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STARTING GENERATORS FOR ABS INTENSITY CALCULATIONS AND MAGNET SYSTEM DESIGN

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Abstract

In his recent thesis, Alexander Nass[1] used the direct simulation monte carlo (DSMC) method to simulate the supersonic expansion of the hydrogen beam of an atomic beam source (ABS), finding good agreement with measured data for both atomic and molecular beams. Because the properties of such expansion cannot be calculated analytically, the potential applications of such simulations are numerous. In particular, when designing the sextupole magnets that both polarize and focus the ABS beam, one needs to know how the speed, direction, and position of the beams' atoms are distributed While the original simulations of Nass provided only the average value of these distributions, a recent extension of the simulation provides the speed, position and direction of every atom simulated. This additional information can be used to test the crude models of the beam previously employed to calculate magnet transmissions. In addition, it is demonstrated that the speed distribution of the atoms predicted by DSMC is very sensitive to the numerical value for the cross section used to simulate collisions.

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1 Introduction

An atomic beam source (ABS) begins with molecular hydrogen or deuterium gas which is then dissociated into atoms with a high frequency discharge. These atoms are accelerated by an expansion from a high pressure to low pressure through a narrow cylindrical aperture called a nozzle. The gas is cooled before exiting the nozzle via collisions with its surface, which is kept at low temperature ($\sim$100 K). A skimmer and collimator select a small portion of the expanding gas, forming a jet of supersonic atomic hydrogen. Sextupole magnets separate the atoms by their electron spin, and hyperfine transitions can be induced with radio-frequency cavities to obtain a final beam of atoms with polarized nuclei.

The sextupole magnets separate the atoms by focusing those with a particular electron spin. The position, aperture and strength of these magnets must be carefully optimized to maximize the intensity and/or the polarization of the atomic beam. A typical calculation of the magnet transmission starts with N atoms, whose initial position, direction and speed at the entrance to the magnet system are randomly selected from known distributions. Each atom's trajectory through the magnetic field is calculated and the fraction of atoms that arrive at the collection tube is the transmission.

The method for producing a list of N atoms and their initial position, direction and speed is called a *starting generator* within the community. Various methods have been used to predict the position and direction of the individual atoms. Two such historic generators, for which the calculated magnet transmission is very different, are discussed in this note, comparing them with both measurements and predictions from DSMC. One is found to disagree with the both the measurements and the predictions while the other is in agreement as long as the aperture of the magnet system is very small. A third generator, appropriate for any aperture magnets, also agrees with both the measurements and the predictions.

The speed distribution of the atoms can be measured, and has been for some ABS systems[1,2]. Because it requires a special experimental setup, often the speed distribution measured on a separate but similar ABS is used calculate the magnet transmissions. However, there are experimental indications that the speed distribution (often called the velocity distribution) is very sensitive to the dissociator conditions such as temperture and geometry, and thus may be system dependent. The speed distribution predicted by DSMC is compared with the measurement performed by Nass, and the predicted width is considerably larger than the measured one. However, it is demonstrated that the DSMC predictions are extremely sensitive to the scattering cross section at low temperatures (10-50K), which must be input into the simulation, and thus some more tuning is necessary

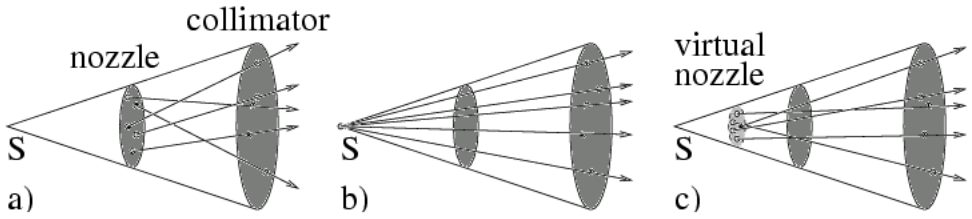

Figure 1:

for the DSMC simulation.

2 Position and Direction of atoms

2.1 Different generators

Many starting generators have evolved within the community in the past few decades. Two are nicely discussed in the doctoral thesis of Bernd Braun[3], who calls them *molecular* and *laminar*. They are depicted in figure 1 as a) and b) respectively.

The laminar generator is a point-like source whose position along the beam axis is determined by connecting the collimator and nozzle apertures and extending this line to its intersecton with the beam axis. Tracks are then created by connecting the point of the source with a randomly chosen point inside the collimator. These tracks give the position and direction of atoms entering the magnet system.

The molecular generator creates tracks by connecting a random point inside the nozzle aperture with one inside the collimator aperture. These two generators give surprisingly different results for the magnet transmission of hydrogen atoms of hyperfine state $|1\rangle$ for the HERMES target: 60% and 45% for the laminar and molecular generators respectively.

In addition to these two generators from the community, two new generators are considered, called *point-like* and *extended*. For the point-like generator, all atoms originate at the nozzle position on the beam axis.

For the extended generator, all atoms originate from a disk of radius equivalent to the nozzle radius, with an equal probability for every position within the disk. In both cases, the direction of the atoms leaving the source is distributed as $\cos^n \theta$ and distributed uniformly in azimuthal angle ϕ. ($n = 1$ corresponds to isotropic distributions, while values larger than 1 accomodate the forward peaking observed in supersonic expansions).

These two generators offer many advantages over the molecular and laminar ones

of Braun. They are independent of the collimator geometry, they are isotropic for n=1, and they also determine the fraction of the initial beam which enters the magnet system, a quantity needed to calculate the intensity of the ABS. Neither the molecular nor the laminar generator is isotropic (each point within the collimator disk is equally probable), a difference that cannot be neglected for a large aperture collimator and magnet system.

There are two important quantities for comparing any starting generator to measurements and/or monte carlo data: the azimuthal component of the direction and the transverse beam size. For the laminar and point-like generators, the azimuthal component of the direction of the atoms entering the collimator is zero by definition. For the molecular and extended generators, non-zero values are possible below a maximum defined by the nozzle-collimator geometry. For more detail, see Appendix A. The azimuthal velocity distribution is difficult to measure, but the distributions from simulations and generators can be compared. The transverse beam size at positions between the source and collimator are predicted by simulations and generators, and can be measured in the laboratory as well.

2.2 DSMC description

DSMC is a technique for the computer modelling of a real gas flow by a sample of simulated particles[4]. The velocity and position coordinates of these particles evolve in time as they experience collisions with other particles and with surfaces in simulated physical space. The time steps of the simulation must be small enough that the motion and the collisions of the particles are decoupled, as they are treated separately in the simulation. It is only in the last few years that such simulations have been feasible (in computing power) for the beam formation system of an ABS.

Nass' work shows that the DSMC method simulates quite well the properties of the expansion and resulting particle beam. He also verified, with simulations and experiment, that the carrier jet method proposed to increase the forward intensity of the hydrogen beam is ineffective. The DSMC software used by Nass provides only the mean and the rms values for the distributions of the position and velocity coordinates of the particles. A recent addition by the author gives access to the position and velocity of every particle simulated, faciltating a comparison of the simulated beam's properties with those predicted by the much simpler generators.

2.3 Azimuthal Direction

Figure 2 shows the distributions of azimuthal direction for tracks created with four different starting generators. For the laminar (effusive) and point-like generators, the direction

has no azimuthal component, whereas for the molecular and extended the distributions are identical. These can be compared with the distribution of the atoms simulated with the DSMC method in figure 3. The long tails of this distribution are excluded from the figure, and come from the background gas: particles that have already collided with a surface, thus randomizing their velocity direction. Clearly, the DSMC results are not compatible with the laminar and point-like generators. The HWHM of the DSMC distribution is slightly larger than the molecular and extended generators.

2.4 Transverse Beam Size

Figure 4 shows the beam density as a function of distance from the axis at a position 20 mm from the skimmer. Again the difference between the point-like source and the laminar model is significant, and the extended source is just a smeared version of the point-like source. Figure 6 contains the DSMC predicitions for beam density as a function of radius (distance from beam axis) at four distances from the skimmer. The upper left plot is compared with the predictions from the four generators in figure 5. For the laminar and point-like generator, the edge of the beam is well-defined. For the extended and molecular, the mid point, where the beam density drops by 50% corresponds to the point-like predictions (dotted line). The solid line indicates the radius for which the density is 0. The points are the DSMC predictions, located at the radius where the beam density falls to 50% of its original value. The error bars indicate the full range of the drop from the original beam density to 0.

Unfortunately, no experimental measurements of the transverse beam size after the skimmer are currently available from the Jade Hall test stand, for which the DSMC simulations were performed. However, we can compare the simulations with the generators. The extended source and molecular generator both agree nicely with the DSMC results. The smearing caused by the non-zero azimuthal velocity changes the beam's radial edge from a sharp drop from the previously constant density near the axis to a more gradual decrease. Note that not only is the smearing absent in the laminar generator, but the beam size is different as well. The conclusions are the same as those for the azimuthal direction distributions: the extend and molecular generators are compatible with the DSMC results while the laminar and point-like are not.

Although the DSMC results clearly favor the extended source, the point-like source should not be completely discarded when designing a magnet system. Placed at the same position as the extended source, it slightly overestimates the magnet transmission. As an example, the magnet transmission of the HERMES ABS, calculated with a point-like generator is 50% for hyperfine states 1 and 2. Using the either the extended or the molec-

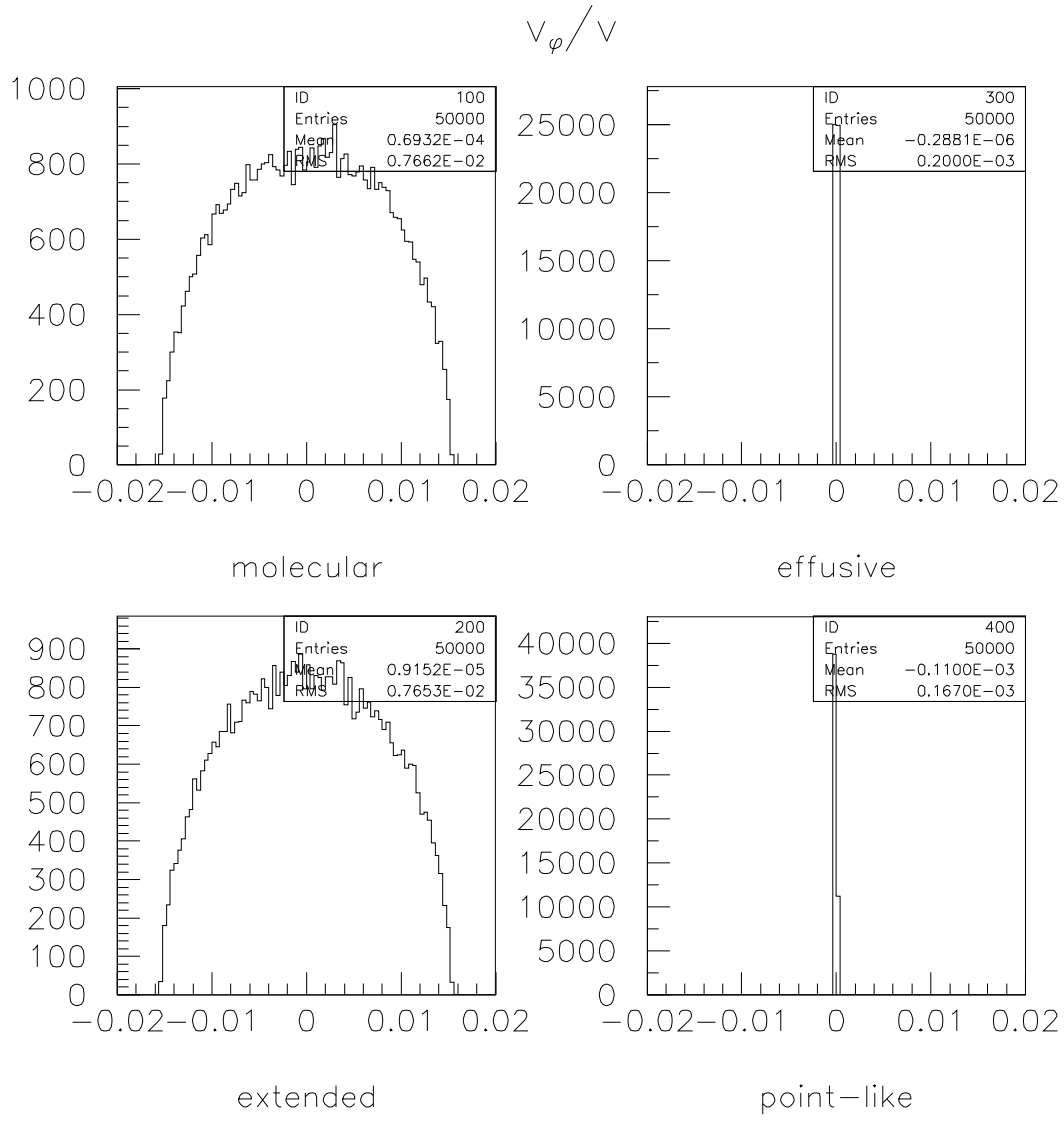

Figure 2: The distributions of the azimuthal direction for tracks created with four different starting generators.

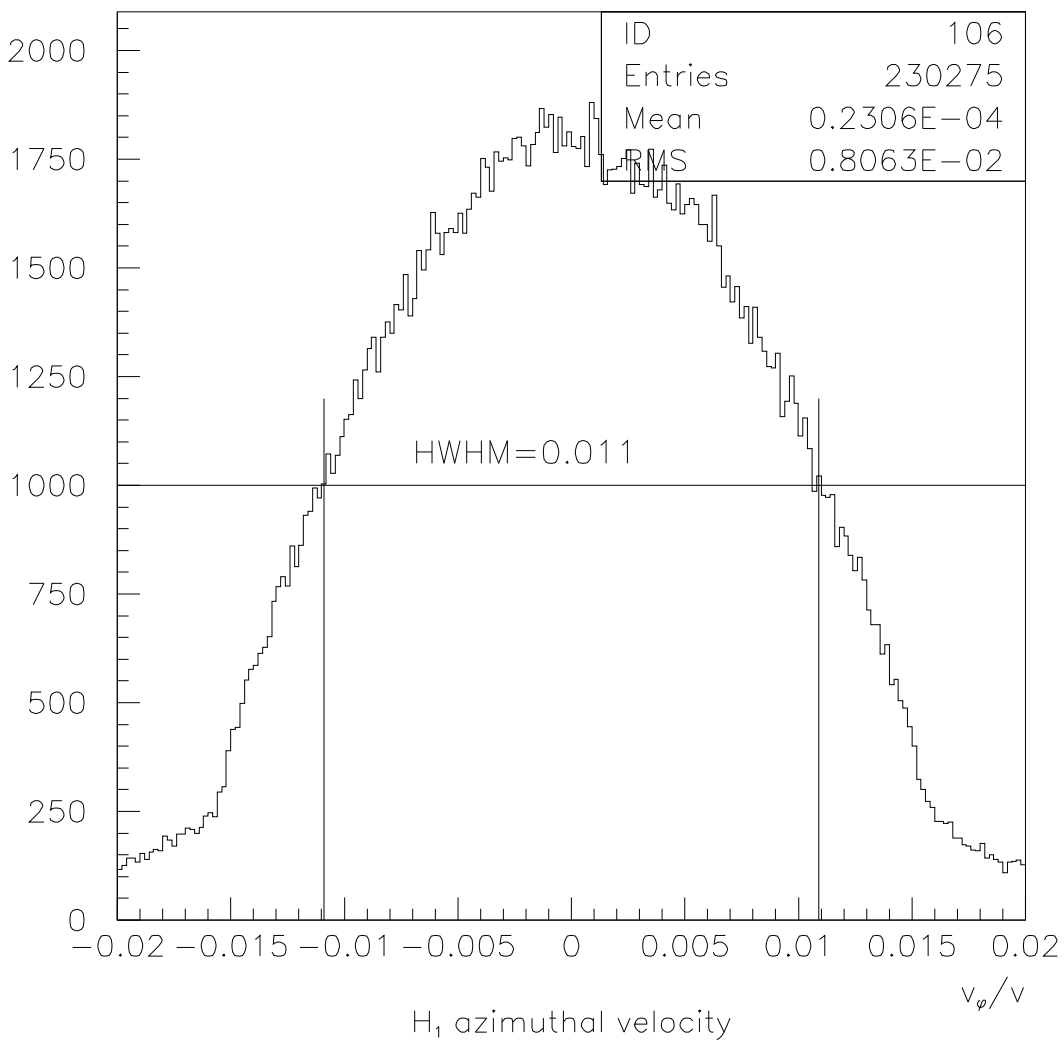

Figure 3: The distribution of azimuthal direction at the collimator aperture for hydrogen atoms simulated with the DSMC method.

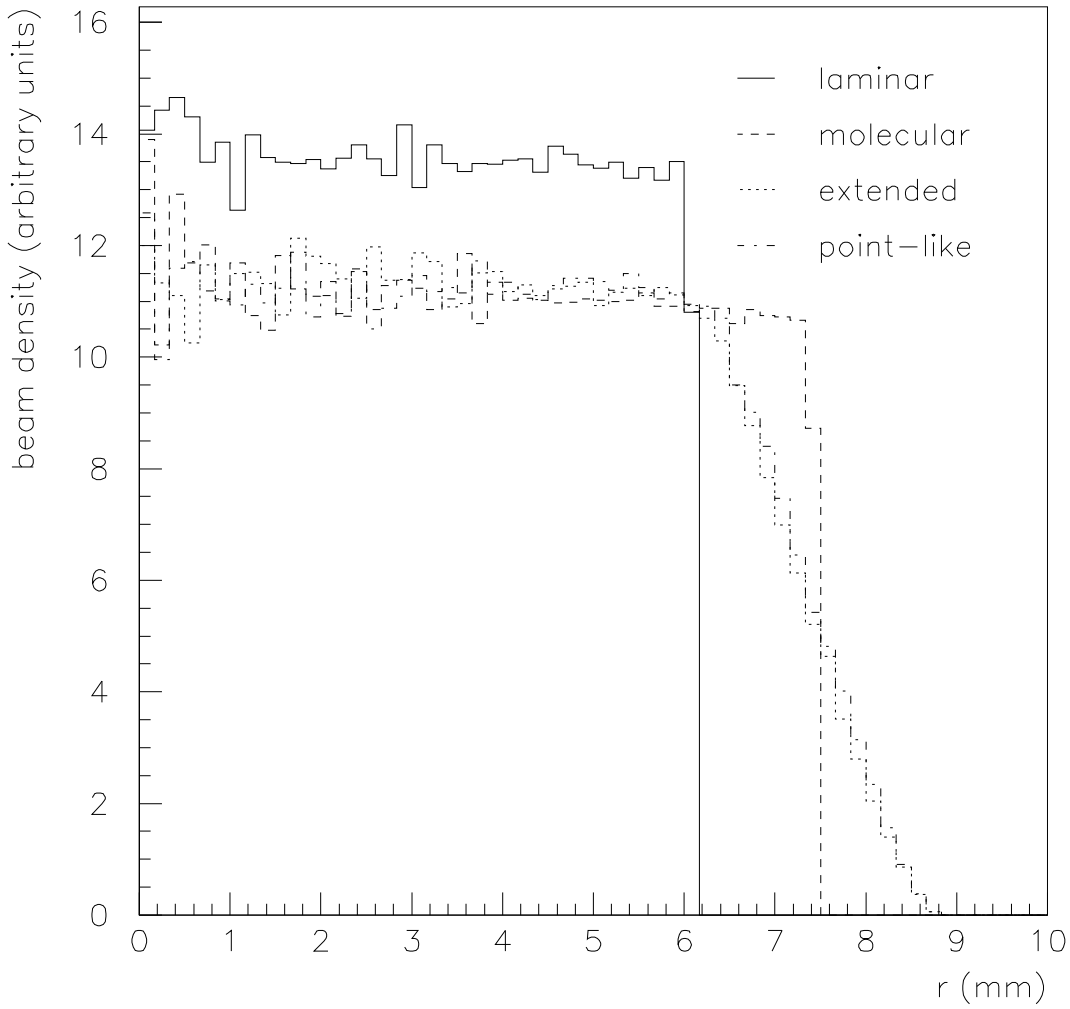

Figure 4: The radial beam profiles from the four starting generators, at a distance of 20 mm from the skimmer.

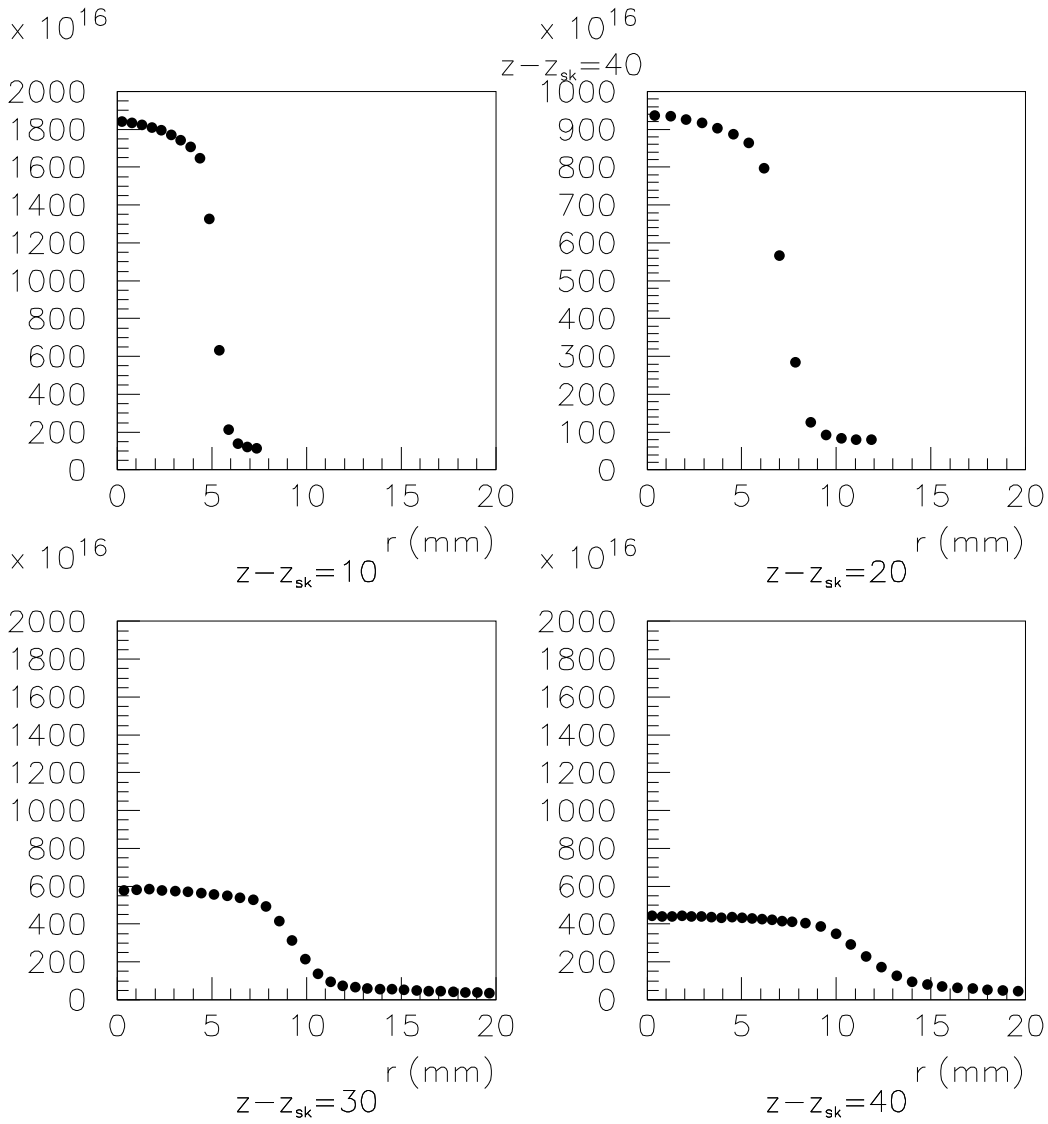

Figure 5: The DSMC predictions for the radial beam profile at various distances from the skimmer.

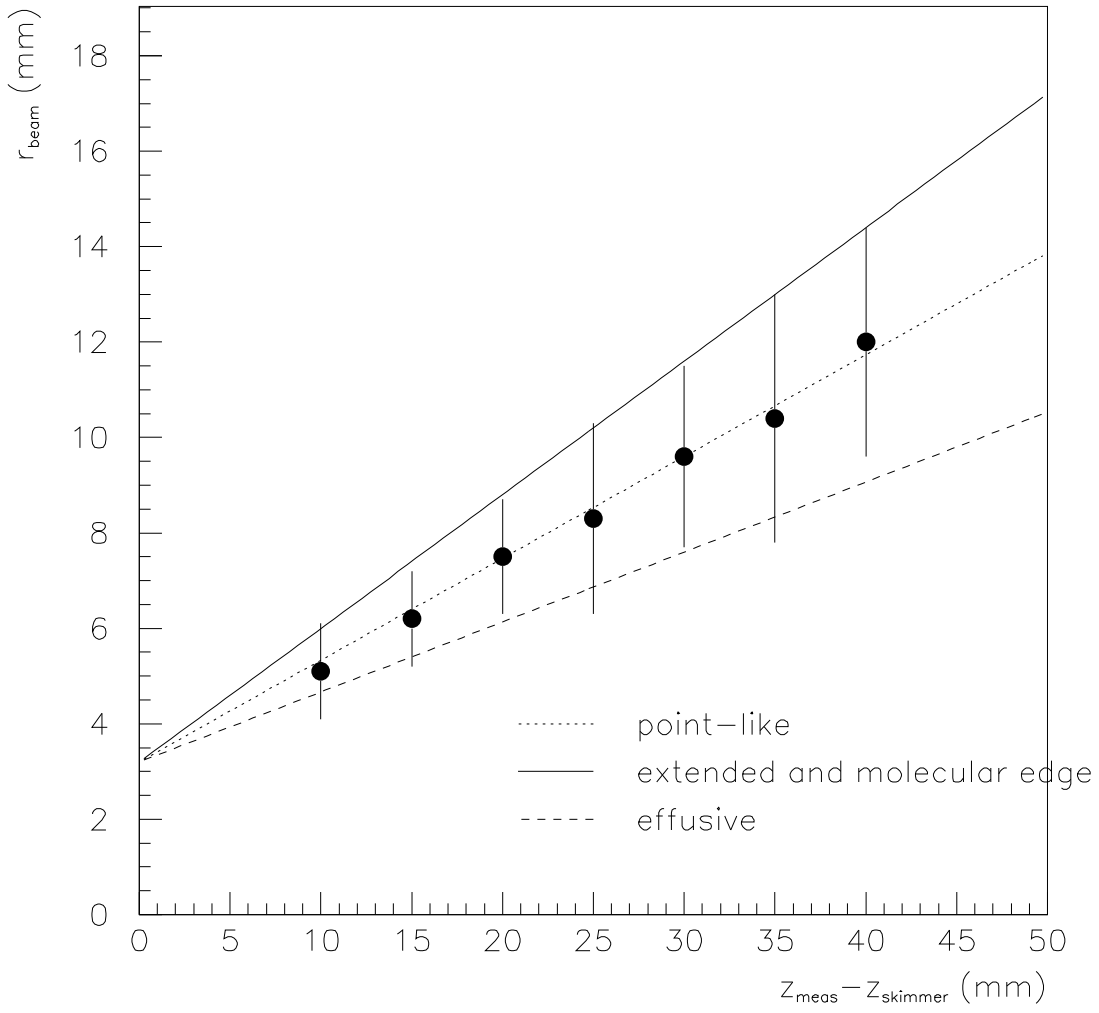

Figure 6: The complete radial beam size as a function of distance from the skimmer, which is 15 mm upstream of the nozzle, for the four starting generators. The points are the DSMC results, taken as the radius where the beam reaches 50% intensity and the error bar indicates the full beam size.

ular generator, the efficiency drops to 45%. However, the computation times is a factor of 50 longer for the extended source, and the small overestimate of the efficiency may be acceptable when searching for the optimal magnet parameters (aperture, length, position, etc), where the acceptance of many thousands of systems must be calculated. If the nozzle-collimator separation and nozzle diameter are kept fixed, precious computation time is saved by starting the parameter search with the point-like source to find the minima, and then refining these results with the extended source.

3 Speed distribution of the atoms

The second piece needed to calculate the transmission of the magnet system is the speed distribution of the atoms entering the magnets. *Speed distribution* is used here instead of the usual term velocity distribution to emphasize that the direction of the atoms has already been discussed. Here instead we are concerned with only the magnitude of their velocity. Again, there is no analytical way to predict the speed distribution that results from expansions charaterized by Mach numbers in the range 1 to 4 (barely supersonic). Until the DSMC simulation results, only measured distributions from other sources were available when designing a magnet system. Given the success of Nass' simulations in reproducing the measured characteristics of the expansion such as beam size and mean velocity, it remains only to demonstrate agreement between the measured and predicted speed distributions before proceeding with DSMC simulations of new nozzle geometries for example, in hopes to increase the forward intensity and/or the magnet efficiency.

The transmission of the magnet system depends not only on the mean speed of the beam, but also on the width of the beam's speed distribution. Nass' measurement of this width is much smaller than simulation predicts - the difference well beyond the quoted errors. Any influence from background atoms (those which collide with a surface and thermalize to 300 K) has been excluded by extending the simulation to the QMA position, 1 meter downstream of the collimator. The speed distribution from the DSMC simulations corresponding to Nass' measurements for a molecular hydrogen beam is shown in figure 7. It has been fit with the traditional modified-Maxwellian shape[1]

$$vf(v) = Av^3 e^{\frac{-m(v-v_{drift})^2}{2kT_{beam}}} \tag{1}$$

where A is an arbitrary normalization constant, and v_{drift} and T_{beam} are the two parameters of the distribution. The distribution is obtained from a dump file placed at the end of

[1]the density distribution $f(v)$ must be multiplied by v because the file records all atoms crossing the boundary during the simulation time, which is equivalent to a flux distribution. The QMA measures the density distribution.

the simulation, and molecules whose transverse velocity exceeds 1% of their total velocity are excluded to ensure a background free sample. The agreement between the best fit curve and the actual distribution is poor - the simulated distribution has a different functional form. Furthermore, the simulated distribution is incompatible with the measured beam parameters, shown as a dashed curve on the same plot.

These discrepancies motivated a more indepth study of the DSMC input parameters. The density of the input stream into the nozzle was adjusted to give the correct simulated flow (within 3%) at the nozzle exit (experimentally fixed by the flowcontroller at the input to the dissociator tube). While doubling the amount of background gas in the chambers has no effect on the velocity of the beam, changing the hydrogen scattering cross section at low temperatures does.

3.1 Scattering Models

The DSMC software used offers three models to calculate collision dynamics: the traditional hard sphere scattering model, the Variable Hard Sphere (VHS) scattering model, and the Variable Soft Sphere (VSS) model.

In the hard sphere scattering model, the scattering cross section and the deflection angle depend only on the atom or molecule diameter.

$$\sigma = \pi d^2 \tag{2}$$

and the deflection angle, χ, of the incident particle (in the frame where the other is at rest) is given by

$$\chi = 2\cos^{-1}(b/d) \tag{3}$$

where b is the impact parameter. The hard sphere model has the disadvantage that the cross section is independent of the relative translational energy, E_t, in the collision, whereas the effective cross section of real molecules decreases as E_t increases. The rate of decrease is related to the change of the coefficient of viscosity with temperature.

The variable hard sphere model (VHS) accounts for this by defining an effective molecule diameter which varies with temperature

$$d = d_{ref}(c_{r,ref}/c_r)^{\omega-0.5} \tag{4}$$

where the subscript ref denotes reference values, usually taken at 273 K, and c_r is the relative speed between the molecules of the collision, the magnitude of which is unchanged during the collision. The dimensionless parameter ω is called the viscosity index, and its value is gas dependent, roughly in the range from 0.5 (simple hard sphere model) to 1.1. The angle of deflection, χ is unchanged from the hard sphere model in VHS.

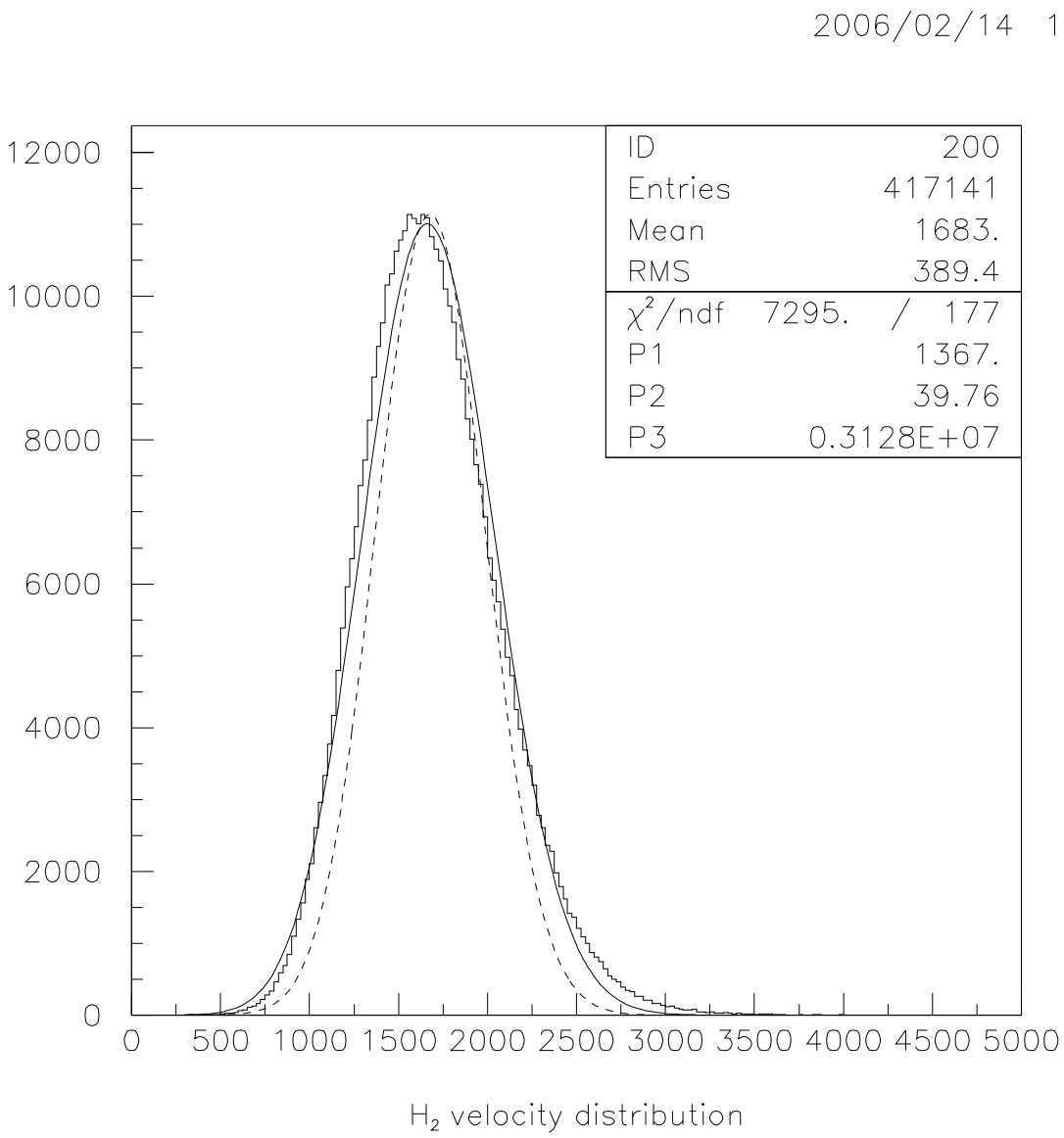

Figure 7: The measured and simulated (original) velocity distributions for molecular hydrogen.

The VSS model is a further refinement of the VHS model in which the deflection angle distribution can be changed via the parameter α,

$$\chi = 2\cos^{-1}[(b/d)^{(\frac{1}{\alpha})}] \tag{5}$$

which allows the ratio of the momentum and the viscosity cross section to move closer to its measured value. The values of α generally lie between 1 and 2. The simulations originally performed by Nass use the VSS model with $\omega = 0.67$ and $\alpha = 1.35$.

3.2 Impact on speed distribution

To investigate the correlation between the parameters of the collision dynamics (d,ω, and α) and the speed distribution predicted by the simulation, the parameters were individually changed from their original values and the effect on the speed distribution noted in table 1. In the fourth and fifth columns of the table are the values reported by the DSMC program for the mean and the rms of the moelcules' velocity. The sixth and seventh columns contain the mean and rms of the distributions after a cut requiring that the transverse velocity of the molecule was less than 1% of its total velocity. All the molecules that enter the QMA ionizing volume also satisfy this requirement, the cut serves to eliminate background gas. Comparing columns 5 and 7, the background gas slightly inflates the width reported by the DSMC program.

Increasing the cross section at low temperature (by increasing either the parameter d or the parameter ω) decreases the width of the speed distribution. In contrast, turning off VSS by setting $\alpha = 1.00$ has no effect on the distribution. Figures 8-10 compare the distributions generated with different parameter sets to Nass' measurement. Also plotted as a solid line is the modified Maxwellian curve that best fits the simulated data.

This exercise is intended only to demonstrate the sensitivity of the speed distribution to these initial parameters. Before using the DSMC method as a tool in future studies, these parameters need to be fine tuned using dedicated measurements with a molecular beam, as well as a through literature search for existing cross section measurements at 20 K. The atomic hydrogen cross section and atom-molecule cross section must also be investigated before extensive simulations with dissociated beams.

4 Conclusions

At Jade Hall in DESY, Hamburg, the properties of the supersonic expansion of the ABS beam formation system have been predicted by the DSMC method and most agree with measurements. The distributions of position and direction for the atoms entering the ABS magnet system is predicted by the DSMC simulations. The predicted distributions and

			DSMC calculated		distribution	
d (10^{-10} m)	ω	α	$\bar{v}$ (m/s)	TTX (K)	$\bar{v}$ (m/s)	rms
2.88	0.67	1.35	1349	32.9	1338	29.0
2.88	0.67	1.00	1353	32.5	1345	28.3
2.16	0.67	1.35	1285	38.9	1280	34.0
3.81	0.67	1.35	1388	28.0	1381	23.6
2.88	1.25	1.35	1396	23.4	1371	19.0

Table 1: The effects of different cross section values on the velocity distributions of a simulated beam of molecular hydrogen. TTX is the parameter from the DSMC simulation that corresponds the beam temperature. The top line corresponds to Nass' original simulation. A cut on the transverse component of the molecule's velocity was applied to the raw distributions before calculating their mean and width to eliminate background.

these predictions can be tested with laboratory measurements. The DSMC simulation itself is too time consuming for repeated use when designing a magnet system; however its predictions for the position distributions allow us to select a simplified model, or starting generator, for the task. Furthermore, simulations of different nozzle, skimmer or dissociator geometries may lead to new improvements to the beam formation system. Dedicated experimental measurements of the transverse beam profile would cement the agreement between data, generator and simulation.

Comparing the speed distributions generated by the DSMC simulation with measured ones reveals that they are not in complete agreement. Although the background gas slightly inflates the width, it does not account for the complete discrepancy. The model used for simulating collisions inside the DSMC software, in particular the parameters which determing the scattering cross section, likely account for the rest. Dedicated studies are needed to determine whether the parameters in the VSS model for low temperature hydrogen collisions can be tuned to match laboratory measurements, or the VSS model itself is inadequate. Collisions involving atomic hydrogen have not yet been studied, but one can expect to do a fair amount of tuning there as well. Such dedicated studies could very well provide an indirect measurement of the scattering cross section in the temperature range 10-50 K.

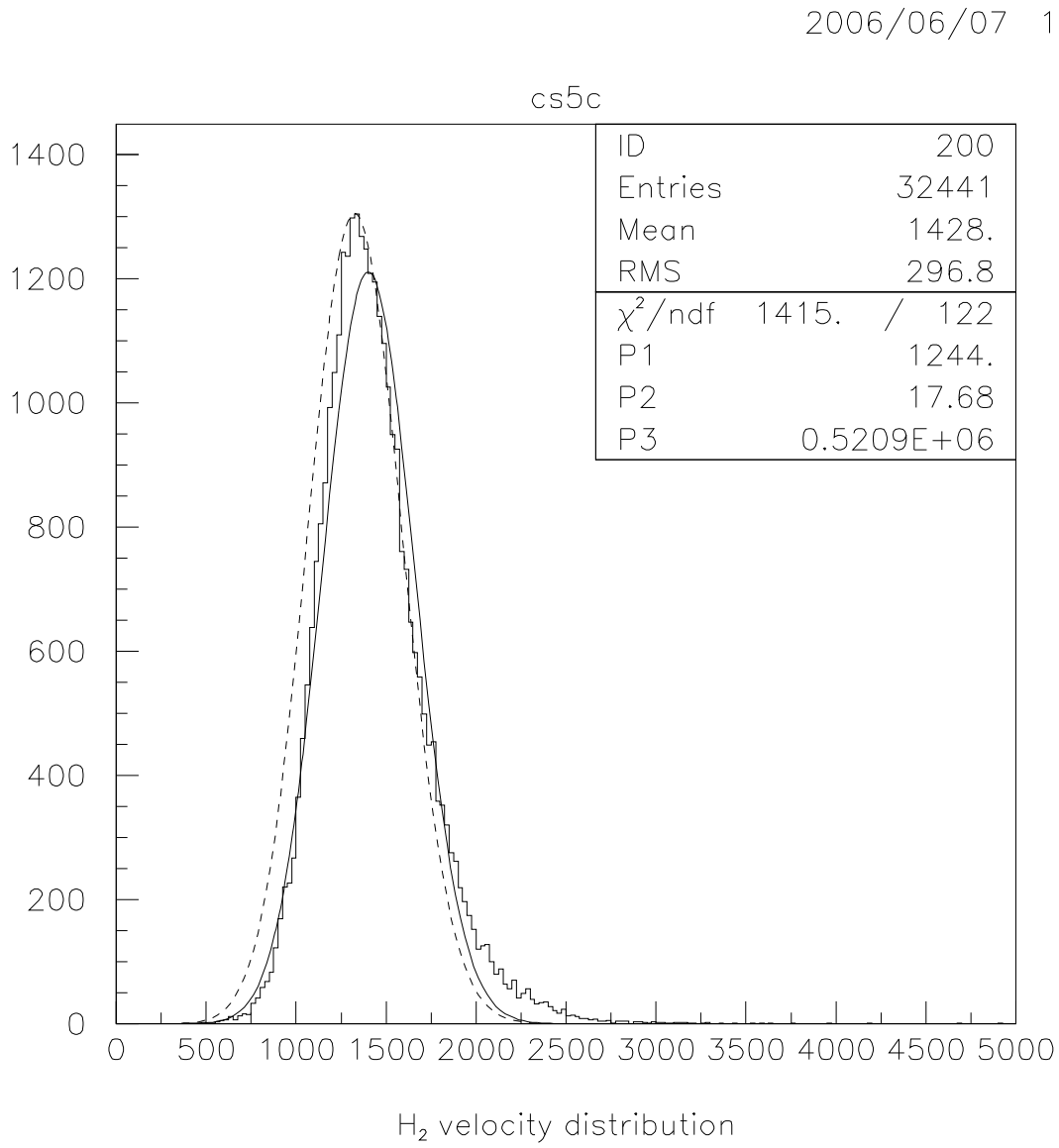

Figure 8: Comparison of the measured (dashed line) and simulated ($\omega = 1.25$) velocity distributions, with the modified Maxwellian that best fits the simulated data plotted as a solid line.

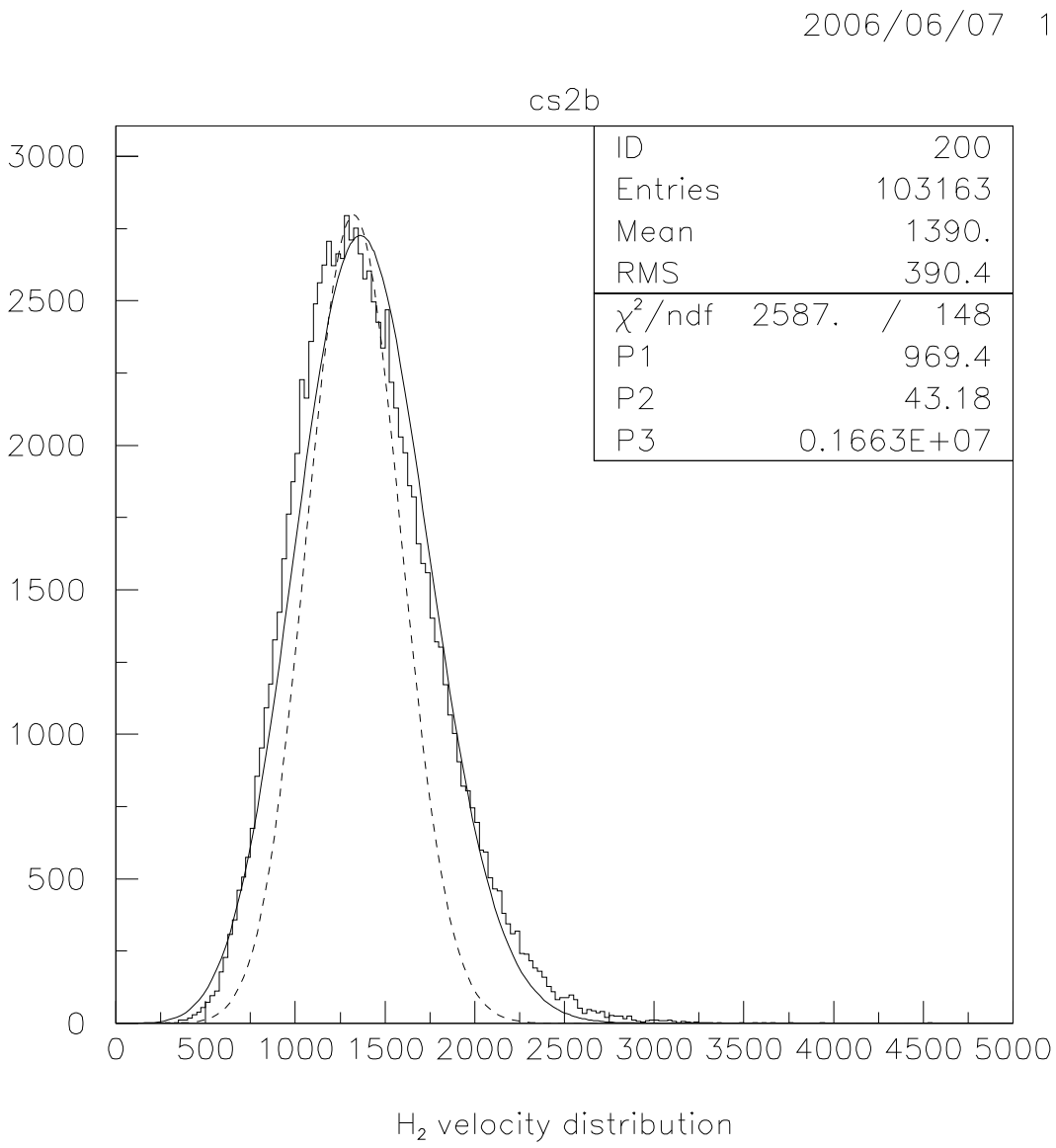

Figure 9: The measured and simulated ($d = 2.16 \times 10^{-10}$ m) velocity distribuitions.

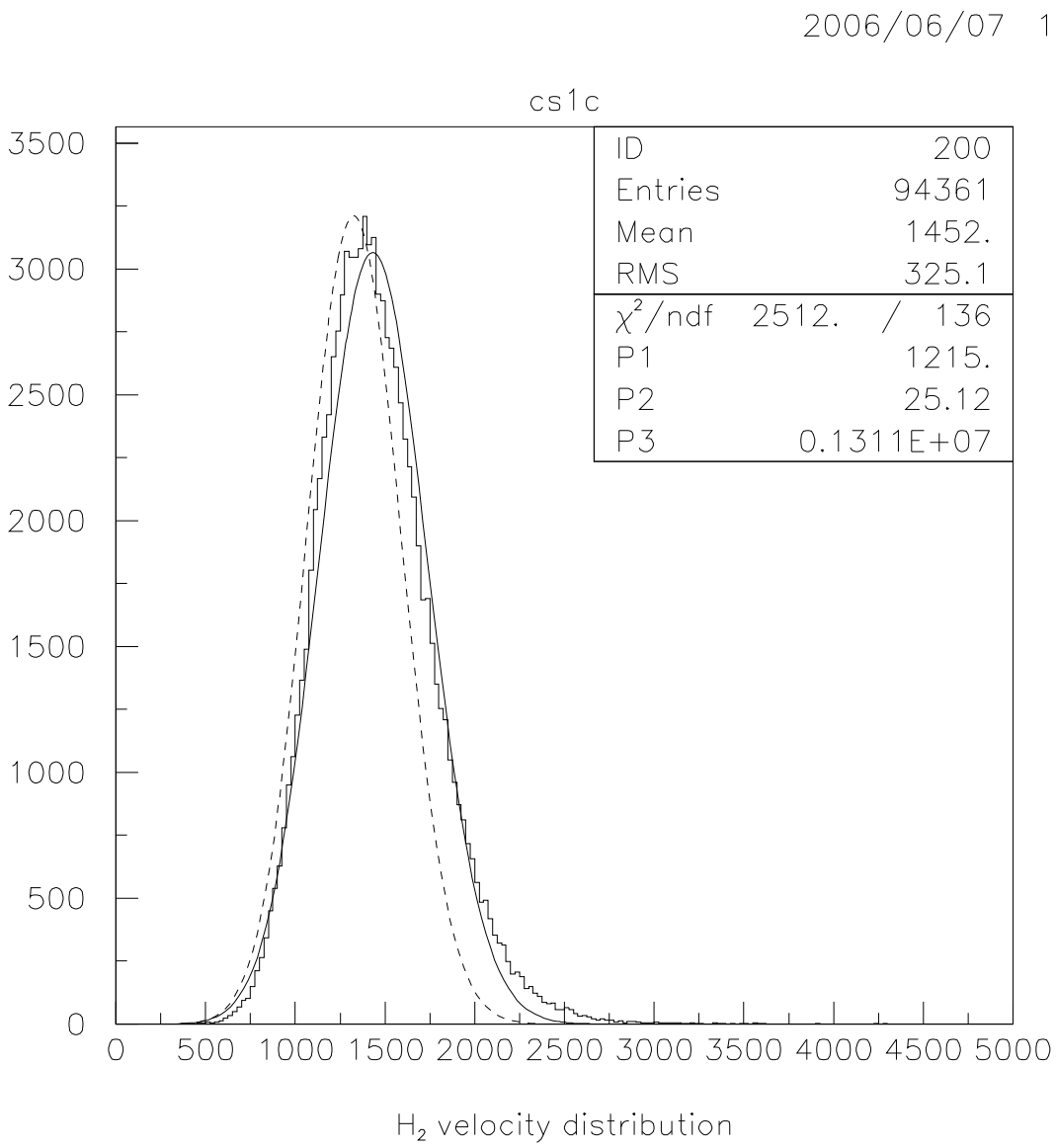

Figure 10: The measured and simulated ($d = 3.81 \times 10^{-10}$ m) velocity distribuitions for molecular hydrogen.

5 References

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