# Non-linear Fitting of Charge Exchange Recombination Spectra with Energy-Dependent Cross Section Included

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# Overview of Poster

- **Poster is about measurements of $T_i$ and $V_{tor}$ via Charge Exchange Recombination (CER) Spectroscopy**
- **Details of the CER cross section affect the observed spectra**
  - **Apparent shifts in $T_i$ and $V_{tor}$ can be obtained if the "cross section effect" is ignored**
- **This poster documents the development of algorithms for fitting of the observed spectra with cross section effect included**
- **Cross section is modeled in non-linear least squares analysis of data, rather than via post-processing**

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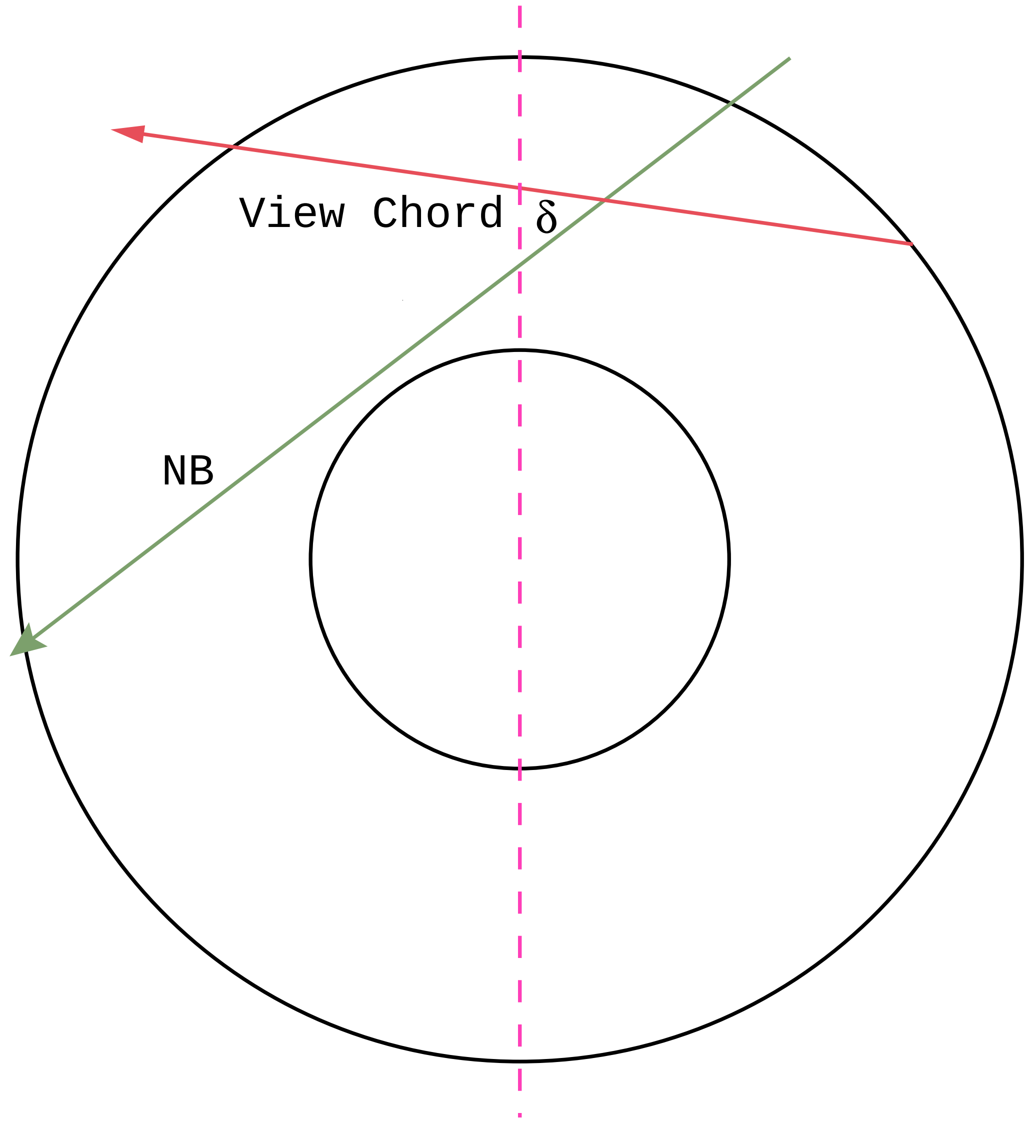
# Energy-Dependent Cross Section Modifies Charge Exchange Recombination Spectra

- **The problem: spectrum produced by charge exchange recombination of a thermal population of plasma ions with the fast neutrals of a neutral beam**
  - **E.g. $D^0 + C^{6+} \rightarrow D^+ + (C^{5+})^* \rightarrow D^+ + C^{5+}$ + photon**
- **To lowest order, the spectrum is a shifted Gaussian in wavelength space**
- **However, cross section for CER process varies as function of relative velocity between ions and beam atoms**
  - **Spectrum is modified - lowest order analysis will have systematic offsets of temperature and rotation velocity**

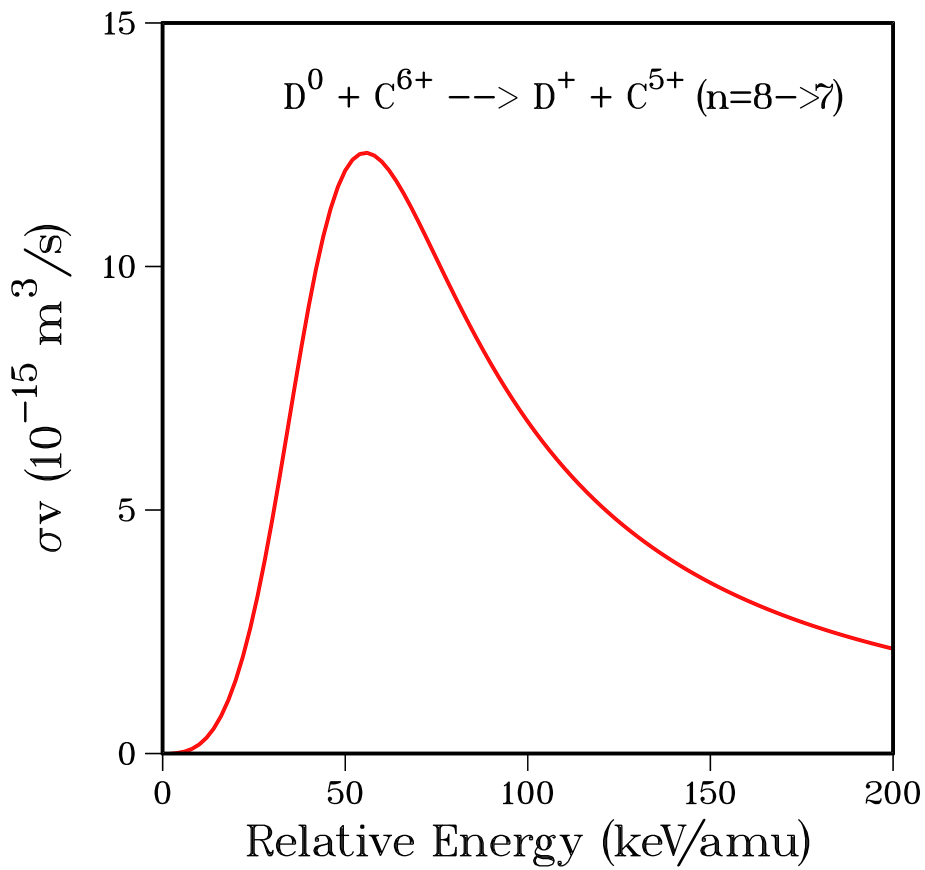
# Geometry for Horizontal View

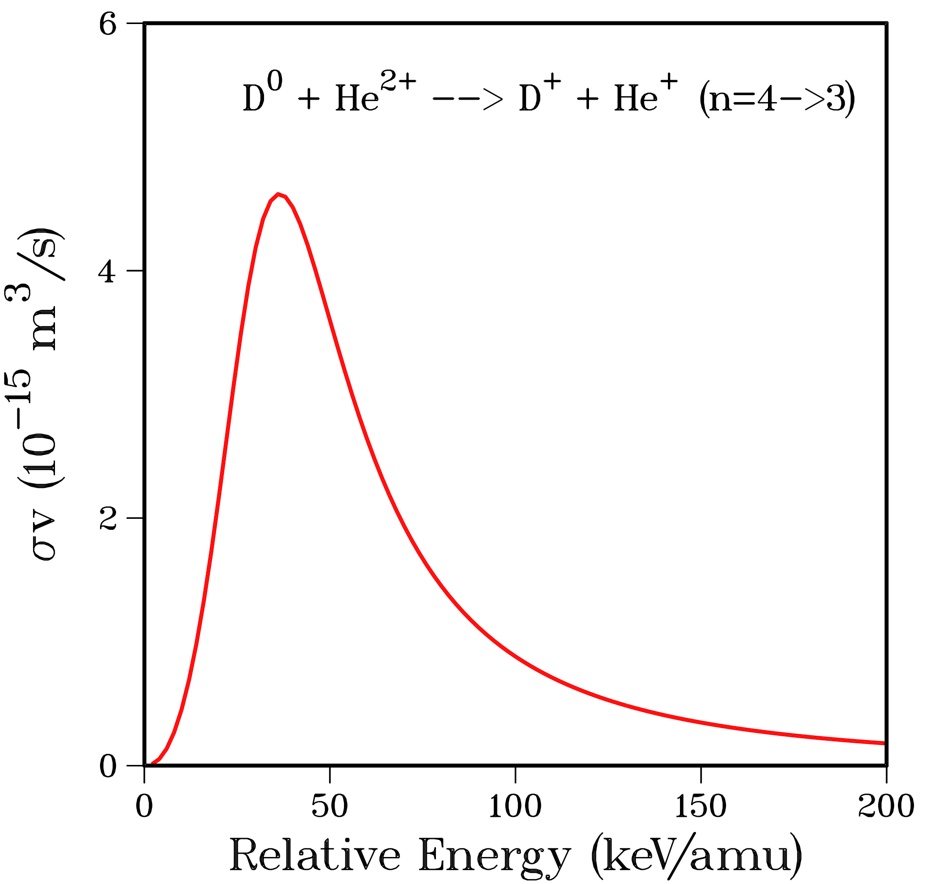
- δ is angle between view chord and neutral beam
- In DIII-D, typical δ for core views is 40-45 °



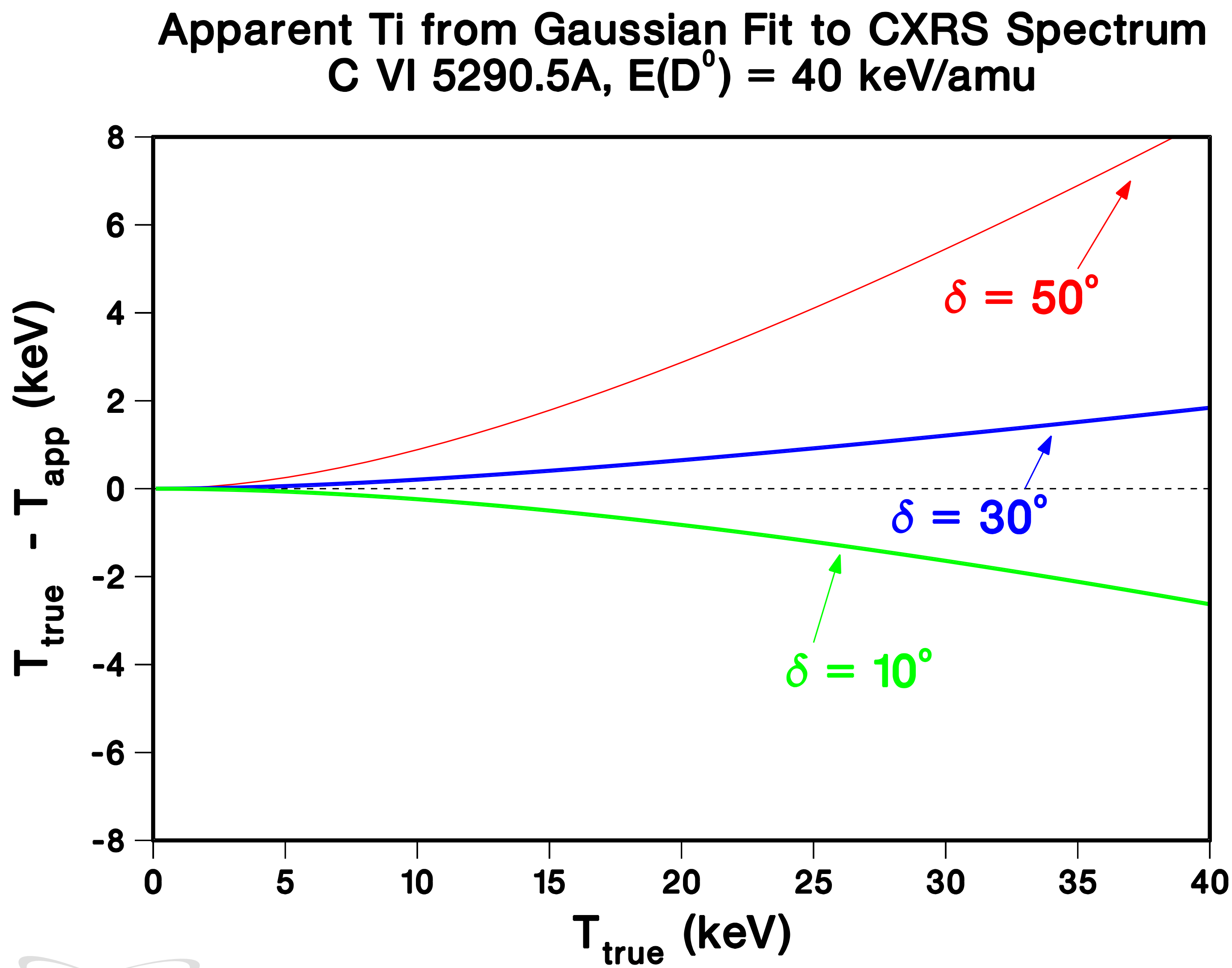
# Effective Emission Rates

**From M. von Hellermann et al., Plasma Phys. Control Fusion 37 (1995), 71.**



# "Cross Section Effect" for $T_i$ for CVI 5290

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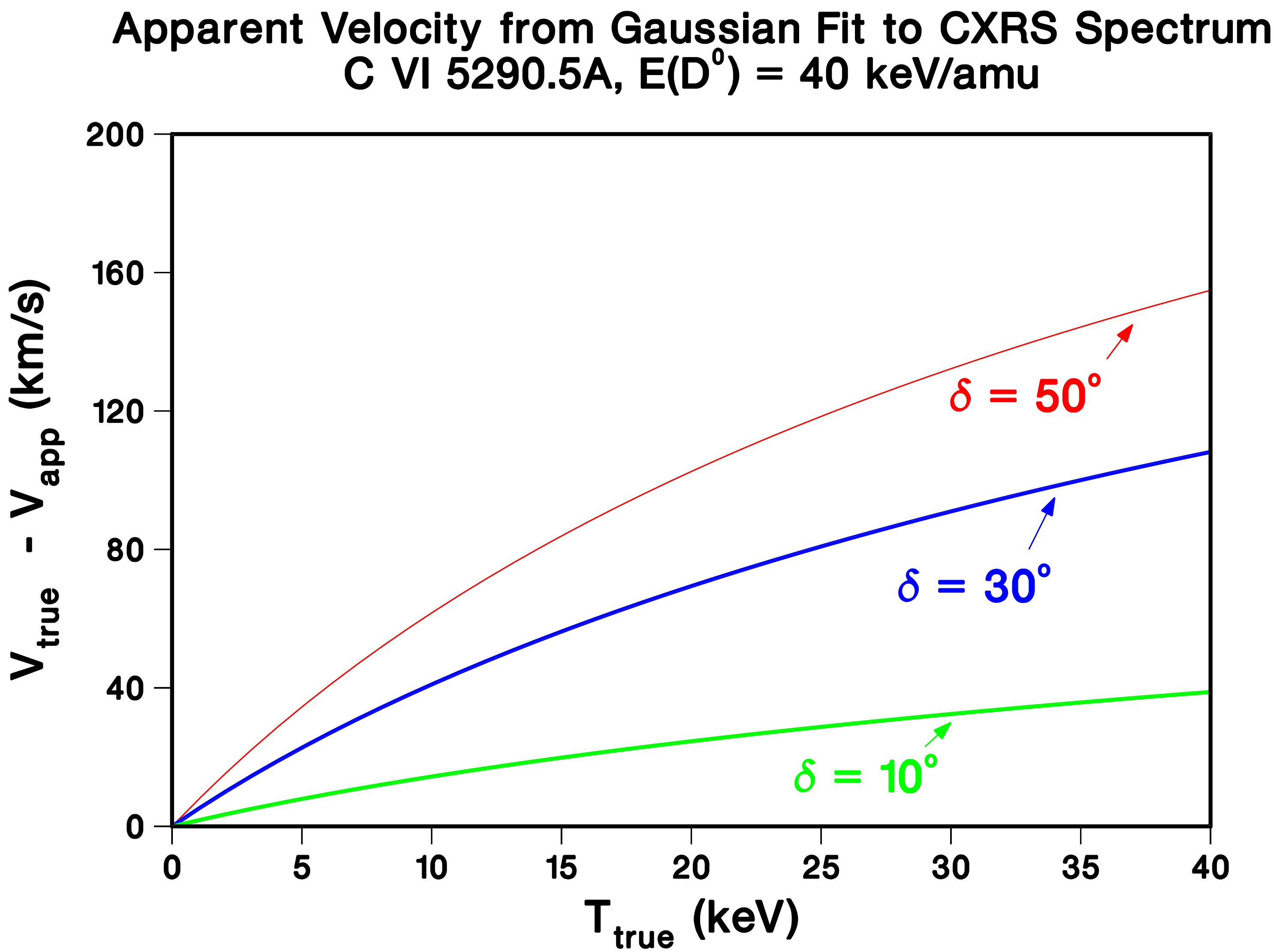
# “Cross Section Effect” for $V_{tor}$ for CVI 5290

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# Post-processing Is Often Used to Account for the "Cross Section Effect"

- **Cross section effect is well known and studied**
  - **R.B. Howell et al., Rev. Sci. Instrum. 59 (1988), 1521.**
  - **M. von Hellermann et al., Plasma Phys. Control Fusion 37 (1995), 71.**
  - **R.E. Bell et al., Rev. Sci. Instrum. 70 (1998), 821.**
- **Typically, this effect produces a spectrum which is very close to Gaussian in shape**
  - **Spectrum exhibits apparent shifts of rotation and temperature relative to true parameters for emitting ions**
- **Post-processing often used to correct cross section effect**
  - **Fit Gaussian to experimental spectrum with least squares and then correct for apparent Ti and rotation shifts**

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# “Cross Section Effect” Can Be Accommodated Directly in Least Squares Fitting of Data

- **Post-processing has potential drawback**
  - **If cross section effect produces spectrum which is not sufficiently Gaussian, post-processing may introduce error**
- **Fitting to a model with cross section effect included avoids this problem**
  - **The price is a more complicated and slower analysis procedure because the fitting model cannot be specified in a completely analytic form**
- **This poster documents the development of algorithms for the direct fitting of the spectrum with cross section effect included**

# Fit Model Based on Velocity Integrals Which Include CER Cross Section

**Following von Hellermann, the spectrum line-shape is:**

$$f(v_z) = \frac{1}{\pi^{3/2} v_{th}^3} \int d^3\vec{v}' \, Q\left(\left|\vec{v}' - \vec{v_b}\right|\right) \delta\left(v_z' - v_z\right) \exp\left[-\left(\vec{v}' - \vec{V}\right)^2 \Big/ v_{th}^2\right]$$

**Where:**

line of sight is along z - axis

$\vec{v_b}$ is the velocity of the beam neutrals

$\vec{V}$ is the flow velocity of the emitting ions

$v_{th}$ is the thermal velocity of the ions

$Q\left(\left|\vec{v}\right|\right) = \sigma_{cx}\left(\left|\vec{v}\right|\right)\left|\vec{v}\right|$ is the effective excitation rate for a charge exchange event with cross section $\sigma_{cx}$

**Use von Hellermann's analytic expression for** $Q$

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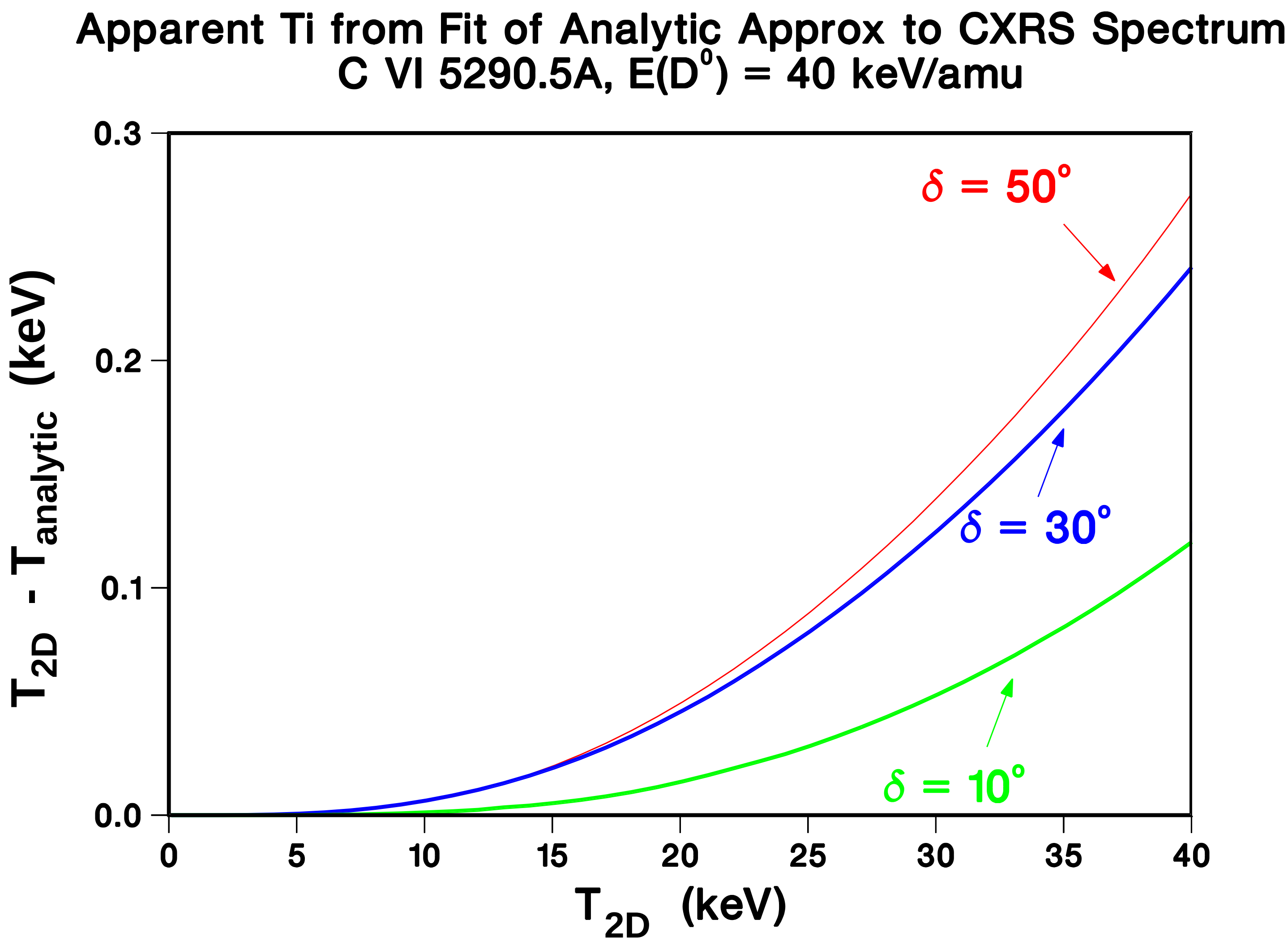
# Evaluation of Velocity Space Integral Has been Performed in Three Ways

- **Evaluation over $v_z'$ is trivial due to delta function**
- **The remaining integral is a 2D integral over $v_x'$ and $v_y'$**
- **Burrell has exploited a symmetry in the problem to turn the 2D integral into an exact 1D integral**
- **Burrell has also obtained an approximate analytic solution for the 1D integral**
- **Thus, integral can be evaluated via**
  - **1) Numerical evaluation of exact 2D form**
  - **2) Numerical evaluation of exact 1D form**
  - **3) Analytic evaluation of approximation 1D form**

# The Three Forms for Velocity Space Integrals Have Been Successfully Implemented

- Testing shows that numerical evaluation of the 2D and 1D forms of the exact integrals agree, as expected
- For C VI 5290, the evaluation of the 1D analytic form of the integral agrees well with the numerical evaluation for $T_i$ up to 15-20 keV
- Evaluation of the 1D analytic form is 2 orders of magnitude faster than numerical evaluation of the exact 2D form

# 1D Analytic Function for C VI 5290 Is Good Approximation to 2D form for $T_i$

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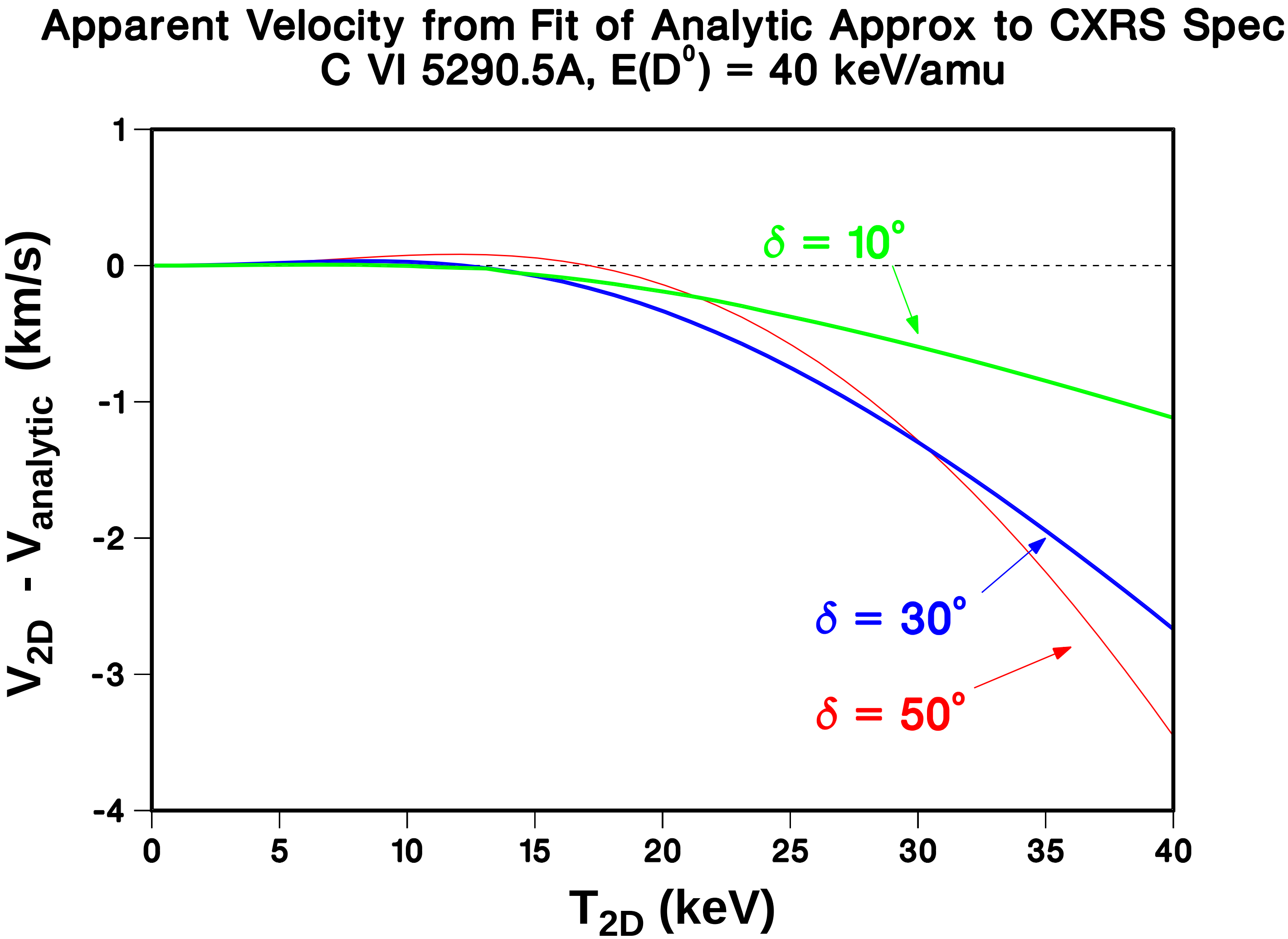
# 1D Analytic Function for C VI 5290 Is Good Approximation to 2D form for $V_{tor}$

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# Implementation of Model for CER Spectrum in Least Squares Fitting

- **The 1D numerical and analytic forms of the velocity integral have been incorporated into least squares fitting of experimental data**
- **Implemented in *CERFIT*, code used to fit experimental DIII-D CER spectra**
  - **To obtain ion temperature, rotation velocity and amplitude**
- ***CERFIT* is a fortran-90 code**
- **Modular programming used to implement the model for CER spectrum**
- **Algorithms developed to maximize speed while retaining required accuracy**

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# Mechanics of Non-Linear Fitting

Perform initial fit using Gaussian model

Estimate cross section effect on $T_i$ and $V_{tor}$

Perform non-linear least-squares minimization

- Fit to model which is sum of CER peak plus Gaussians
- Perform numerical convolution of instrumental function with model spectrum
- Compute chi-squared

Compute error bars

# Perform initial fit using Gaussian model

- Problem initialized with standard Gaussian fit to experimental spectrum
- This model treats the spectrum as sum of Gaussians
  - Includes the CER line
  - May include a passive edge line from same ion
  - May include other edge lines

# Estimate Cross Section Effect on $T_i$ and $V_{tor}$

- Gaussian model produces good fit to CER spectrum
- However, the $T_i$ and $V_{tor}$ which are produced by the fit will have apparent shifts
- These apparent shifts are estimated from t he 1D analytic model for the spectrum
- The $T_i$ and $V_{tor}$ parameters are corrected for apparent shifts and used as initial guesses for the next step of the fit
- Amplitude parameter from Gaussian fit is passed through to the next step

# Perform Least-squares Minimization with CER Model

- **Fit to a model in which CER line is modeled with CER spectrum and other lines are treated as Gaussians**
  - **In fact, CER line is sum of 3 (6) CER spectra due to 3 energy components of 1 (2) neutral beams**
  - **Ratios of energy components obtained from beam attenuation calculations which are available from a database**
- **Instrumental function is convoluted numerically with model spectrum**
  - **Convolution performed with *QUADPACK* routine *DQNG*, a non-adaptive definite integral routine**
  - **Speed-up (~100X) obtained by evaluating model spectrum once and fitting with spline for use in the convolution**

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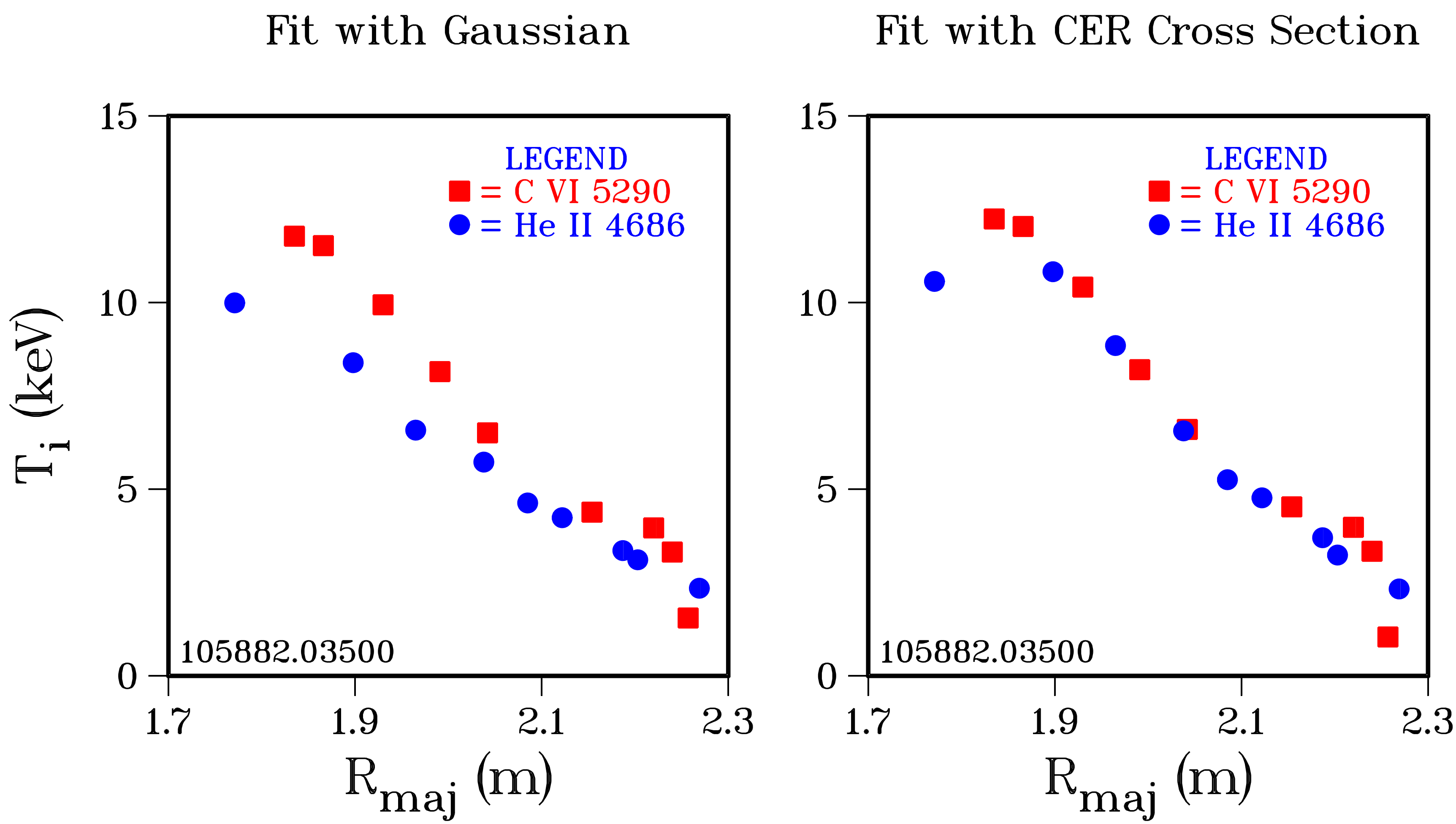
# Perform Least-squares Minimization - continued

- **Non-linear minimization is performed with *SLATEC* routine *DNLS1E***
  - **A Levenberg-Marquardt routine**
  - **Performs numerical derivatives of chi-squared with respect to the fit parameters**
- **After fit is completed, error bars are computed from covariance matrix**
  - **Covariance matrix obtained with *SLATEC* routine *DCOV***
  - ***DCOV* numerically obtains the Jacobian, required for the covariance matrix**

# Model with Cross Section Effect Brings He II and C VI Temperatures into Agreement

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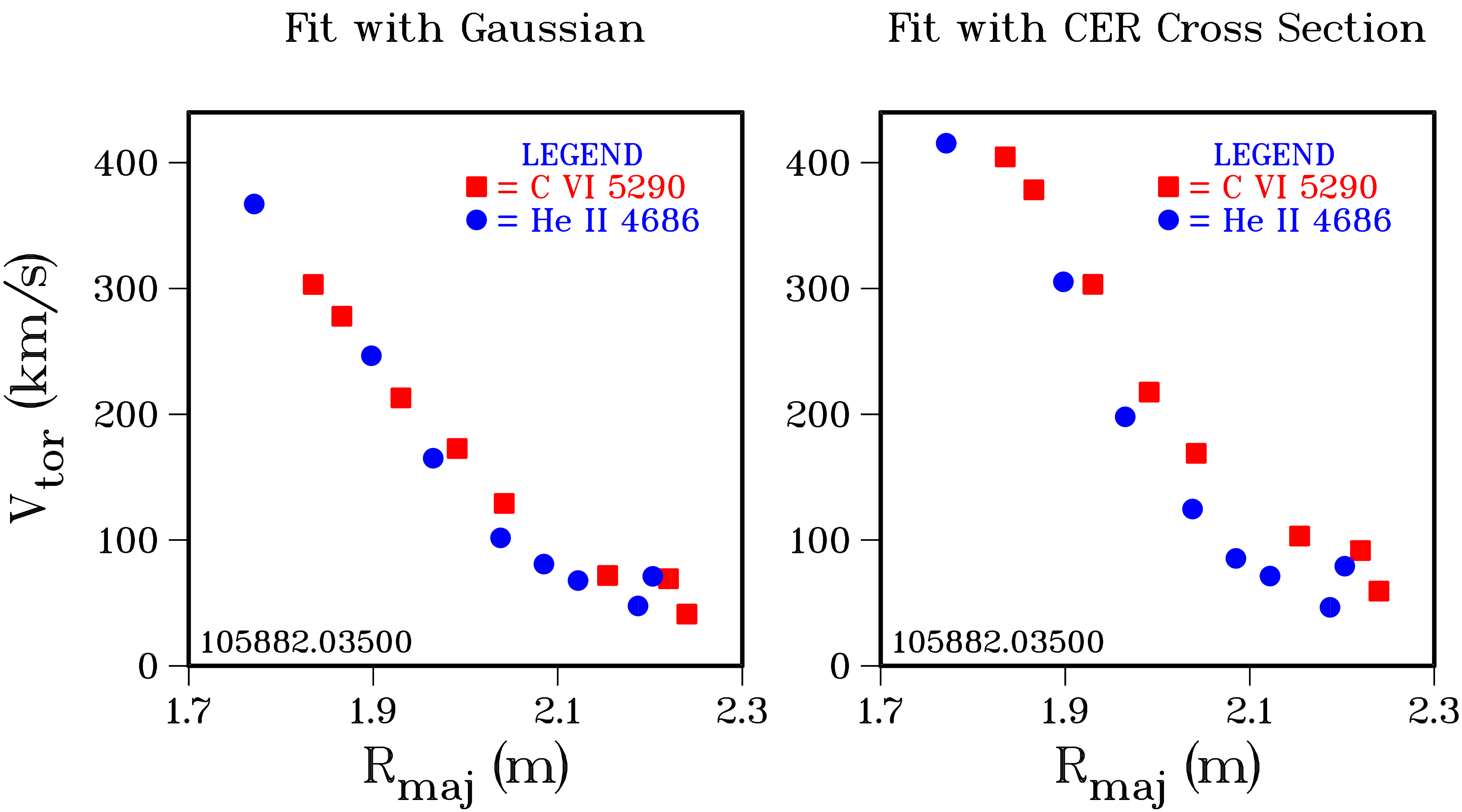
# Model with Cross Section Effect Increases Rotation Velocities Substantially



# Initial Conclusions

- **For ion temperature, use of CER cross section vs pure Gaussian model (for DIII-D geometry) →**
  - **Small increases of $T_i$ for C VI**
  - **Moderate increases $T_i$ for He II**
  - **Tends to bring $T_i$ for He II and C VI into agreement**
- **For toroidal rotation, use of CER cross section vs pure Gaussian model (for DIII-D geometry) →**
  - **Moderate increases of $V_{tor}$ for C VI and for C VI**
  - **Does not bring $V_{tor}$ for He II and C VI into full agreement**
    - This result is potentially a neoclassical effect
    - **See Baylor, RP1.030, this session**

# Status

- Software and testing have been completed for direct least squares fitting of CER spectrum with a model which includes the CER cross section effect
  - For horizontal views
- Benchmarking of results against post-processing technique has not yet been performed