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1. REPORT DATE (DD-MM-YYYY) 17 July 2016		2. REPORT TYPE Briefing Charts		3. DATES COVERED (From - To) 07 June 2016 – 17 July 2016	
4. TITLE AND SUBTITLE Comparison of DSMC Reaction Models with QCT Reaction Rates for Nitrogen				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) I. Wysong, S. Gimelshein				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER Q1MK	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/RQRC 10 E. Saturn Blvd. Edwards AFB, CA 93524-7680				8. PERFORMING ORGANIZATION REPORT NO.	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/RQR 5 Pollux Drive Edwards AFB, CA 93524-7048				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S) AFRL-RQ-ED-VG-2016-146	
12. DISTRIBUTION / AVAILABILITY STATEMENT Approved for Public Release; Distribution Unlimited. The U.S. Government is joint author of the work and has the right to use, modify, reproduce, release, perform, display, or disclose the work.					
13. SUPPLEMENTARY NOTES For presentation at AFOSR Aerothermochemistry Program Review; Arlington VA and Symposium on Rarefied Gas Dynamics; Victoria BC Canada (2 different meetings) (13-17 July) PA Case Number: #16299 ; Clearance Date: 6/14/2016 Prepared in collaboration with ERC					
14. ABSTRACT Viewgraph/Briefing Charts					
15. SUBJECT TERMS N/A					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT SAR	18. NUMBER OF PAGES 20	19a. NAME OF RESPONSIBLE PERSON I Wysong
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NO (include area code) N/A

Comparison of DSMC Reaction Models with QCT Reaction Rates for Nitrogen

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Introduction

- Comparison with measurements is final goal
- Validation challenge: many parameters and assumptions needed to model shock experiments
- Need to examine them for chemistry and vibrational relaxation models
- Recent years: many detailed QCT computations, especially for $\text{N}_2\text{-N}_2$ and $\text{N}_2\text{-N}$
- These data provide basis for benchmarking and accuracy analysis of fast empirical models

Objective

- Our project seeks to recommend and improve simplified microscopic models and connect them to macroscopic counterparts
- This work is first step: use recent high quality QCT calculations for model verification and parameter adjustment
- Four chemistry models: total collision energy (TCE), quantum kinetic (QK), vibration-dissociation favoring (VFD), and weak vibrational bias (Bias)

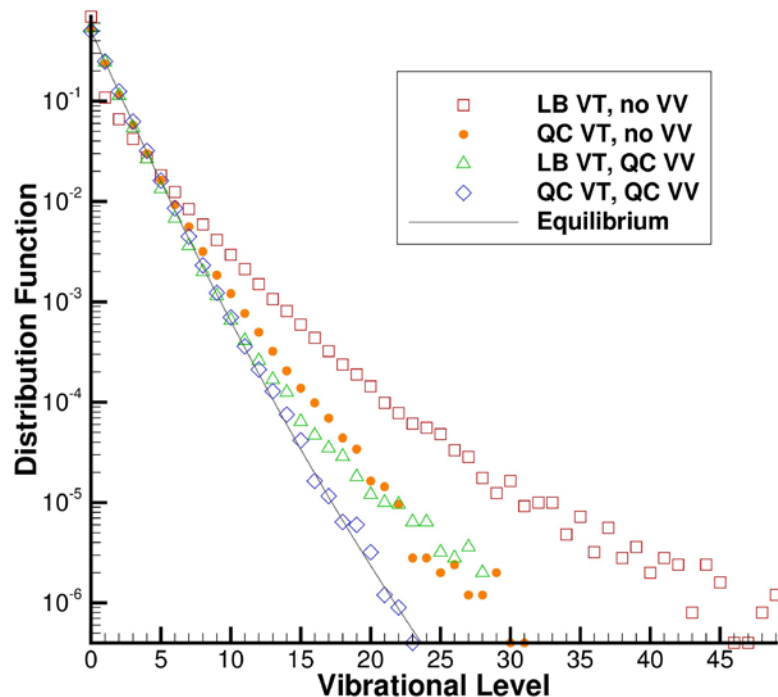
Numerical Approach

- **DSMC method:** SMILE tool extended to include Bias and QK models
- **Homogeneous bath:** N_2 and N
- **Translationally isothermal:** velocities re-sampled every time step
- **Majorant frequency scheme:** modified to correct for larger than 1 reaction probability in Bias model
- **VHS model:** d and ω to match high-T viscosity
- **Diameter** of N_2 depends on internal state (v, J)
- **Internal energy modes:** continuum rotational, discrete vibrational (AHO)

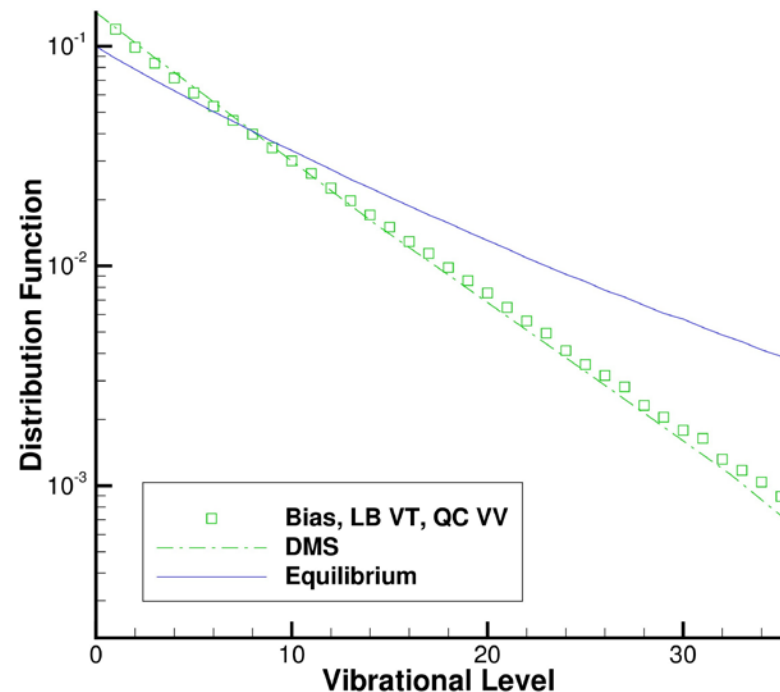
Vibrational Energy Transfer

VT: Larsen-Borgnakke model with $Z_v(T)$ prohibiting double relaxation - matching QCT for all T

VV: QC model



VV reduces unphysical overrepresentation of ground level (transient state at $T_v=4,500\text{K}$)



Reasonable agreement with QCT (QSS state at $T=30,000\text{K}$)

Non-Coupled Dissociation Models

TCE model: reaction occurs when $E = E_t + E_r + E_v > D$
with probability

$$P = a_1 \frac{(E - D)^{b_1}}{E^{c_1}}$$

a_1, b_1, c_1 depend on Arrhenius and VHS/VSS
parameters and molecular properties

TCE is tied to VHS/VSS interaction model

QK model: reaction occurs during VT energy
transfer when

$$\text{Integer} \left[\frac{E_t + E_v}{k \theta_v} \right] > \frac{D}{k \theta_v}$$

QK is integrated with Larsen-Borgnakke VT transfer

Models Coupled with Vibrations

VFD model: reaction occurs when $E - E_v > D$ with

a_2, b_2, c_2 depend on Arrhenius and VHS/VSS
 ϕ is free parameter that controls vibration coupling

Bias model: reaction occurs when $E_t + E_v > D$ with

$$P = A \left(1 - \frac{D - E_v}{E_t} \right) \exp \left(\lambda \left(\frac{E_v}{D} \right) \right)$$

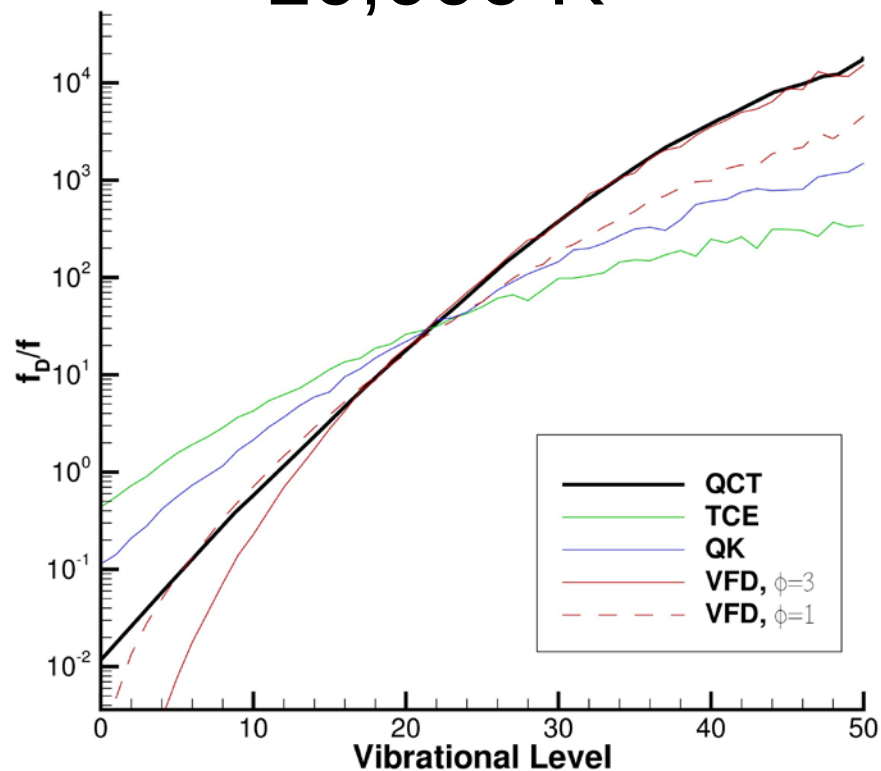
λ controls vibration coupling

A is adjusted to match thermal reaction rate

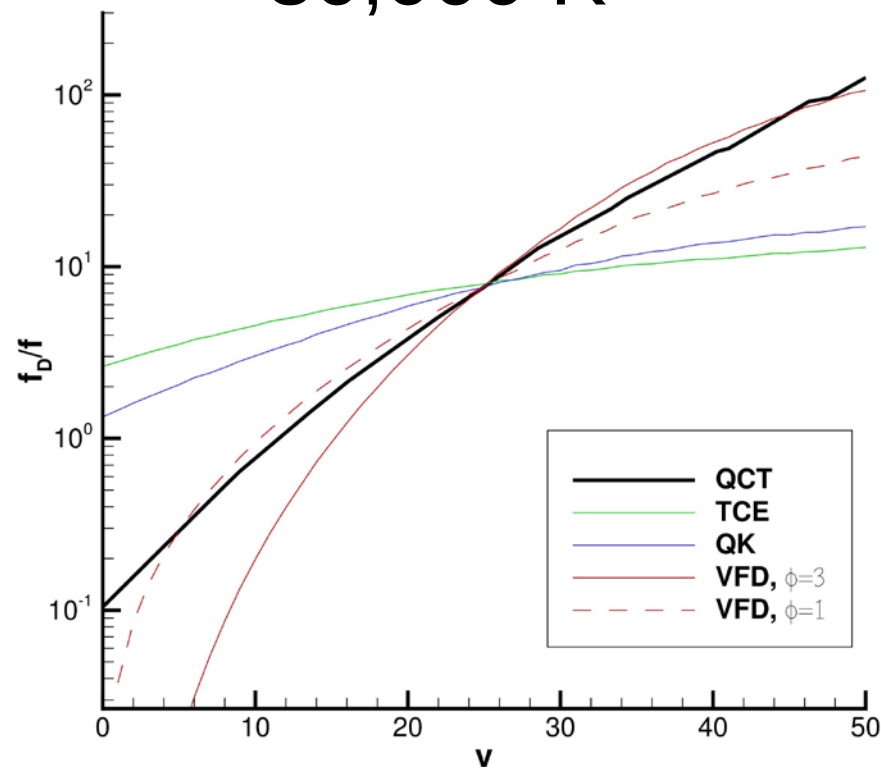
Simplest to implement, not tied to any other model

Dissociating-to-Total Vibrational Distribution Ratio, N_2-N_2 at QSS

10,000 K



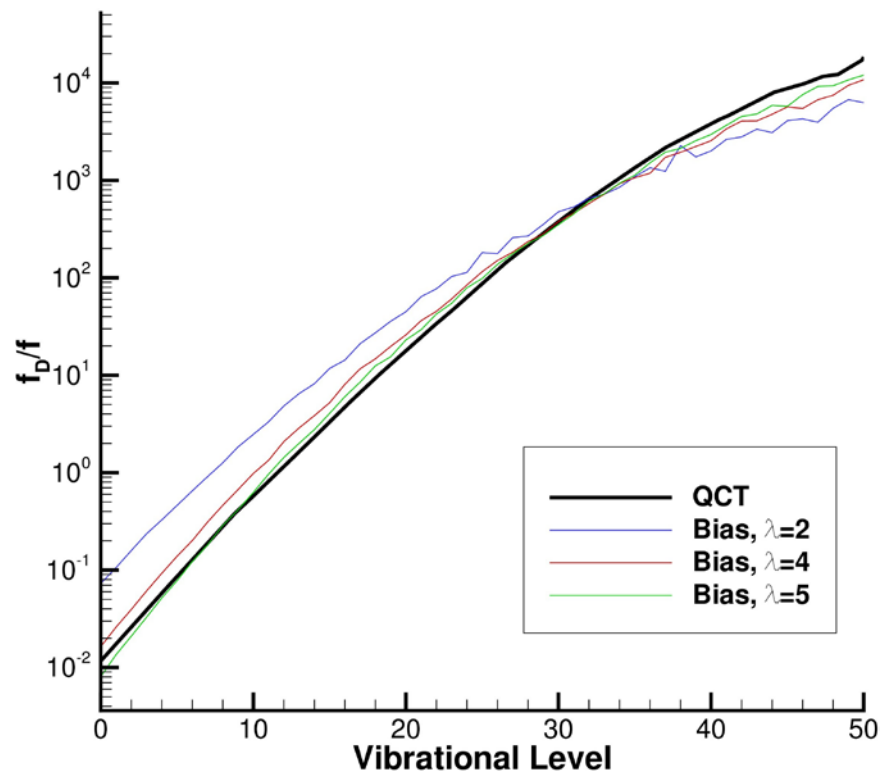
30,000 K



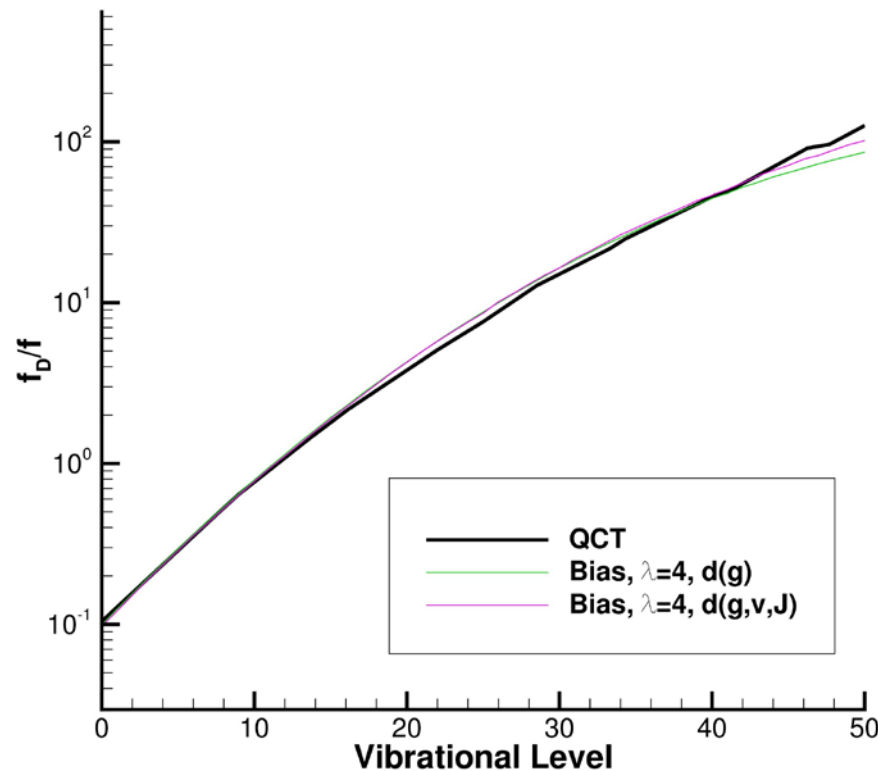
- **General trend:** reaction rate increases with v
- **TCE, QK:** lack of vibrational favoring results in much lower slope as compared to the benchmark QCT
- **VFD:** $\phi=1$ only works for lower levels, $\phi=3$, for high levels

Vibrational Distribution for Bias Model

10,000 K

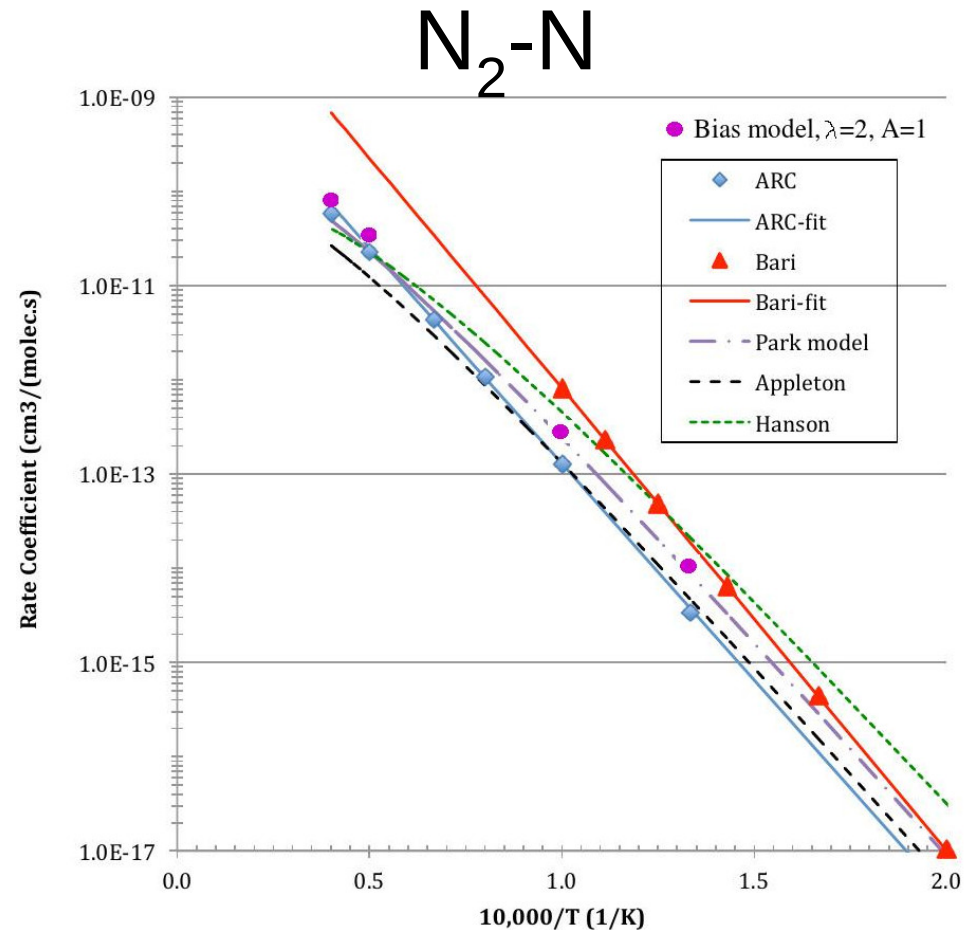
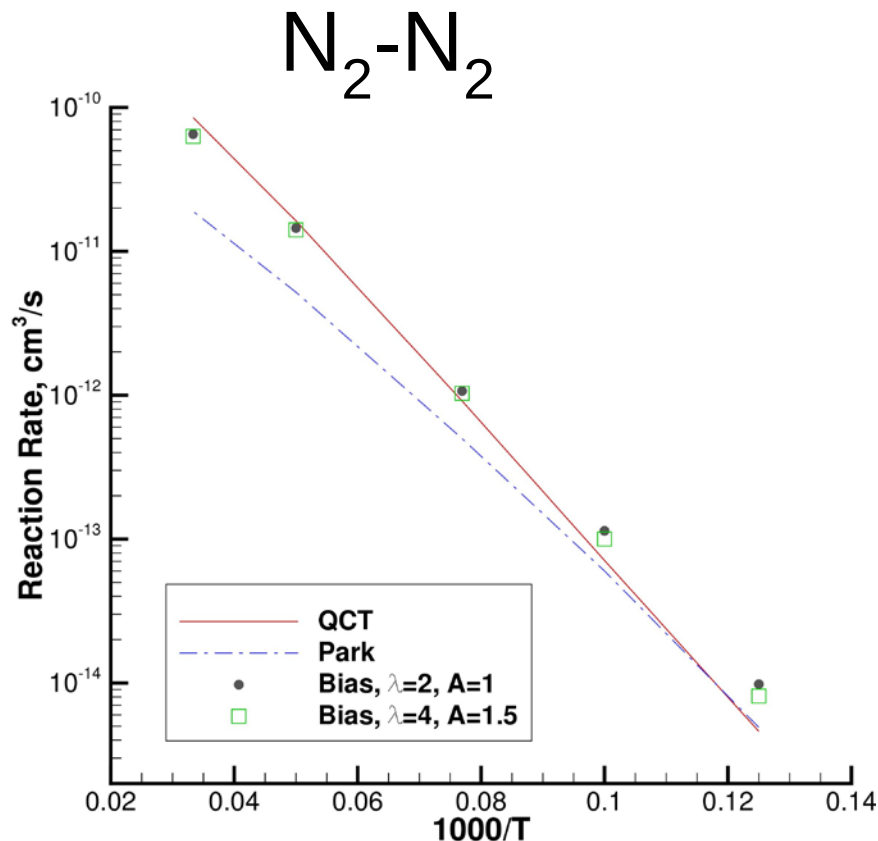


30,000 K



- Excellent fit
- 10,000 K: $\lambda=4$ and $\lambda=5$ work well
- 30,000 K: $\lambda=4$ provides best fit
- Impact of diameter increasing with v and J is small

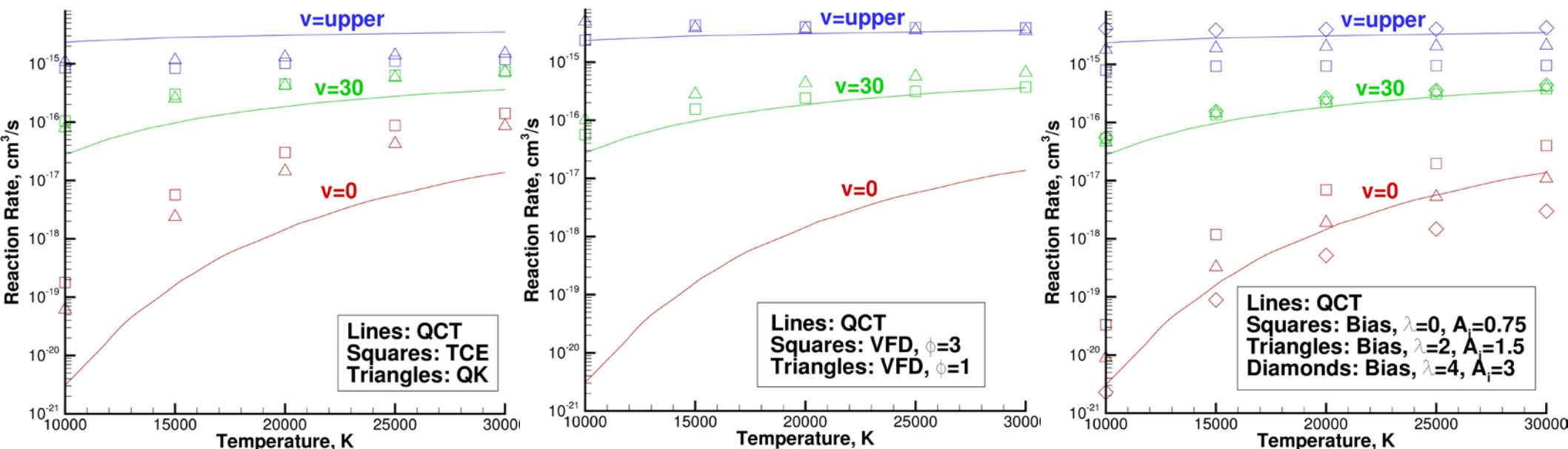
Total Equilibrium Reaction Rates



Adapted from Jaffe et al AIAA 2016-0503

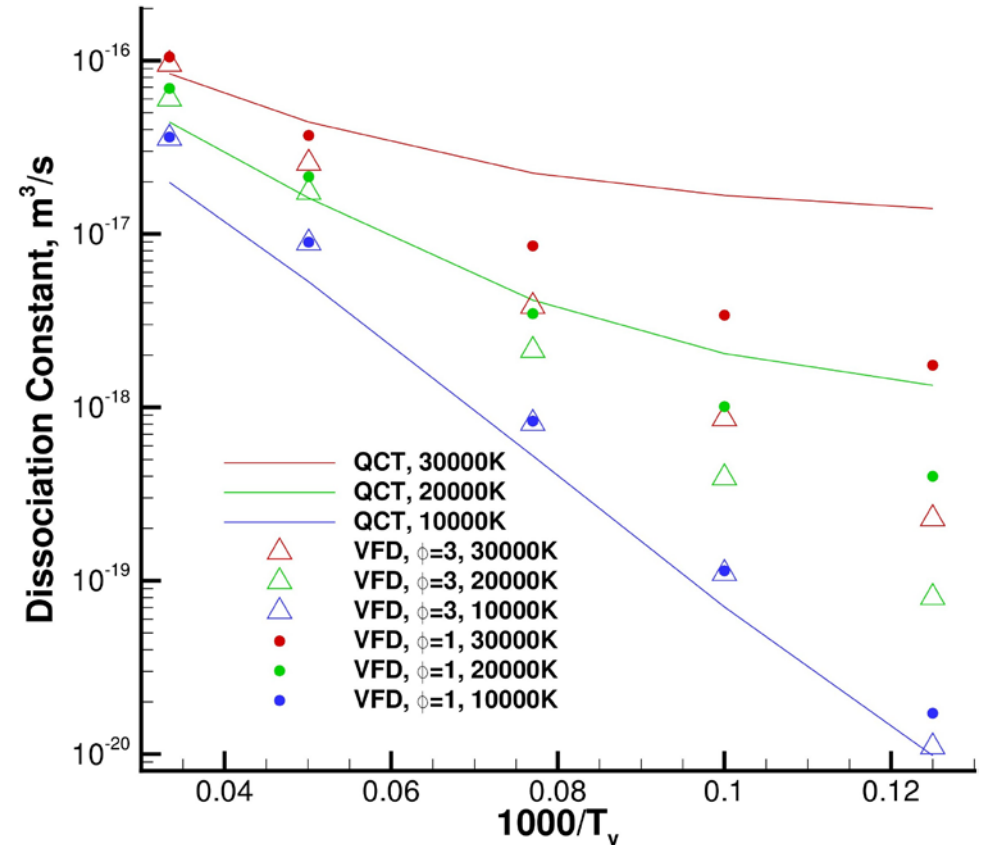
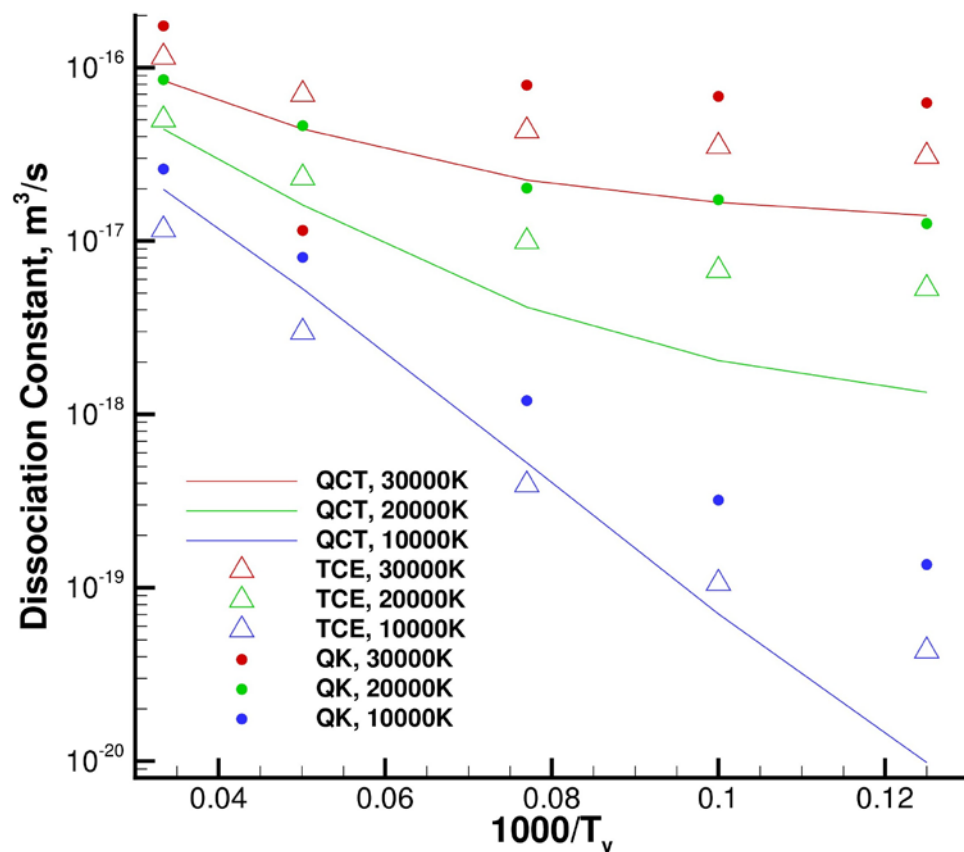
- TCE and VFD: explicitly match total reaction rate written in Arrhenius form
- Bias model: A needs to be adjusted, but captures rates well for $A \sim 1$

Level Specific N₂-N Reaction Rates



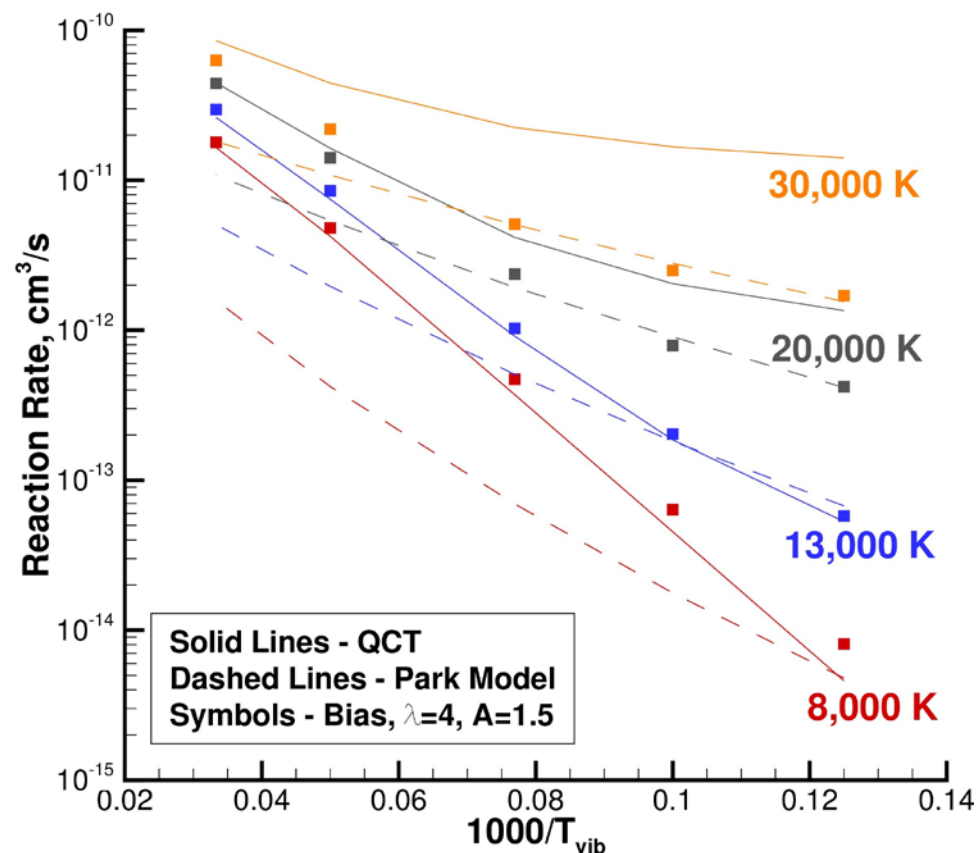
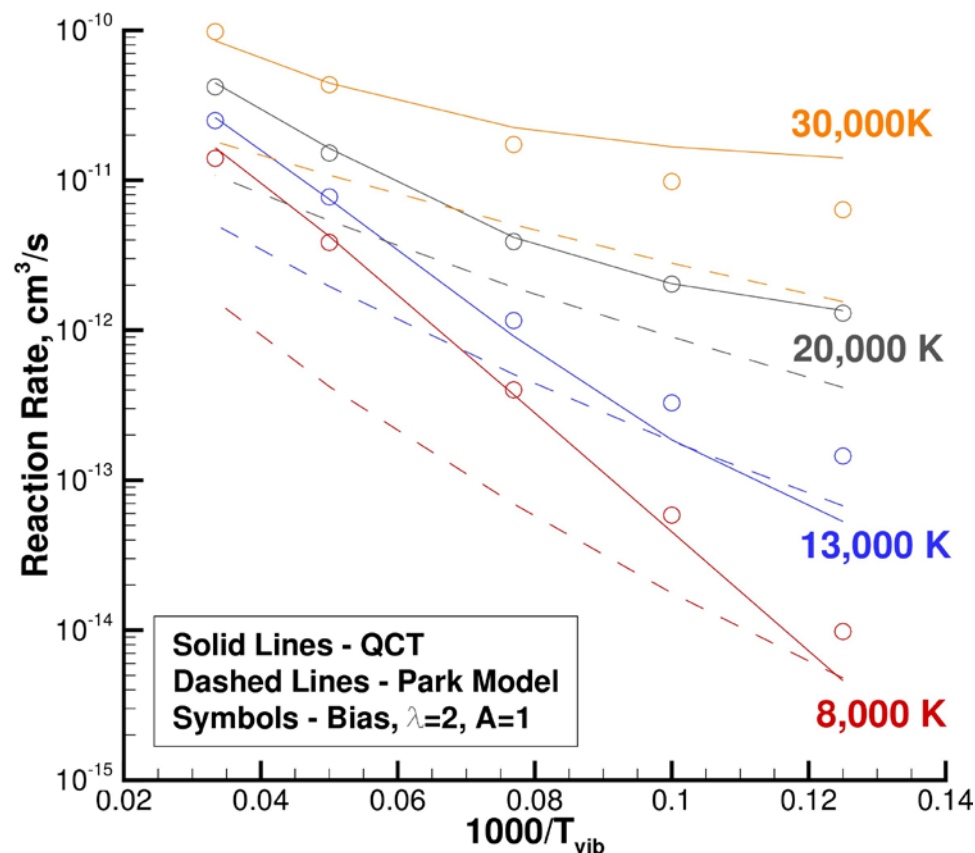
- **TCE, QK:** lack of vibrational favoring results in much weaker dependence of the reaction rate on v as compared to QCT
- **VFD:** $\phi=3$ provides reasonable agreement with QCT for $v>30$, but for the first few levels it is orders of magnitude lower
- **Bias:** very good agreement for $\lambda=2$

Non-Equilibrium Reaction Rates



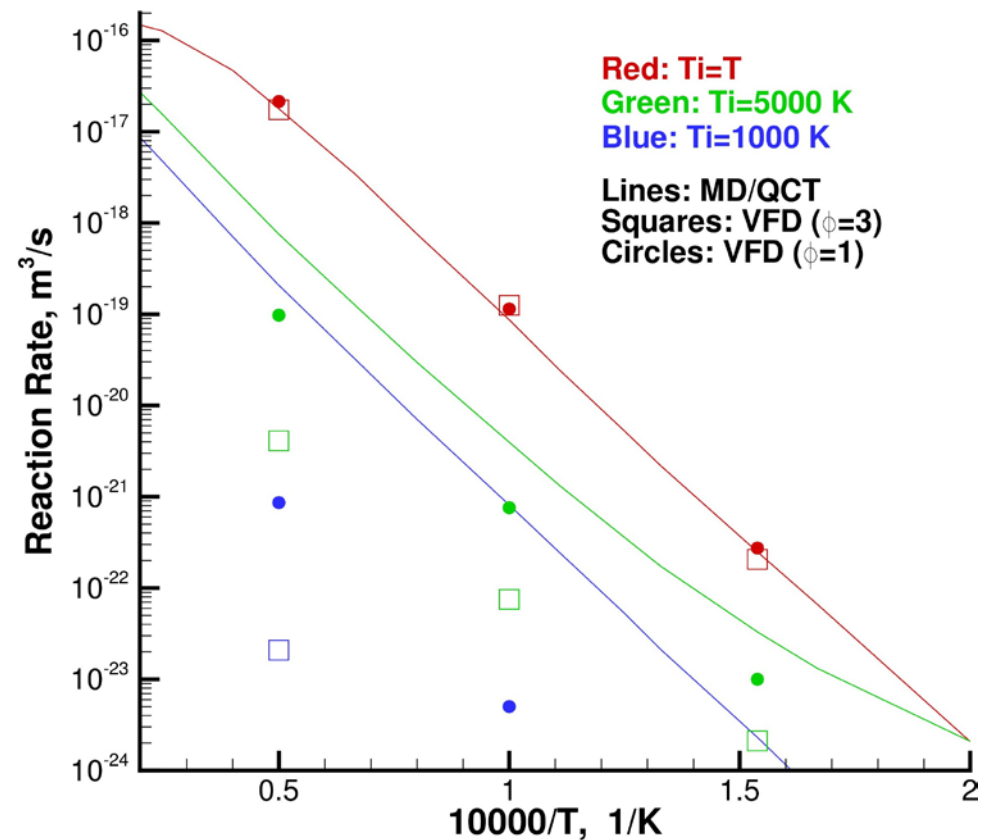
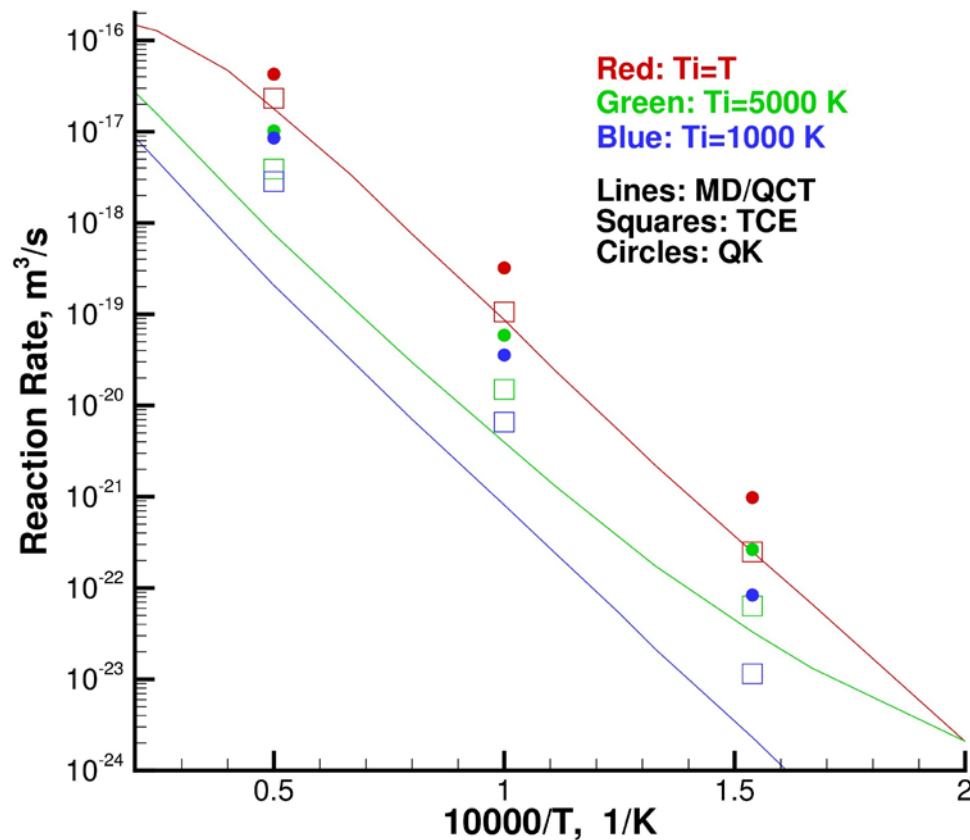
- TCE, QK, and VFD are over an order of magnitude off at lower T_v
- Of these three models, TCE provides somewhat better agreement with QCT

Non-Equilibrium Rates for Bias Model



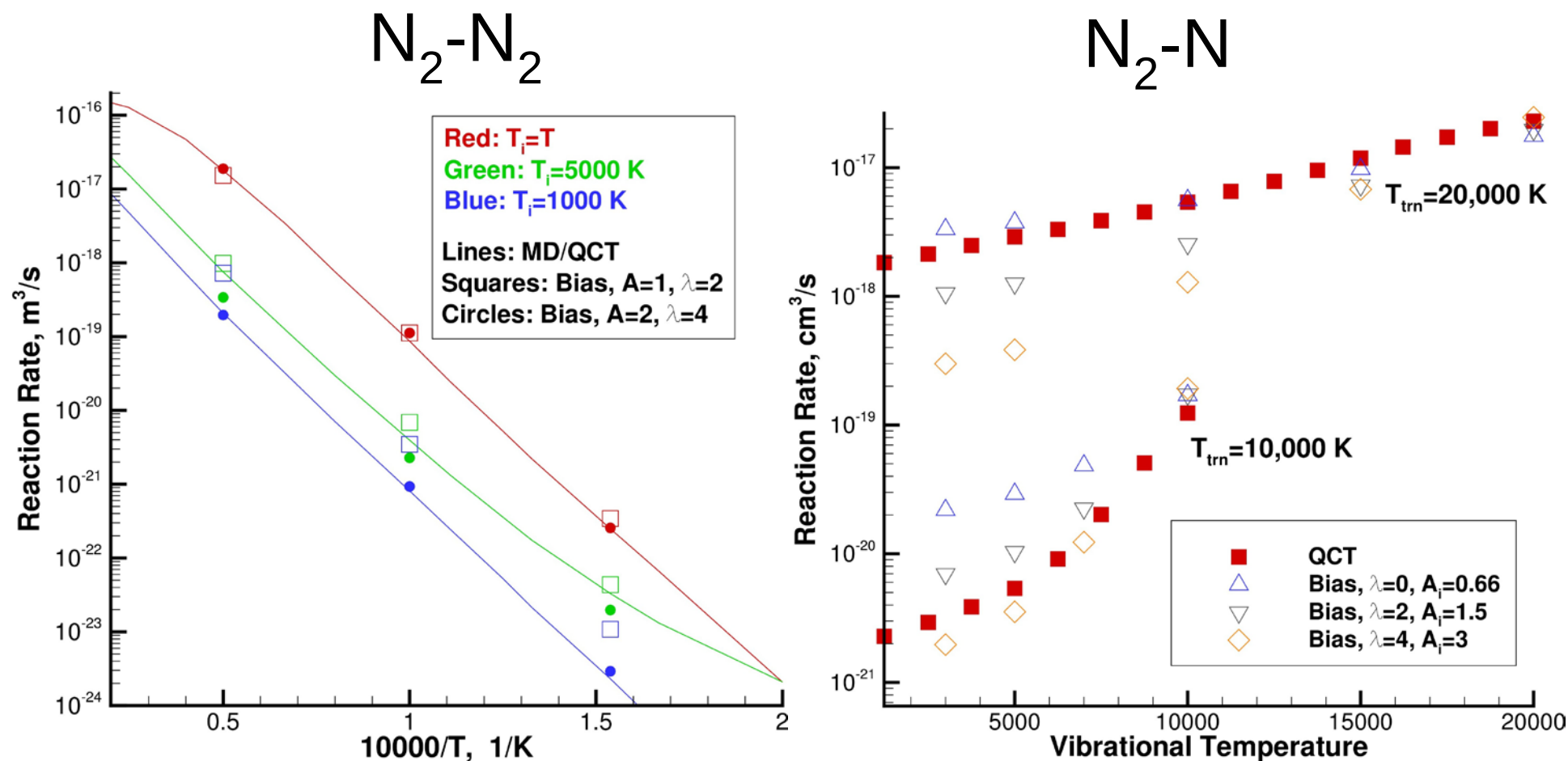
- Bias model provides much better fit than Park 2-T model
- Higher vibrational favoring for lower T_t : $\lambda > 2$ works better than $\lambda = 4$ for $T_t > 20,000$ K

Non-Equilibrium N₂-N₂ Reaction Rates for Low Internal Temperatures



- TCE within one order of magnitude
- VFD model fails at low T_v

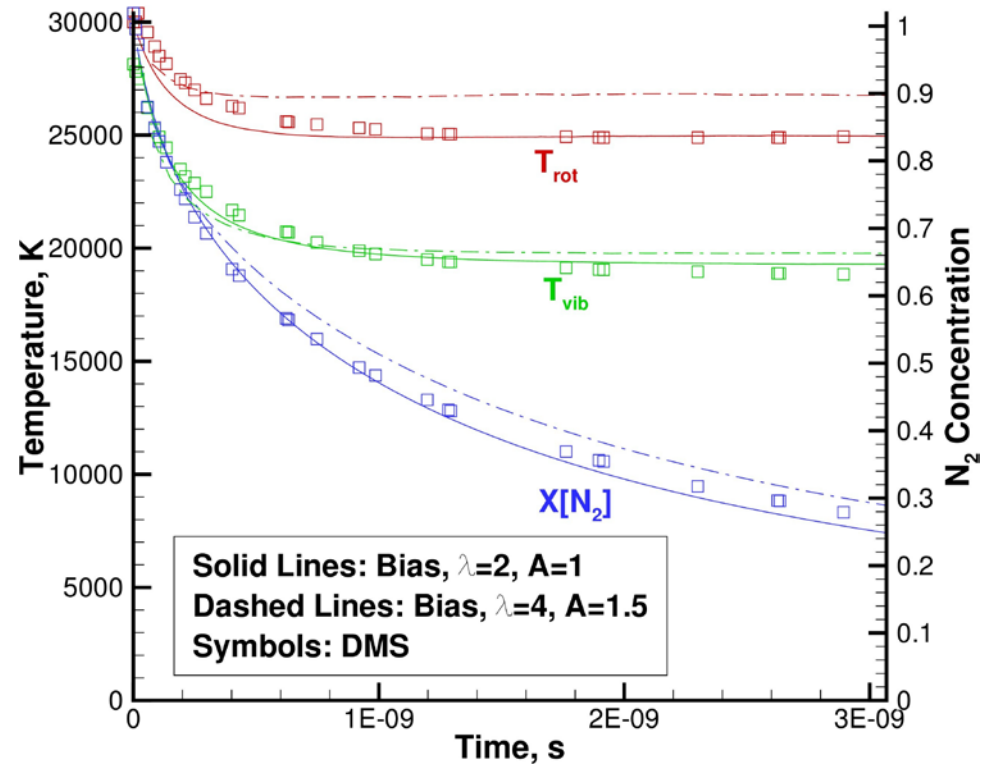
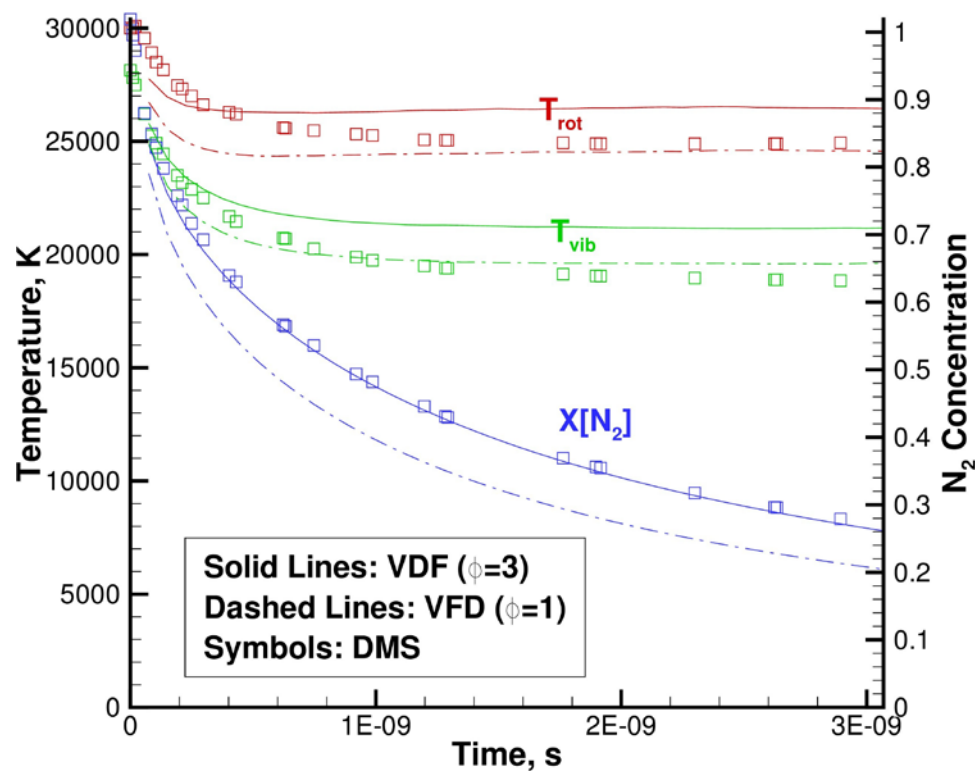
Non-Equilibrium Rates for Low Internal Temperatures: Bias Model



$\lambda = 4$ for N₂-N₂ and $\lambda = 2$ for N₂-N provide good agreement with QCT

Relaxation from Equilibrium to QSS

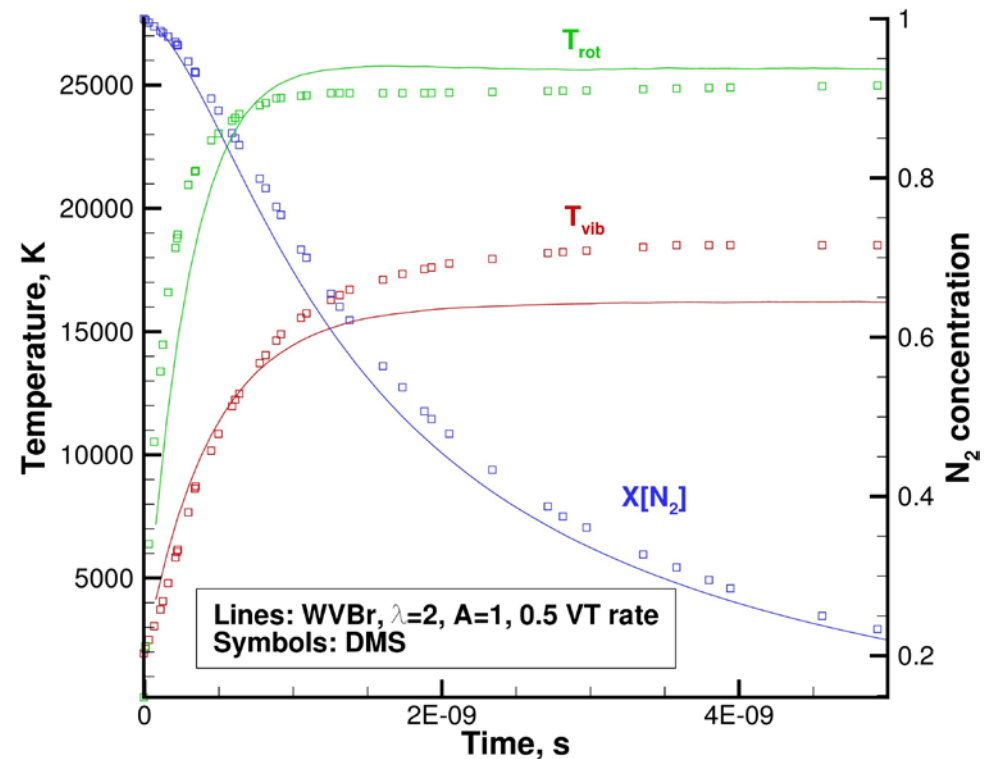
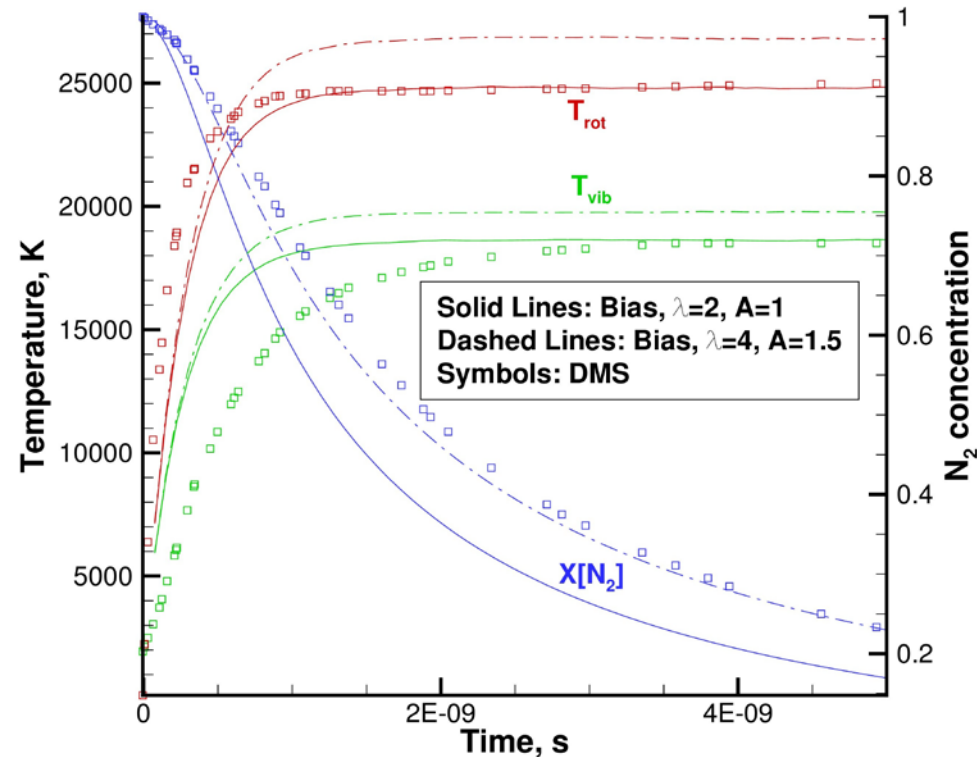
Initial state: $T_v = T_r = T_t = 30,000$ K



Bias model agrees well with QSS

Relaxation from Non-Equilibrium to QSS

Initial state: $T_v = T_r = 2,000$ K, $T_t = 30,000$ K



- QSS state for $\lambda=2$ is close to QSS, but initial rotational relaxation is faster and vibrational, slower
- Possible reason: LB model, where relaxation numbers are determined from local T_t
- VT rate reduced by 2 gives better agreement over the first ns

Conclusions

- Accuracy of four DSMC dissociation models is analyzed through comparison of $\text{N}_2\text{-N}_2$ and $\text{N}_2\text{-N}$ with recent QCT calculations
- TCE, QK, and VFD models do not capture key reaction features related to the vibration-dissociation coupling
- Bias model performs very well, and the adjustable parameters $\lambda = 4$, $A = 1.5$ for $\text{N}_2\text{-N}_2$ and $\lambda = 2$, $A = 1.5$ for $\text{N}_2\text{-N}$ provide good agreement with
- These preliminary results set the stage for more extensive comparisons of this promising reaction model, to include more realistic cases

Acknowledgement

The work was supported by the Air Force Office of Scientific Research (Program Officer Dr. Ivett Leyva).