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*Form Approved*  
*OMB No. 0704-0188*

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<b>1. REPORT DATE (DD-MM-YYYY)</b> 30-08-2011		<b>2. REPORT TYPE</b> Briefing Charts		<b>3. DATES COVERED (From - To)</b>	
<b>4. TITLE AND SUBTITLE</b>  <b>Comparison of Reaction Cross Sections for Two DSMC Models and Sensitivity in Non-Equilibrium Flow</b>				<b>5a. CONTRACT NUMBER</b>	
				<b>5b. GRANT NUMBER</b>	
				<b>5c. PROGRAM ELEMENT NUMBER</b>	
<b>6. AUTHOR(S)</b> Ingrid Wysong, Sergey Gimelshein, Natalia Gimelshein, William McKeon, and Fabrizio Esposito				<b>5d. PROJECT NUMBER</b>	
				<b>5f. WORK UNIT NUMBER</b> 23080532	
<b>7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)</b>  Air Force Research Laboratory (AFMC) AFRL/RZSA 10E. Saturn Blvd. Edwards AFB CA 93524-7680				<b>8. PERFORMING ORGANIZATION REPORT NUMBER</b>  AFRL-RZ-ED-VG-2011-369	
<b>9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)</b>  Air Force Research Laboratory (AFMC) AFRL/RZS 5 Pollux Drive Edwards AFB CA 93524-7048				<b>10. SPONSOR/MONITOR'S ACRONYM(S)</b>	
				<b>11. SPONSOR/MONITOR'S NUMBER(S)</b> AFRL-RZ-ED-VG-2011-369	
<b>12. DISTRIBUTION / AVAILABILITY STATEMENT</b>  Approved for public release; distribution unlimited (PA #11667).					
<b>13. SUPPLEMENTARY NOTES</b> For presentation at DSMC 11, Santa Fe, NM, 25-28 Sep 2011.					
<b>14. ABSTRACT</b>  This is a presentation to DSMC 11 on comparing reaction cross sections for two DSMC models and sensitivity in a non-equilibrium flow.					
<b>15. SUBJECT TERMS</b>					
<b>16. SECURITY CLASSIFICATION OF:</b>			<b>17. LIMITATION OF ABSTRACT</b>	<b>18. NUMBER OF PAGES</b>	<b>19a. NAME OF RESPONSIBLE PERSON</b>
<b>a. REPORT</b>	<b>b. ABSTRACT</b>	<b>c. THIS PAGE</b>			Andrew D. Ketsdever
Unclassified	Unclassified	Unclassified	SAR	21	<b>19b. TELEPHONE NUMBER</b> <i>(include area code)</i> N/A



# COMPARISON OF REACTION CROSS SECTIONS FOR TWO DSMC MODELS AND SENSITIVITY IN NONEQUILIBRIUM FLOW

Ingrid Wysong, Sergey Gimelshein,  
Natalia Gimelshein, William McKeon,  
Fabrizio Esposito





# Acknowledgements



- **Wysong AFRL**
- **Gimelshein, Gimelshein, McKeon ERC, AFRL**
- **Esposito IMIP-CNR, Bari**
- **Support from the Air Force Office of Scientific Research, Dr. Mitat Birkan program manager, is gratefully acknowledged.**



# Introduction: DSMC Chemistry Models



- Important for hypersonic reacting flows (re-entry): strong nonequilibrium, large effect on heating, radiation
- Long history of proposed simplified models; realism can be improved **if** reaction behavior is well understood
- After flurry of work inspired by BSUV data, many felt that without new measurements, further work unfruitful
- New(ish) Quantum Kinetic (QK) model proposed by Bird has generated renewed interest



# QK Model



- See G.A. Bird, Gallis, references therein
- Very appealing simplicity
- Impressively predicts thermal rate coefficients  $k(T)$  over wide  $T$  range in good agreement with measured/recommended values
- The present paper investigates the behavior of  $\sigma(E)$ , or reaction probability per collision, important for strongly nonequilibrium flows
- Available detailed quasi-classical trajectory (QCT) results for  $\sigma(E)$  for 2 important reactions are used to evaluate



# Model Definitions



- **QK dissociation:  $P_{\text{react}} = 1$  for  $E_c > E_a$ ,  $= 0$  otherwise**
- **QK exchange:**
- **Total Collision Energy (TCE)\*: reproduces**
  - $k(T) = AT^B \exp(-E_a/T)$  for given values of A, B,  $E_a$  and  $\zeta$
- **Both models need total collision cross section values: VHS model parameters selected so that collision-pair viscosity matches values predicted by Capitelli (ref) in 5,000 – 15,000K range**
- **\* Bird, 1994.**



# Vibrational Energy Levels



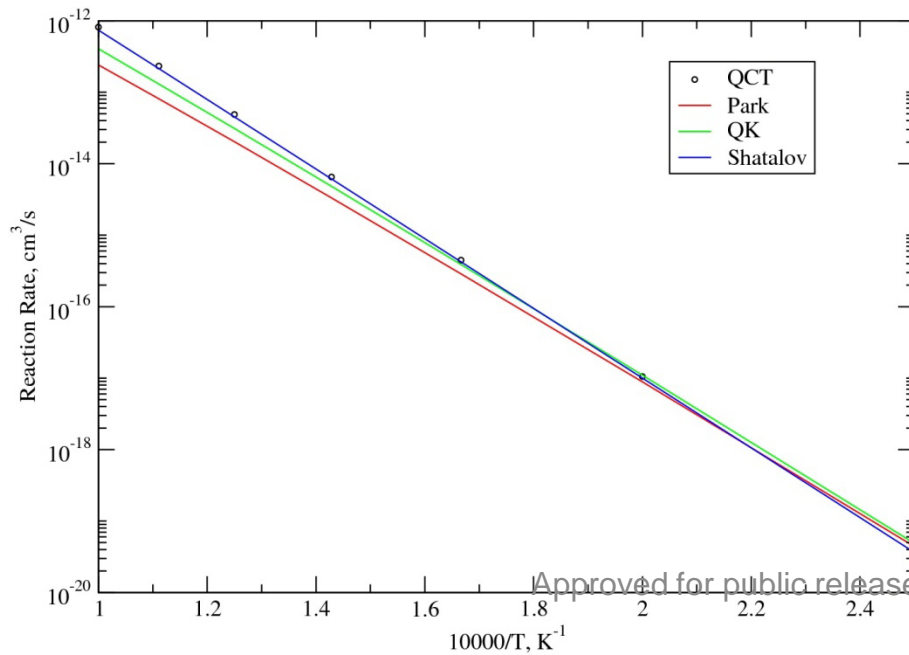
- **Original TCE model used continuous internal energy modes**
- **Later work adapted it for quantized internal energy levels, see esp Gimelshein (ref) and discussion of small correction factor to use for simple harmonic oscillator (SHO) levels; zero-point vibrational energy (ZPE) is included in total collision energy**
- **QCT calculations of course use real vibrational energy level values (closer to AHO)**
- **This work compares DSMC results for SHO levels to QCT results for AHO levels which have same  $E_{vib}$**



# $N_2+N$ Dissociation Reaction



- Plot of thermal reaction rate coefficients
- TCE model uses published Arrhenius parameters as input and will match QCT  $k(T)$  by definition
- QK model uses no adjustable parameters and matches QCT (and expt)  $k(T)$  quite closely



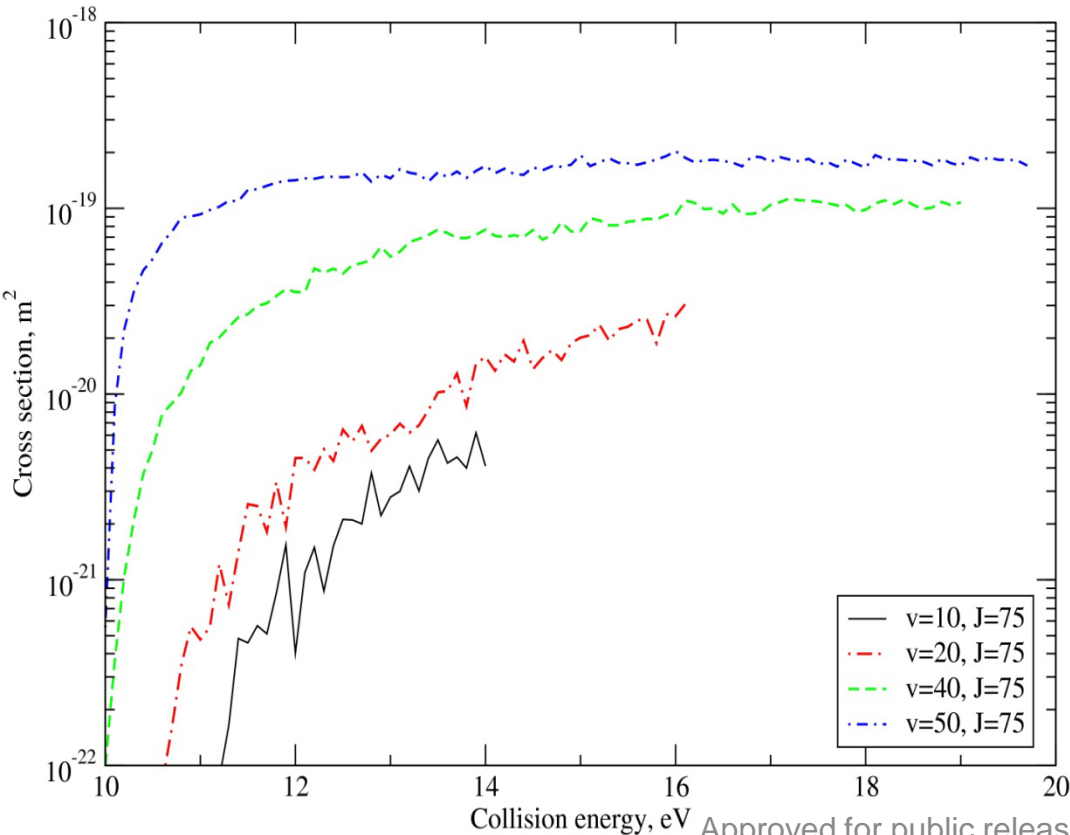
QCT results from Esposito et al., (Chem Phys. 331 2006)



# $N_2+N$ Dissociation Reaction



- **QCT  $\sigma$  results from Esposito** (Chem Phys Lett 302, 1999 and unpublished)
- **Dissociation reaction, as is well-known, has strong vibrational favoring**



**QCT cross sections at same  $E_c$  show  $>100x$  difference in  $\sigma$ !**

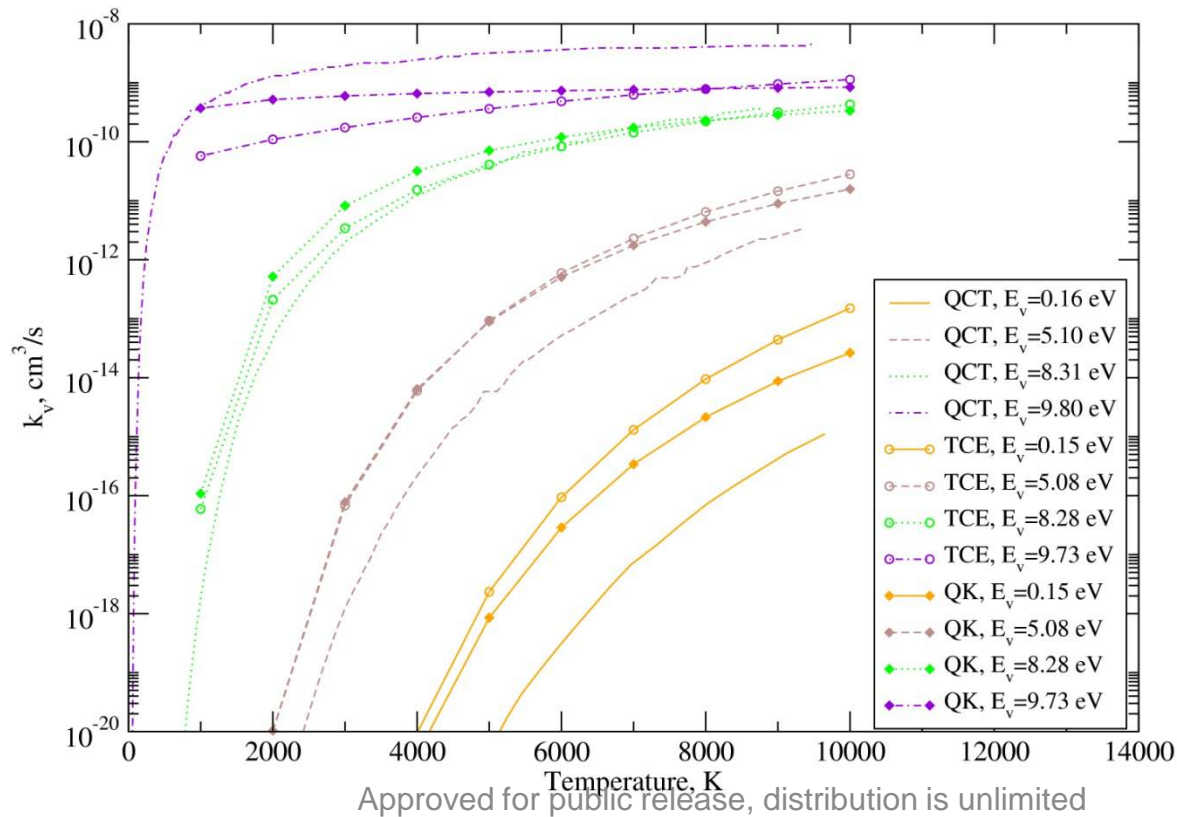
**No simplified DSMC reaction model includes this effect**



# $N_2+N$ Dissociation Reaction



- State-specific thermal rates  $k_v(T)$
- TCE and QK models both have  $k_v(T)$  that are high for low- $v$  and low for high- $v$  levels. No surprise.

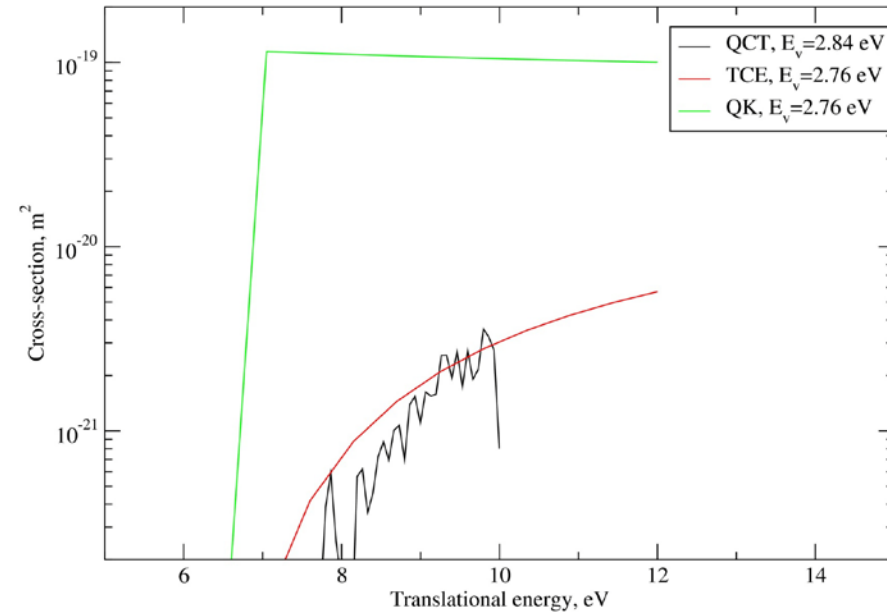




# $N_2+N$ Dissociation Reaction



- QK assumes that each collision above threshold energy has unity reaction probability
- TCE matches realistic QCT  $\sigma$  surprisingly closely

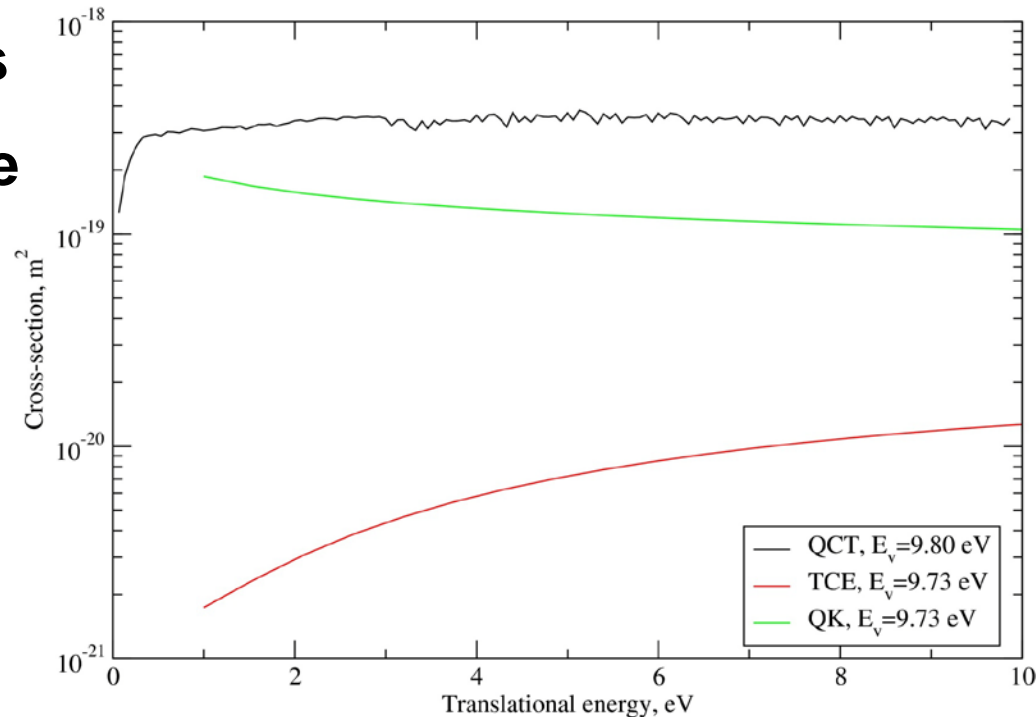




# $N_2+N$ Dissociation Reaction



- For  $v=60$ , QCT has  $\sigma_{\text{diss}} \geq \sigma_{\text{total}}$  ; QK very close to this
- TCE far underestimates the probability for very high  $v$
- For flows with mainly low  $v$  populated, QK may be problematic

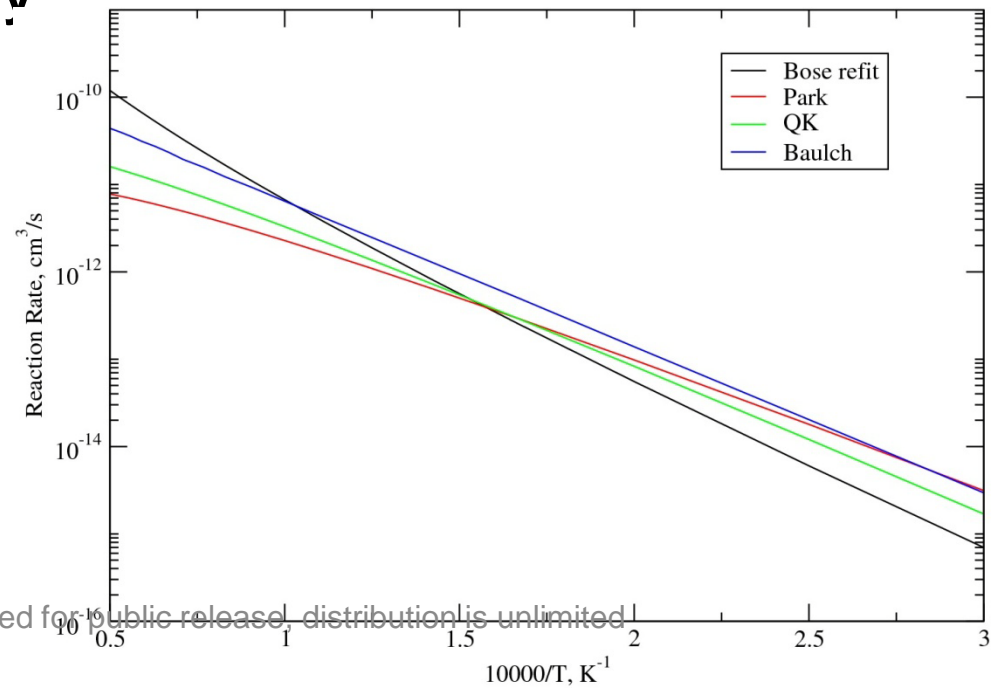




# $N_2+O$ Exchange Reaction $k(T)$



- $N_2+O \rightarrow NO + N$  QCT results from Bose and Candler, unpublished
- Plot of thermal reaction rate coefficients
- TCE model uses published Arrhenius parameters as input and will match QCT  $k(T)$  by definition
- QK model uses no adjustable parameters and matches QCT (and expt)  $k(T)$  reasonably



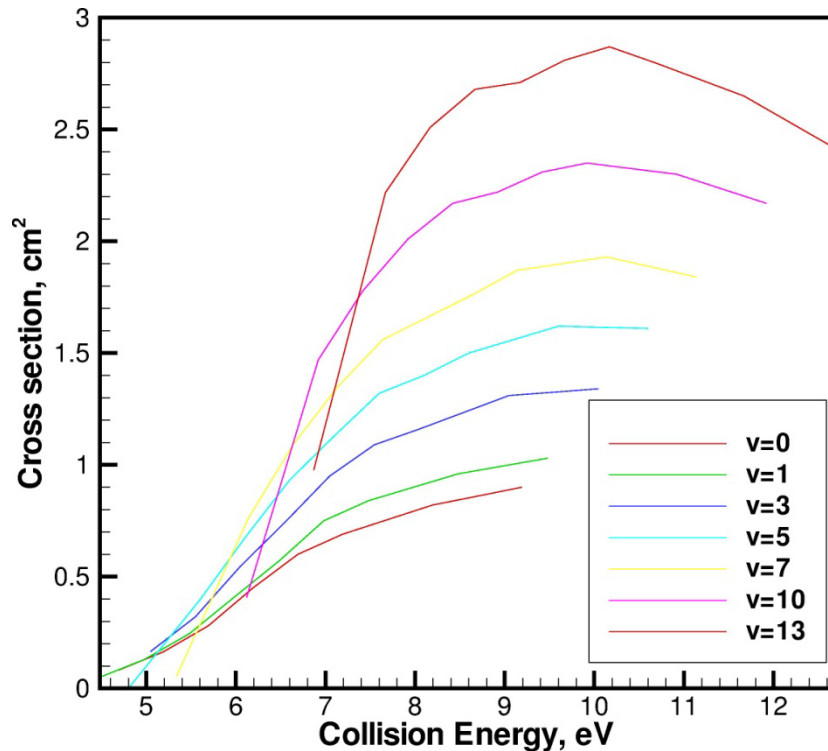
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# $N_2+O$ Exchange Reaction



- This (and many other) exchange reactions have no strong vibrational favoring



**QCT cross sections at same  $E_c$  show  $\sim 3x$  difference in  $\sigma$**

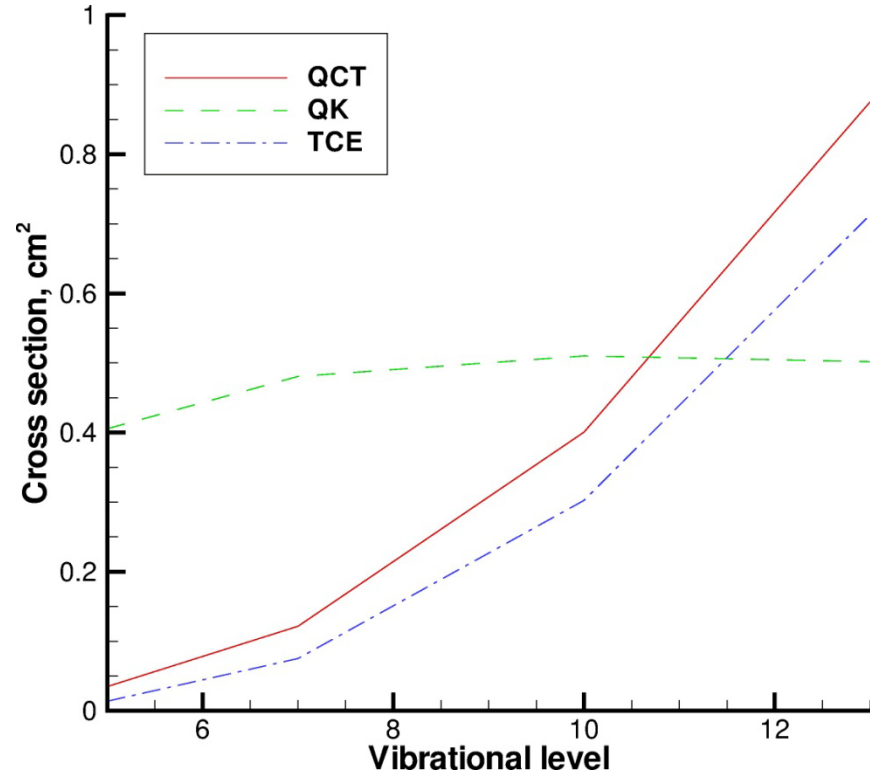
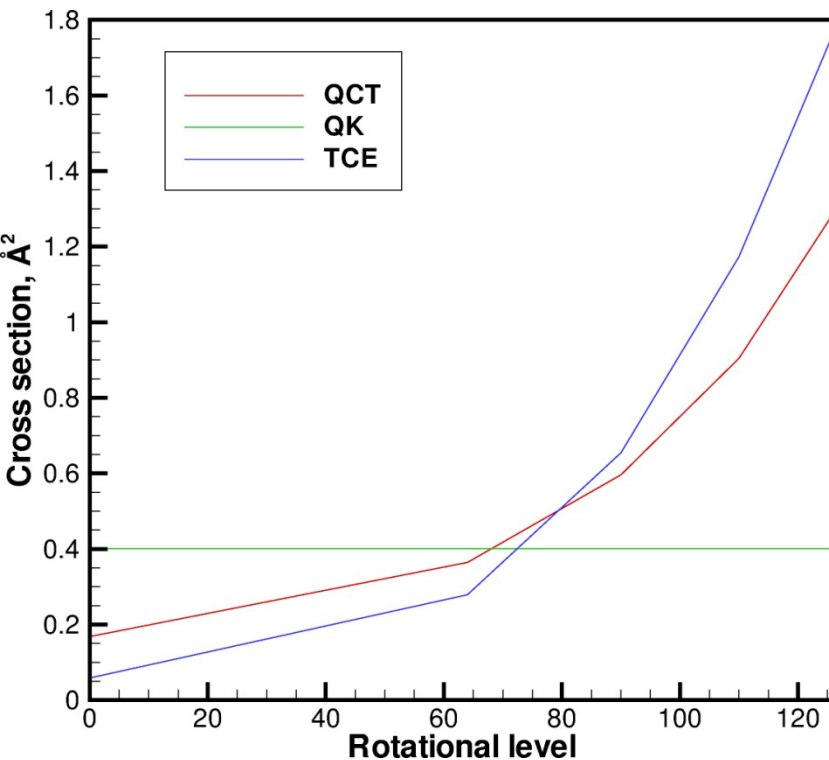
**Lends itself more readily to a simplified DSMC model**



# $N_2+O$ Exchange Reaction



- Overall shape of  $\sigma(E)$  much better represented by TCE model



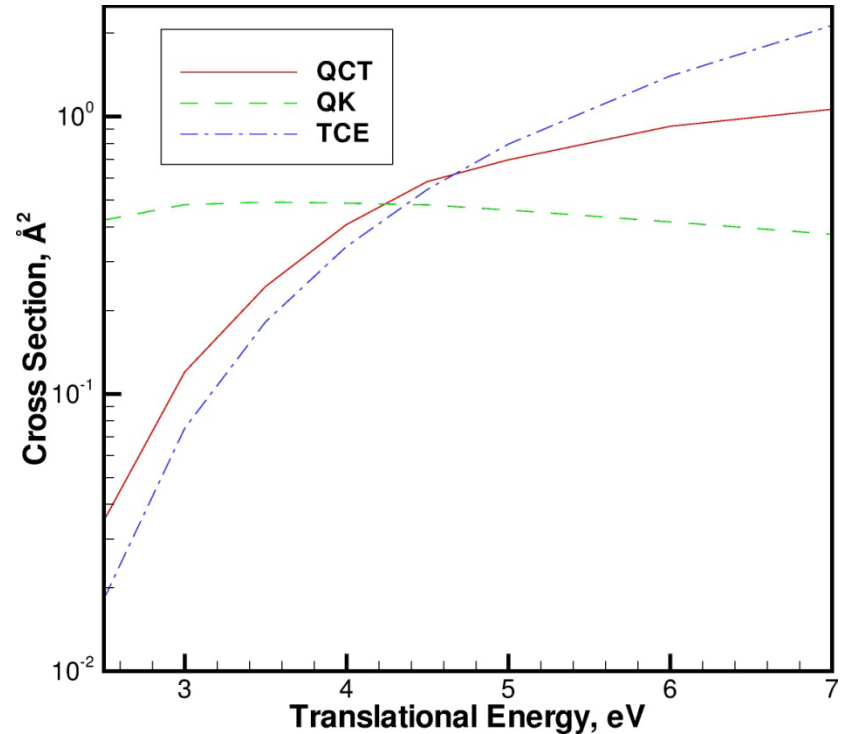
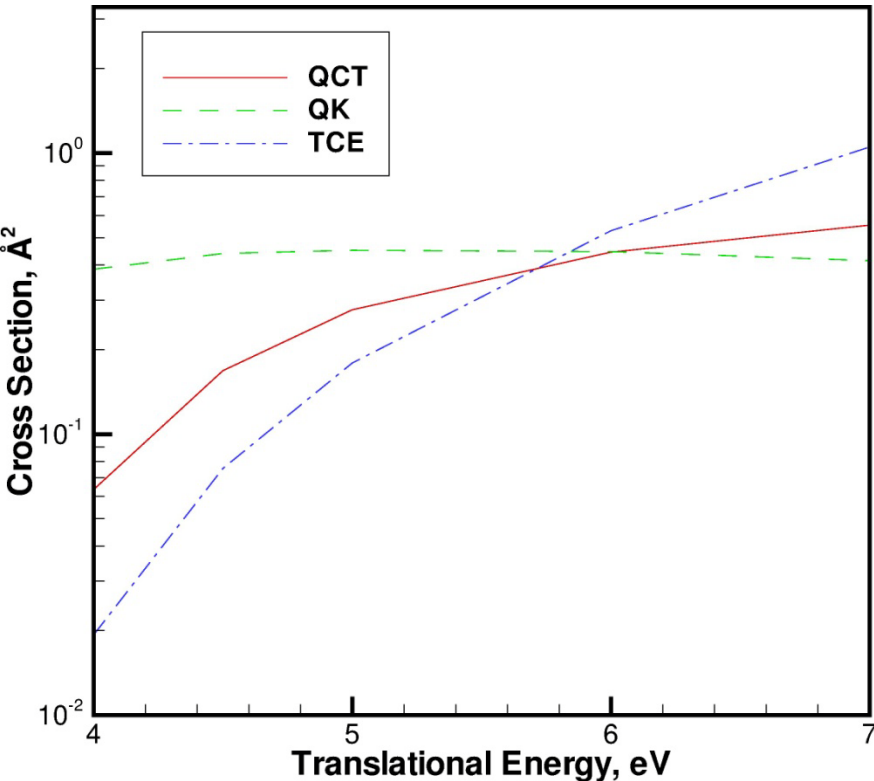
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# $N_2+O$ Exchange Reaction



- Overall shape of  $\sigma(E)$  much better represented by TCE model,  $v=0$  and  $v=5$  examples ( $J=0$ )

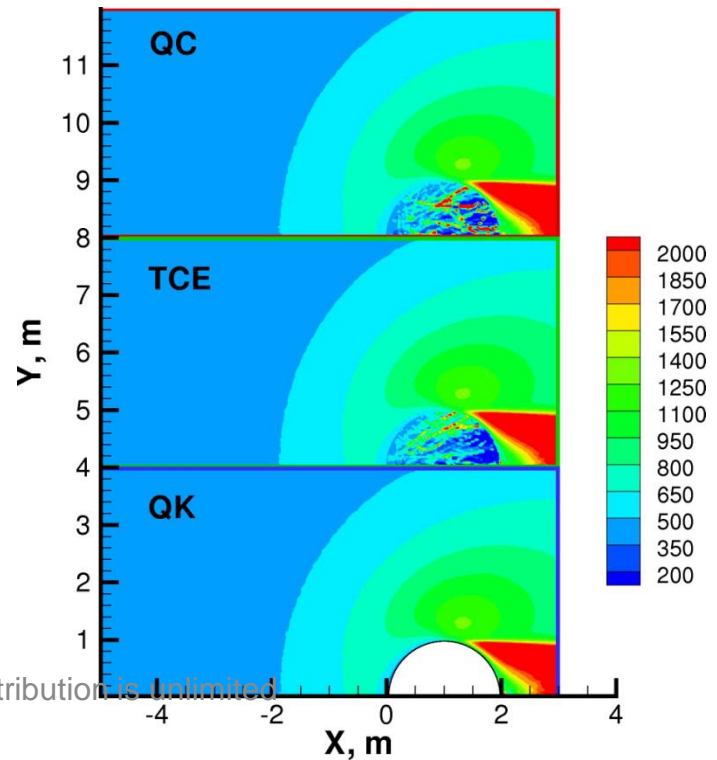
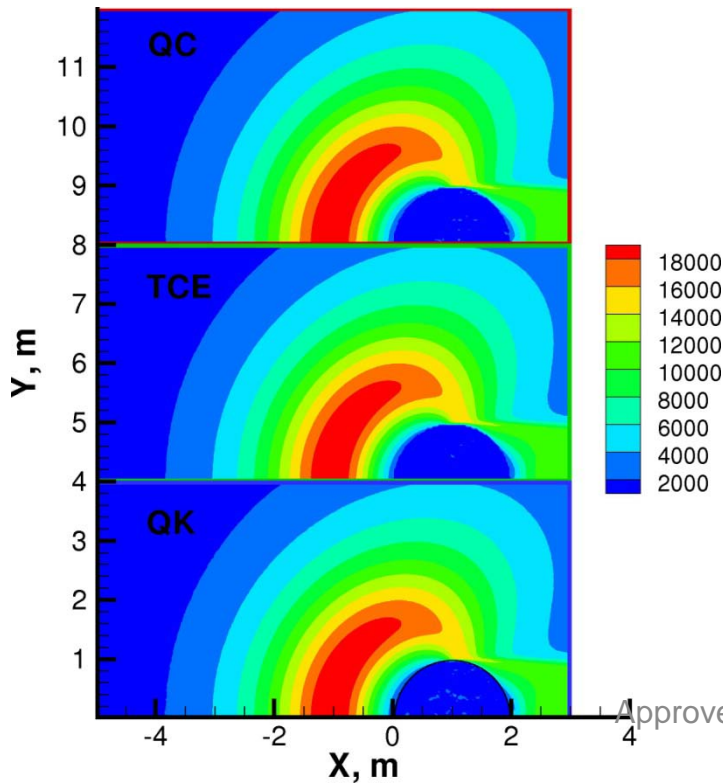




# Sensitivity of Flowfield Results to N<sub>2</sub>+O reaction model



- Simple axisymmetric flow over cylinder, **8 km/s**, 120 km (fractions of N<sub>2</sub>, O?) nearly single-collision
- QCT cross sections were used in one run as look-up table with interpolation for comparison



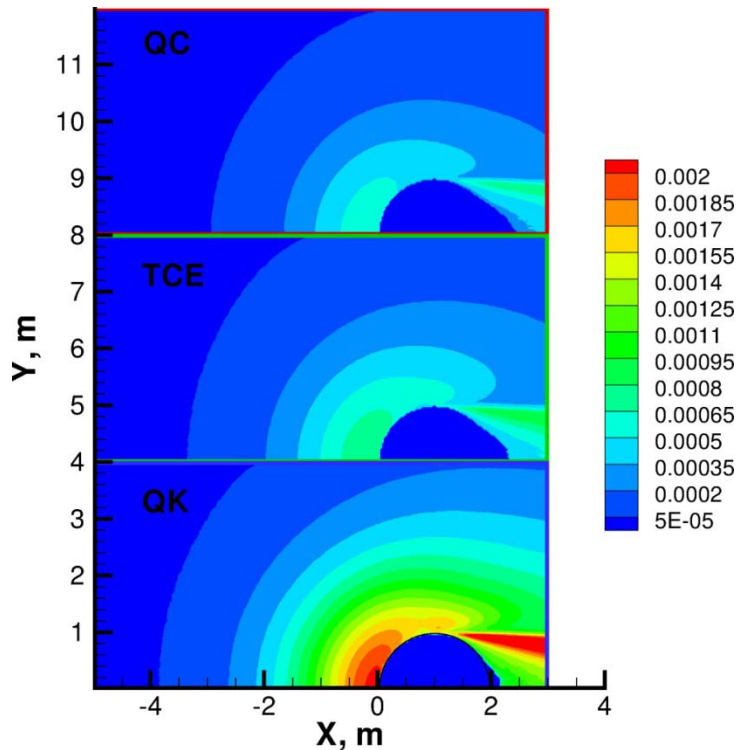
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# Sensitivity of Flowfield Results



- NO product mole fraction, 8 km/s



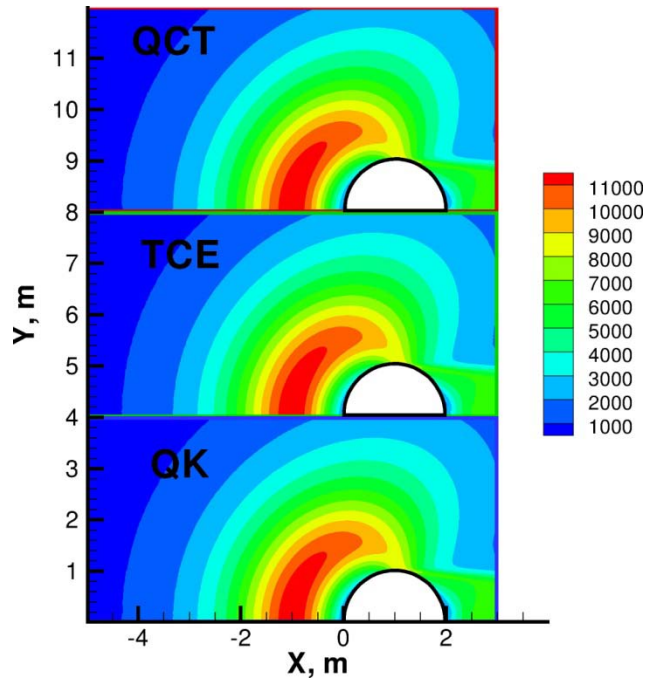
- **Conclusion:** As indicated by  $\sigma$  plot, QK model significantly overpredicts reaction probability near threshold
- **QK NO fraction is 3x high**



# Sensitivity of Flowfield Results to N<sub>2</sub>+O reaction model



- Simple axisymmetric flow over cylinder, **6 km/s**, 120 km (fractions of N<sub>2</sub>, O?) nearly single-collision



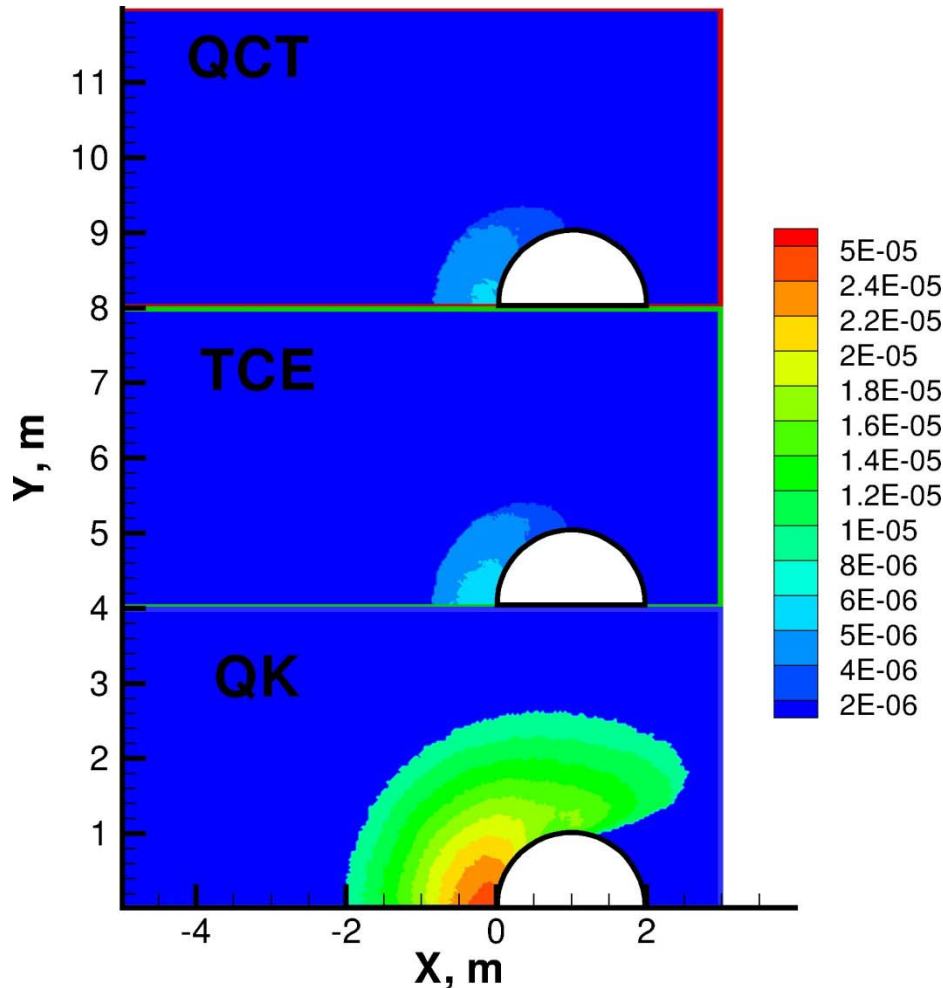
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# Sensitivity of Flowfield Results



- NO product mole fraction, 6 km/s



**Conclusion: As indicated by  $\sigma$  plot, QK model significantly overpredicts reaction probability near threshold**



# Summary and Recommendations



- **Present results are complementary to previous publications on QK model, focusing on noneq aspects**
- **for strongly nonequilibrium flows, the probability of reaction is sensitive to the shape of the energy-dependent cross section; TCE more realistic than QK model in this respect**
- **Possibly explore gaining the best of both?**