

N-shield, description

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I. Overview

(A) Motivation for N-SHIELD

N-SHIELD is a simple hadron cascade FORTRAN Monte Carlo program whose purpose is to evaluate dose equivalent from (primarily) neutrons arising from the interaction of hadrons in bulk matter. Its existence stems from this author's experience with two other Monte Carlo programs, CASIM,¹ and MCNPX.² CASIM has been used for many years at BNL for shielding calculations. However, it has several deficiencies when used for shielding calculations. One problem is that low energy neutrons are not transported, so that an "equilibrium spectrum" assumption is needed to estimate dose equivalent (hereafter referred to as "dose") from the actual quantity calculated, namely the star density for hadrons above 0.3 GeV/c (~47 MeV for neutrons). It is somewhat difficult to judge when the equilibrium spectrum assumption is a good one. Another significant problem is that CASIM gets dose "too far forward" in comparison with both other codes and measurements.³ On the other hand, CASIM's transport enables good statistical precision for "deep penetration" calculations, which will be *assumed* to be a virtue,⁴ and has magnetic field capability.

MCNPX, by contrast, has extremely detailed low energy neutron transport, and high energy physics approximations that are generally recognized as reasonably good (although a suite of careful measurements for comparison to code predictions is notably lacking.) Other than lacking magnetic field capability, MCNPX is in many ways the perfect tool for shielding calculations.⁵ However, one drawback and one "pseudo-drawback" exist in using this code. The drawback is the opposite of the assumed virtue of CASIM, namely that deep penetration calculations (usually encountered in a complex 3-D geometry) can be difficult, at least for a user as naïve as this author. The "pseudo-drawback" of MCNPX is the immensity and complexity of the code. This author has made serious errors in misguided attempts to use some of the variance reduction techniques available in this code. MCNP itself is used for reactor design, and it is by no means obvious that obtaining "reasonable estimates" of the radiation field around an accelerator – at least in many geometric configurations – requires a code of this complexity. It is very easy, by contrast, to understand what CASIM is doing, if not the exact details. Many physicists at BNL have run CASIM over the years with a high "comfort level," and no need for special training. This is also assumed, without proof, to be a virtue of the CASIM code. N-SHIELD is certainly not intended to be an alternative to MCNPX, but may have some advantages as an alternative to CASIM.

(B) The N-SHIELD Code in Brief

Many aspects of the CASIM code have been blatantly copied (sometimes literally) into N-SHIELD. The principal similarities between CASIM and N-SHIELD are the following.

1. The approximation is made that the hadronic world is composed entirely of nucleons and pions.
2. The code is simplistically “on mass shell,” meaning that differences in the actual masses of spallation products is ignored. All energy comes from the incident kinetic energy of the beam. As an example of this simple behavior, 8 MeV is subtracted from the incident kinetic energy for each evaporation nucleon created.
3. The transport of (“high energy”, i.e., cascade-propagating) particles is essentially copied from CASIM. This is briefly explained further in the next section, but the reader is referred to Ref. [1] for a detailed explanation.

The principal differences between CASIM and N-SHIELD are the following.

1. The “high energy” physics modeling is, of course, *different* than that in CASIM, not necessarily better.
2. An approximation of low energy (< 20 MeV) neutron creation and transport exists in N-SHIELD.
3. The quantities estimated are derived from hadrons crossing user-specified surfaces, not the star density calculated by CASIM. Furthermore, no other quantities (energy deposition or dose from muons) are estimated in the current version of N-SHIELD)
4. Mixtures are allowed in N-SHIELD.

Additional differences exist, which will be touched on in subsequent sections of this note. The incident energy range over which N-SHIELD might be used is not clear. There is a hard upper limit to the current version of the code at about 500 GeV, and a hard lower limit of 20 MeV. (All energies mentioned in connection with N-SHIELD are kinetic energies.) However, very little testing has been done above 100 GeV, and none at all above 250 GeV. Comparisons between N-SHIELD, CASIM, and MCNPX over a wide range of energies for some simple geometries are given in Section VIII below.

II. Excitation Energy

The first step in the code simulating an interaction of a particle with a nucleus is to subtract the “excitation energy” from the incident particle’s energy. The starting point for the prescription for this energy was taken from the original approximations of Ranft.⁶ The distribution of this energy into nucleons, de-excitation photons etc. is supposed to roughly account for virtually all of the “nuclear physics” envisaged to take place during a collision, i.e., the “intra-nuclear” cascade.⁷ The first step in the development of N-SHIELD was to “tune” the prescription of Ranft to the number of neutrons < 10 MeV (mostly evaporation neutrons) and the number of neutrons > 10 MeV (mostly cascade neutrons) to MCNPX calculations for 3 values of atomic weight A and 3 energies. The intent was to make as few changes as possible to the original prescription to obtain roughly the right numbers of neutrons. In the end, besides the threshold, which was changed to 20 MeV from 50 MeV, only two significant changes were made

which corresponded to the most sensitive parameters to this somewhat arbitrary comparison to MCNPX. The first change was that the total excitation energy, instead of being proportional to A, contains one term proportional to A, corresponding to the evaporation process, and another term proportional to $A^{2/3}$, corresponding to the (higher energy) cascade process. The other (rather modest) change was that the ratio of sampling of cascade nucleon energies from two distributions described by Ranft was changed slightly. The excitation energy was normalized to the original version of Ranft at A = 56.

A brief description of the excitation energy and its distribution in N-SHIELD is as follows. The excitation energy is taken to be

$$\begin{aligned}
 &= T_0 \text{ for } T_0 < E_{th} \\
 E_{ex} &= E_{th} + \frac{(T_0 - E_{th}) \times (B - E_{th})}{3 - E_{th}} \\
 &= B \text{ for } T_0 > 3 \text{ GeV}
 \end{aligned}$$

where T_0 is the incident energy, E_{th} is .020 GeV, and B is $1.54 \times (.001A + .021A^{2/3})$. A portion of this energy is assigned to heavy fragments and photons, following which cascade nucleons and finally evaporation nucleons are selected. The energy “allocated” to the cascade selection corresponds to the $A^{2/3}$ part of the energy remaining after subtracting the heavy fragment and photon energy. Protons are selected with probability less than Z/A due to Coulomb barrier effects. With the current prescription of excitation energy assignment, the comparison to the MCNPX neutron spectrum is shown in Table 1.

Table 1 Average number of neutrons (MCNPX/N-SHIELD)

A	T_0 (GeV)	n < 10 MeV	n 10 < E < 50	Total n
12	0.5	.25/.26	.24/.48	1.0/1.2
12	2.5	.35/.68	.50/.94	1.9/2.3
12	5.0	.82/.67	1.4/1.0	3.4/2.4
56	0.5	1.4/.9	.6/.9	2.5/2.4
56	2.5	3.0/3.0	2.5/2.3	7.3/6.5
56	5.0	4.4/3.3	2.3/2.2	8.1/6.9
208	0.5	6.0/3.7	1.1/2.1	7.7/6.7
208	2.5	14.5/14.8	6.2/7.0	23.2/24.1
208	5.0	21.3/16.8	9.9/6.7	34.0/26.4

This table compares the number of neutrons in the energy ranges indicated as a function of the 3 materials and energies chosen. Other materials and energies would presumably disagree much more since this table represents the tuning performed.

The result of the subroutine that handles the excitation process is a certain amount of “local energy,” which in principle accounts for photons, heavy fragments, and protons < 20 MeV, and two “stacks” of particles – a low energy stack containing neutrons \leq 20 MeV, and a “high energy” stack containing nucleons > 20 MeV.

III. The Cascade Process & High Energy Cross-Sections

Optionally, the second step in the life of an incident particle is that its direction can be (slightly) changed by considering the (already selected) cascade nucleons to be the result of the incident particle scattering with nucleons. This is in the spirit of a very crude “wounded nucleon” model. A target nucleon is then selected and given a Fermi Momentum from a simple Fermi Gas distribution. Finally, a particle-particle interaction is simulated as elaborated in the next section.

As mentioned above, the transport in N-SHIELD mimics that of CASIM. One difference is that, in each interaction, complete events are constructed. In the cascade process, as distinguished from the “recording” of the cascade process,¹ here called scoring, a single particle, appropriately weighted, is selected from the complete event stack to propagate the cascade. The cascade terminates when the particle selected is below threshold or exits the confines of the geometry during transport. The reader is referred to Ref. [1] for further details.

The change of the cascade threshold to 20 MeV necessitates cross sections that also change. In the current code, inelastic cross sections are considered to be constant above 70 MeV for nucleon-nucleus interactions and above 300 MeV for pi-nucleus interactions. In the region of constant cross sections, the cross section is assumed to have a Brant-Peters form, i.e. $C1 \times (1. + A^{1/3} - C2)^2$, where $C1$ and $C2$ are constants. The constants were fixed for nucleon-nucleus by adopting the CASIM cross section for $A = 56$ and taking 33 mb. for the high energy pp cross section. Pi-nucleus cross sections are currently set at 0.65 of the nucleon-nucleus cross section.

Nucleon-nucleus cross sections rise linearly from 70 MeV to 1.7 times the high energy value at 30 MeV, are then constant to 20 MeV, and drop to 0 at 8 MeV where, in the simplicity of the on mass shell model, a nucleon can no longer be liberated. (The relevance of the cross section below 20 MeV will be explained in Section VI below.)

The rise in the pi-nucleus cross section is the only account taken of the resonance region for incident pions. The threshold corresponds to the beginning of the Δ region, and the assumption is made that the rise in the pi-nucleus cross section is relatively the same as that in the pi-nucleon cross section. The peak of the cross section is flat between 190 and 210 MeV (lab pion energy) and goes linearly to the high energy value at 300 MeV, and zero at 20 MeV. Higher mass resonances in the particle-particle spectrum are totally ignored at the present time.

IV. Particle-Particle Physics and Event Creation

The particle selection starts from expressions that are intended to approximate inclusive distributions in the “scaling region,” i.e., above 8 GeV or so, with very crude extrapolation to lower energies as explained below. No exhaustive examination of the literature has been undertaken – both the starting and ending points of the approximations currently used are (non-recent) publications known to this author. The final product of the particle selection process is

that the created particles are added to the high energy event stack, joining the high energy cascade products described in Section II above.

(A) Nucleon-Nucleon Collisions

The first step in particle selection in a nucleon-nucleon collision is that one nucleon is sampled from an approximation of a distribution which itself approximates inclusive proton spectra in pp collisions.⁸ Then pions are selected from a similar distribution^{9,10} until either energy is exhausted or the mean multiplicity is reached.¹¹ As an example, the expression for the pion invariant cross section is given by:

$$f = E \frac{d\mathbf{S}}{d^3p} = \frac{A}{(1 + P_T^2 / m^2)^q} \left\{ (1 - x_r)^{n(P_T)} \times \left(1 + \frac{A_l}{x_r}\right) \right\}$$

Where x_r is the radial scaling variable (E/E_{\max}), and the parameters are $A=77.5$ (for $pp \rightarrow \pi^+$), $m^2 = 0.2$, $q = 3$, $n(P_T) = 3.2 + 1.28(P_T - 1)^2$, and $A_l = .003$. It should be clear that this is simply a by-hand parameterization of data, most of which is a compilation given in a single publication. At the end of the pion selection process, the second nucleon is chosen. (In all selections P_T is ≤ 2.0 GeV/c.) At this point a “check” is made on the event as a whole. If both energy and the parallel component of momentum (in the CM frame) are conserved within some criteria,¹² the event is considered acceptable. If this is not the case, a loop is made over the created particles wherein each particle is replaced by a particle “made up” to best balance the energy and momentum of the other particles. If the criteria is satisfied by substituting the single “best” made-up particle, the substitution is made and the event (although clearly biased from the non-correlated single particle function) is accepted. If substituting a single particle does not satisfy the criteria, the entire event selection process is iterated.

The selection process in fact proceeds in two steps. In the first step, P_T is selected from distributions which approximate the integral of the invariant cross section expression over Feynman x . Only after P_T is specified is x selected from the distribution as given above. This was found to be much faster than attempting to select both variables simultaneously.

The selection process is extended to lower \sqrt{s} than the distribution functions are intended to apply. When \sqrt{s} is so low that no pions are produced, and half the time when a single pion is produced, a separate particle generator is called that assumes that the production is quasi-two body, i.e, dominated by N^*N production followed by $N^* \rightarrow N\pi$. However, no physics, other than the existence of a single pion in the final state, is simulated – the decay is simply isotropic in the N^* center of mass. The mass of the (so-called) N^* is simply picked uniformly over the allowable kinematic region.

(B) Pion-Nucleon Collisions

The selection of pions at high energy from incident pions is very similar to that from nucleons. Here, however, two distributions are used, one for Leading pions (e.g., $\pi^+ N \rightarrow \pi^+$), and one for Non-Leading pions ($\pi^+ N \rightarrow \pi^-$). The by-hand distributions are derived primarily from data at 100 GeV.¹³ They are, excluding normalization, the same as the expression given above with the exception that additional terms are added to describe the asymmetry in Feynman

x. Similar to what was described immediately above, pions are picked until the multiplicity is obtained, and then a single nucleon is chosen.¹⁴ Again, the imbalance in energy and parallel momentum conservation is examined, and the same “trial substitution” method as described above is attempted and the same criteria is used determine whether an event is acceptable.

In pi-N collisions, no account of the resonance region exists until the 300 MeV cross section threshold is reached. Below this energy, the angular distributions of the final state pion and nucleon are more-or-less correct.

V Scoring

In the scoring transport, every neutron in the high energy stack is transported, along with a single (weighted, in a manner similar to the single cascade hadron) charged hadron. Here, the particles are transported to the end of the geometry¹⁵ in steps of fixed length specified by the user. What is actually transported is a weight, which corresponds to the probability that the hadron did not interact between its creation and a given point in the geometry, and the transport can also be terminated by a user specified weight cut-off. This technique is how CASIM achieves its good statistical precision (for cascade-propagating hadrons) in deep penetration geometries.

At each step in the scoring transport, if the user has selected to transport low energy neutrons also, a single low energy neutron is created, and transported as described in the next section. The creation of low energy neutrons, as a stochastic process, is a part of the nucleus “excitation” described in Section II above. In order to reduce fluctuations, however, the scoring subroutine calls a subroutine that emulates the stochastic process. The average multiplicity and parameters for describing the neutron energy spectrum are stored for 5 atomic weight values and 7 incident energy values. At each step (in material) of each high energy cascade “scoring particle,” a call is made to the emulation routine which returns an energy (< 20 MeV of course) and a weight obtained by interpolation in pre-stored tables.

The scoring process is schematically shown in Fig. 1. In this figure a high-energy hadron goes a distance S from point (a) to point (b) in some material medium (assumed for simplicity). Let the probability that the hadron had actually gotten to point (a) without interacting be denoted by $P1$. Then the probability that point (b) was reached without interaction is $P2 = P1 \times \exp(-S/\lambda(E))$. As shown in the figure, a “scoring plane” happens to exist between (a) and (b), so a “high energy” contribution to the score on the plane would be recorded with a weight proportional to $P2$. Now at point (b), a low energy neutron is created with a weight proportional to $P3 = P1 \times (1 - \exp(-S/\lambda(E)))$. This neutron may or may not “score” one or more times by crossing the plane shown, depending on its transport history which is described in the next section.

Thus, in N-SHIELD, the high energy cascade particles are explicitly “carriers” of low energy neutrons. In general, the step length S (Fig. 1) is intended to be several cm., with the first step “randomized” so that, on average, spatial biases do not exist.

VI. Low Energy Neutron Physics & Transport

At each interaction in the cascade, and at each scoring step corresponding to an interaction, a single neutron with some weight and energy < 20 MeV is created. The transport for these is simple elastic scattering in an analog manner using non-relativistic kinematics. Thus, a random distance to the next elastic collision is repeatedly sampled from an energy dependent approximation for the elastic scattering cross section. At each collision, the neutron loses some energy. In the approximation made here, the nucleus from which the neutron recoils is considered free and motionless. Given this approximation, it makes no sense to transport the neutrons all the way down to thermal energies. In N-SHIELD, 50 ev is *called* thermal. The meaning of this statement is that, when the neutron reaches 50 ev, subsequent collisions are simply a random walk in the laboratory frame and thermal absorption cross sections are *turned on*.

The elastic cross sections are shown in Fig. 2. The lowest curve in this figure gives the elastic cross sections at 10 MeV.¹⁶ The higher curve gives the “geometric” cross section,¹⁷ which is used for the elastic cross section at 50 ev in the absence of “thermal” elastic cross sections from measurements.¹⁸ These are shown also in Fig. 3 and include most atoms of interest.

Fig. 3 shows the “absorption” cross sections, which are usually (but not always) (n,γ) cross sections. Again, in the absence of data, which actually exists for most atoms of interest, an approximation to the curve shown in this figure is used. The “off-scale” absorption cross section for Boron illustrates one aspect of the materials specification which should be mentioned here, although a more complete description is given in a companion *Users Guide* to this document. In N-SHIELD, the atomic weight of all material components are specified as whole numbers; for Boron it is 11.0. However, the low energy cross sections assume that the isotopic content is as found in nature. The 729 barns for what is called B11 is, in fact, 19% of the B10 absorption cross section.

Elastic scattering differential cross sections are very complicated. In N-SHIELD, tables from which the cosine of the scattering angle are created and stored which represent crude approximations to data cited in a standard Nuclear Physics text.¹⁹

There are five ways that the transport of a neutron can be terminated. If the neutron begins its life above 8 MeV, the reader should recall from Section III above that a finite inelastic cross section exists. At each transport step between elastic collisions if the energy is above 8 MeV, an inelastic interaction is allowed to occur. If one in fact does, the transport is simply terminated, which is the approximation that inelastic interactions below 8 and 20 MeV do not themselves produce neutrons. The other four ways are (1) degradation by elastic scattering followed by absorption as described above, (2) going out of bounds, (3) exceeding a user-specified number of elastic scatters, and (4) explicitly being killed by the user. In most applications, the last method of termination is expected to be important. The transport of low energy neutrons is very slow, and the user is expected to kill neutrons that are created in, or wander to, “uninteresting” regions.

VII User Routines

Any interested user must consult the N-SHIELD *Users Guide* which explains the input, output, and the one routine that must be provided for any calculation. The only routine that must be provided is the routine “Where,” which is analogous to the “Hitorm” routine in CASIM. However, “Where” is slightly more complicated because the user must distinguish calls made to Where from both the high energy and low energy transport. If the variety of scoring surfaces built into the code is satisfactory, and no magnetic field is present, no other routines are required.

VIII. Comparison to MCNPX and CASIM

In the comparisons made below, MCNPX is used in a very naïve manner – no attempt is made to use it optimally. As an example, one form of variance reduction available employs “point detectors” to obtain dose from (in this author’s code and cross-section configuration) neutrons below 20 MeV. However, here only results from particles crossing surfaces are quoted. It should also be mentioned that the MCNPX results were obtained from the transport of only protons, neutrons, and pions.

(A) A Simple Transverse Geometry

Fig. 4 (a) shows a simple cylindrical transverse geometry. An Fe target, with radius 3 cm. exists between $Z = 0$ and $Z = 150$ cm. The only additional material is a concrete²⁰ cylinder between $R = 100$ cm. and $R = 300$ cm., and between $Z = -100$ cm. and $Z = 1000$ cm. A proton beam with no transverse size is incident along the Z axis.

Results in 100 cm. Z bins at $R = 300$ cm. are shown in Fig. 5 at 100 GeV and Fig. 6 at 20 GeV.²¹ In these figures, low energy neutron transport in N-SHIELD was “turned on” for $R > 200$ cm. Even with this cut, N-SHIELD is very slow in comparison with the other codes.

Before discussing the results, an important digression on the statistical errors is needed. The errors – shown only for N-SHIELD in Figs. 5 and 6 – are simply the standard deviation estimated from 4 runs. What matters is the error per unit computer time. The average error (averaged over the 11 Z bins) estimated in this way is shown in Table 2.

Table 2 Statistics for the Runs Represented in Figs. 3 and 4

Energy	Code	Ave. Error (%)	No. cpu hrs.	No. Incidents
100	CASIM	5.71	1.7	500K
100	MCNPX	8.24	11.0	2500
100	N-SHIELD	18.4	6.0	150K
20	CASIM	5.45	1.3	500K
20	MCNPX	12.1	7.3	6000
20	N-SHIELD	14.0	6.1	200K

Even though estimating the error from only 4 arbitrary runs is itself fraught with error, the numbers are widely enough distinguished to determine that CASIM is a statistical winner and that N-SHIELD is worse than MCNPX by some modest factor.²² Although the number of primaries is given, note that it is not terribly relevant. However, when used in the same manner as CASIM, N-SHIELD is competitive, as illustrated in Fig. 7. This shows the same N-SHIELD data as in Fig 4, but also shows a high statistics N-SHIELD run without low energy neutron transport multiplied by 4. *This corresponds to the equilibrium spectrum assumption of CASIM.* This run, with errors shown in Fig. 7, took 2.3 hours for 1.5M primaries. The average error is 5.19%. N-SHIELD is slightly faster than CASIM per primary, but (averaged over more comparisons than shown here) slightly worse in the quantity that counts – statistical fluctuations per hour of computer time.

Also shown in Figs. 5 and 6 the Tesch value,²³ which is based on measurements, and is generally considered to be correct within a factor of 2. All three codes pass this criteria. As mentioned in Section I, CASIM is considered to give results which are “too far forward.” Although N-SHIELD gives results which are more forward than MCNPX, it is considerably less forward than CASIM.

In a further investigation, a slightly “more backward” geometry was explored. The geometry of Fig. 4(a) was changed such that the concrete between $R = 200$ and $R = 300$ was changed to soil,²⁴ and the Z bin size was changed to 50 cm. The fluence > 20 MeV (corresponding to a typical activation threshold) was calculated at 5 cm into the soil ($R=205$ cm.), and Table 3 shows this quantity in the first (most backward) bin, and at the maximum value (without regard to Z position) at 20 GeV incident energy.

Table 3 Fluence (n/cm^2 -p) in Soil at $R = 205$ cm

Z Interval	MCNPX (> 20 MeV)	CASIM (> 47 MeV)	N-SHIELD (> 20 MeV)
$-100 < Z < -50$	1.1×10^{-6}	5.9×10^{-9}	2.0×10^{-7}
(at maximum)	4.8×10^{-6}	2.0×10^{-6}	3.4×10^{-6}

The maximum fluences are essentially in agreement, given CASIM’s higher threshold. However, CASIM drastically underestimates the flux in the backwards direction. The N-SHIELD result is a factor of 33 higher than CASIM, but a factor of 5 lower than MCNPX. Estimates are often made at BNL of essentially this quantity as a part of evaluating possible soil contamination due to the production of 3H and ^{22}Na . N-SHIELD would appear to be much better in the backwards direction for this purpose than CASIM, although some caution is still mandated.

Fig 8 shows the same quantities as Figs. 5 and 6 at 2 GeV incident energy. In this instance N-SHIELD “out-performs” MCNPX somewhat in that the average error for N-SHIELD is 8.9% for 5.0 hr. runs vs. an average error of 20.6% for 3.8 hr. MCNPX runs. The same general character of the distributions is observed, but, unlike the comparisons at higher energies, N-SHIELD gives the largest dose.

“Just for fun” a comparison was made to MCNPX at 200 MeV. The result is shown in Fig. 9. N-SHIELD gets the position of the peak about right, but is too low by a factor of 3 at this

point, and quickly by orders of magnitude at larger Z values. Here MCNPX runs of 6.4 hours are compared to N-SHIELD runs of 5.7 hours.²⁵ MCNPX runs out of steam for the run times chosen at the larger Z values. The two very large error bars on the MCNPX data were faked; the rms actually exceeded the mean values on these points. N-SHIELD demonstrates the CASIM deep penetration ability here, but what the demonstration most likely illustrates is that good precision is not necessarily correlated with accuracy.

(B) A Simple Forward Geometry

Fig. 4(b) was chosen to illustrate a deep geometry in the very forward direction. Here the cylindrical concrete shell of the previous comparison is replaced by an “end plug” cylinder extending from $Z = 600$ cm. to $Z = 1000$ cm., where $Z = 0$ is still the beginning of the same target, and to $R = 100$ cm.. The goal was to make comparisons at $Z = 1000$ cm., with the end surface divided into 5 radial bins. Figs. 10, 11, and 12 show the comparisons at 100 GeV, 20 GeV, and 2 GeV respectively.

The differences are very large here. CASIM always gives much higher values than MCNPX, with N-SHIELD somewhere in between. At 2 GeV, the rms of the 4 MCNPX runs (of 4.8 hrs each) exceeded the mean in many of the radial bins, but the average behaved sensibly for this length of run, so this quantity is compared in the inset of Fig. 12. The discrepancies at 2 GeV are particularly large.²⁶

Also shown in these figures is a high statistics run of N-SHIELD in the High Energy mode only multiplied by 2.5. This is a reasonable approximation (in concrete) of the “equilibrium spectrum” at this very forward geometry. The difference between this value of 2.5 and the transverse value of 4.0 simply reflects the obvious fact that the hadron spectrum is stiffer in the forward direction. This is a part (though not a very large part) of the high estimate of CASIM results, namely that a single number, more appropriate for a transverse geometry than this one, multiplies the star density to obtain the dose estimate.

(C) A Simple Penetration

Fig. 13 shows a simple penetration in a tunnel surrounded by 30 cm. of soil.²⁴ The target is the same as in the previous comparisons. The intent was to compare N-SHIELD to MCNPX in a geometry sensitive to neutrons “bouncing” in the tunnel as well as along the walls of the penetration. The dose due to neutrons < 20 MeV was calculated at the entrance of the penetration and at a position 2.1m “deep” as indicated in Fig. 13 (a). In MCNPX, the dose estimate was made with the very powerful “point detector” technique. In N-SHIELD, the estimate was derived from the flux of neutrons crossing a disk of 15 cm. radius. The comparison, whose results are shown in the first 2 rows of Table 4, was done only at 20 GeV.

Table 4. Comparison of MCNPX and N-SHIELD at 20 GeV in Fig. 13 Geometry

Code/Position	Z=50 cm, R=30 cm.	Z=100 cm, R=30 cm.	Z=150 cm., R=15 cm.
MCNPX ----- Entrance	$5.70 \pm .12 \times 10^{-12}$	$5.56 \pm .09 \times 10^{-12}$	$5.27 \pm .11 \times 10^{-12}$
MCNPX ----- at 2.1m	$8.63 \pm .26 \times 10^{-13}$	$4.16 \pm .15 \times 10^{-13}$	$3.30 \pm .40 \times 10^{-14}$
N-SHIELD --- Entrance	$5.90 \pm .55 \times 10^{-12}$	$5.21 \pm .20 \times 10^{-12}$	$5.37 \pm .33 \times 10^{-12}$
N-SHIELD --- at 2.1m	$1.30 \pm .13 \times 10^{-12}$	$7.71 \pm .78 \times 10^{-13}$	$5.50 \pm 1.3 \times 10^{-15}$
N-SHIELD --- Entrance (bad physics) – at 2.1m	–	–	$7.12 \pm .28 \times 10^{-12}$ $3.30 \pm 1.4 \times 10^{-16}$

The results in the first two positions are in quite good agreement. In the third position however, where the (small) penetration does not “look at” the source, N-SHIELD underestimates the dose by a nominal factor of 6.²⁷ Following this result, a simple “test” was made with the N-SHIELD code, wherein the elastic CM scattering angle of neutrons was simply chosen uniformly (refer to Section VI above). The result is shown as the 3rd row of Table 4, labeled “bad physics.” In this case, the result at 2.1m is low by 2 orders of magnitude.

This comparison shows clearly that great caution must be used when using the low energy neutron option available in N-SHIELD. It is intended to be useful for deriving the “equilibrium spectrum,” which in this case simply means the ratio of total dose to the dose from neutrons > 20 MeV, as a function of geometric configuration and material.²⁸ It would appear to also be useful in deriving the “entrance dose” in penetration configurations where well known labyrinth formula are applicable. However, N-SHIELD is not accurate if applied to geometries which are sensitive to accuracy in low energy neutron transport.

IX Conclusions and Caveats

Above (say) 2 GeV, N-SHIELD would appear to have characteristics which make it a reasonable alternative to CASIM. When used in the “high energy mode,” i.e., when transporting hadrons above 20 MeV, the statistical precision is “almost” as good as CASIM, but use of an optional low energy transport allows a more direct method of estimating total dose than the single number multiplication of CASIM. For reasons that are certainly not clear, the dose distribution appears to be better (or at least closer to MCNPX distributions) than that of CASIM. Also, having the threshold at 20 MeV rather than 0.3 GeV/c is more appropriate for activation estimates.

The total time that has been invested in this code (which is not this author’s “day job”), excluding documentation, is probably not more than 20 man-weeks. Although the vast majority of this time was spent in de-bugging, it is not unlikely that bugs may still be present. No guarantee can be made that the code actually does what this documentation claims. This document describes what the author *intended* to do which, if past experience can serve as a guide, may be perhaps only loosely correlated with the actual product.

Even ignoring possible blunders, the code has many shortcomings, among which are the complete lack of visual tools, and its limited scope.

X. Acknowledgement

The author would like to acknowledge his extreme debt to Andy Van Ginneken of FNAL. Only the fact that CASIM was copied in large chunks enabled the code to progress to its current state with a very limited effort. It should be noted that no originality is present in N-SHIELD. The author is also very grateful for the advice and “tutoring” on radiation transport received from Andy over many years.

XI. Functionality of Modules

In this last section, a list of all the routines currently comprising N-SHIELD is given, along with a very short description of the routine’s functionality. No attempt has been made to provide as much detail as the CASIM manual, for example.

1. Nsprogram

This is the trivial main program. It is intended to contain all the machine dependent code. At the moment this is just how file names are passed and calls to a routine that gives the time of execution. This program just calls Nscascade.

2. Nscascade

This is the primary driver routine of the code. Initialization calls, cascade transport, calls to the particle creation routines, etc. are all called from Nscascade. Its structure was essentially copied from the main CASIM routine.

3. Inputdat

Called from Nscascade. Does what it says – reads the problem specification in the input file.

4. Initialize

Called from Nscascade. This routine performs or oversees initialization, and writes out the problem specification.

5. Init55, Setnnxsec, Setpinxsec, Setlexsec, Ngammax, Elaspams, Buildrtables, Initlescore, Initlescat, Initheselect.

These are all initialization routines. Init55 (filename Ran0init.f) is called from Inputdat. Ngammax and Elaspams are called by Setlexsec. The remainder are called by Initialize.

6. Getprimary

Called from Nscascade. Does what it says – gets a primary particle into Nscascade.

7. Lowep

Called from Nscascade. This is the Monte Carlo version of the routine that generates low energy particles intended to “describe” the intra-nuclear cascade.

8. Pbeamsc

Called from Nscascade. This (optional) routine scatters incident particles as described at the beginning of Section III above.

9. Fermip

Called from Nscascade. Selects a Fermi momentum for a target nucleon.

10. Hegen

Called from Nscascade. Driver for the particle-particle interaction routines.

11. Pifromngen

Called from Hegen. This routine “oversees” generation of particles in nucleon, nucleon collisions.

12. Selnucleon, Piongen, Quasitbody

Called from Pifromngen. Selnucleon selects nucleons and Piongen generates pions. In the resonance region, Quasitbody may replace the particles selected by the “high energy” routines.

13. Getmult, Selpion, Chargenn

Called from Piongen. Getmult gets the pion multiplicity, Selpion selects a pion (in nucleon-nucleon collisions), and Chargenn the charge of the next pion to be selected.

14. Pifrompigen

Called from Hegen. This routine oversees generation of particles in pion, nucleon collisions.

15. Piresregion, Pireschannel

Piresregion called from Hegen, and Pireschannel is called from Piresregion. These relate to the pion-nucleon resonance region below 300MeV.

16. Selpifrompi, Selpperpn, Chargenp

Called from Pifrompigen. Selpifrompi actually selects pions (in pion-nucleon collisions). Chargenp obtains the charge of the next pion to be selected and whether it should be selected from the leading or non-leading distribution. Selpperpn selects a P_T value for the nucleon.

17. Getppfpil, Getppfpinl

Called from Selpifrompi. These are used in the process of selecting pions in pion-nucleon collisions. They select P_T from the leading and non-leading distributions.

18. Cmxyz

Called from Hegen. This constructs X,Y,Z momentum components (in the CM system) from P_T and $P_{||}$ components.

19. Labtocm, Cmtolab

Called from Nscascade. Labtocm sets up parameters for transforming from the CM system to the lab. System. The transformation is done by Cmtolab.

20. Selectnewp

Called from Nscascade. Selects a new cascade particle from an interaction.

21. Score

Called from Nscascade. This oversees the transport of scoring particles.

22. Lowetrack, Getlowepart, Surfacecross, Zcylinder

These are called from Score. Lowetrack tracks low energy neutrons. Getlowepart is the tabular version of Lowep, i.e., it returns a single low energy neutron and weight obtained from a parameterization of the Lowep code. Surfacecross looks for scoring surfaces. Surfacecross is also called from Lowetrack. Zcylinder is a subroutine called by Surfacecross.

23. Elasl, Ngamma, Nucabsorb, Elscat.

These are called by Lowetrack. Elasl calculates the elastic scattering length. Ngamma determines whether a “thermal” neutron is absorbed, Nucabsorb determines whether a neutron > 8 MeV is absorbed, Elscat performs an elastic scattering.

24. Getelca

This routine, called from Elscat, returns the scattering angle in a neutron elastic scattering.

25. Getcompp, Tarnuc, Getmu, Step, Field, Trac

These are routines involved in the transport in one way or another. Getcompp selects the component of a material which is a mixture. Tarnuc simply selects the charge of the target nucleon. Getmu returns the absorption (energy dependent) coefficient in the high energy transport. Field and Trac are invoked only when magnetic fields are present. (See the *Users Guide* for more information on specifying both materials and magnetic field.)

26. Scatter, Rgivene, Egivenr

These “miscellaneous physics” routines are used in multiple scattering simulation and range-energy relations.

27. Gplots, Geom.

Used for geometry printer plots.

28. Trans, Sortdn, Fluxtodose, Getrandr, Ran0

These are all “utility routines.” Getrandr creates a particle with random direction in the lab frame. The Ran0 routine (filename Ran0fnal.f) and Trans are “borrowed” from a late 80’s version of CASIM.

29. Errorsub, Summary

Both of these routines are called from Nscascade. Errorsub is modeled after a part of CASIM used to very crudely estimate the statistical error on each segment of a scoring surface. Summary is called at the end of execution to write out the results. The reader is again referred to the Users Guide for more details.

References/Footnotes

1. A. Van Ginneken, "CASIM; Program to Simulate Hadron Cascades in Bulk Mater," Fermilab FN-272 (1975). See also A. Van Ginneken, FN-250 (1972).
2. H.G. Hughes, R.E. Prael, R.C. Little, "MCNPX – The LAHET/MCNP Code Merger," X Division Research Note, 4/22/97. The version number of the code whose results are reported later in this note is 2.1.5. MCNPX has various physics options; only the default options have been used. In the default option, FLUKA (circa 1990) is "phased in" for particle production between 2500 and 5000 MeV. This code is considered a beta-test version released by LANL for testing and validation purposes. This author is responsible for validation procedures in the present application.
3. For a comparison of CASIM and FLUKA, see K. Tesch and H. Dinter, "Estimation of Radiation Fields at High Energy Proton Accelerators." Rad. Prot. Dosimetry Vol. 15, No. 2 pp. 89-107 (1986). Two measurements at BNL, one direct and one indirect, are in conflict with CASIM simulations. The first was an old measurement by D. Beavis of dose equivalent above a target in the C-line at the AGS. Although the maximum dose measured agreed with the CASIM maximum (within a factor of 2.5), the position of the maximum dose was much closer to 90° than CASIM would predict. The "indirect" measurement relates to a recent problem concerning soil activation upstream of a magnet in the V-line at the AGS. The ^3H concentration measurements are consistent with activating flux in the backward direction predicted by MCNPX due to scraping on this magnet, but not with CASIM.
4. The problem with getting good statistical precision very far from the initiating interaction in a hadron cascade is that simple systematic errors (like not-perfectly-correct physics) become magnified.
5. The physics in the ~ 1 GeV energy region is presumably very good in MCNPX. Although CASIM works (i.e., gives answers) for primaries whose energy is in this region, it was not really intended to be "correct" here. Comparisons at 2 GeV are given in Section VIII.
6. J. Ranft, and J.T. Routti, "Monte Carlo Programs for Calculating Three-Dimensional High-Energy (50 MeV – 500 GeV) Hadron Cascades in Matter," Computer Physics Communications 7, pp. 327 – 342, North Holland (1974). See also "Hadron Cascade Calculations of Angular Distribution of Integrated Secondary Particle Fluxes from External Targets and Description of Program FLUKU," CERN LABII-RA/72-8 (1972). The first of these references is certainly one of the first references to FLUKA. How the description of the excitation energy has evolved in FLUKA is not known to this author.
7. The conceptual picture adopted here is that the cascade "proper" is caused by multiple hadron interactions. After (in some sense) the hadronic interactions are over, an excited residual nucleus de-excites into photons, heavy fragments, and evaporation nucleons.
8. See both Ref. [10] below and M. Perl, "High Energy Hadron Physics," John Wiley & Sons, New York, 1974, Fig. 8-6.

9. F.E. Taylor, et. al., Phys. Rev. D 14, p. 1217 (1976).
10. K. Guettler, et. al. Phys. Lett. 64B, p. 111 (1976). This references reports ISR data where simple Feynman scaling is dramatically violated near $x = 0$. Use of x_F , rather than Feynman x , seems advantageous to account for this effect.
11. The mean multiplicity is of course not an integer. In a manner similar to (but cruder than) what is described in Ref. [7], the code attempts to get the “correct” multiplicity averaged over both events and bins of \sqrt{s} .
12. The current criteria is that the imbalance in both cm energy and P_T should not exceed $.25\sqrt{s}$. Approximately 75% of the events satisfy the criteria on the first pass.
13. J. Whitmore, et. al., Phys. Rev. D 16, p. 3137 (1977).
14. G. W. Brandenburg, “Experimental Low Pt Inclusive Scattering and Comparison with Quark-Parton Models,” Proc. 14th Recontre de Morland, J. Tran Thanh Van Ed., Vol. 1 p 507 (1979). This reference gives the x distribution of protons from $\pi^+ p$ interactions at 100 GeV.
15. The transport of charged particles usually terminates when the particles exceed their range, but they *may* go to the end of the geometry. In most applications, neutrons dominate.
16. Neutrons greater than 10 MeV are assigned the 10 MeV cross section.
17. $4\pi R^2$. See E. Segre, Ed., “Experimental Nuclear Physics,” John Wiley & Sons, NY (1953).
18. S.F. Mughabghab and D.I. Garber, “Neutron Cross Sections,” BNL325, Third Edition (1973).
19. M. A. Preston, “Physics of the Nucleus,” Addison-Wesley, Palo Alto, 1962. The data approximated are given in Fig. 18.4. The approximation of $d\sigma/d\Omega$ is simply a parameterization of two hand-drawn exponentials in the cosine of the scattering angle.
20. Concrete is taken to have a density of 2.35 g/cc and an atomic composition of .17 H, .5833 O, .1935 Si, .032 Ca, .021 Al. For CASIM, the average Z and A values are taken from this mixture excluding the hydrogen.
21. If the MCNPX results were being used for an estimation of the radiation field, (as opposed to being shown for comparison purposes), this author would multiply the results shown at the peak and forward of the peak by 1.1 to make a first order “allowance” for the fact that K’s etc. have been neglected.
22. N-SHIELD was run with the constraint of using the same scoring step size (5 cm.) as used in CASIM. A larger choice would have made N-SHIELD “look better” since low energy neutrons are “emitted” at each step.

23. K. Tesch and H. Dinter, "Estimation of Radiation Fields at High Energy Proton Accelerators," Radiation Protection Dosimetry, Vol. 15, No. 2, pp. 89-107 (1986). The expression is $H = 1.5 \times 10^{-12} E^{0.8} \exp(-d/107)/R^2$ where H is dose in rem per incident, E is energy in GeV, d is shield thickness in g/cm², and R is the transverse distance in m.
24. BNL soil was taken to be .10 H, .617 O, and .285 Si with density 1.8 g/cc.
25. No geometry cuts were made on low energy neutrons in N-SHIELD in these runs.
26. Runs were made at Z = 800 cm. at this energy. The R averaged values at this Z at 2 GeV were 1.56×10^{-13} (CASIM), 3.0×10^{-14} (N-SHIELD) and 1.45×10^{-14} (MCNPX). The rms values are always less than 3% in CASIM. In these runs, and for the values shown in the inset of Fig. 12, the rms values were at least 10% for N-SHIELD and MCNPX.
27. The discrepancy is actually "only" a factor of 5, because the average over the N-SHIELD disk in this case is supposed to be slightly lower than in the center of the hole. If the entrance dose is used together with the 1-st leg labyrinth expression of Goebel, the result at 2.1m would be about 1.3×10^{-14} rem/p.
28. Clearly some materials (e.g., pure Fe) are also sensitive to accuracy in transporting low energy neutrons.

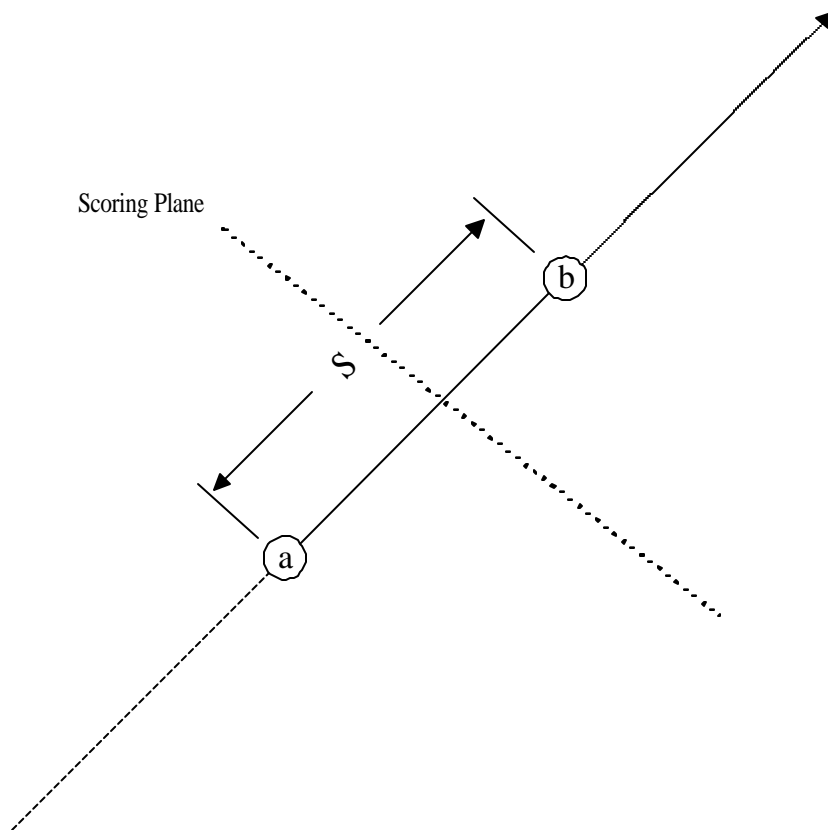


Fig. 1 Illustration of the Scoring Transport

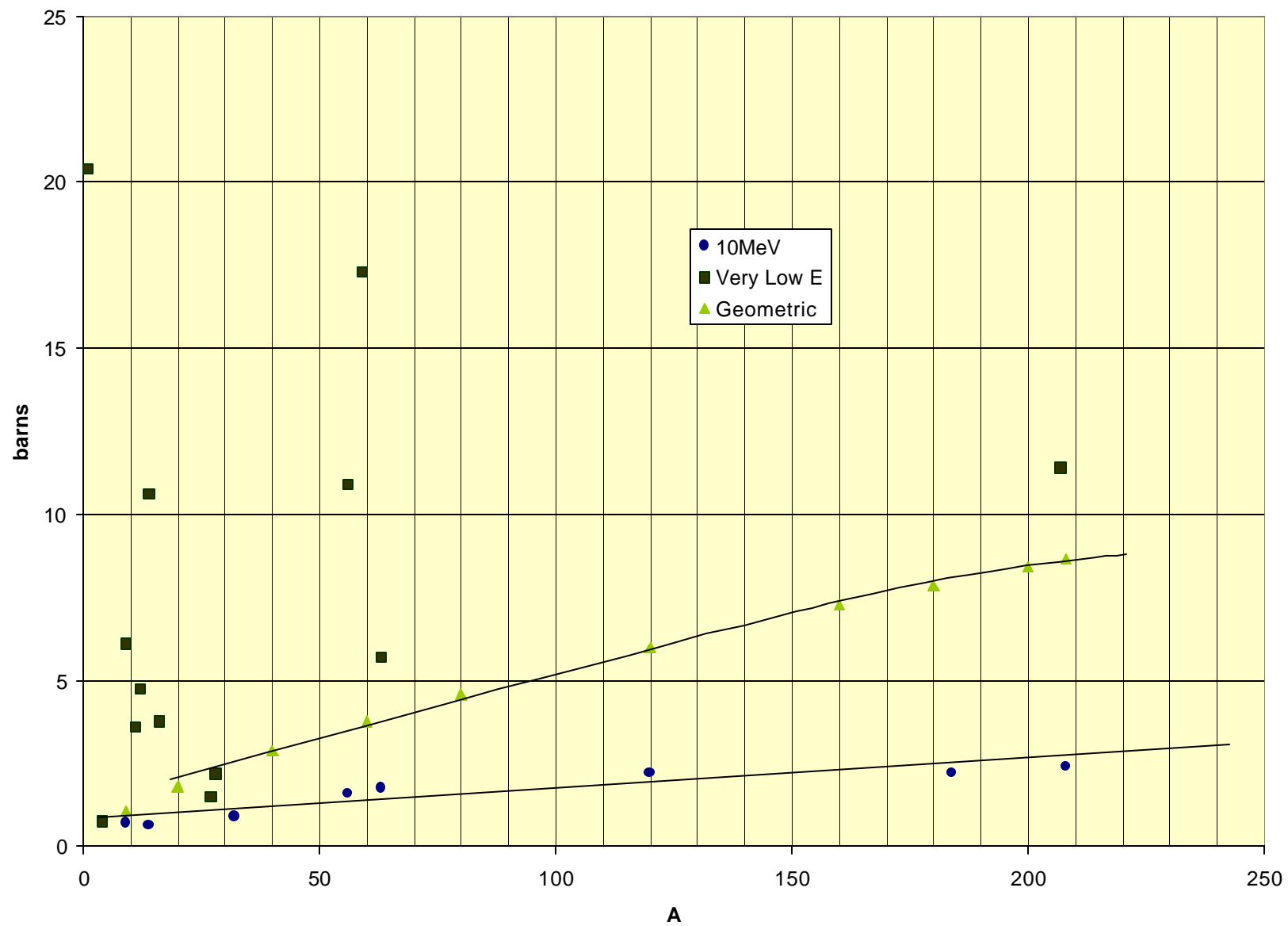


Fig. 2 Elastic Scattering Cross Sections (see text)

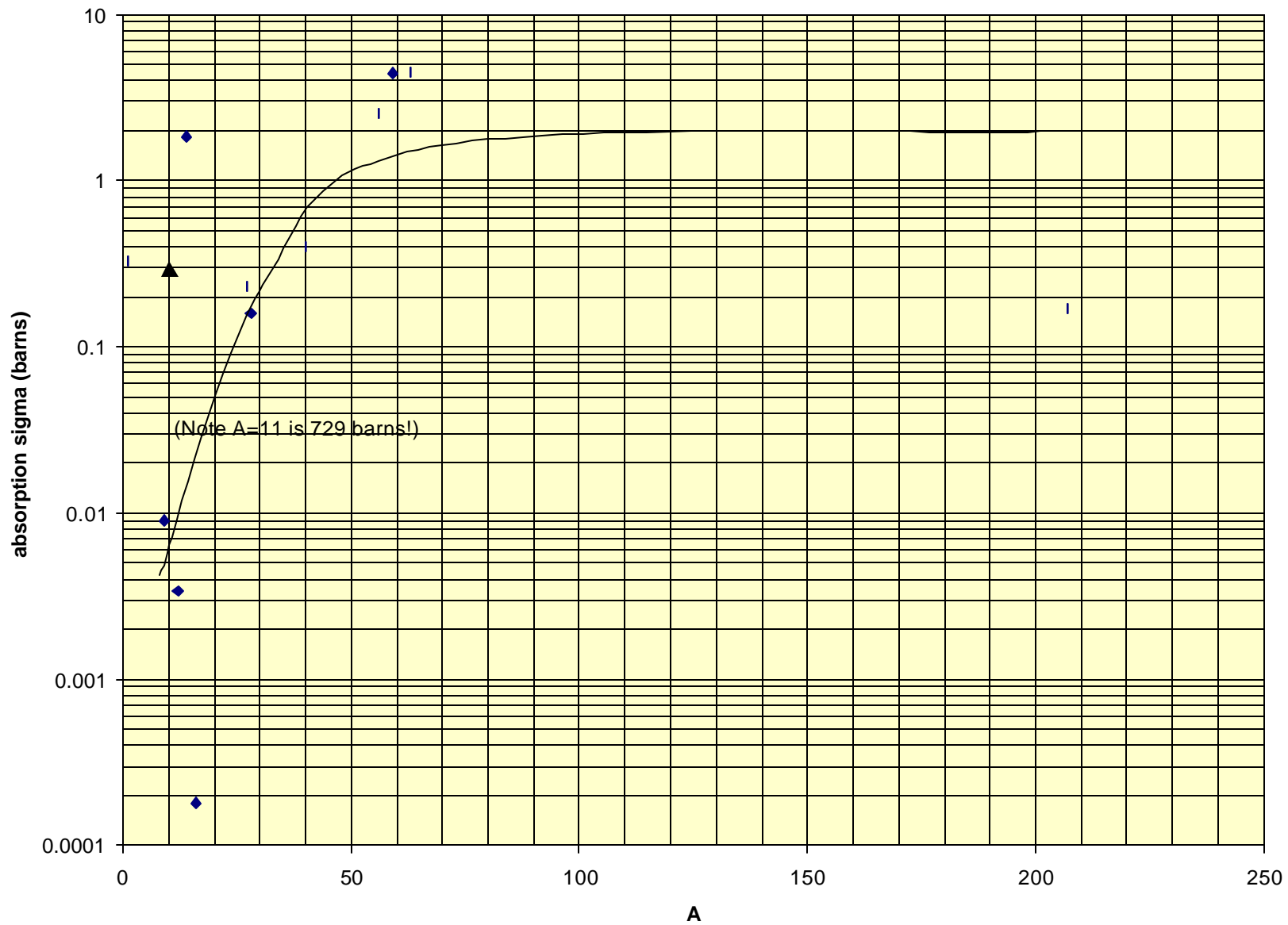
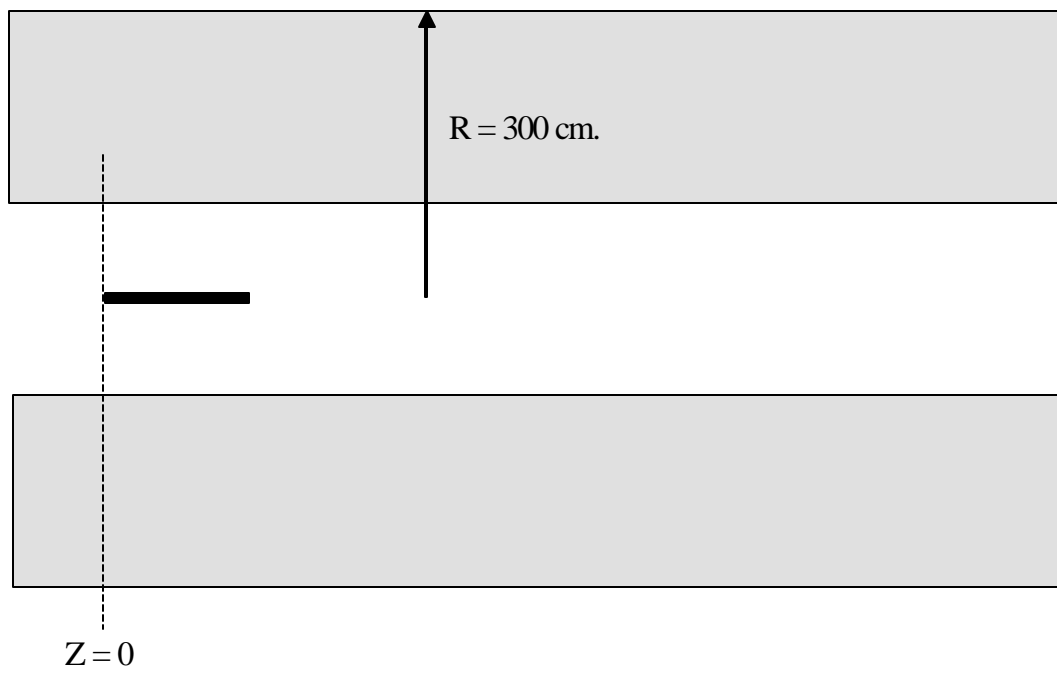
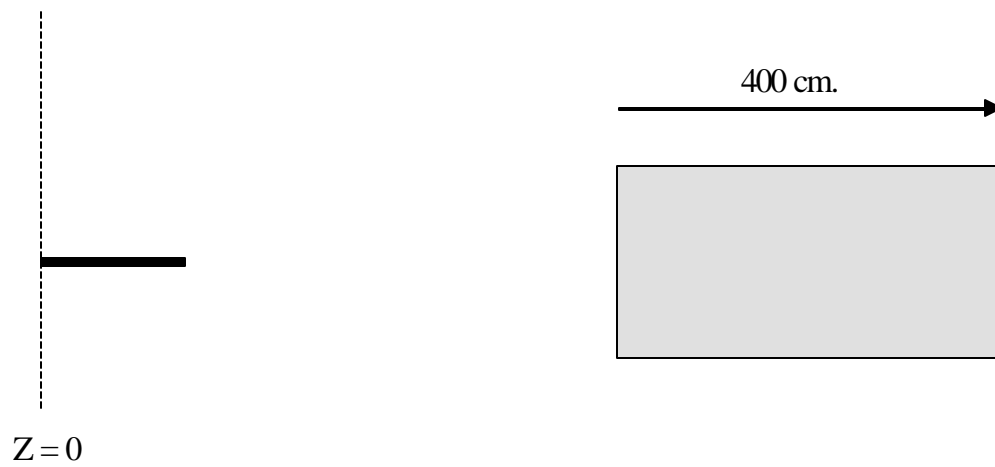


Fig. 3 Absorption Cross Sections at “Thermal” Energy (see text)



(a) Transverse Geometry



(b) Forward Geometry

Fig. 4. Simple Geometries for Code Comparisons
(Target Diameter not to Scale)

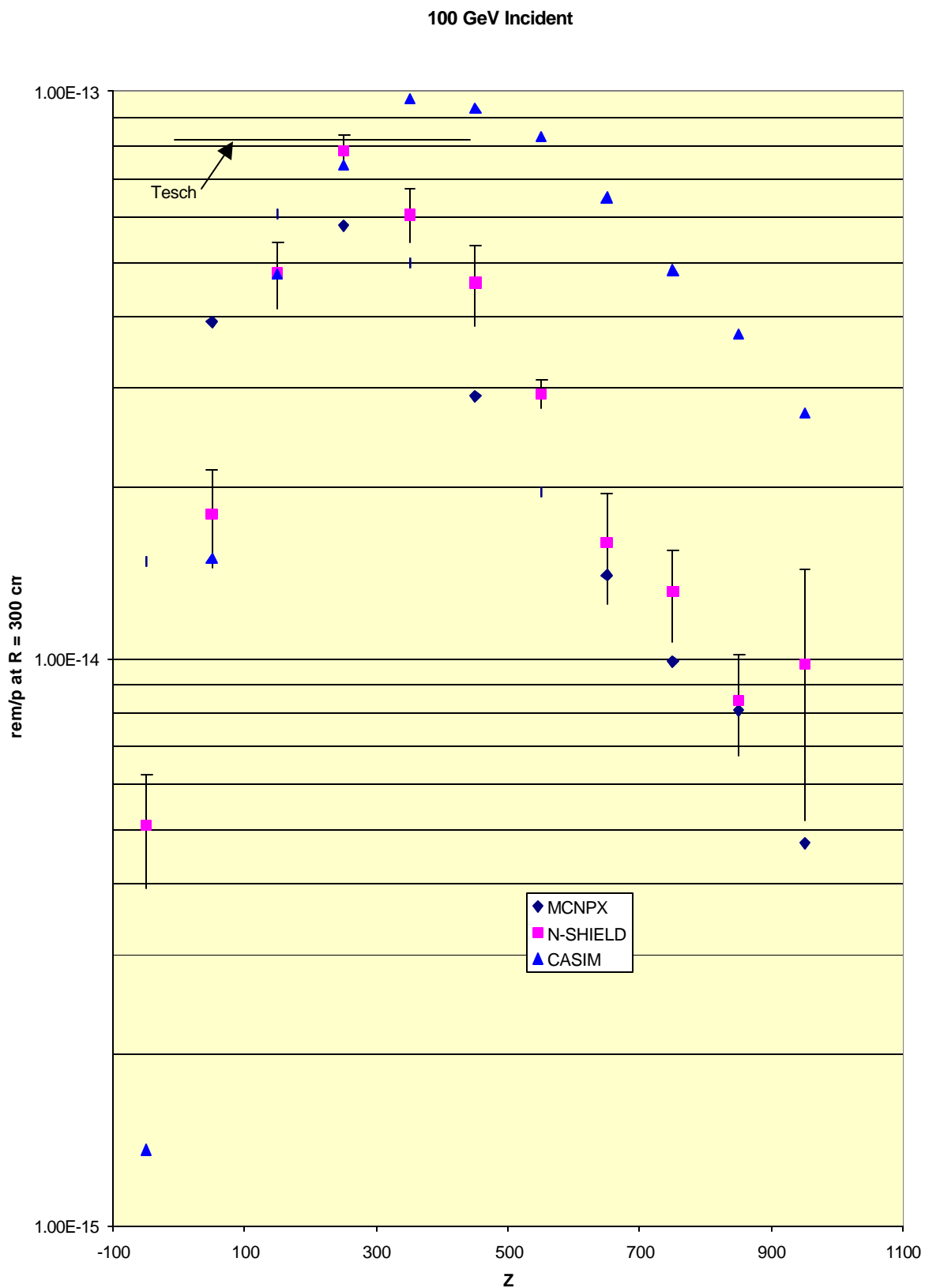


Fig. 5 Code Comparison in the Transverse Geometry at 100 GeV (See Text)

20 GeV Incident

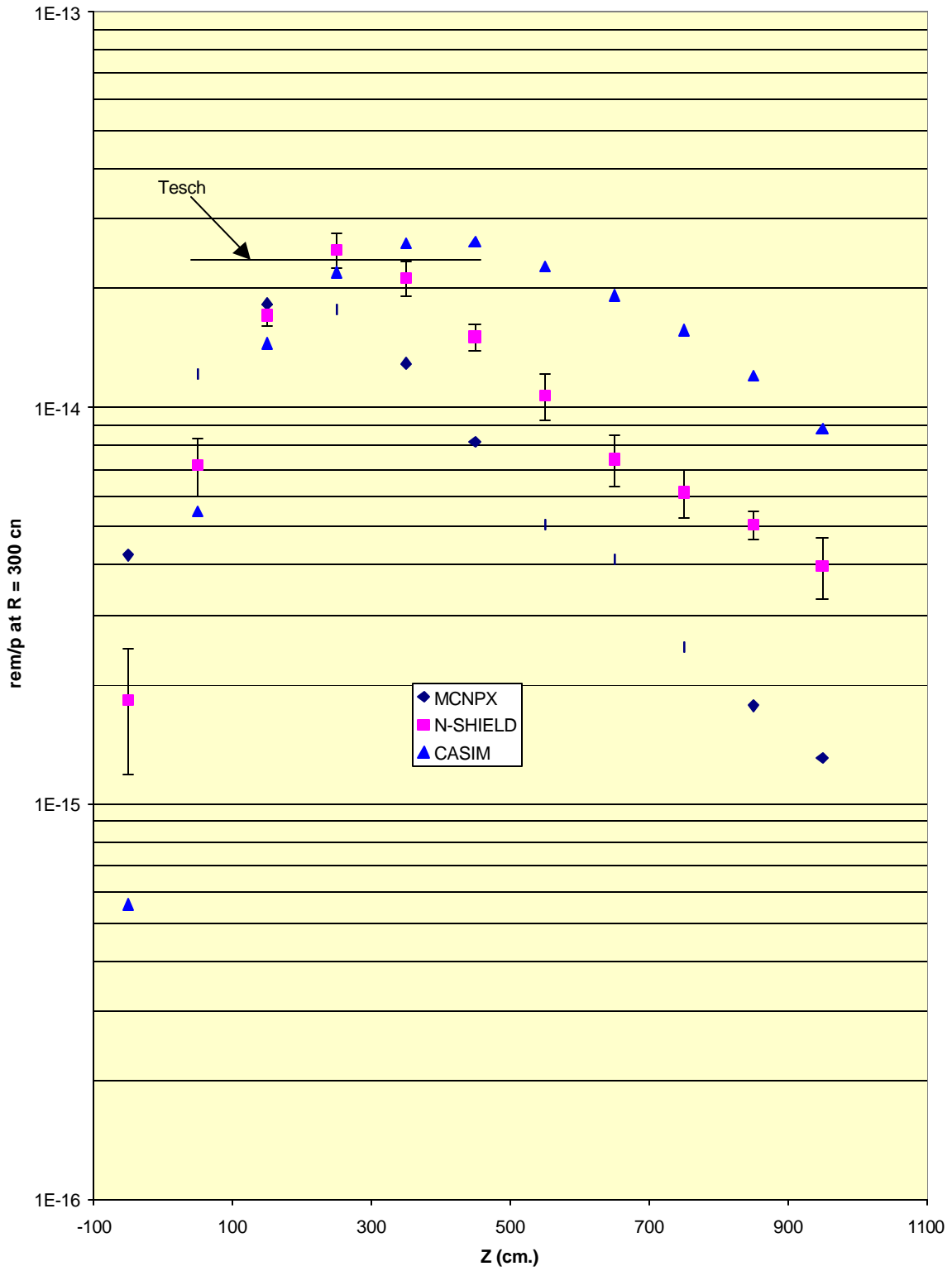


Fig. 6 Code Comparison in the Transverse Geometry at 20 GeV (See Text)

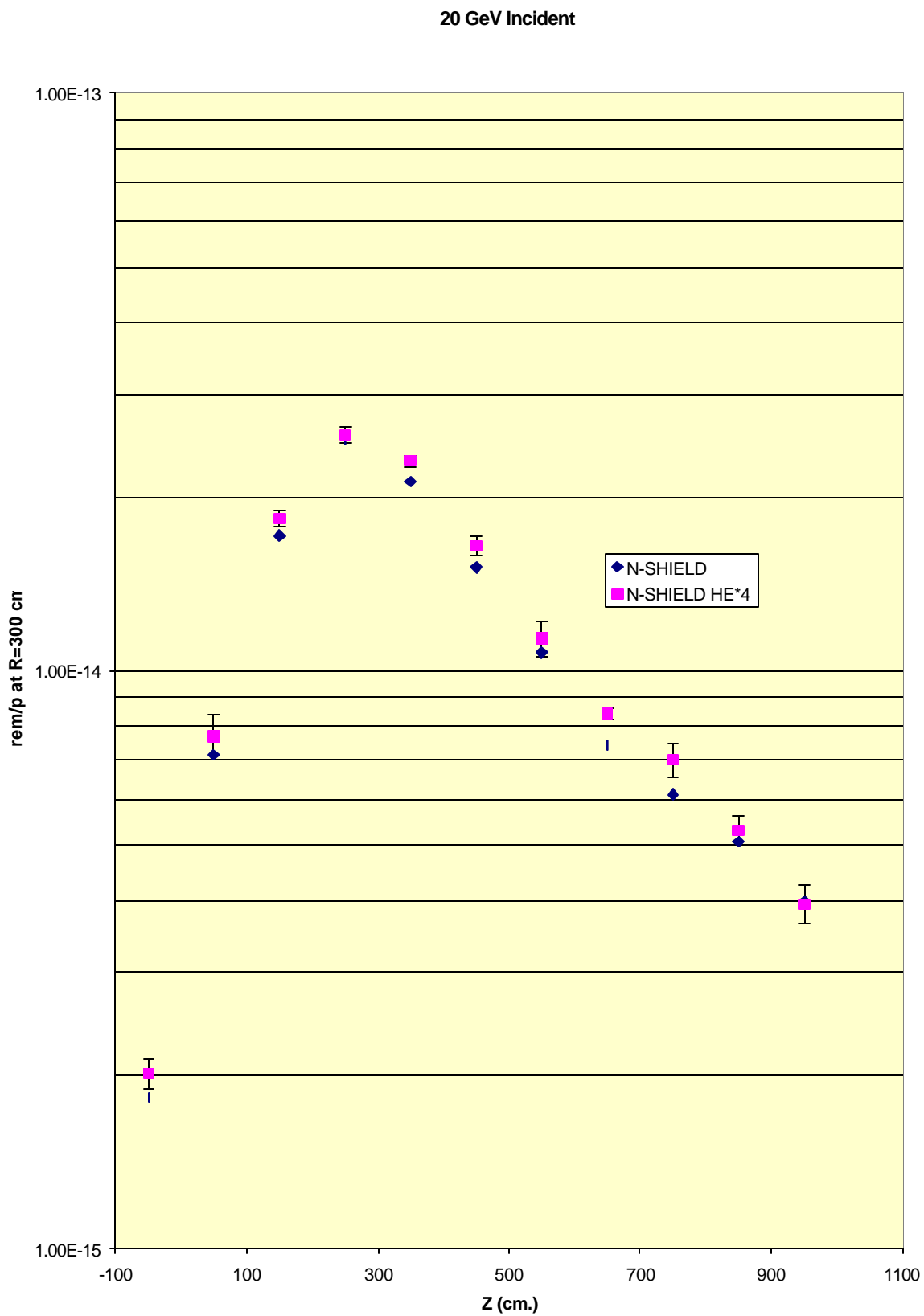


Fig. 7. N-SHIELD HE Only times 4 Compared to Fig. 6 N-SHIELD

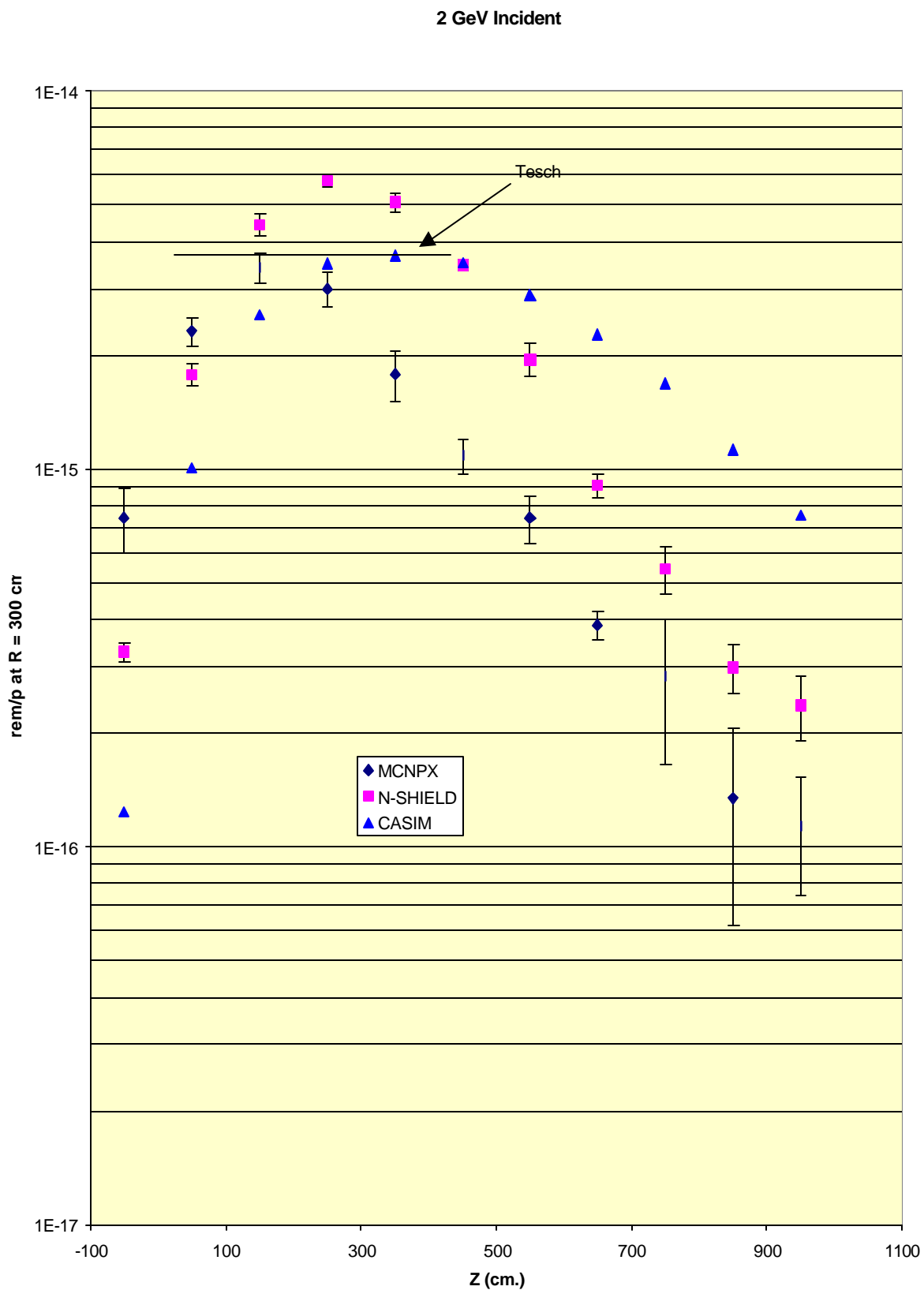


Fig. 8 Code Comparison in the Transverse Geometry at 2 GeV (See Text)

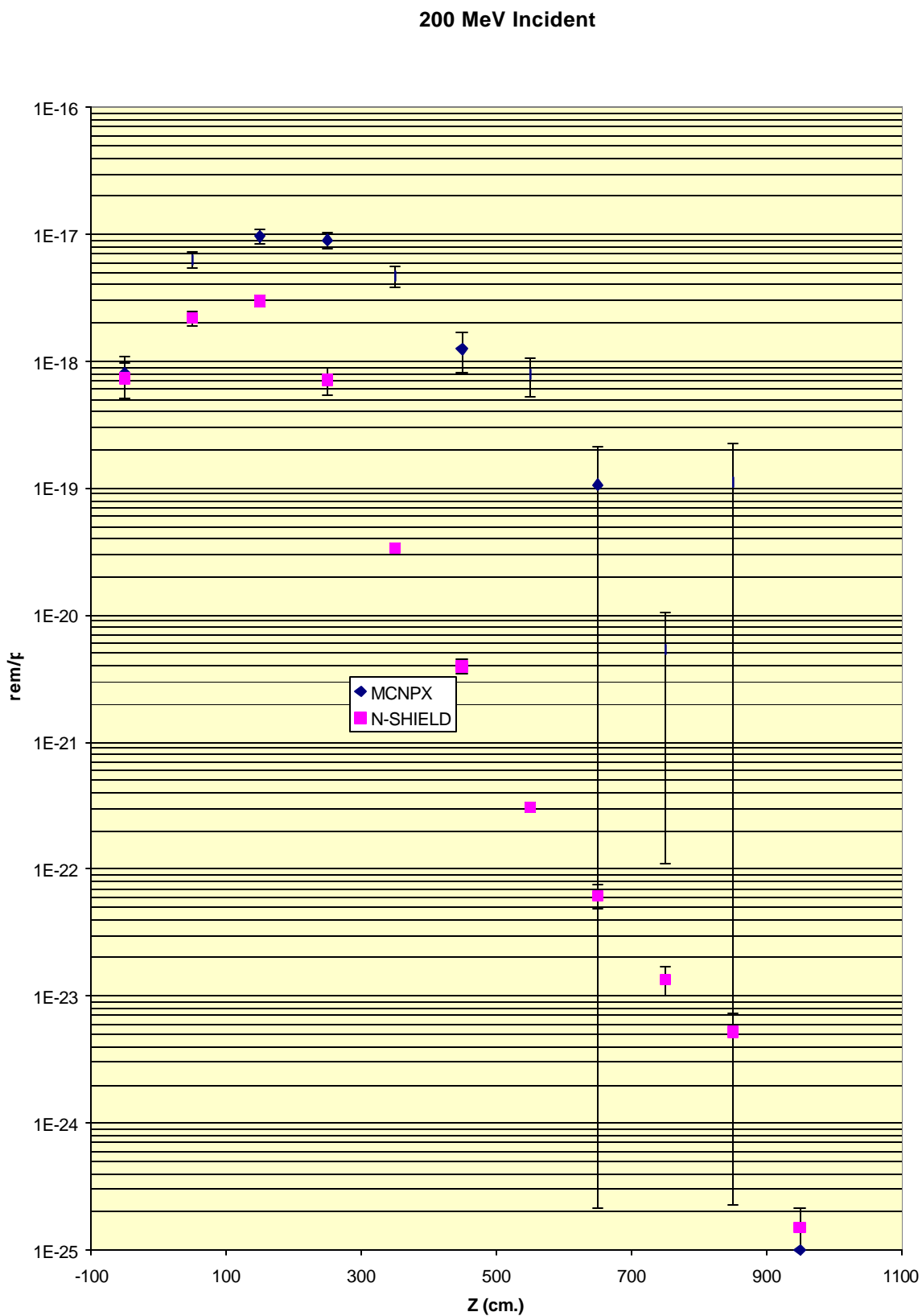


Fig. 9 Code Comparison in the Transverse Geometry at 200 MeV (See Text)

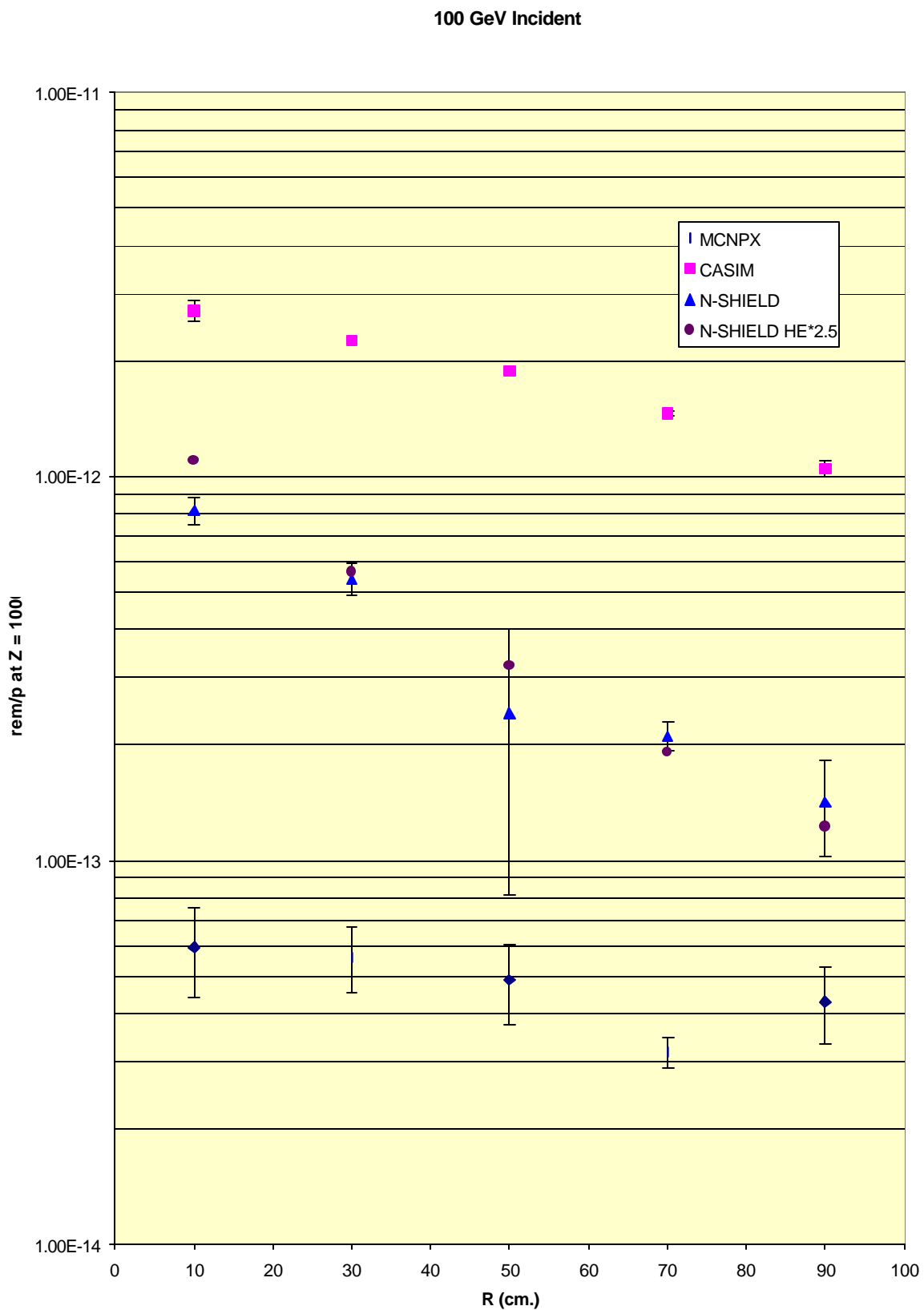


Fig. 10 Code Comparison in the Forward Geometry at 100 GeV (See Text)

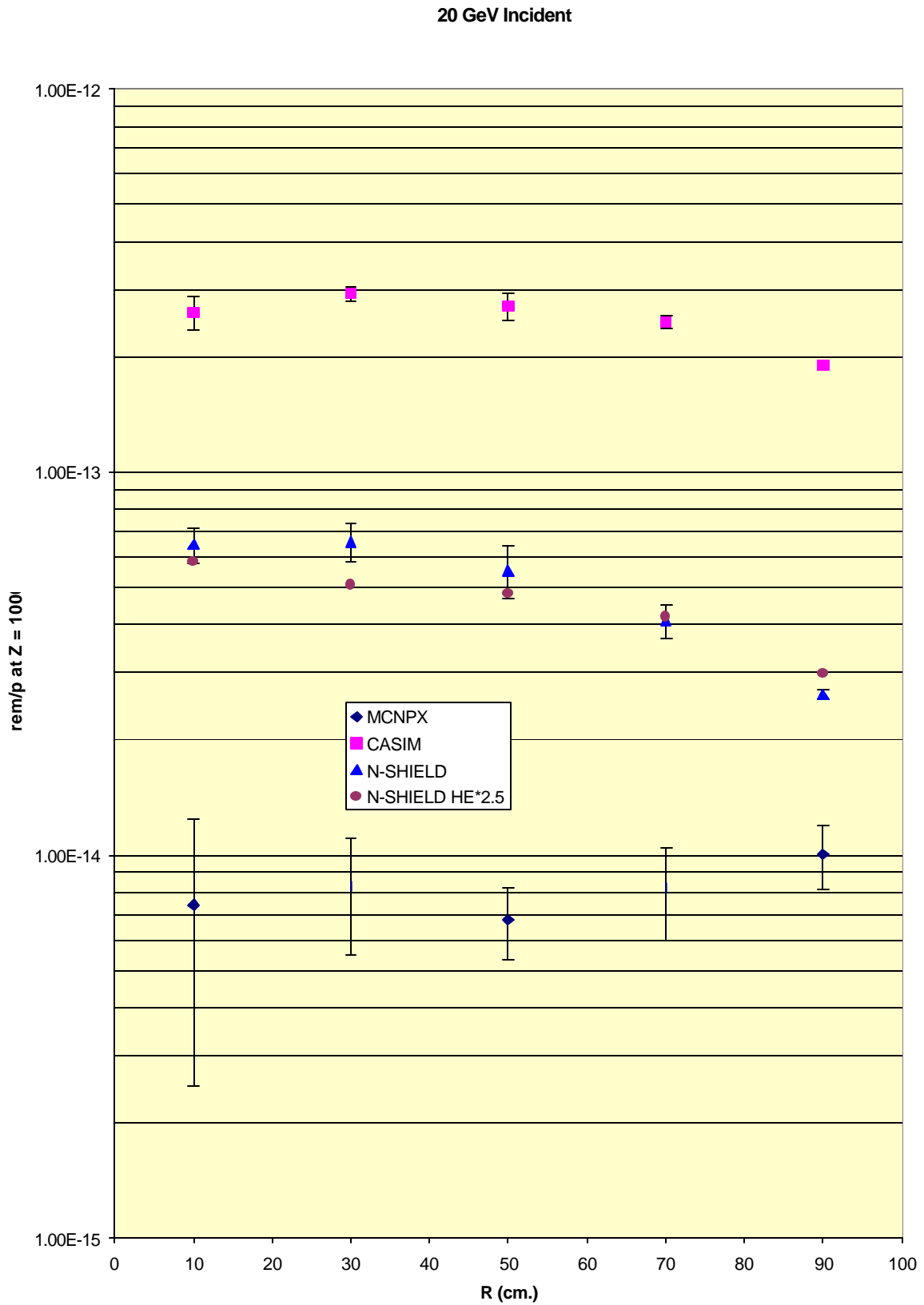


Fig. 11 Code Comparison in the Forward Geometry at 20 GeV (See Text)

Dose at Z=1000 for 2 GeV Incident

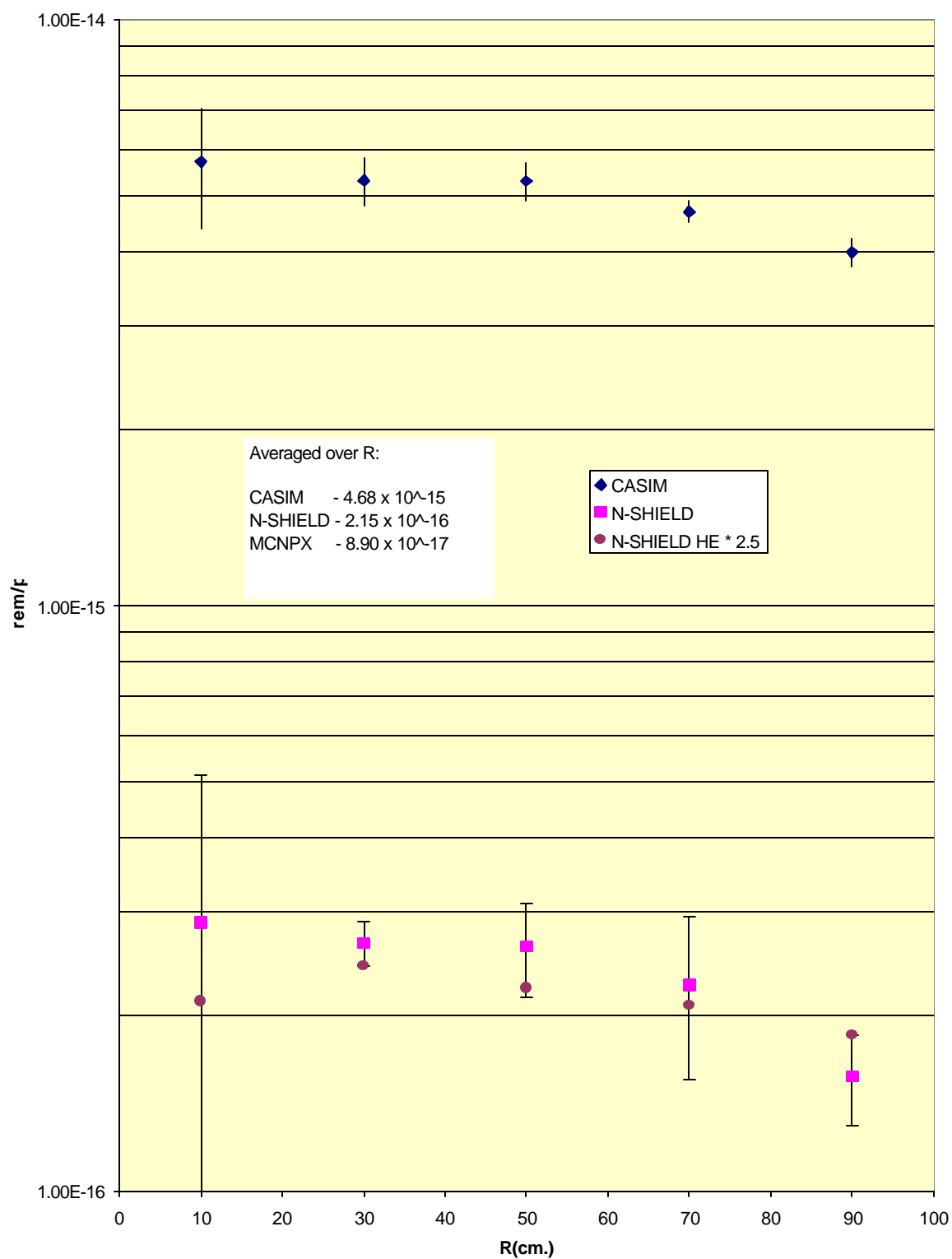
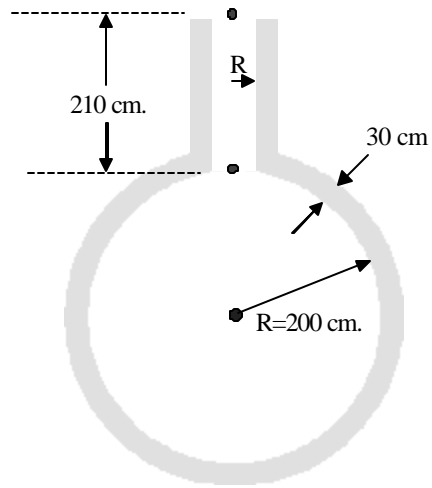
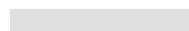
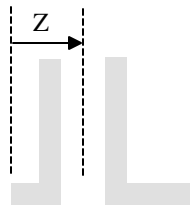


Fig. 12 Code Comparison in the Forward Geometry at 20 GeV (See Text)



(a) End View



(b) Side View

Fig. 13 Sketch of Penetration Calculation