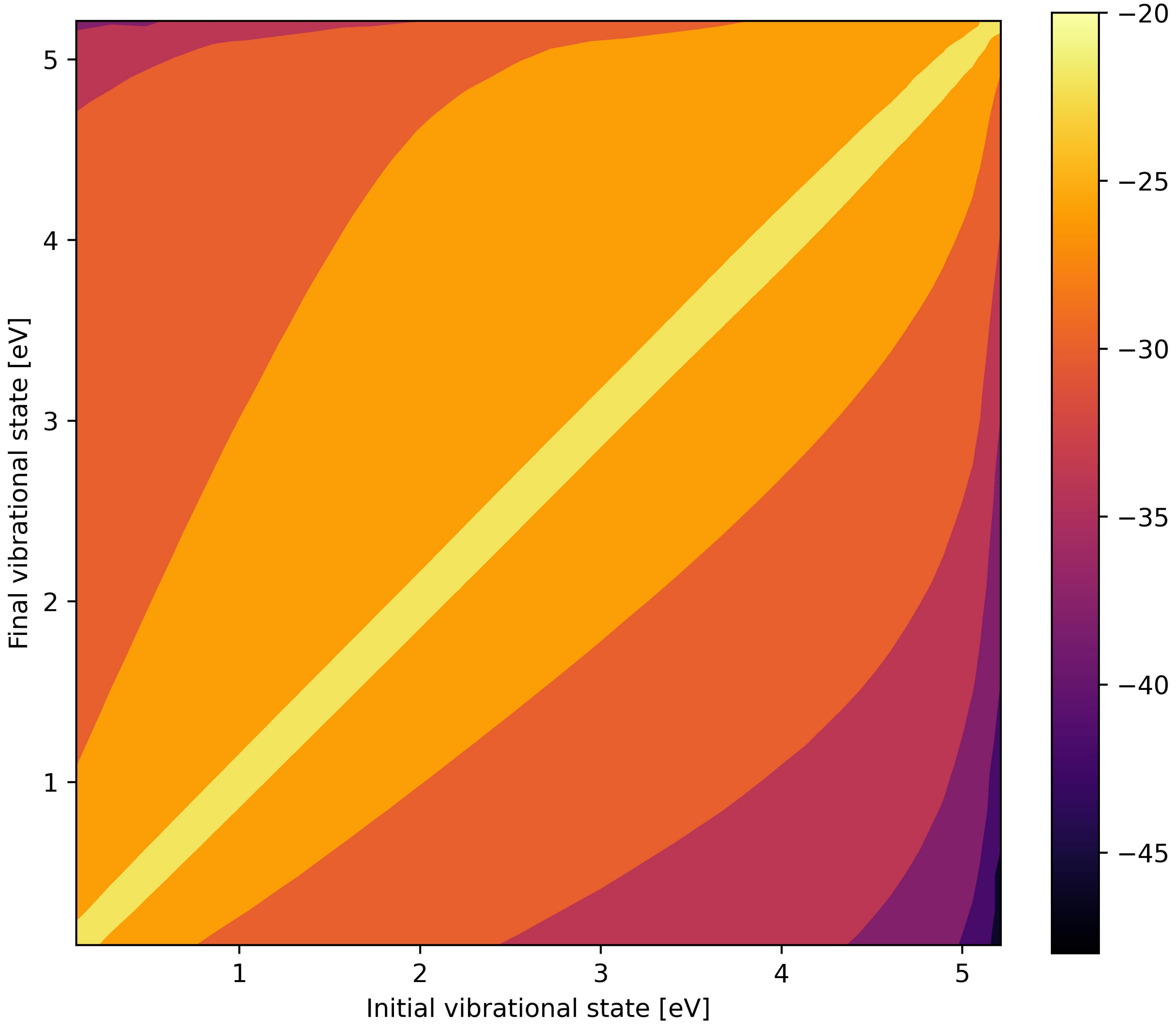


Mapped/Unknown - Varandas (46 state ladder)

O_2-Ar bound-bound **log**(rates) at 10000 K

OBJECTIVE 2: PERFORM STATE-TO-STATE SIMULATIONS OF OXYGEN-ARGON FLOWS

Approach – State-to-State Modeling

- Approach 1: perform state-to-state simulations in 1D code designed for argon-oxygen mixtures[1]
  - It works!
  - Difficult to test different configurations/mixtures

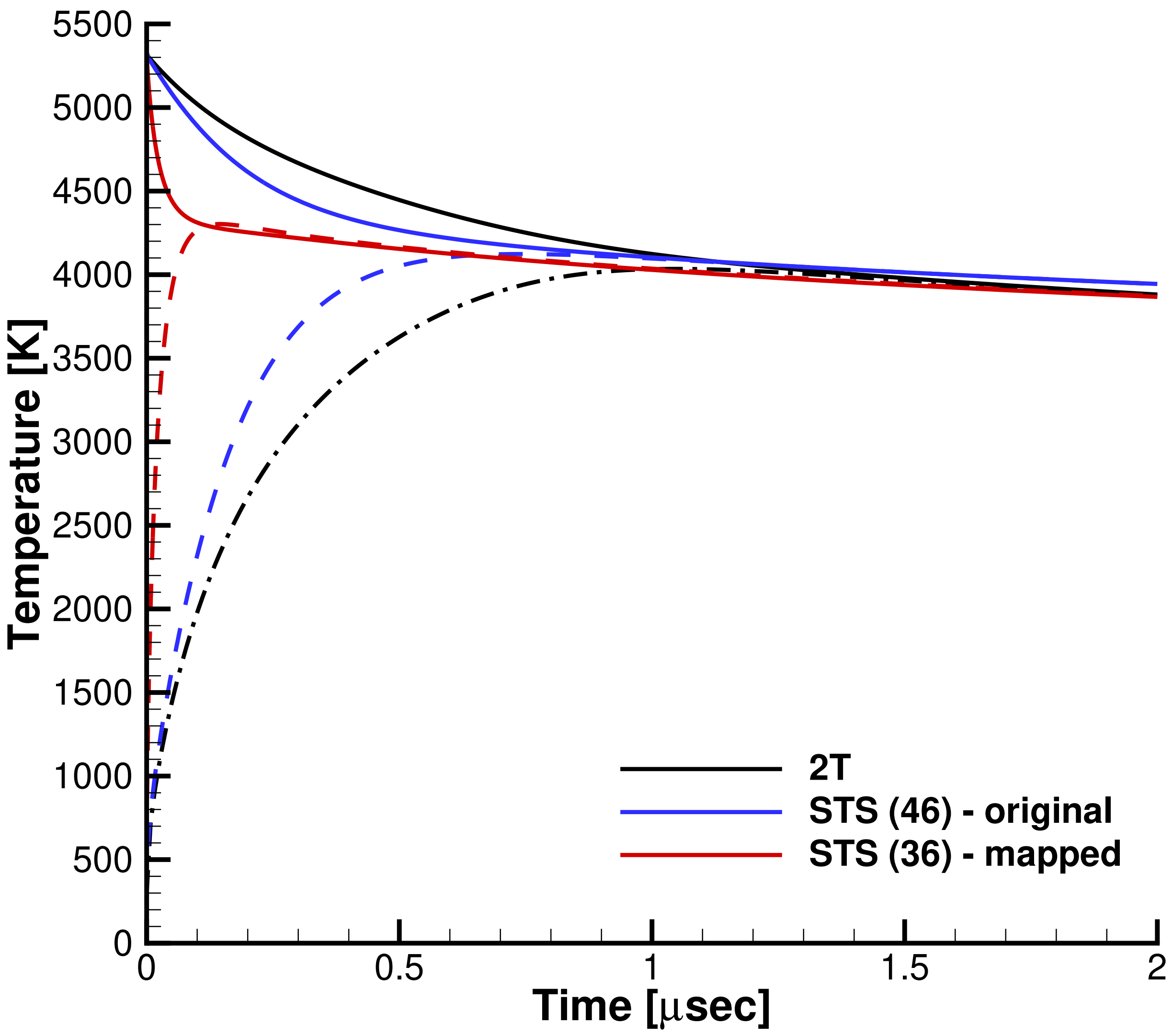
$$\frac{dn_v}{dx} = \sum_s \left(R_{v,s} n_O^2 n_s - D_{v,s} n_v n_s\right) + \sum_s \left(K_{v',v} n_v' n_s - K_{v,v'} n_v n_s\right), \qquad v = 0, \ldots, v_{max}$$

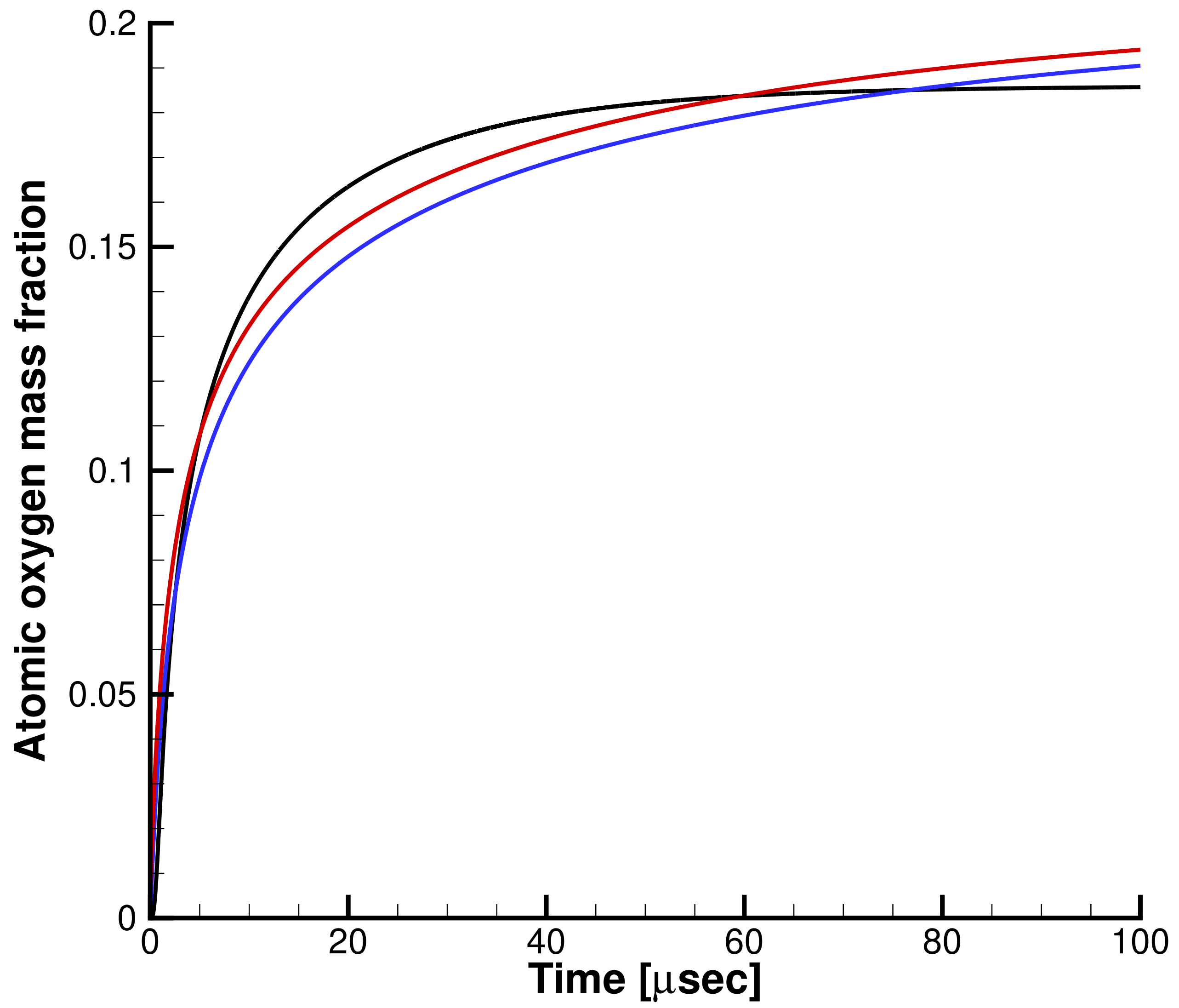
- Approach 2: implement state-to-state capabilities into Mutation++, which is coupled to existing CFD codes
  - In development
  - More easily extended to different configurations/mixtures

[1]Hanquist, Chaudhry, Boyd, Streicher, Krish, and Hansen, "Detailed Thermochemical Modeling of O2-Ar Mixtures in Reflected Shock Tube Flows," AIAA Paper 2020-3275.
[2]Scoggins, Leroy, Bellas-Chatzigeorgis, Dias, and Magin. "Mutation++: MUlticomponent Thermodynamic And Transport properties for IONized gases in C++". SoftwareX 12, 2020.

Results – Assess RBF mapping approach

- Mach 9.44 oxygen flow at ~40 km altitude [1]
- O2-O2 and O2-O rates[2]

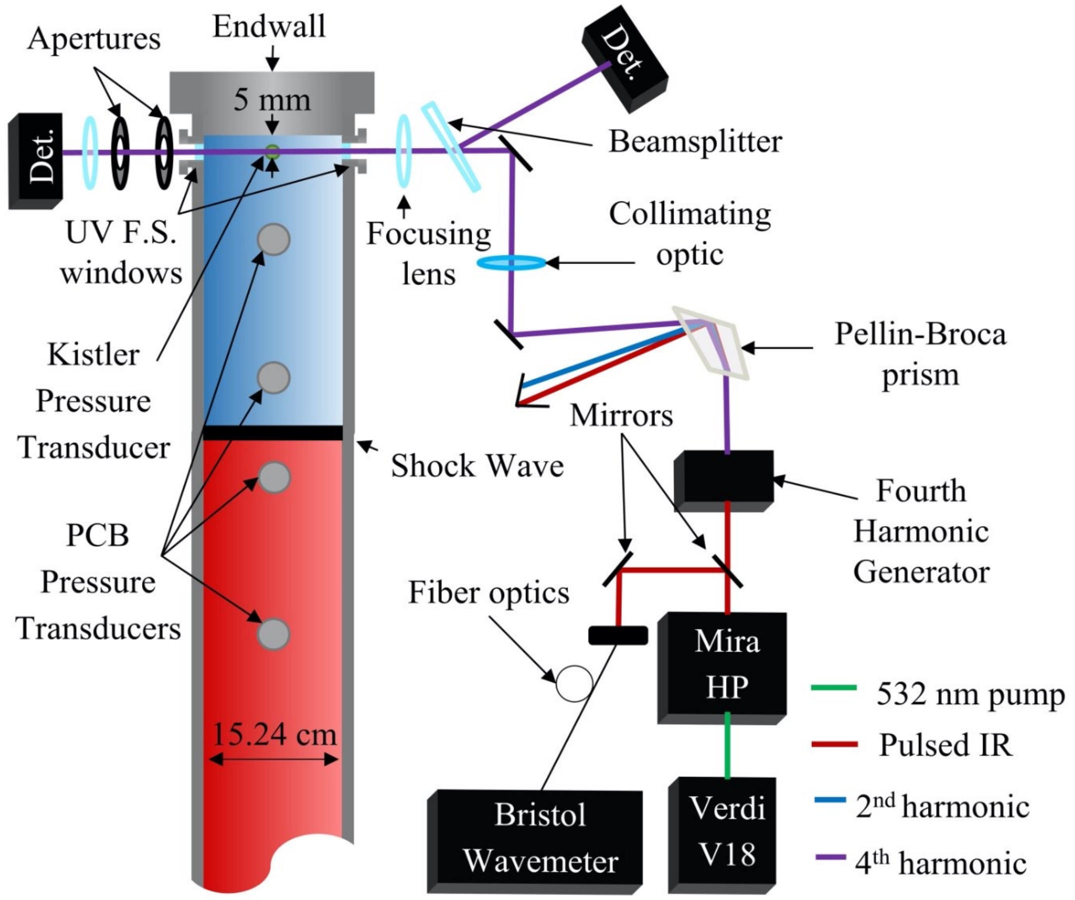




[1]Ibraguimova, Sergievskaya, Levashov, Shatalov, Tunik, and Zabelinkii, The Journal of Chemical Physics, 2013.
[2]Andrienko and Boyd, Physics of Fluids, 2015; Chemical Physics, 2017; The Journal of Chemical Physics, 2016.

Approach 1 – State-to-State Modeling

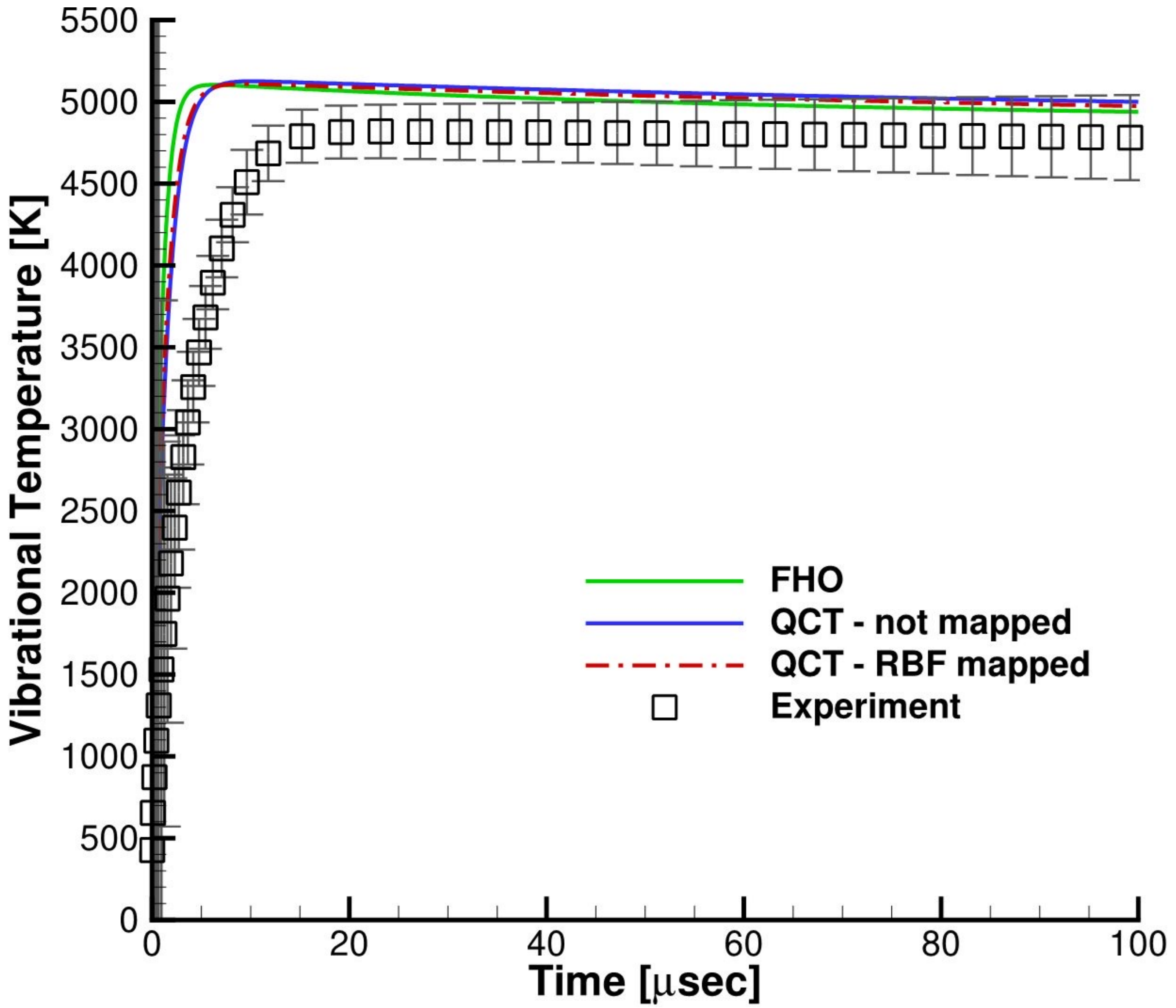
- Oxygen diluted in argon flows[1]
- O_2-O_2 and O_2-O rates[2]
- O2-Ar rates[3]



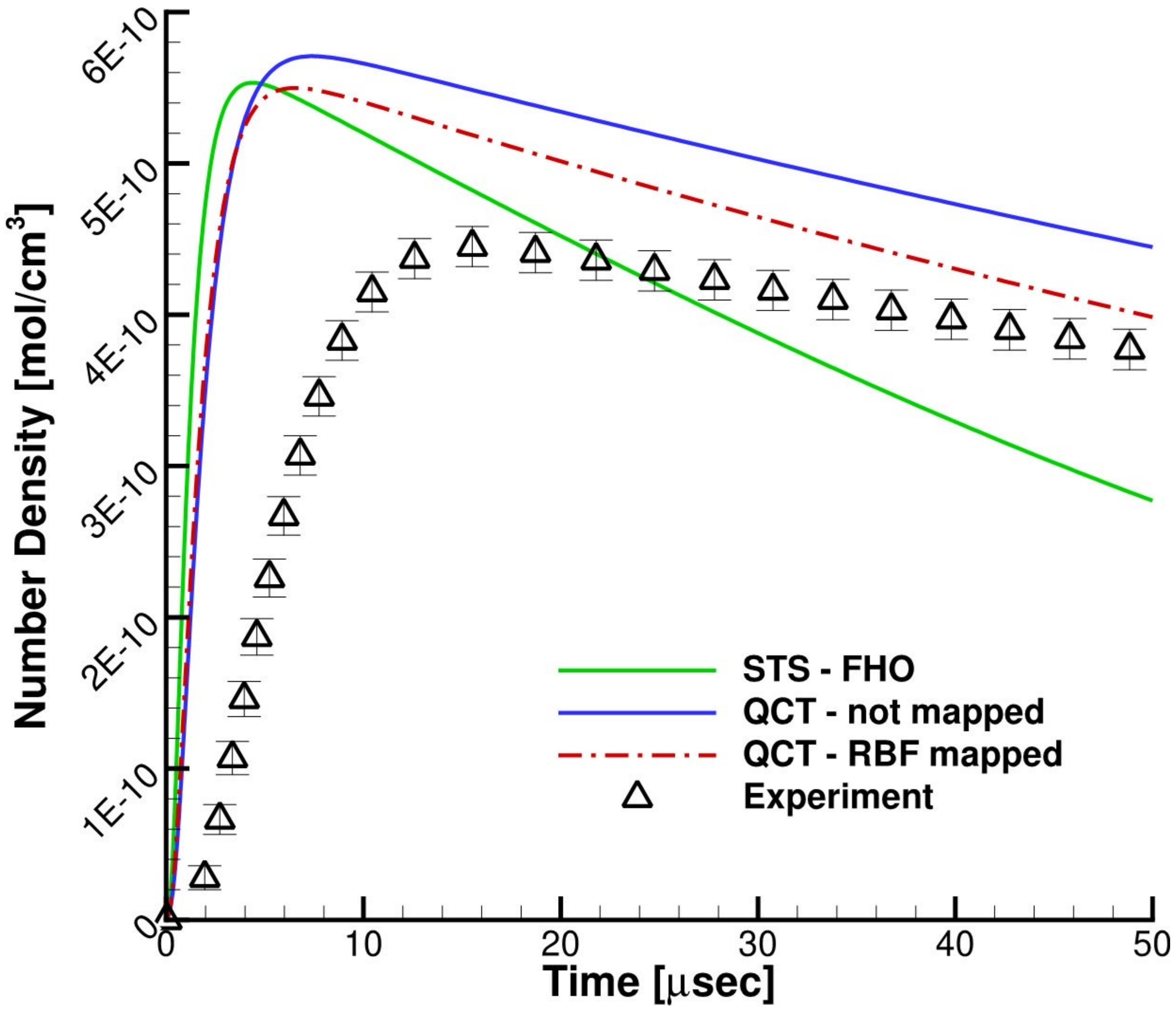
Case	*5280 K Case*	*10710 K Case*
Shock Velocity		
Incident [km/s]	1.55	2.24
Reflected [km/s]	0.79	1.09
Before Incident Shock		
Composition [mol fraction O_2]	0.02	0.05
Pressure [torr]	2.25	0.08
Temperature [K]	296	296
Between Incident/Reflected Shock		
Composition [mol fraction O_2]	0.02	0.05
Pressure [torr]	65.4	4.56
Temperature [K]	2,400	4,700
After Reflected Shock		
Pressure [torr]	344	28
Temperature [K]	5,300	10,700

[1]Streicher, Krish, Hanson, Hanquist, Chaudhry, and Boyd, "Shock-tube measurements of coupled vibration-dissociation time-histories and rate parameters in oxygen and argon mixtures from 5,000-10,000 K," Physics of Fluids, 2020.
[2]Andrienko and Boyd, Physics of Fluids, 2015; Chemical Physics, 2017; The Journal of Chemical Physics, 2016.
[3]Kim and Boyd, Chemical Physics, 2014.

Results – Diluted Oxygen Flows – 5280 K case

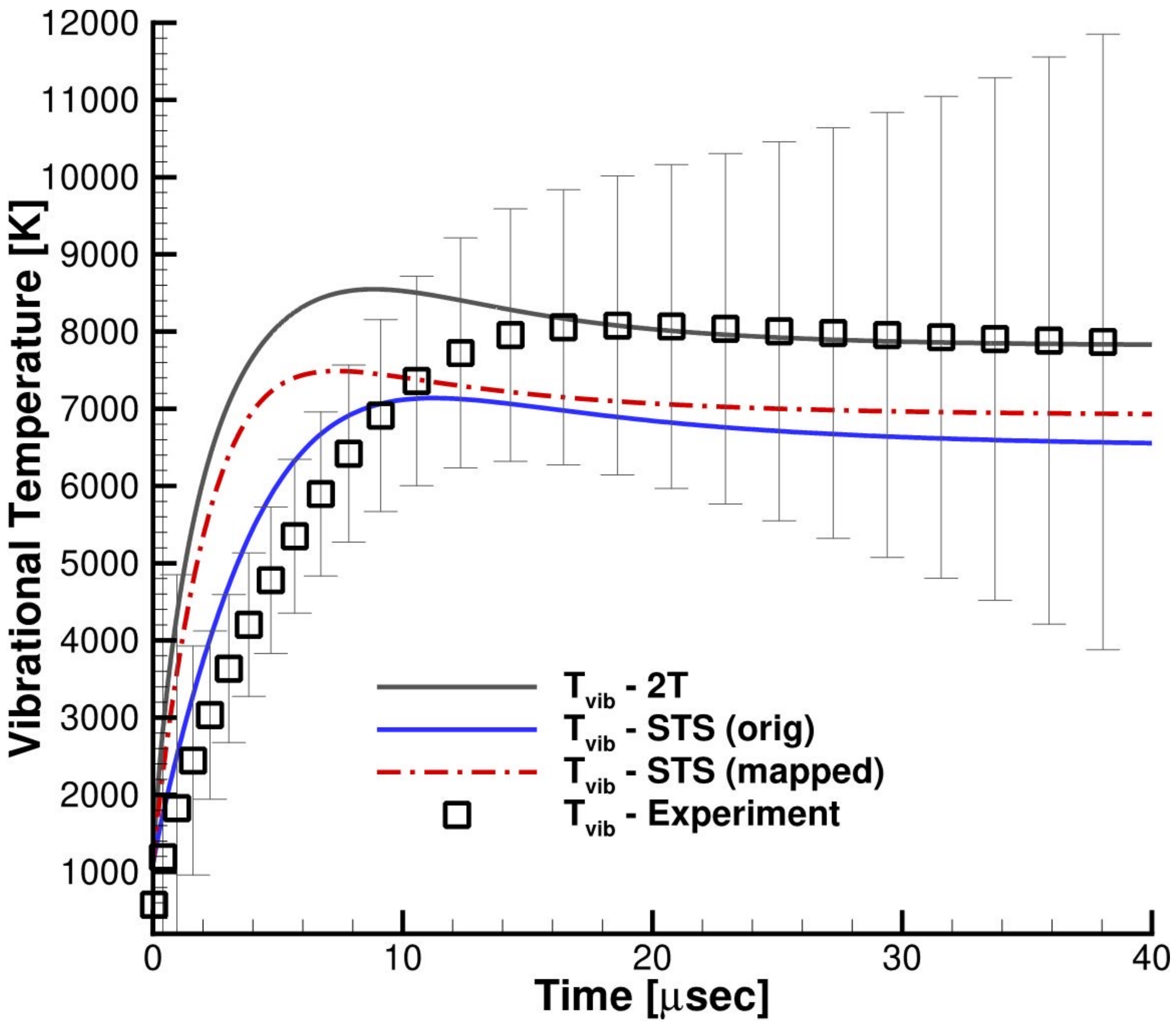


Vibrational temperature

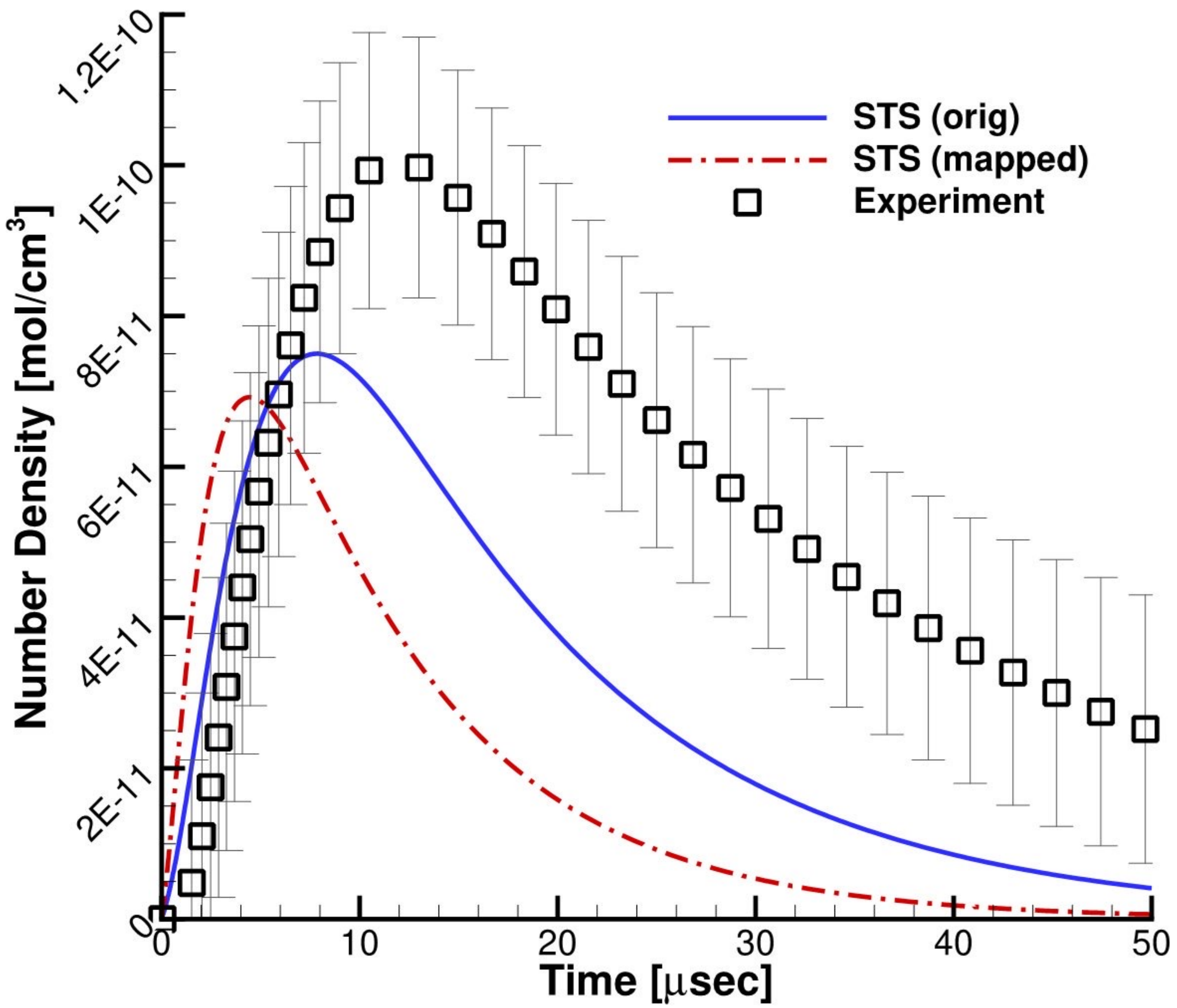


6th vibrational state of O_2

Results – Diluted Oxygen Flows – 10,710 K case

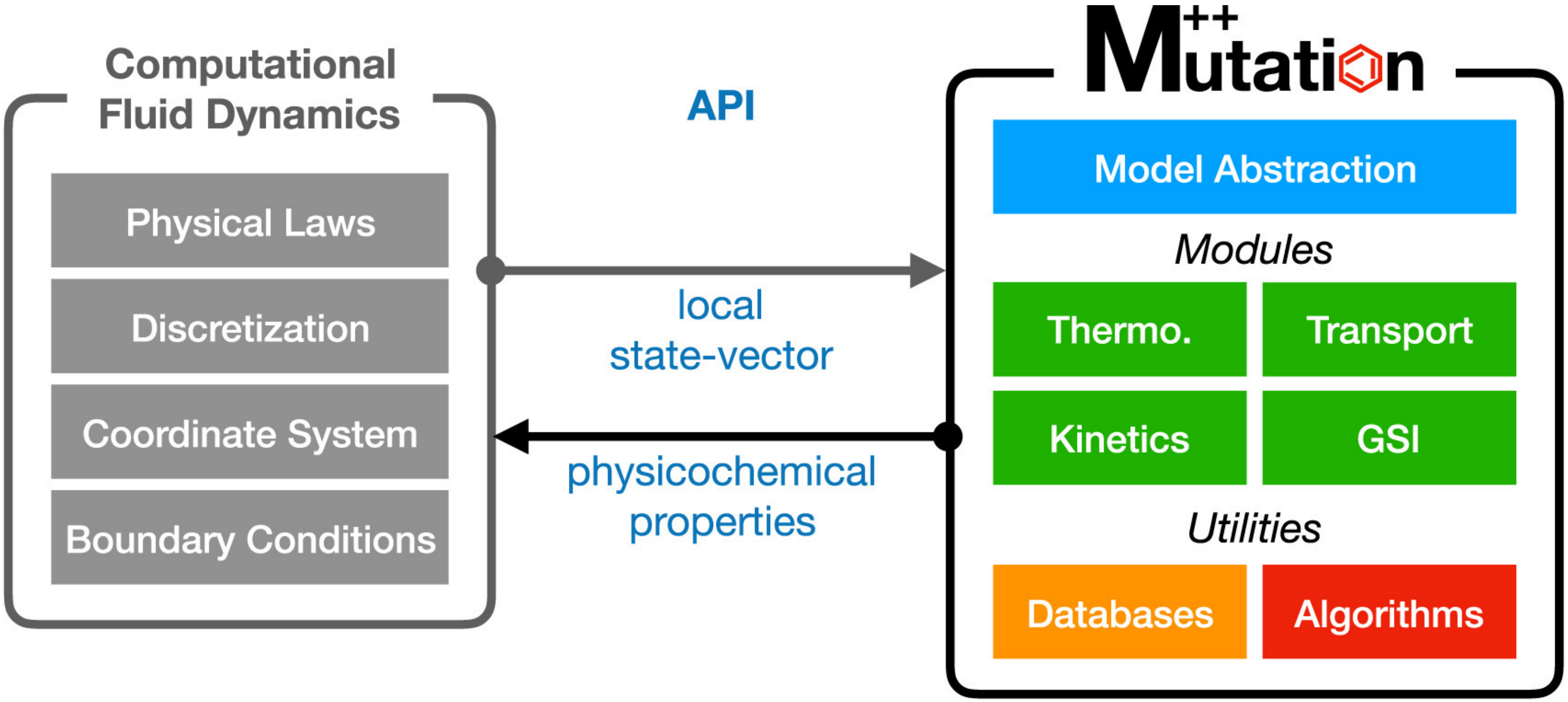


Vibrational temperature



6th vibrational state of O_2

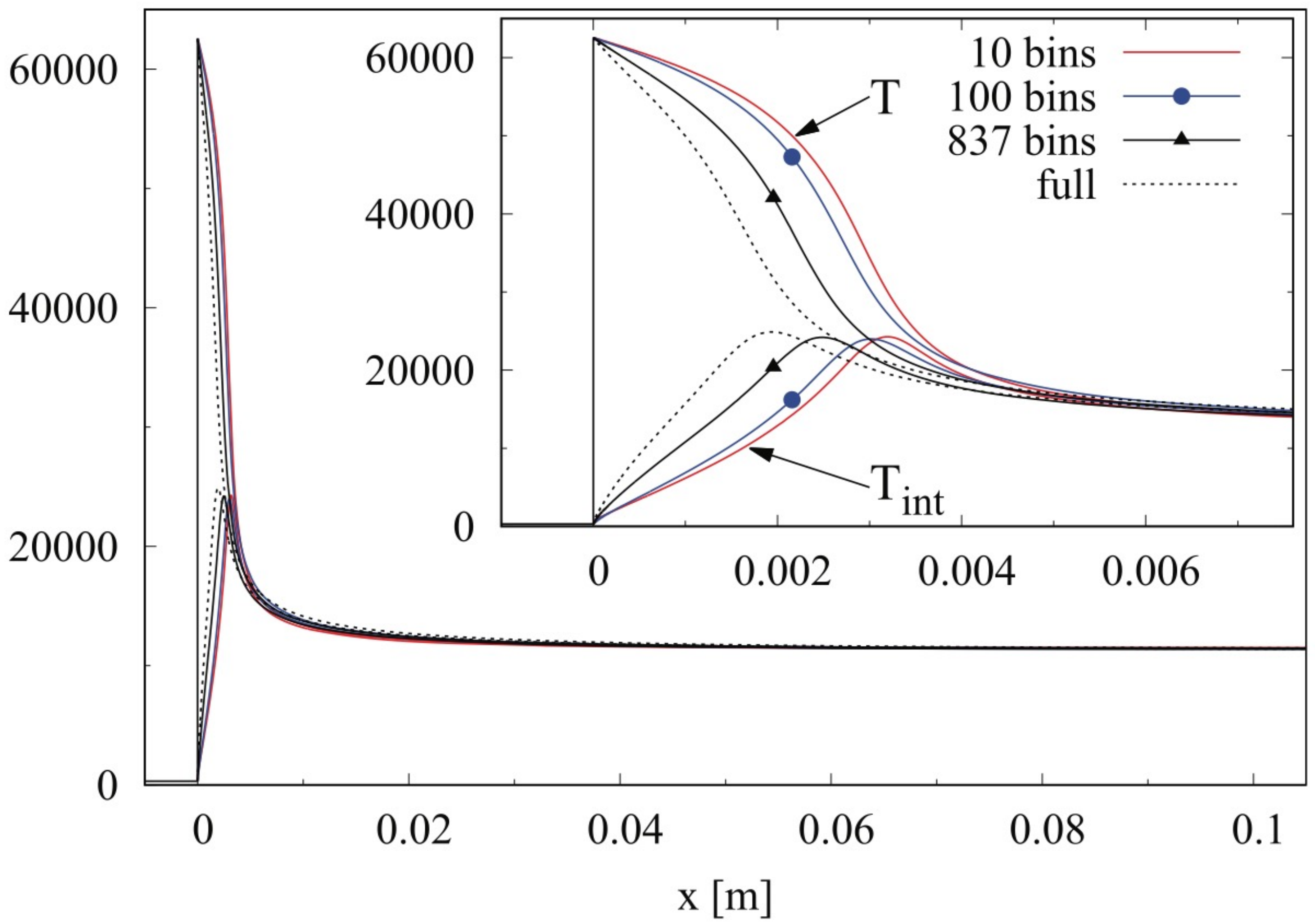
Approach 2 – State-to-State and Mutation++

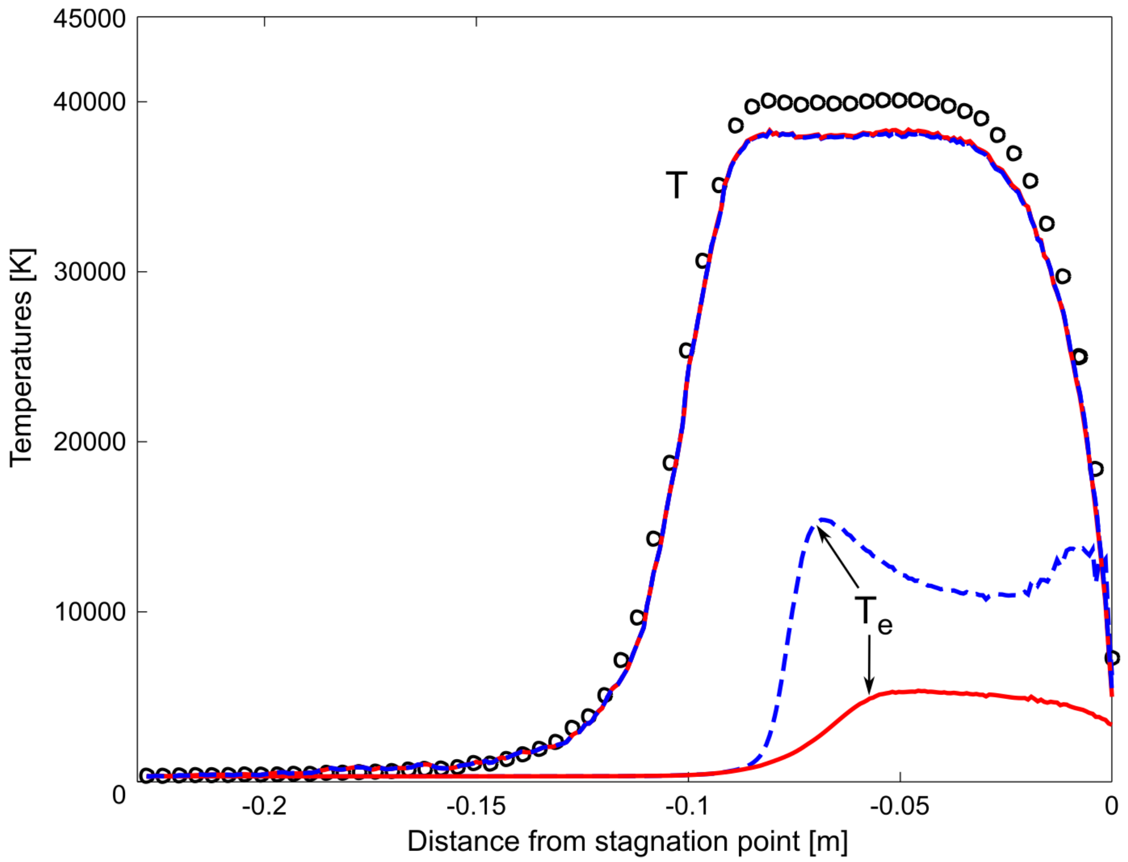


Scoggins, Leroy, Bellas-Chatzigeorgis, Dias, and Magin. ”Mutation++: MUlticomponent Thermodynamic And Transport properties for IONized gases in C++”. SoftwareX 12, 2020.

Approach 2 – State-to-State and Mutation++

- We are not the first to perform state-to-state in Mutation++
  - Rovibrational binning of nitrogen - Torres et al.
  - Collisional radiative of electronically excited argon flows - Boccelli et al.
  - *But we are trying to create a generic state-resolved framework in Mutation++*





[1]Torres, Bellas-Chatzigeorgis, and Magin, "How to build coarse-grain transport models consistent from the kinetic to fluid regimes ," Physics of Fluids, 2020.

[2]Boccelli, Bariselli, Dias, and Magin, "Lagrangian diffusive reactor for detailed thermochemical computations of plasma flows ," Plasma Sources Sci. Technol., 2019.

Approach 2 – State-to-State and Mutation++

- Mutation++ requires:
  - Mixtures ✓
  - Rates ✓
  - Thermodynamic database
    - Specific Heat
    - Enthalpy
    - Entropy
    - Gibbs Free Energy

Approach 2 – State-to-State and Mutation++

$$s_{\text{tr}} = NK\left[1 + \ln\left(\frac{Q}{N}\right) + T\partial_T\left[\ln\left(Q\right)\right]\right]$$
$$e_{\text{tr}} = RT^2\partial_T\left[\ln\left(Q\right)\right]$$
$$h_{\text{tr}} = e_{\text{tr}} + pv$$
$$(c_p)_{\text{tr}} = \left(\frac{\partial e_{\text{tr}}}{\partial T}\right)_V + R$$
$$g_{\text{tr}} = h_{\text{tr}} - Ts_{\text{tr}}$$

$$s_{\text{int}} = NK\left[\ln\left(\frac{Q}{N}\right) + T\partial_T\left[\ln\left(Q\right)\right]\right]$$
$$e_{\text{int}} = RT^2\partial_T\left[\ln\left(Q\right)\right]$$
$$h_{\text{int}} = e_{\text{int}}$$
$$(c_p)_{\text{int}} = \left(\frac{\partial e_{\text{int}}}{\partial T}\right)_P$$
$$g_{\text{int}} = h_{\text{int}} - Ts_{\text{int}}$$

Approach 2 – State-to-State and Mutation++
Translational Mode

$$Q_{\mathrm{tr}} = \sum_{a \in \mathcal{A}} \exp\left(-\frac{(\varepsilon_{\mathrm{tr}})_a}{kT}\right) = \sum_{n_1, n_2, n_3} \exp\left(-\frac{h^2}{8mkT}\left[\frac{n_1^2}{a_1^2} + \frac{n_2^2}{a_2^2} + \frac{n_3^2}{a_3^2}\right]\right)$$

$$\begin{aligned} s_{\mathrm{tr}} &= Nk\left[1 + \ln\left(\frac{Q_{\mathrm{tr}}}{N}\right) + T\partial_T[\ln(Q_{\mathrm{tr}})]\right] \\ &= R\left[\frac{5}{2}\ln(kT) - \ln(P) + \ln\left(\left[\frac{2\pi m}{h^2}\right]^{3/2}\right) + \frac{5}{2}\right] \end{aligned}$$

$$h_{\mathrm{tr}} = e_{\mathrm{tr}} + pv = RT^2\partial_T[\ln(Q_{\mathrm{tr}})] + RT = \frac{5}{2}RT$$

$$(c_p)_{\mathrm{tr}} = \left(\frac{\partial e_{\mathrm{tr}}}{\partial T}\right)_V + R = \frac{3}{2}R + R = \frac{5}{2}R$$

Approach 2 – State-to-State and Mutation++

Rotational Mode

$$Q_{\text{rot}} = \sum_{j=0}^{\infty} (2J+1)\exp\left(-\frac{\theta_{\text{rot}} J(J+1)}{T}\right) \approx \int_0^{\infty} (2J+1)\exp\left[-\frac{\theta_{\text{rot}}}{T} J(J+1)\right] dJ = \frac{T}{\sigma\theta_{\text{rot}}}$$

$$s_{\text{rot}} = -\frac{\partial}{\partial T}\left[-NkT\ln\left[Q_{\text{rot}}\right]\right] = R\left[\ln\left(\frac{T}{\sigma\theta_{\text{rot}}}\right)+1\right]$$

$$h_{\text{rot}} = RT^2\frac{\partial}{\partial T}\left[\ln\left(\frac{T}{\theta_{\text{rot}}}\right)\right] = RT$$

$$(c_p)_{\text{rot}} = \left(\frac{\partial e_{\text{rot}}}{\partial T}\right)_V = R$$

Approach 2 – State-to-State and Mutation++

Vibrational Mode

$$Q_{\text{vib}} = \exp\left(-\frac{\varepsilon_i}{kT}\right)$$

$$s_{\text{vib}} = -\frac{\partial}{\partial T}\left[-NkT\ln\left[\exp\left(-\frac{\varepsilon_i}{kT}\right)\right]\right] = -\frac{\partial}{\partial T}\left[-NkT\left[-\frac{\varepsilon_i}{kT}\right]\right] = 0$$

$$h_{\text{vib}} = RT^2\frac{\partial}{\partial T}\left[\ln\left(\exp\left(-\frac{\varepsilon_i}{kT}\right)\right)\right] = RT^2\left(\frac{\varepsilon_i}{kT^2}\right) = R\varepsilon_i$$

$$(c_p)_{\text{vib}} = \left(\frac{\partial e_{\text{vib}}}{\partial T}\right)_V = 0$$

Approach 2 – State-to-State and Mutation++

Electronic Mode

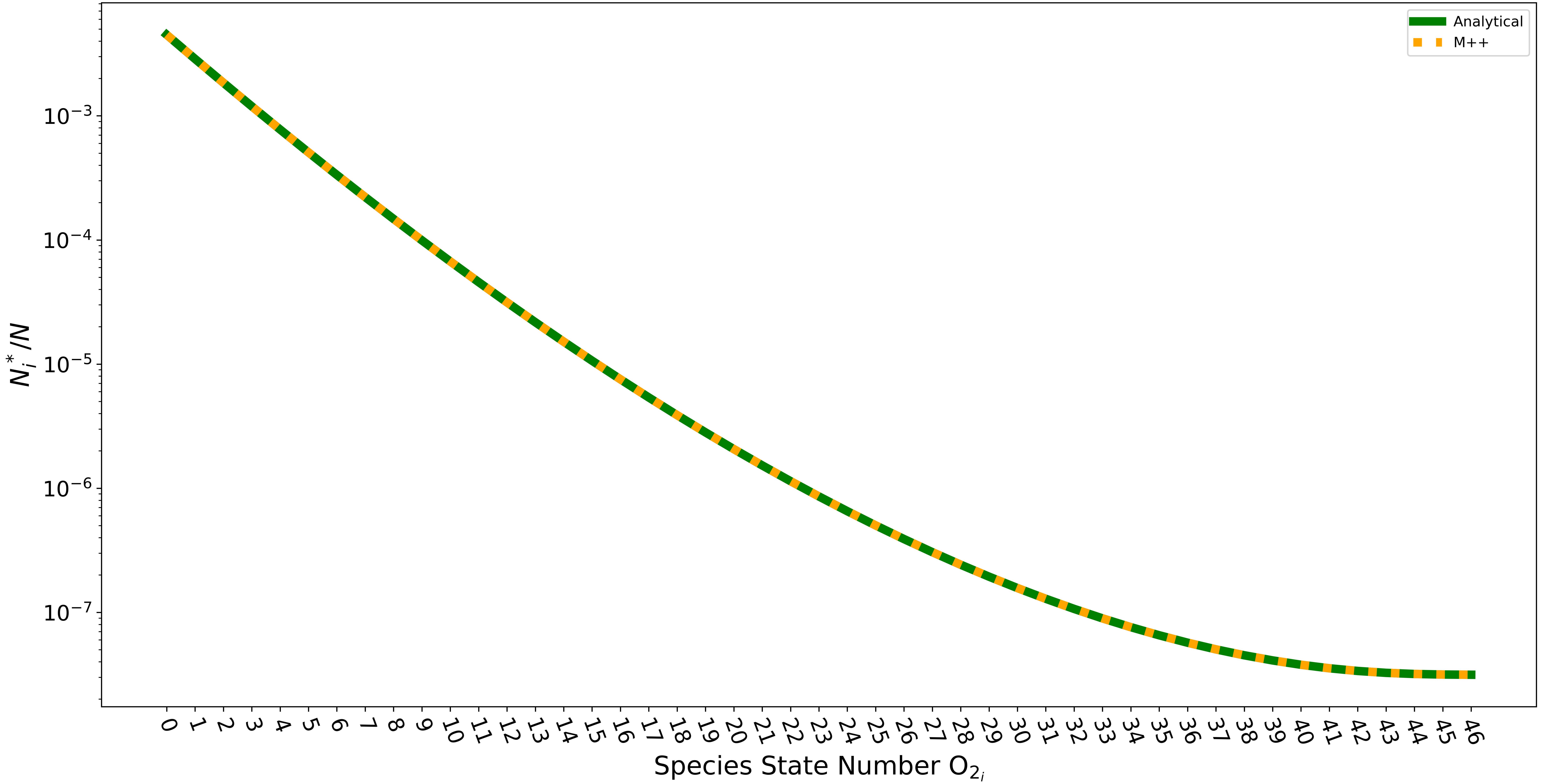
$$Q_{\mathrm{el}} = \sum_i g_i \exp\left(-\frac{\theta_i}{kT}\right)$$

$$\begin{aligned} s_{\mathrm{el}} &= -\frac{\partial}{\partial T}\left[-NkT \ln\left[g_0 \exp\left(-\frac{\theta_0}{T}\right) + g_1 \exp\left(-\frac{\theta_1}{T}\right)\right]\right] \\ &= R\left[\ln(g_0) + \ln\left\{1 + \frac{g_1}{g_0}\exp\left(-\frac{\theta_1}{T}\right)\right\} + \frac{(g_1/g_0)(\theta_1)(T)\exp(-\theta_1/T)}{1 + (g_1/g_0)\exp(-\theta_1/T)}\right] \end{aligned}$$

$$h_{\mathrm{el}} = RT^2 \frac{\partial}{\partial T}\left[g_0 + g_1 \exp\left(-\frac{\theta_1}{T}\right)\right] = RT^2\left[-\frac{g_1\theta_1\left(-\frac{1}{T^2}\exp\left(-\frac{\theta_1}{T}\right)\right)}{g_0 + g_1\exp\left(-\frac{\theta_1}{T}\right)}\right] = \frac{R\theta_1\left(\frac{g_1}{g_0}\right)\exp\left(-\frac{\theta_1}{R}\right)}{1 + \frac{g_1}{g_1}\exp\left(-\frac{\theta_1}{T}\right)}$$

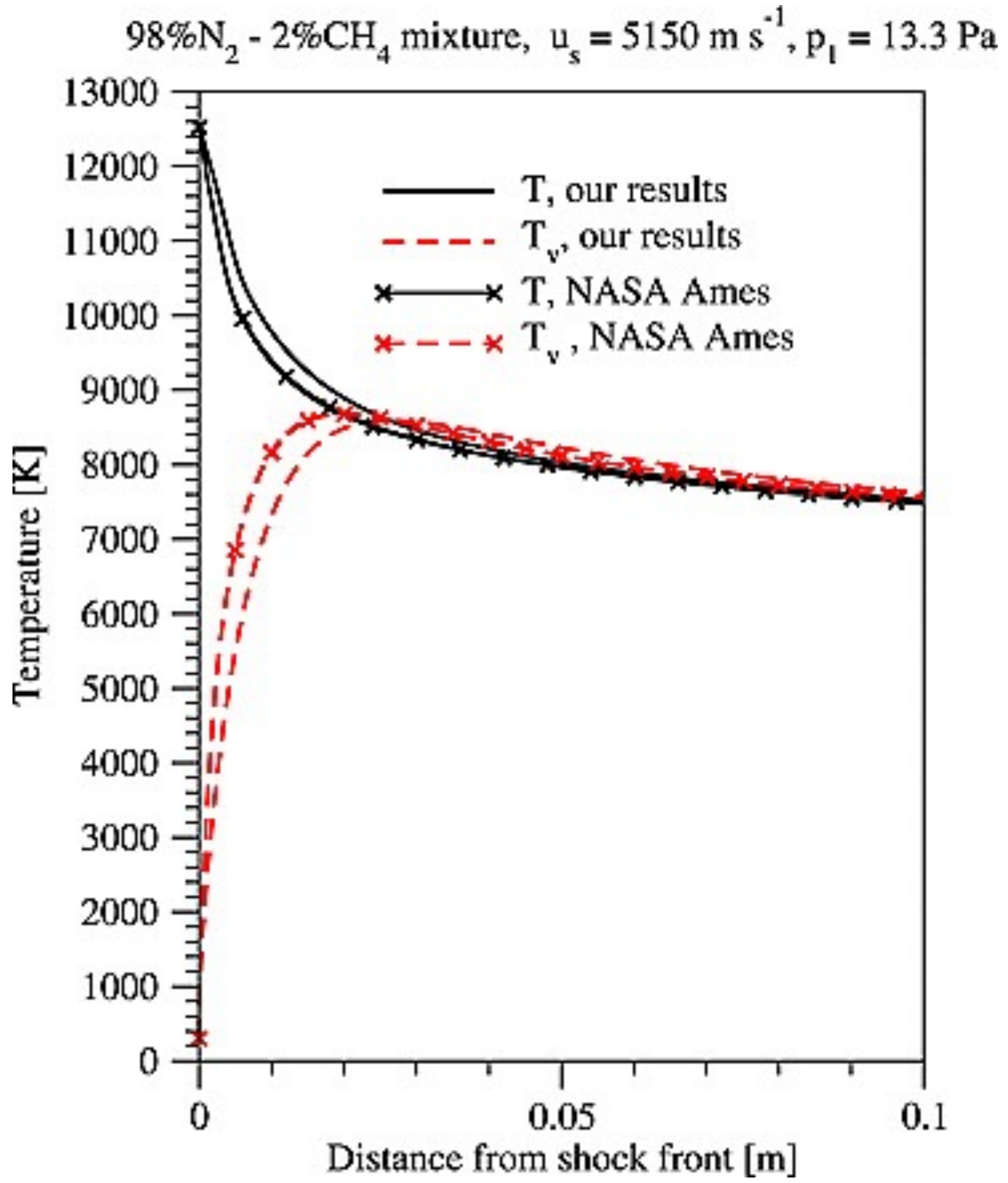
$$(c_p)_{\mathrm{el}} = \left(\frac{\partial e_{\mathrm{el}}}{\partial T}\right)_V = R\left(\frac{\theta_1}{T}\right)^2 \frac{\frac{g_1}{g_0}\exp\left(-\frac{\theta_1}{T}\right)}{\left[1 + \frac{g_1}{g_0}\exp\left(-\frac{\theta_1}{T}\right)\right]^2}$$

Boltzmann Distribution at Equilibrium using Thermodynamic Database at 5000 K



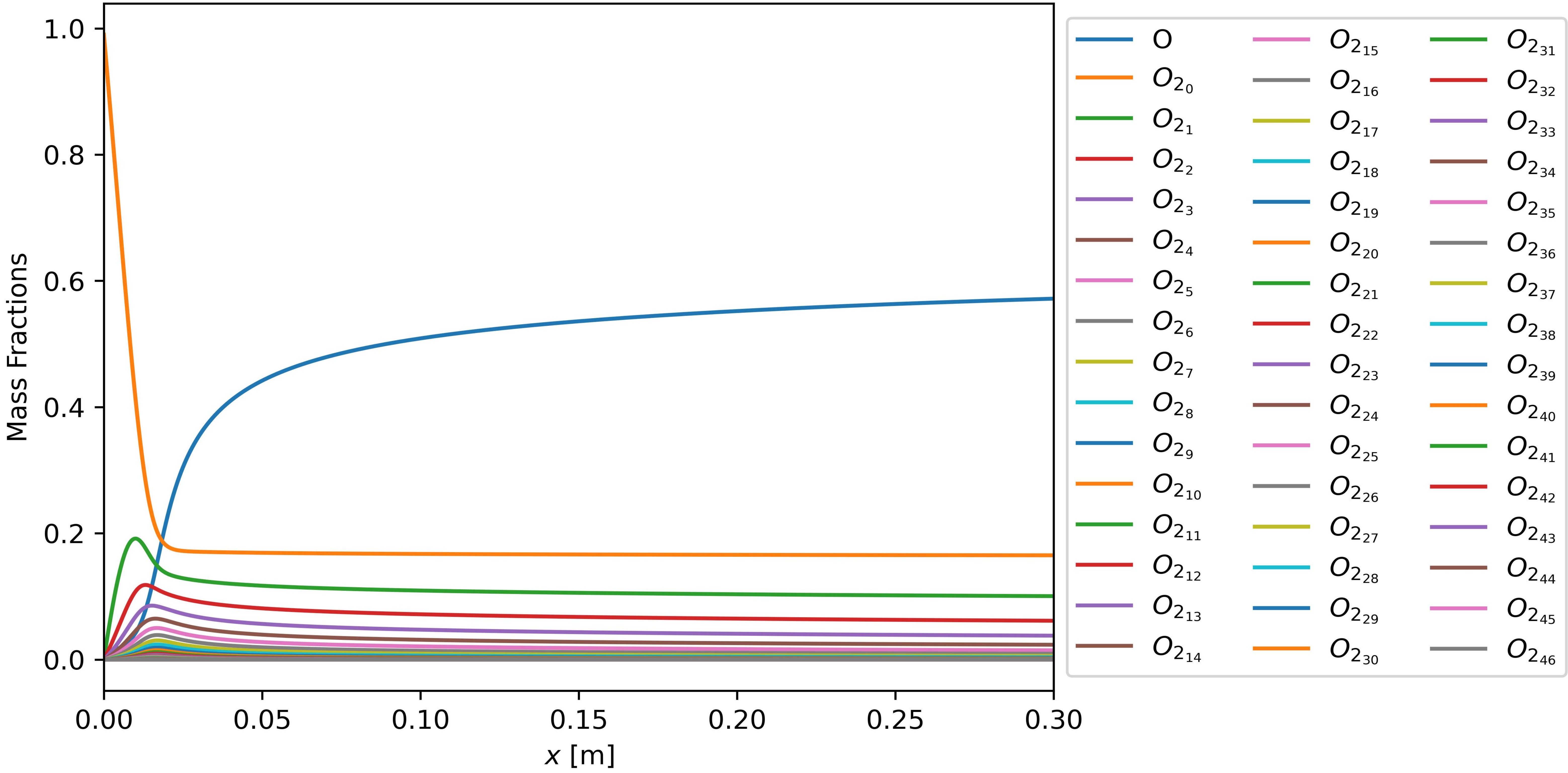
brODErs

- 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 = 31.18 Pa
  - Freestream Temperature = 250 K
  - Freestream Velocity = 5255 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



Mass Fractions
1.0
0.8
0.6
0.4
0.2
0.0
0.00
0.05
0.10
0.15
0.20
0.25
0.30
x [m]
O
$O2_0$
$O2_1$
$O2_2$
$O2_3$
$O2_4$
$O2_5$
$O2_6$
$O2_7$
$O2_8$
$O2_9$
$O2_{10}$
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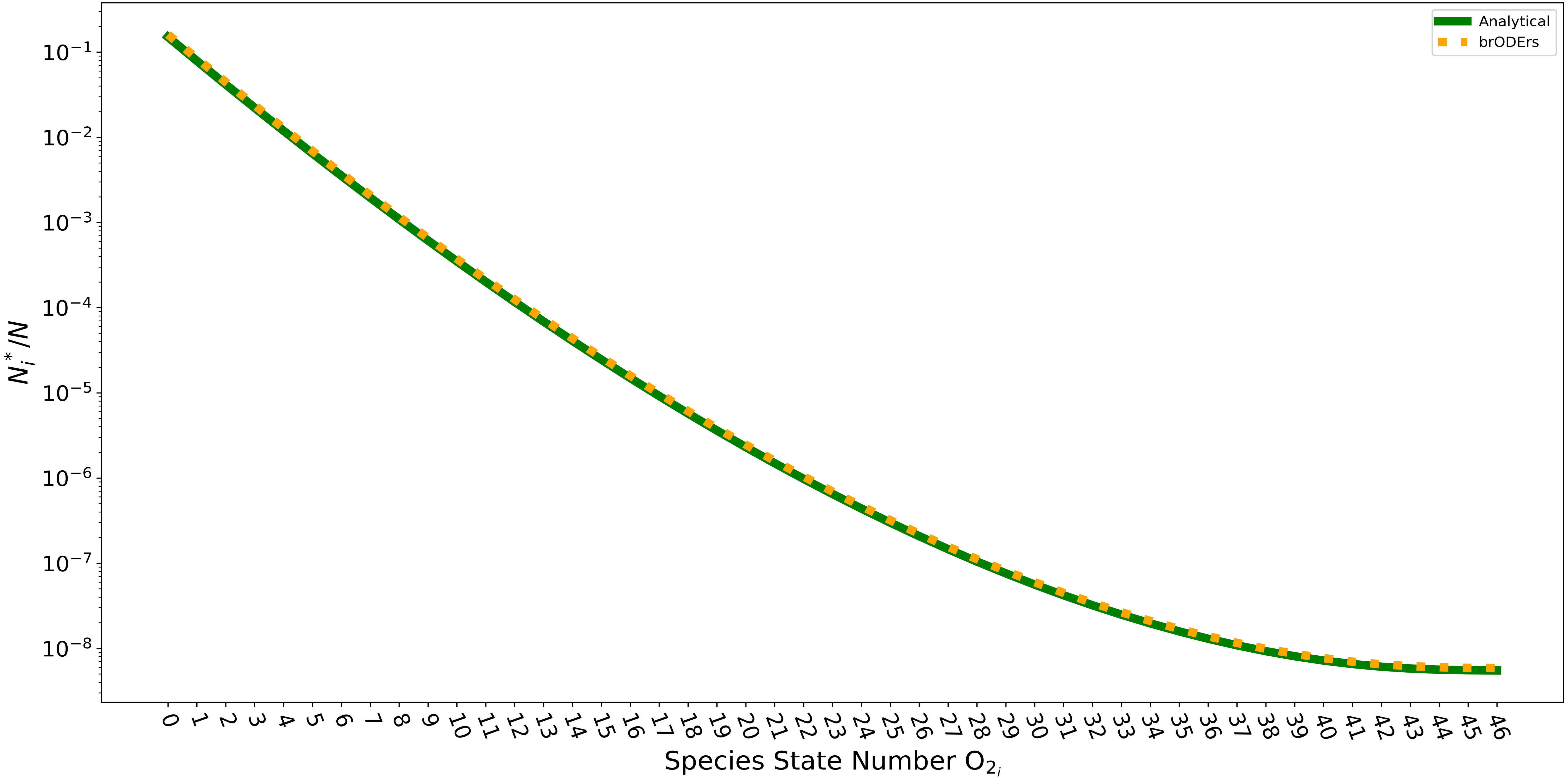
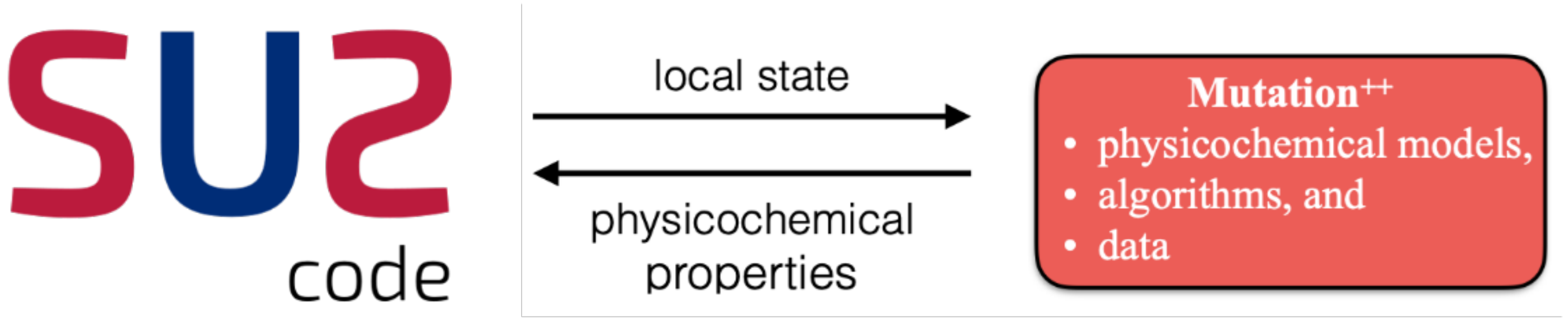
$O2_{44}$
$O2_{45}$
$O2_{46}$

brODErs



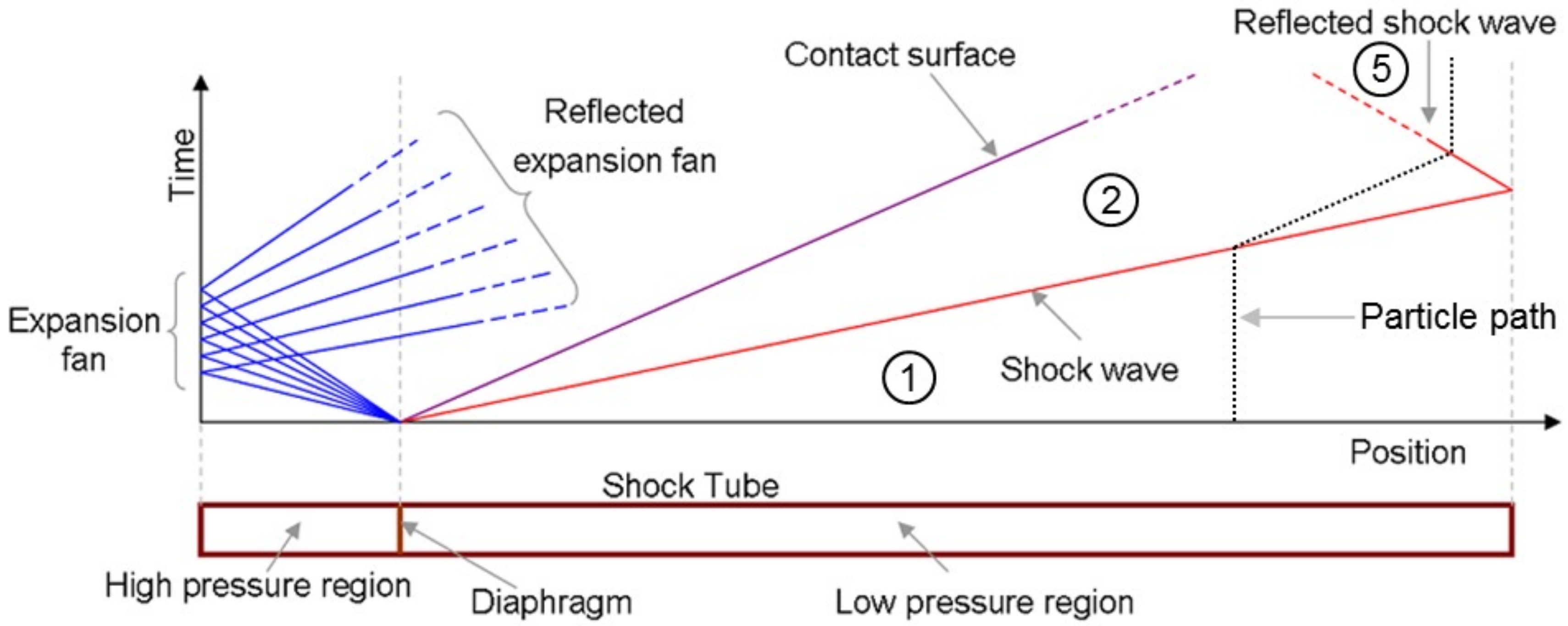
Analytical
brODErs
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
N_i^*/N
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46
Species State Number O_{2_i}

CFD – Unsteady

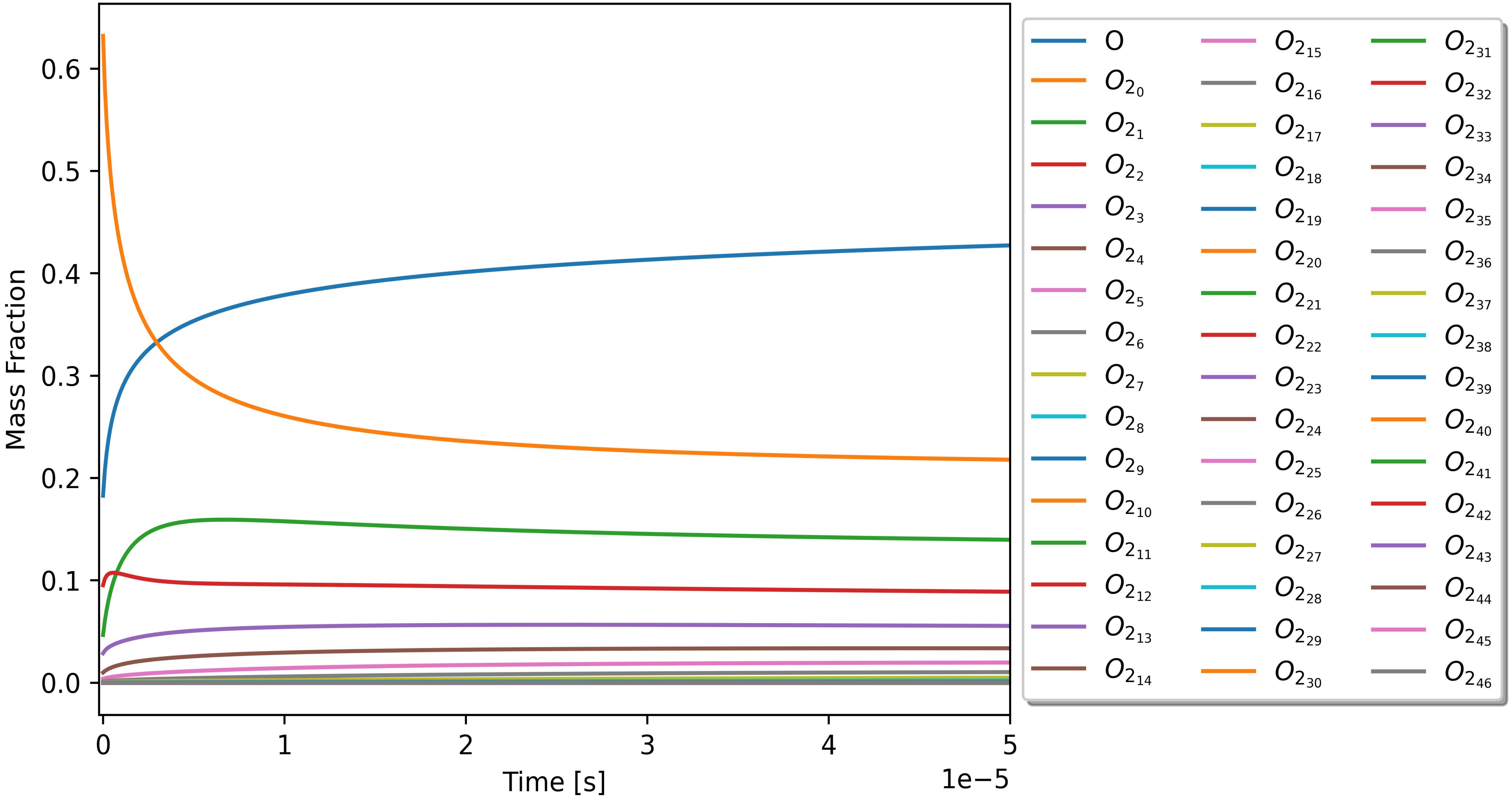


Maier, et al., AIAA Paper 2023-3488

- Euler Solver
- Mesh: 5x5 Grid
- Boundary Conditions
  - Symmetry walls (no boundary layer effects)
- SU2-NEMO CFD Code
- Test Case: Heat Bath (section 5 of reflected shock tube)
- T = 15,000 K, P = 11040 Pa

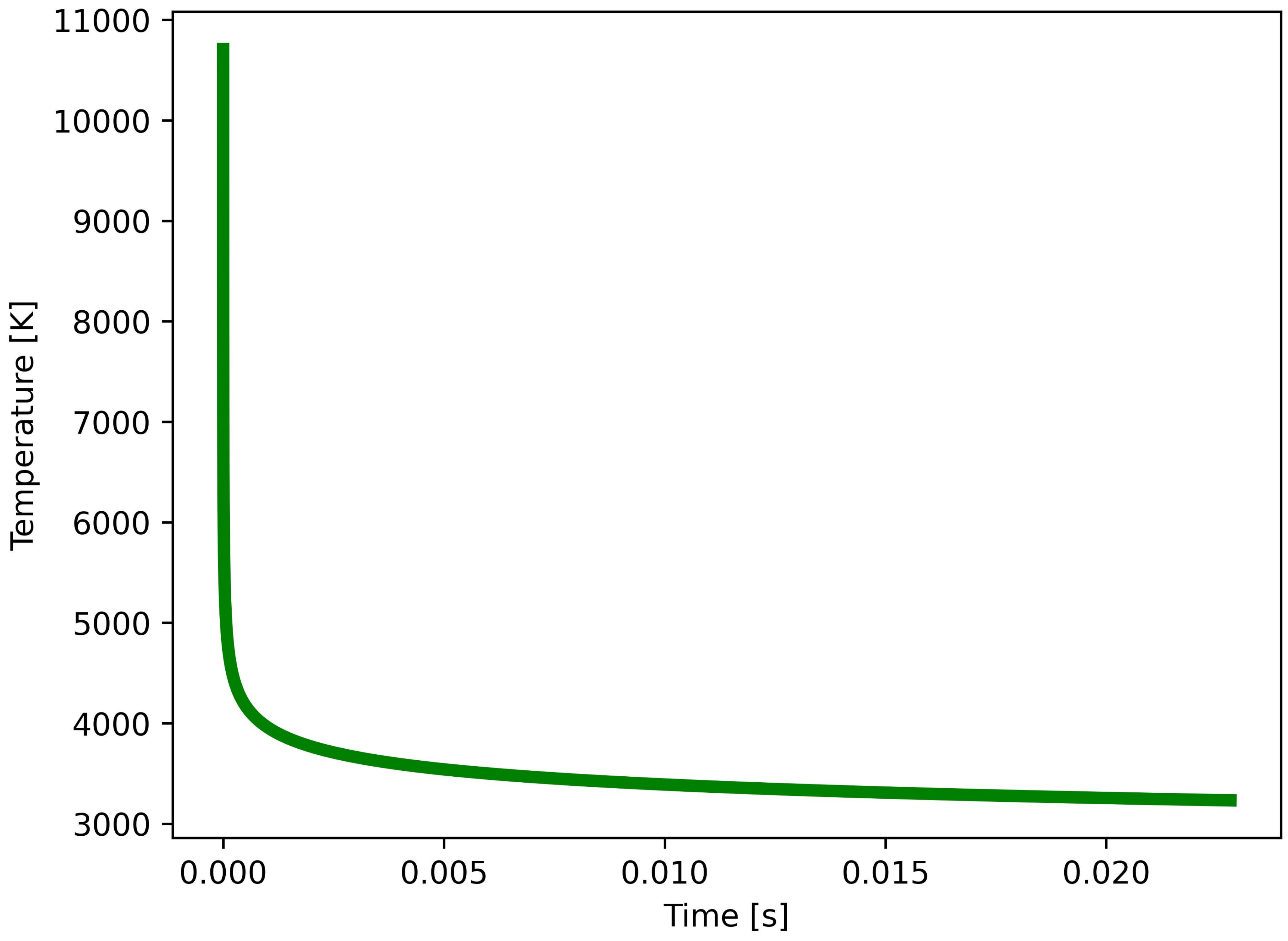


CFD – Unsteady

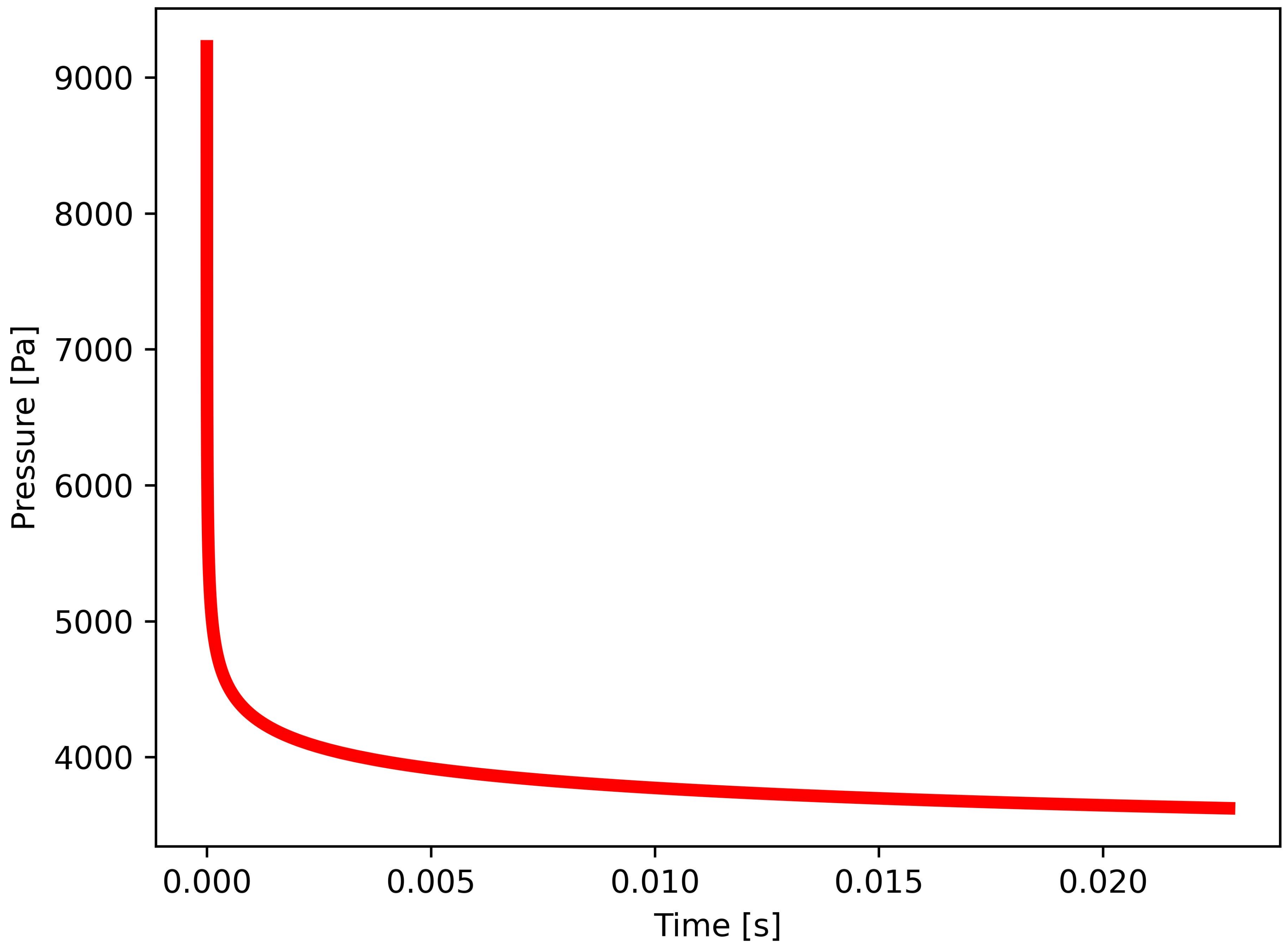


CFD – Unsteady

Translational Temperature

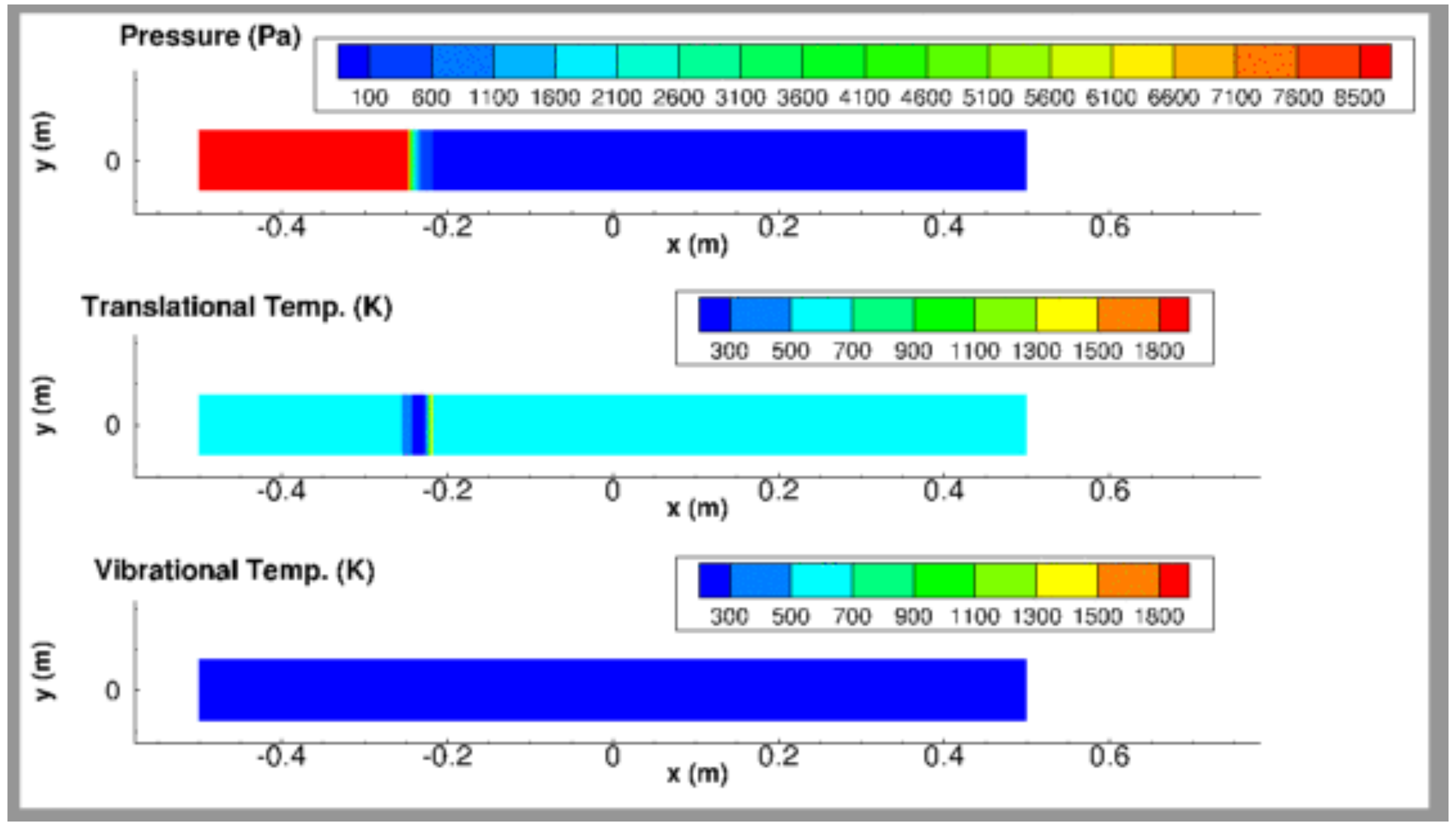


Pressure



Future work

- Refine mapping appraoch
    - Binning approach (10 state?)
    - Machine learning/physics informed for rates
- Run in shock tube to assess thermal bath assumption
    - Are we not matching experimental data due to rates or assumptions (e.g., heat bath)?
    - Our talk on Monday
- Assess modeling approach with recent Hansen group data



Coupled vibration-dissociation time-histories and rate measurements in shock-heated, nondilute O_2 and O_2–Ar mixtures from 6000 to 14 000 K

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  - Georgios Bellas

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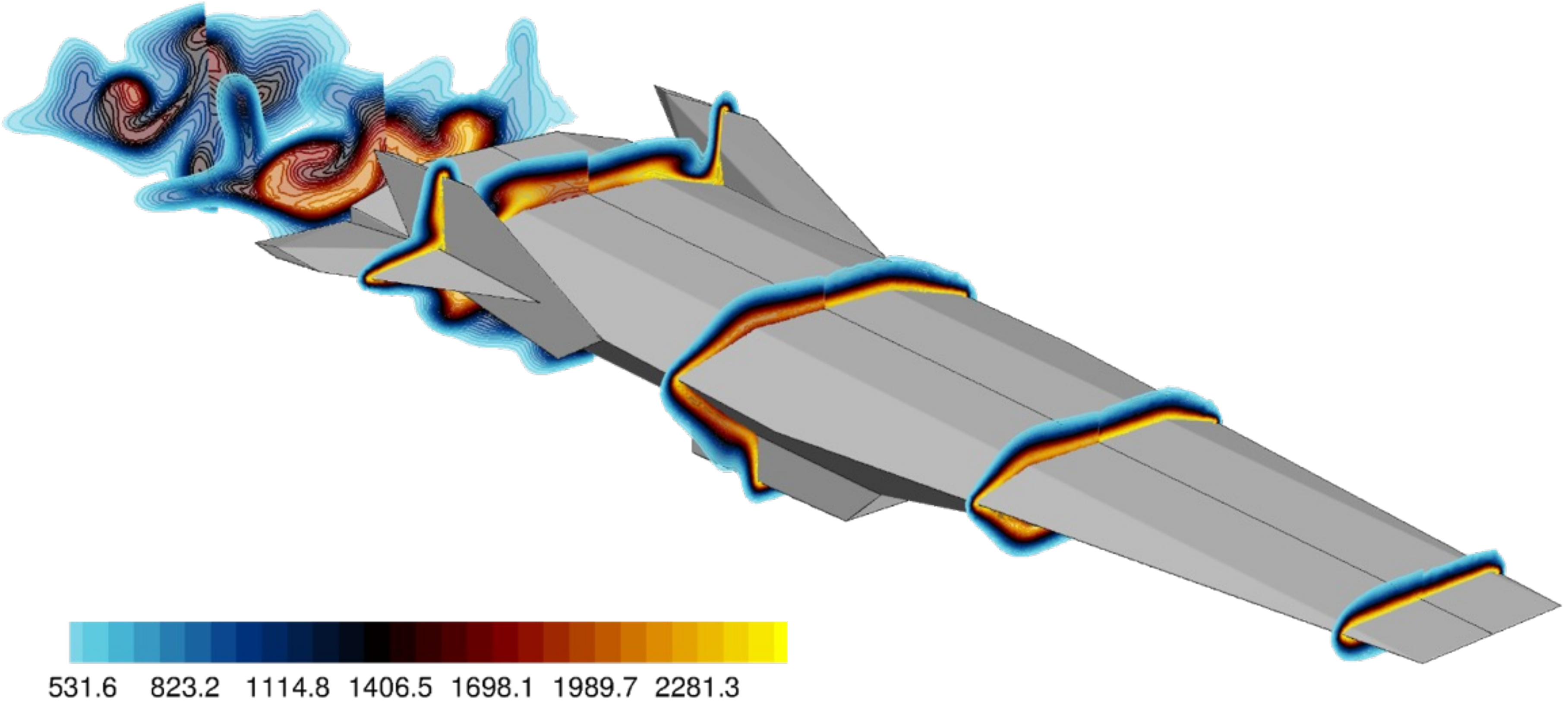
  - AFRL Summer Faculty Program (cleared for public distribution under case AFRL-2022-4769)
  - Computational resources and services provided by the University of Arizona's Research Data Center (RDC)



QUESTIONS/DISCUSSION

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