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1. PURPOSE

The purpose of this document is to evaluate the potential for criticality for the fissile material that could accumulate in the near-field (invert) and in the far-field (host rock) beneath the U.S. Department of Energy (DOE) spent nuclear fuel (SNF) codisposal waste packages (WPs) as they degrade in the proposed monitored geologic repository at Yucca Mountain. The scope of this calculation is limited to the following DOE SNF types: Shippingport Pressurized Water Reactor (PWR), Enrico Fermi, Fast Flux Test Facility (FFTF), Fort St. Vrain, Melt and Dilute, Shippingport Light Water Breeder Reactor (LWBR), N-Reactor, and Training, Research, Isotope, General Atomics reactor (TRIGA). The results of this calculation are intended to be used for estimating the probability of criticality in the near-field and in the far-field. There are no limitations on use of the results of this calculation.

The calculation is associated with the waste package design and was developed in accordance with the technical work plan, *Technical Work Plan for: Department of Energy Spent Nuclear Fuel and Plutonium Disposition Work Packages* (Bechtel SAIC Company, LLC [BSC], 2002a). This calculation is subject to the Quality Assurance Requirements and Description (QARD) per the activity evaluation under work package number P6212310M1 in the technical work plan TWP-MGR-MD-000010 REV 01 (BSC 2002a).

2. METHOD

The Monte Carlo N-Particle (MCNP) transport code (Briesmeister 1997) is used to calculate the effective neutron multiplication factor (k_{eff}) for the configurations with fissile material that could accumulate in the near-field and in the far-field beneath the degraded DOE SNF codisposal WPs. The MCNP calculations use continuous-energy cross sections processed from the evaluated nuclear data files ENDF/B-V (Briesmeister 1997, App. G). These cross section libraries are part of the MCNP code system that has been obtained from the Software Configuration Management (SCM) in accordance with appropriate procedures. For each of the configurations modeled, the results reported from the MCNP calculations are the combined average values of k_{eff} from the three estimates (collision, absorption, and track length) and the standard deviation of these results (σ) listed in the final generation summary in the MCNP output.

For the configurations represented the following parameters were varied:

- Infiltration rate
- Saturation levels in the fractures and lithophysae
- Fracture porosity
- Lithophysae porosity

The above factors affect k_{eff} for the configurations in which fissile material accumulation occurs. High infiltration rates tend to spread out accumulation over a larger radius, but into a thinner layer. High fracture intensity reduces the volume of accumulation. The lithophysae porosity tends to decrease the accumulation volume.

3. ASSUMPTIONS

All the following assumptions are used in Section 5.

3.1 The tuff matrix, fractures and lithophysae are assumed fully saturated with water for the criticality evaluations. Additionally, the emplacement drift is assumed filled with water. The rationale for this assumption is that episodic fully saturated conditions are possible. This assumption is conservative since better neutron moderation and reflection enhances the potential for criticality.

3.2 The WP is assumed to be breached immediately after emplacement. The rationale for this assumption is that it is conservative since it allows for the least decay of Pu-239 to the less neutronically reactive U-235. Thus a higher Pu-239 to U-235 ratio will lead to higher k_{eff}.

3.3 The fissile material is assumed to distribute uniformly throughout the volume of the accumulation. The rationale for this assumption is that it is conservative for intermediate to highly enriched systems. Configurations with homogeneous distributions of fissile material result in higher k_{eff} values.

3.4 The critical limit is assumed to be 0.92. The rationale for this assumption is that this value was used as lowest (therefore most conservative) critical limit for internal criticality evaluations for all DOE fuel types investigated.

4. USE OF COMPUTER SOFTWARE AND MODELS

4.1 SOFTWARE

4.1.1 MCNP

The MCNP 4B2LV (Civilian Radioactive Waste Management System [CRWMS M&O] 1998b) code is used to calculate the k_{eff} of the fissile material external accumulation configurations. The software specifications are as follow:

- Software name: MCNP
- Software version/revision number: Version 4B2LV
- Software tracking number (computer software configuration item [CSCI]): 30033 V4B2LV
- Computer type: Hewlett Packard (HP) 9000 Series Workstations

- Status/Operating system: Qualified/HP-UX 10.20

- Computer processing unit number: Software is installed on the BSC workstation "bloom" whose CPU number is 700887.

The input and output files for the various MCNP calculations are documented in Attachments I and II. Attachment II provides the list of the files in Attachment I. The calculation files described in Sections 5 and 6 are such that an independent repetition of the software use may be performed.

The MCNP software used is: (a) appropriate for the application of k_{eff} calculations, (b) used only within the range of validation as documented in CRWMS M&O (1998a) and Briesmeister (1997), (c) obtained from the Software Configuration Management in accordance with the appropriate procedures.

5. CALCULATION

This section describes the bounding configurations and parameters for external fissile material accumulations that have a potential for criticality. The fissile material accumulation external to WPs containing DOE spent nuclear fuel was described in BSC (2002b). As fissile material leaves the WP it can either accumulate directly beneath the WP in the near-field or in the far-field. Section 5.1 discusses the near-field accumulation. The far-field accumulation is presented in Section 5.2.

Avogadro's number and atomic masses are taken from Parrington et al. (1996), this information is established fact, therefore considered accepted due to the nature of the reference cited therein.

The number of digits in the values cited herein may be the result of a calculation or may reflect the input from another source; consequently, the number of digits should not be interpreted as an indication of accuracy.

5.1 ACCUMULATION IN THE NEAR-FIELD

The invert consists of crushed tuff with 0.545 porosity (DTN: SN9908T0872799.004). This tuff corresponds to Topopah Spring tuff, which will be prepared from rock removed from the emplacement drift, access drift, etc. The invert height is 80.6 cm (CRWMS M&O 2000a, p. 24). In the simplest representation used, the fissile material accumulated in the invert beneath the WP and was assumed to distribute uniformly in the volume defined by the footprint of the WP (see Assumption 3.3 and Table 5-1). This volume is 6.523 m^3 for the footprint of a 5-DHLW/DOE long WP, and 4.295 m^3 for the footprint of a 5-DHLW/DOE short WP (footprint volumes are calculated in cells H17 to H26 in worksheet 'Main', spreadsheet 'Tab6_1&2.xls'). In all configurations, the tuff rock is conservatively assumed fully saturated with water and the emplacement drift is filled with water (see Assumption 3.1).

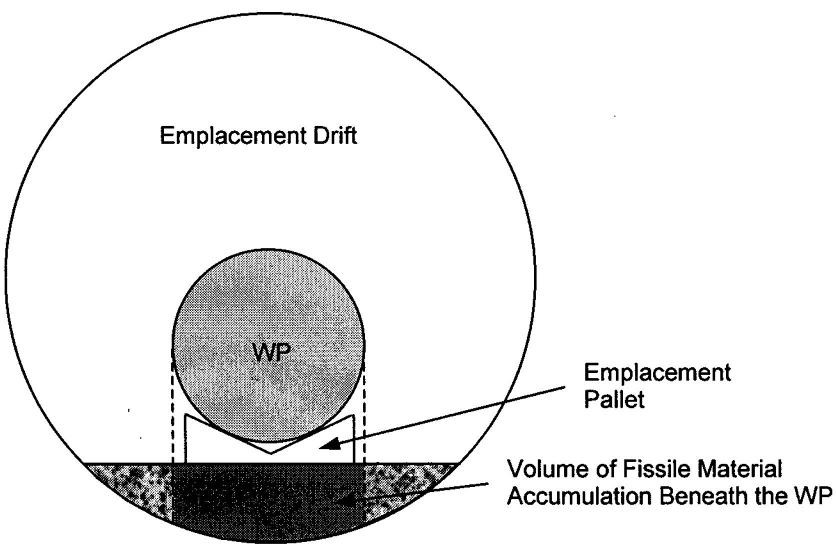


Figure 5-1. Footprint Configuration of Near-Field External Accumulation of Fissile Material from a WP

The near-field footprint configurations for each DOE fuel type external accumulations, which have the highest potential for criticality, were selected for investigation. They are presented in Table 5-1.

Table 5-1. Near-Field Footprint Configurations for the External Accumulation of Fissile Material from a WP

Fuel Type	WP Type	PHREEQC Case	MCNP Case	Time after WP Breach (years)	U-235 (moles)	Pu-239 (moles)
Shippingport PWR	long	sm1r1432	s1nf	10,000[a]	94.5[a]	0.00
Enrico Fermi	short	nt1x1432	n1nf	47,466[b]	458.2[b]	0.00
Enrico Fermi	short	nc2x1402	n2nf	84,536[c]	598.5[c]	0.00
Enrico Fermi	short	nc2x1402	n3nf	84,536[c]	598.5[c]	0.00
FFTF	long	f11xf21x	f1nf	76,551[d]	174.5[d]	32.3[d]
Fort Saint Vrain	long	fm1t3422	v1nf	38,000[a]	21.8[a]	0.00
Melt and Dilute	short	mm1x3332	m1nf	92,982[e]	179.9[e]	0.00
Shippingport LWBR	long	sm1t1031/sm2t1402	l1nf	77,000[a]	49.3[a]	0.00
N-Reactor	long	nm1o2131	r1nf	634,000[a]	22.9[a]	0.00
TRIGA	short	tt1y13h1	t1nf	430,000[a]	74.2[a]	0.00

Sources: [a] BSC 2002b, Table 6-1.
[b] BSC 2002b, 'nt1x1432_20_10_CritIn_SAT=0.8.xls', worksheet 'From_Acc_with_decay'.
[c] BSC 2002b, 'nc2x1402_20_10_CritIn_SAT=0.8.xls', worksheet 'From_Acc_with_decay'.
[d] BSC 2002b, 'f11xf21x_20_10_CritIn_SAT=0.8.xls', worksheet 'From_Acc_with_decay'.
[e] BSC 2002b, 'mm1x3332_20_10_CritIn_SAT=0.25.xls', worksheet 'From_Acc_with_decay'.

The conical configuration for near-field external accumulation, which is potentially more conservative (shown in Figure 5-2), was also investigated. The conical configurations and their characteristics for each DOE fuel type are presented in Table 5-2.

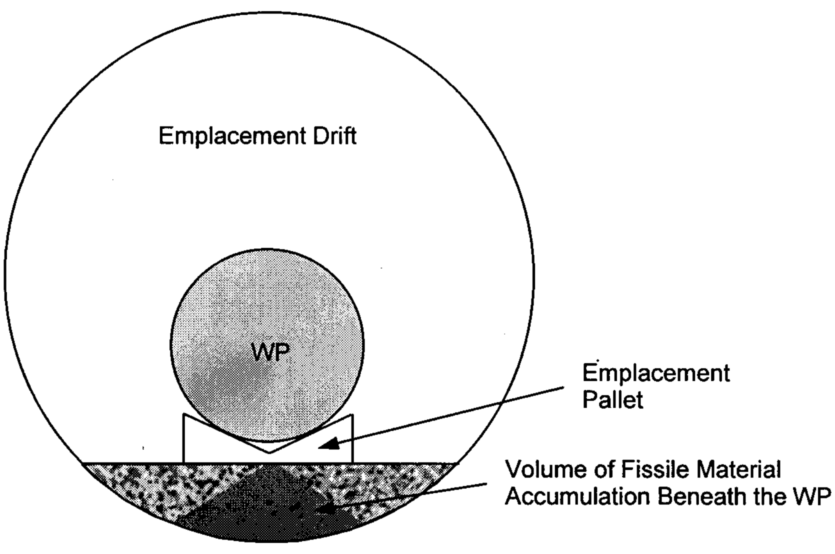


Figure 5-2. Cone-Shaped Near-Field External Accumulation of Fissile Material from a WP

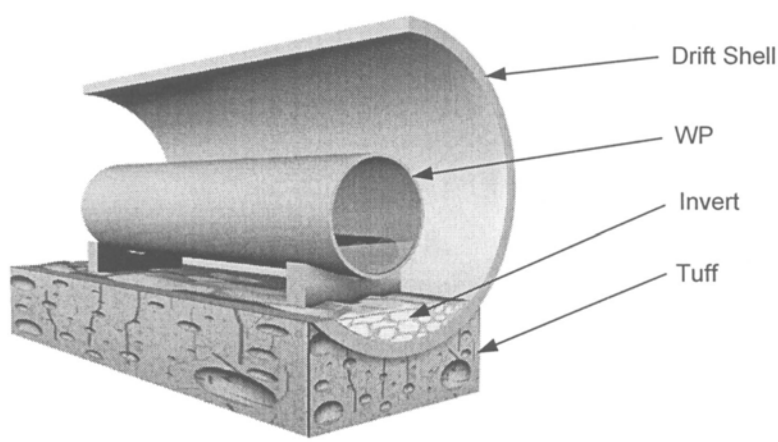
Table 5-2. Near-Field Cone-Shaped Configurations for the External Accumulation of Fissile Material from a WP

Fuel Type	PHREEQC Case	WP Type	MCNP Case	Time after WP Breach (years)	U-235 (moles)	Pu-239 (moles)
Shippingport PWR	sm1r1432	long	N/A[e]	10,000[a]	94.50[a]	0.00
Enrico Fermi	nt1x1432	short	ncnf	47,466[b]	458.17[b]	0.00
FFTF	ft1x1321	long	fcnf	343,748[c]	174.54[c]	32.34[c]
Fort Saint Vrain	fm1t3422	long	N/A[e]	38,000[a]	21.80[a]	0.00
Melt and Dilute	mm1x3332	short	mcnf	92,982[d]	179.9[d]	0.00
Shippingport LWBR	sm1t1031/sm2t1402	long	N/A[e]	77,000[a]	49.3[a]	0.00
N-Reactor	nm1o2131	long	N/A[e]	634,000[a]	22.9[a]	0.00
TRIGA	tt1y13h1	short	N/A[e]	430,000[a]	74.2[a]	0.00

Sources: [a] BSC 2002b, Table 6-1.
[b] BSC 2002b, 'nt1x1432_20_10_CritIn_SAT=0.8.xls', worksheet 'From_Acc_with_decay'.
[c] BSC 2002b, 'f11xf21x_20_10_CritIn_SAT=0.8.xls', worksheet 'From_Acc_with_decay'.
[d] BSC 2002b, 'mm1x3332_20_10_CritIn_SAT=0.25.xls', worksheet 'From_Acc_with_decay'.
NOTE: [e] The external accumulation information for these fuel types as provided in BSC 2002b does not include the details needed to construct the MCNP cases as done for Enrico Fermi, FFTF, and Melt and Dilute fuel types.

5.2 ACCUMULATION IN THE FAR-FIELD

Fissile material accumulates in the far-field along the walls of the fractures and in lithophysae. The far-field consists of several meters (maximum 10 m) of rock beneath the drift. Due to its volcanic origin, the rock has many fractures and a distribution of cavities (lithophysae). Figure 5-3 shows the WP and an idealized representation of fractures and lithophysae in the tuff rock beneath. The composition of the tuff rock is given in Table 5-3. The porosity of the tuff is 15.7 % (average of nominal porosities + two standard deviations, for TMN TLL TM2 hydrological units in DTN: MO0111RIB00040.001, Table 1), which is conservatively assumed to be fully saturated with water (see Assumption 3.1).



NOTE: Figure not to scale.

Figure 5-3. Far-Field Representation

Table 5-3. Tuff Composition

Element	Wt.%[a]
SiO_2	76.83
Al_2O_3	12.74
FeO	0.84
MgO	0.25
CaO	0.56
Na_2O	3.59
K_2O	4.93
TiO_2	0.1
P_2O_5	0.02
MnO	0.07
Particle Density[b] = 2.54 g/cm^3	

NOTES: [a] The wt.% values are the averages for rhyolite, locations no. 8, 9, 10, 12, 13, 14 in Lipman et al. 1966, Table 2.
[b] The tuff's density is the average of rock grain density values for TMN, TLL, TM2 hydrological units in MO0111RIB00040.001, Table 1.

Section 5.2.1 describes criticality calculations of fissile accumulations in fractures. The criticality calculations for the fissile accumulations in lithophysae are discussed in Section 5.2.2.

5.2.1 Accumulation in Fractures

Fissile material can accumulate along the walls of the fractures. The main condition to allow for accumulation is sufficient mixing between effluent water and enough fresh water to neutralize the mixture and lower the pH levels enough for uranium and plutonium to become insoluble and precipitate. Due to the nature of the flow from the waste package and through the fractures, geochemistry calculations show that the accumulation will spread out as the fissile materials flow deeper into the tuff. This results in a conical accumulation volume, which is represented using cylindrical layers as shown in Figure 5-4. The number of layers, their depth, and their radii vary based on the PHREEQC accumulation representation (BSC 2002b). PHREEQC is a geochemical transport code developed by the United States Geological Survey, which was used in BSC 2002b to calculate accumulation of minerals external to the WP. For purposes of criticality calculations, the fissile material accumulated in each layer is homogenized throughout that layer according to Assumption 3.3. In all cases investigated fracture porosity used was between 0.010 and 0.065, and all fractures and rock porosities were assumed filled with water (Assumption 3.1).

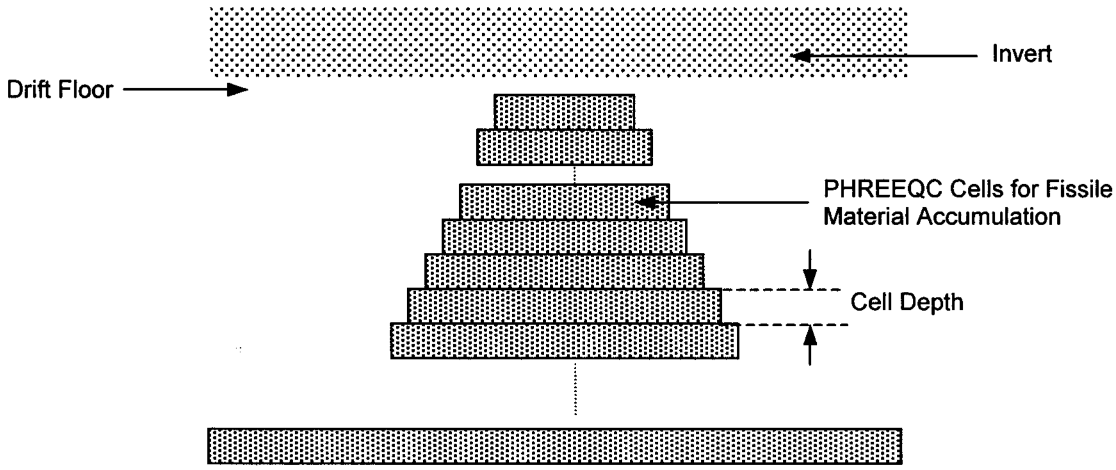


Figure 5-4. Accumulation Volumes in Fractures Representation

Table 5-4 is a summary of the accumulation cases in fractures only that resulted in significant fissile material accumulations in relatively optimum volumes to pose a criticality concern. Results for the most conservative configurations showed that only FFTF, Melt and Dilute, and Enrico Fermi fuel types had k_{eff} values close to 0.6 and above. Since the most conservative accumulations for the rest of the DOE fuel types have approximately half or less fissile material of the lowest amount for the three types mentioned (see Table 5-5), it is expected that k_{eff} for similar accumulations for the remaining DOE fuel types be smaller than 0.6, therefore subcritical, and no futher investigation is necessary.

Table 5-4. Summary of External Accumulation Cases in Fractures Only for the Most Reactive DOE Fuel Types

Fuel Type	PHREEQC Case	MCNP Case	Time (Years)	Infiltration Rate (L/year)	Fracture Porosity	Cell Depth (m)	Top Cell Radius[g] (m)	Saturation	Pu-239[a] (Moles)	U-235[a] (Moles)
FFTF[b]	f21c1402	f1ff	83,400	10000	0.065	0.1205	0.823	1	2.69	5.56
FFTF[b]	f21c1402	f11ff	83,400	10000	0.010	0.1205	2.098	1	2.69	5.56
FFTF[b]	f21c1402	f2ff	83,400	50	0.065	0.3030	0.519	1	2.69	5.56
FFTF[b]	f21c1402	f21ff	83,400	50	0.010	0.3030	1.323	1	2.69	5.56
FFTF[c]	f21x1402	f3ff	76,550	10000	0.065	0.1205	0.823	1	0.44	2.20
FFTF[c]	f21x1402	f4ff	76,550	50	0.065	0.3030	0.519	1	0.44	2.20
Melt and Dilute[d]	mm1x3332	m1ff	92,982	10000	0.065	0.1205	0.823	1	0.00	33.67
Melt and Dilute[d]	mm1x3332	m11ff	92,982	10000	0.030	0.1205	1.212	1	0.00	33.67
Melt and Dilute[d]	mm1x3332	m12ff	92,982	10000	0.020	0.1205	1.484	1	0.00	33.67
Melt and Dilute[d]	mm1x3332	m13ff	92,982	10000	0.065	0.1205	1.164	0.5	0.00	33.67
Melt and Dilute[d]	mm1x3332	m14ff	92,982	10000	0.065	0.1205	1.646	0.25	0.00	33.67
Melt and Dilute[d]	mm1x3332	m2ff	92,982	50	0.065	0.3030	0.519	1	0.00	33.67
Melt and Dilute[d]	mm1x3332	m21ff	92,982	50	0.030	0.3030	0.764	1	0.00	33.67
Melt and Dilute[d]	mm1x3332	m22ff	92,982	50	0.020	0.3030	0.936	1	0.00	33.67
Melt and Dilute[d]	mm1x3332	m23ff	92,982	50	0.065	0.3030	1.038	0.25	0.00	33.67
Enrico Fermi[e]	nt1x1331	n1ff	382,523	10000	0.065	0.1205	0.260	1	0.00	4.93
Enrico Fermi[e]	nt1x1331	n11ff	382,523	10000	0.065	0.1205	0.368	0.5	0.00	4.93
Enrico Fermi[e]	nt1x1331	n12ff	382,523	10000	0.030	0.1205	0.383	1	0.00	4.93
Enrico Fermi[e]	nt1x1331	n13ff	382,523	10000	0.010	0.1205	0.664	1	0.00	4.93
Enrico Fermi[e]	nt1x1331	n14ff	382,523	10000	0.020	0.1205	0.664	0.5	0.00	4.93
Enrico Fermi[e]	nt1x1331	n2ff	382,523	50	0.065	0.3030	0.164	1	0.00	4.93
Enrico Fermi[e]	nt1x1331	n21ff	382,523	50	0.065	0.3030	0.232	0.5	0.00	4.93
Enrico Fermi[e]	nt1x1331	n22ff	382,523	50	0.030	0.3030	0.242	1	0.00	4.93
Enrico Fermi[e]	nt1x1331	n23ff	382,523	50	0.010	0.3030	0.418	1	0.00	4.93
Enrico Fermi[e]	nt1x1331	n24ff	382,523	50	0.030	0.3030	0.342	0.5	0.00	4.93
Enrico Fermi[e]	nt1x1331	n25ff	382,523	50	0.020	0.3030	0.418	0.5	0.00	4.93
Enrico Fermi[f]	nc2x1402	n3ff	84,536	10000	0.065	0.1613	0.711	1	0.00	8.14
Enrico Fermi[f]	nc2x1402	n31ff	84,536	10000	0.010	0.1205	2.098	1	0.00	8.14
Enrico Fermi[f]	nc2x1402	n32ff	84,536	10000	0.030	0.1613	1.047	1	0.00	8.14
Enrico Fermi[f]	nc2x1402	n33ff	84,536	10000	0.065	0.1613	0.795	0.8	0.00	8.14
Enrico Fermi[f]	nc2x1402	n4ff	84,536	50	0.065	0.8333	0.313	1	0.00	8.14
Enrico Fermi[f]	nc2x1402	n41ff	84,536	50	0.010	0.8333	0.798	1	0.00	8.14
Enrico Fermi[f]	nc2x1402	n42ff	84,536	50	0.030	0.8333	0.461	1	0.00	8.14

NOTE: [a] This information is applicable only to the top cell of the accumulation.
[g] Calculated in Attachment I, spreadsheet :\far_field\spreadsheets\Tab6_3.

Sources: [b] BSC 2002b, spreadsheet 'f11cf21c_20_10_Critln_SAT=0.8.xls,' worksheet 'Density no lith.'
[c] BSC 2002b, spreadsheet 'f11xf21x_20_10_Critln_SAT=0.8.xls,' worksheet 'Density no lith.'
[d] BSC 2002b, spreadsheet 'mm1x3332_20_10_Critln_SAT=0.25.xls,' worksheet 'Density no lith.'
[e] BSC 2002b, spreadsheet 'nt1x1331_20_10_Critln_SAT=0.5.xls,' worksheet 'Density no lith.'
[f] BSC 2002b, spreadsheet 'nc2x1402_20_10_Critln_SAT=0.8.xls,' worksheet 'Density no lith.'

Table 5-5. Summary of External Accumulations with High Total Fissile Content

Fuel Type	PHREEQC Case	U-235 (moles)	U-238 (moles)	Pu-239 (moles)
Shippingport PWR	sm1r1432	94.5	1066.6	0
Enrico Fermi	nt1x1432	481.8	2106.2	0
Enrico Fermi	nc2x1402	613.1	2257.0	0
FFTF	f21c1402	159.3	737.8	33.4
FFTF	f21x1402	174.5	1976.7	32.3
Fort Saint Vrain	fm1t3422	21.8	896.5	0
Melt and Dilute	mm1x3332	180.5	928.8	0
Shippingport LWBR	st1n1432	49.4	1181.7	0
N-Reactor	nm1o2131	22.9	2195.2	0
TRIGA	tt1y13h1	74.2	718.8	0

Source: BSC 2002b, Table 6-1.

It can be seen from Table 5-5 that the lowest total amount of fissile material among external accumulations for FFTF, Melt and Dilute, and Enrico Fermi (180.5 moles for Melt and Dilute), is almost twice the highest total amount of fissile material for the remaining DOE fuel types (94.5 moles for Shippingport PWR).

5.2.2 Accumulation in Lithophysae

In order to account for accumulation in lithophysae, two representations were considered: the equivalent fracture representation and the spherical representation. The equivalent fracture representation treats the lithophysae as if they were wide fractures where accumulation occurs only along the walls of the lithophysae with film flow of effluent and fresh water. In the cases where large lithophysae are considered, the surface area of the lithophysae does not compensate for the reduction of fractures due to the void volume occupied by the lithophysae. In other words the smaller the lithophysae the more conservative the calculation. The lithophysae porosity was varied between 0.027 and 0.27. The spherical representation of lithophysae requires some ponding and enough dilution in a single lithophysae such that fissile materials accumulate at the bottom of a single and relatively large lithophysae. Table 5-6 is a summary of the configurations investigated for equivalent fracture representation of lithophysae.

Table 5-6. Summary of Accumulation in Fractures and Lithophysae as Equivalent Fractures

Fuel Type	PHRREQC Case	MCNP Case	Infiltration Rate (L/year)	Porosity of Fractures	Porosity of Lithophysae	Saturation	Cell Thickness (m)
FFTF[a]	f11cf1021/f21c1402	f1ffl	10000	0.020	0.27	1	0.1205
FFTF[a]	f11cf1021/f21c1402	f11fl	10000	0.011	0.18	1	0.1205
FFTF[a]	f11cf1021/f21c1402	f12fl	10000	0.020	0.27	0.8	0.1205
FFTF[a]	f11cf1021/f21c1402	f13fl	1000	0.020	0.27	1	0.1639
FFTF[a]	f11cf1021/f21c1402	f2ffl	50	0.020	0.27	1	0.3030
Melt and Dilute[b]	mm1x3332	m1ffl	10000	0.020	0.27	1	0.1205
Melt and Dilute[b]	mm1x3332	m11fl	10000	0.011	0.18	1	0.1205
Melt and Dilute[b]	mm1x3332	m12fl	10000	0.020	0.27	0.5	0.1205
Melt and Dilute[b]	mm1x3332	m13fl	1000	0.020	0.27	1	0.1639
Melt and Dilute[b]	mm1x3332	m2ffl	50	0.020	0.27	1	0.3030
Melt and Dilute[b]	mm1x3332	m21fl	50	0.011	0.18	1	0.3030
Melt and Dilute[b]	mm1x3332	m22fl	50	0.009	0.071	1	0.3030
Melt and Dilute[b]	mm1x3332	m23fl	50	0.020	0.027	0.5	0.3030
Enrico Fermi[c]	nt1x1331	n1ffl	10000	0.020	0.27	1	0.1205
Enrico Fermi[c]	nt1x1331	n11fl	10000	0.011	0.18	1	0.1205
Enrico Fermi[c]	nt1x1331	n12fl	10000	0.009	0.071	1	0.1205
Enrico Fermi[c]	nt1x1331	n13fl	10000	0.020	0.27	0.5	0.1205
Enrico Fermi[c]	nt1x1331	n14fl	1000	0.020	0.27	0.5	0.1639
Enrico Fermi[c]	nt1x1331	n15fl	10000	0.009	0.071	0.5	0.1205
Enrico Fermi[c]	nt1x1331	n2ffl	50	0.020	0.27	1	0.3030
Enrico Fermi[c]	nt1x1331	n21fl	50	0.011	0.18	1	0.3030
Enrico Fermi[c]	nt1x1331	n22fl	50	0.009	0.071	1	0.3030
Enrico Fermi[c]	nt1x1331	n23fl	50	0.020	0.27	0.5	0.3030
Enrico Fermi[c]	nt1x1331	n24fl	50	0.011	0.18	0.5	0.3030
Enrico Fermi[d]	nc2x1402	n3ffl	10000	0.020	0.27	1	0.1639
Enrico Fermi[d]	nc2x1402	n31fl	10000	0.011	0.18	1	0.1639
Enrico Fermi[d]	nc2x1402	n4ffl	50	0.020	0.27	1	0.8333
Enrico Fermi[d]	nc2x1402	n41fl	50	0.011	0.18	1	0.8333

Sources: [a] BSC 2002b, spreadsheet 'f11cf21c_20_10_Critln_SAT=0.8.xls,' worksheet 'Density no lith.'
[b] BSC 2002b, spreadsheet 'mm1x3332_20_10_Critln_SAT=0.25.xls,' worksheet 'Density no lith.'
[c] BSC 2002b, spreadsheet 'nt1x1331_20_10_Critln_SAT=0.5.xls,' worksheet 'Density no lith.'
[d] BSC 2002b, spreadsheet 'nc2x1402_20_10_Critln_SAT=0.8.xls,' worksheet 'Density no lith.'

Table 5-7 is a summary of the configurations investigated for the spherical representation of lithophysae.

Table 5-7. Cases for Accumulation in Large Spherical Lithophysae

Fuel Type	MCNP Case	PHREEQC Case Name	Time (Years)	Lithophysae Diameter (cm)	Percentage of Lithophysae Filled	Water Content (vol%)	Number of Fractures per Lithophysae	Pu-239 (Moles)	U-235 (Moles)
FFTF[a]	fl	ft1x1321	-	25	100	0	18	0	98.1
FFTF[a]	fl2	ft1x1321	-	2x25	100	0	18	0	98.1
FFTF[a]	fl3	ft1x1321	-	50	21.2	0	42	0	122.1
Enrico Fermi[b]	nt051	nt1x1331	438,249	50	46.8	0	24	0	318.5
Enrico Fermi[b]	nt052	nt1x1331	438,249	50	42.3	0	36	0	321.9
Enrico Fermi[b]	nt055	nt1x1331	438,249	50	50.5	0	18	0	307.7
Enrico Fermi[b]	nt52w	nt1x1331	438,249	50	50.8	20	36	0	321.9
Enrico Fermi[b]	nt58w	nt1x1331	438,249	50	76.1	4	6	0	136.1

Sources: [a] BSC 2002b, spreadsheet 'ft1x1321c_Critln_lith.xls.'
[b] BSC 2002b, spreadsheet 'nt1x1331_Critln_lith_times6.xls,' worksheet 'Results.'

6. RESULTS

This section presents the results of the calculation. The outputs of this calculation are reasonable compared to the inputs, and the results are suitable for the intended use. The uncertainties are taken into account by consistently using the most conservative approach; the calculations, therefore, yield a conservatively bounding set of results.

The results of external criticality evaluation due to fissile material accumulation from waste packages containing DOE SNF in the fractures and lithophysae are presented in Sections 6.1 and 6.2, respectively. The k_{eff} results represent the average collision, absorption, and track length estimator from the MCNP calculations. The standard deviation (σ) represents the standard deviation of k_{eff} about the average combined collision, absorption, and track length estimate due to Monte Carlo calculation statistics.

6.1 NEAR-FIELD ACCUMULATION

This section presents the results for the near-field configurations described in Section 5.1. The results for k_{eff} evaluations of the accumulation calculation corresponding to the footprint configurations (presented in Table 5-1) in the invert are listed in Table 6-1.

Table 6-1. Results for Near-Field Footprint Configurations for the External Accumulation of Fissile Material from a WP

Fuel Type	Case Name	k_{eff}	$k_{eff}+2\sigma$
Shippingport PWR	s1nf	0.46746	0.46836
Enrico Fermi	n1nf	1.29975	1.30201
Enrico Fermi	n2nf	1.38908	1.39114
Enrico Fermi	n3nf	1.39814	1.40002
FFTF	f1nf	0.82757	0.82911
Fort Saint Vrain	v1nf	0.13435	0.13461
Melt and Dilute	m1nf	0.91407	0.91547
Shippingport LWBR	l1nf	0.27681	0.27729
N-Reactor	r1nf	0.13721	0.13747
TRIGA	t1nf	0.53133	0.53215

Table 6-2 presents the k_{eff} results for evaluations of the accumulation calculation for the most conservative conical-shaped configurations described in Table 5-2.

Table 6-2. Results for Conical-Shaped Near-Field Configurations for the External Accumulation of Fissile Material from a WP

Fuel Type	Case Name	k_{eff}	$k_{eff}+2\sigma$
Enrico Fermi	ncnf	1.14573	1.14891
FFTF	fcnf	0.82390	0.82700
Melt and Dilute	mcnf	0.61591	0.61881

The remaining DOE fuel types are expected to have lower k_{eff} values than those shown in Table 6-2 since the amount of fissile material in the external accumulation is significantly lower (see Table 5-2).

6.2 FAR-FIELD ACCUMULATION

6.2.1 Accumulation in Fractures

This section presents the results for the configurations described in Section 5.2.1. The k_{eff} evaluations of the external accumulation calculation in non-lithophysal zone taking into account fractures only (which add up to 6.5% to the tuff porosity) are listed in Table 6-3.

Table 6-3. Summary of k_{eff} Results for Accumulation in Fractures and Lithophysae as Equivalent Fractures

Fuel Type	MCNP Case	Time (Years)	Infiltration Rate (L/year)	Fracture Porosity	Saturation	k_{eff}	$k_{eff}+2\sigma$
FFTF	f1ff	83,400	10000	0.065	1	0.72797	0.72989
FFTF	f11ff	83,400	10000	0.010	1	0.19848	0.19900
FFTF	f2ff	83,400	50	0.065	1	0.79998	0.80172
FFTF	f21ff	83,400	50	0.010	1	0.25520	0.25584
FFTF	f3ff	76,550	10000	0.065	1	0.57456	0.57594
FFTF	f4ff	76,550	50	0.065	1	0.62519	0.62673
Melt and Dilute	m1ff	92,982	10000	0.065	1	1.12875	1.13113
Melt and Dilute	m11ff	92,982	10000	0.030	1	0.92527	0.92757
Melt and Dilute	m12ff	92,982	10000	0.020	1	0.78663	0.78845
Melt and Dilute	m13ff	92,982	10000	0.065	0.5	0.96400	0.96598
Melt and Dilute	m14ff	92,982	10000	0.065	0.25	0.72468	0.72622
Melt and Dilute	m2ff	92,982	50	0.065	1	1.18145	1.18383
Melt and Dilute	m21ff	92,982	50	0.030	1	1.02004	1.02208
Melt and Dilute	m22ff	92,982	50	0.020	1	0.89173	0.89379
Melt and Dilute	m23ff	92,982	50	0.065	0.25	0.83086	0.83252
Enrico Fermi	n1ff	382,523	10000	0.065	1	1.30540	1.30794
Enrico Fermi	n11ff	382,523	10000	0.065	0.5	1.23732	1.24014
Enrico Fermi	n12ff	382,523	10000	0.030	1	1.20853	1.21145
Enrico Fermi	n13ff	382,523	10000	0.010	1	0.90716	0.90912
Enrico Fermi	n14ff	382,523	10000	0.020	0.5	0.90947	0.91173
Enrico Fermi	n2ff	382,523	50	0.065	1	1.21030	1.21288
Enrico Fermi	n21ff	382,523	50	0.065	0.5	1.15964	1.16242
Enrico Fermi	n22ff	382,523	50	0.030	1	1.12903	1.13161
Enrico Fermi	n23ff	382,523	50	0.010	1	0.85953	0.86165
Enrico Fermi	n24ff	382,523	50	0.030	0.5	0.98441	0.98689
Enrico Fermi	n25ff	382,523	50	0.020	0.5	0.86360	0.86556
Enrico Fermi	n3ff	84,536	10000	0.065	1	0.97840	0.98040
Enrico Fermi	n31ff	84,536	10000	0.010	1	0.30552	0.30626
Enrico Fermi	n32ff	84,536	10000	0.030	1	0.67567	0.67699
Enrico Fermi	n33ff	84,536	10000	0.065	0.8	0.89363	0.89521
Enrico Fermi	n4ff	84,536	50	0.065	1	0.89290	0.89484
Enrico Fermi	n41ff	84,536	50	0.010	1	0.32400	0.32476
Enrico Fermi	n42ff	84,536	50	0.030	1	0.65356	0.65502

The most conservative configurations for remaining DOE fuel types are expected to have lower k_{eff} values than 0.8 (which is the lowest k_{eff} for the most conservative case for each of the three DOE fuel types in Table 6-3) since the amount of fissile material in the external accumulation is significantly lower (see Table 5-5).

6.2.2 Accumulation in Lithophysae

This section presents the results for the configurations described in Section 5.2.2. The k_{eff} evaluations of the external accumulation calculation in the lithophysal zone for the equivalent fracture representation are listed in Table 6-4.

Table 6-4. Far-Field Cases Investigated for the External Accumulation of Fissile Material from a WP

Fuel Type	MCNP Case	Infiltration Rate (L/year)	Porosity as Fractures	Porosity as Lithophysae	Saturation	k_{eff}	k_{eff}+2σ
FFTF	f1ffl	10000	0.020	0.27	1	0.63782	0.63891
FFTF	f11fl	10000	0.011	0.18	1	0.38574	0.38664
FFTF	f12fl	10000	0.020	0.27	0.8	0.55513	0.55635
FFTF	f13fl	1000	0.020	0.27	1	0.67402	0.67552
FFTF	f2ffl	50	0.020	0.27	1	0.72416	0.72532
Melt and Dilute	m1ffl	10000	0.020	0.27	1	1.15148	1.15324
Melt and Dilute	m11fl	10000	0.011	0.18	1	0.87753	0.88145
Melt and Dilute	m12fl	10000	0.020	0.27	0.5	0.90376	0.90534
Melt and Dilute	m13fl	1000	0.020	0.27	1	1.18613	1.18859
Melt and Dilute	m2ffl	50	0.020	0.27	1	1.20837	1.21017
Melt and Dilute	m21fl	50	0.011	0.18	1	0.96898	0.97070
Melt and Dilute	m22fl	50	0.009	0.071	1	0.73465	0.73619
Melt and Dilute	m23fl	50	0.020	0.027	0.5	0.98816	0.98966
Enrico Fermi	n1ffl	10000	0.020	0.27	1	1.37558	1.37760
Enrico Fermi	n11fl	10000	0.011	0.18	1	1.20015	1.20235
Enrico Fermi	n12fl	10000	0.009	0.071	1	0.99648	0.99818
Enrico Fermi	n13fl	10000	0.020	0.27	0.5	1.22195	1.22381
Enrico Fermi	n14fl	1000	0.020	0.27	0.5	1.20609	1.20855
Enrico Fermi	n15fl	10000	0.009	0.071	0.5	0.73311	0.73449
Enrico Fermi	n2ffl	50	0.020	0.27	1	1.29597	1.29817
Enrico Fermi	n21fl	50	0.011	0.18	1	1.12829	1.13047
Enrico Fermi	n22fl	50	0.009	0.071	1	0.94468	0.94648
Enrico Fermi	n23fl	50	0.020	0.27	0.5	1.15859	1.16047
Enrico Fermi	n24fl	50	0.011	0.18	0.5	0.92238	0.92416
Enrico Fermi	n3ffl	10000	0.020	0.27	1	0.84332	0.84448
Enrico Fermi	n31fl	10000	0.011	0.18	1	0.54684	0.54792
Enrico Fermi	n4ffl	50	0.020	0.27	1	0.81347	0.81501
Enrico Fermi	n41fl	50	0.011	0.18	1	0.54636	0.54748

The most conservative configurations for remaining DOE fuel types are expected to have significantly lower k_{eff} values than 0.96 (which is the lowest k_{eff} for the most conservative case for each of the three DOE fuel types in Table 6-4) since the amount of fissile material in the external accumulation is significantly lower (see Table 5-5).

The k_{eff} evaluations of the external accumulation calculation in the lithophysal zone for the spherical lithophysae representation are listed in Table 6-5.

Table 6-5. Cases for Accumulation in Large Spherical Lithophysae

Fuel Type	MCNP Case	Lithophysae Diameter (m)	Percentage of Lithophysae Filled	Water Content (vol.%)	Number of Fractures per Lithophysae	Pu-239 (Moles)	U-235 (Moles)	k_{eff}	$k_{eff}+2\sigma$
FFTF	fl	25	100	0	18	0	98.1	0.79026	0.79218
FFTF	fl2	2x25[a]	100	0	18	0	98.1	0.79331	0.79528
FFTF	fl3	50	21.2	0	42	0	122.1	0.48243	0.48471
Enrico Fermi	nt051	50	46.8	0	24	0	318.5	0.92646	0.92894
Enrico Fermi	nt052	50	42.3	0	36	0	321.9	0.95296	0.95526
Enrico Fermi	nt055	50	50.5	0	18	0	307.7	0.89860	0.90120
Enrico Fermi	nt52w	50	50.8	20	36	0	321.9	1.39575	1.39855
Enrico Fermi	nt58w	50	76.1	4	6	0	321.9	0.94576	0.94814

NOTE: [a]This case had two tangent spherical lithophysae with diameters of 0.25 m each.

The most conservative configurations for remaining DOE fuel types are expected to have lower k_{eff} values than 0.8 (which is the lowest k_{eff} for the most conservative case for each of the two DOE fuel types in Table 6-5) since the amount of fissile material in the external accumulation is significantly lower (see Table 5-5).

7. REFERENCES

7.1 DOCUMENTS CITED

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Parrington, J.R.; Knox, H.D.; Breneman, S.L.; Baum, E.M.; and Feiner, F. 1996. *Nuclides and Isotopes, Chart of the Nuclides.* 15th Edition. San Jose, California: General Electric Company and KAPL, Inc. TIC: 233705.

7.2 INPUT DTNS

SN9908T0872799.004. Tabulated In-Drift Geometric and Thermal Properties Used in Drift-Scale Models for TSPA-SR (Total System Performance Assessment-Site Recommendation). Submittal date: 08/30/1999.

MO0111RIB00040.001. RIB Item 0040: Matrix Hydrologic Properties. Submittal date: 11/01/2001.

8. ATTACHMENTS

Attachment I: One Compact Disk (CD) containing the archived MCNP output files, and Excel Spreadsheets used to generate the MCNP inputs.

Attachment II: Description of archived files contained in Attachment I (CD), 3 pages.

ATTACHMENT II

This attachment contains the listing and description of the files archived in 'att.zip' file in Attachment I (CD) of this calculation. The archive file was created using WINZIP 8.1 on 10/17/2002, 3:18 pm, and copied on the CD using the CD writer unit of the BSC personal computer whose CPU number is 150411. The 'att.zip' file size is 6,489,557 bytes and contains 145 files. Upon file extraction, the files with extension 'io' are the MCNP output files, and the files with extension 'xls' are the Excel spreadsheets used for generating the MCNP inputs.

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f1ff.io	08/19/2002	05:16p	357,954
f21ff.io	08/19/2002	05:16p	354,635
f2ff.io	08/19/2002	05:16p	375,661
f3ff.io	08/19/2002	05:16p	416,438
f4ff.io	08/19/2002	05:16p	352,692
m11ff.io	08/19/2002	05:16p	345,698
m12ff.io	08/19/2002	05:16p	345,717
m13ff.io	08/19/2002	05:16p	345,864
m14ff.io	08/19/2002	05:16p	345,772
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m22ff.io	08/19/2002	05:16p	346,214
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m2ff.io	08/19/2002	05:16p	303,827
n11ff.io	08/19/2002	05:16p	349,517
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n13ff.io	08/19/2002	05:16p	349,859
n14ff.io	08/19/2002	05:17p	349,794
n1ff.io	08/19/2002	05:17p	370,336
n21ff.io	08/19/2002	05:17p	345,064
n22ff.io	08/19/2002	05:17p	345,883
n23ff.io	08/19/2002	05:17p	344,981
n24ff.io	08/19/2002	05:17p	344,981
n25ff.io	08/19/2002	05:17p	345,094
n2ff.io	08/19/2002	05:17p	365,879
n31ff.io	08/19/2002	05:17p	348,335
n32ff.io	08/19/2002	05:17p	364,884
n33ff.io	08/19/2002	05:17p	350,567
n3ff.io	08/19/2002	05:17p	349,931
n41ff.io	08/19/2002	05:17p	234,376
n42ff.io	08/19/2002	05:17p	234,257
n4ff.io	08/19/2002	05:17p	345,250
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f13fl.io	08/19/2002	05:17p	359,160
f1ffl.io	08/19/2002	05:17p	379,285
f2ffl.io	08/25/2002	03:55p	375,899
m11fl.io	08/19/2002	05:17p	346,938
m12fl.io	08/19/2002	05:17p	351,475
m13fl.io	08/19/2002	05:17p	336,022
m1ffl.io	08/19/2002	05:17p	301,591

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m23fl.io	08/19/2002	05:17p	260,658
m2ffl.io	08/19/2002	05:17p	265,102
n11fl.io	08/19/2002	05:17p	349,826
n12fl.io	08/19/2002	05:17p	350,590
n13fl.io	08/19/2002	05:17p	347,895
n14fl.io	08/19/2002	05:17p	350,166
n15fl.io	08/19/2002	05:17p	348,589
n1ffl.io	08/19/2002	05:17p	370,793
n21fl.io	08/19/2002	05:17p	345,877
n22fl.io	08/19/2002	05:17p	345,978
n23fl.io	08/19/2002	05:17p	344,164
n24fl.io	08/19/2002	05:17p	345,009
n2ffl.io	08/19/2002	05:17p	366,068
n31fl.io	08/19/2002	05:17p	345,454
n3ffl.io	08/19/2002	05:17p	345,423
n41fl.io	08/19/2002	05:17p	345,331
n4ffl.io	08/19/2002	05:17p	346,488
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fl2.io	08/19/2002	05:17p	171,057
fl3.io	08/19/2002	05:17p	190,398
nt051.io	08/19/2002	05:17p	172,864
nt052.io	08/19/2002	05:17p	172,784
nt055.io	08/19/2002	05:17p	172,784
nt52w.io	08/19/2002	05:17p	172,953
nt58w.io	09/20/2002	03:15p	173,271
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Tab6_5.xls	10/08/2002	04:16p	90,624
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f2ff.xls	06/07/2002	04:46p	104,960
f3ff.xls	07/31/2002	01:00p	129,024
f4ff.xls	07/31/2002	01:00p	102,400
m11ff.xls	08/04/2002	05:32p	99,840
m12ff.xls	08/07/2002	01:16p	99,840
m13ff.xls	08/07/2002	01:32p	99,840
m14ff.xls	08/07/2002	02:34p	99,840
m1ff.xls	08/07/2002	01:23p	102,912
m21ff.xls	08/04/2002	06:24p	99,840
m22ff.xls	08/04/2002	09:59p	99,840
m23ff.xls	08/08/2002	08:19a	99,328
m2ff.xls	08/07/2002	05:14p	99,328
n11ff.xls	08/07/2002	05:00p	104,448
n12ff.xls	08/08/2002	08:58a	104,448
n13ff.xls	08/08/2002	09:20a	104,448
n14ff.xls	08/08/2002	11:13a	104,448
n1ff.xls	08/07/2002	04:28p	104,448
n21ff.xls	08/07/2002	04:53p	99,328
n22ff.xls	08/07/2002	04:58p	99,328
n23ff.xls	08/08/2002	10:11a	99,328
n24ff.xls	08/08/2002	10:57a	99,328

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n32ff.xls	08/04/2002	02:56p	113,152
n33ff.xls	08/07/2002	03:00p	104,448
n3ff.xls	09/05/2002	05:15p	104,448
n41ff.xls	08/04/2002	10:31p	69,120
n42ff.xls	08/04/2002	03:29p	69,120
n4ff.xls	08/07/2002	02:24p	99,328
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f12fl.xls	08/05/2002	11:03a	110,080
f13fl.xls	08/06/2002	02:41p	110,080
f1ffl.xls	08/06/2002	02:18p	110,080
f2ffl.xls	06/07/2002	01:14a	105,472
m11fl.xls	08/22/2002	05:52p	103,424
m12fl.xls	08/05/2002	12:39p	103,424
m13fl.xls	08/05/2002	03:06p	94,720
m1ffl.xls	08/05/2002	02:24p	103,424
m21fl.xls	08/05/2002	02:35a	76,288
m22fl.xls	08/05/2002	10:12a	76,288
m23fl.xls	08/05/2002	03:52p	75,776
m2ffl.xls	06/10/2002	01:28a	76,288
n11fl.xls	08/05/2002	09:19a	104,448
n12fl.xls	08/05/2002	10:49a	104,448
n13fl.xls	08/06/2002	02:08p	104,448
n14fl.xls	08/06/2002	04:37p	104,448
n15fl.xls	08/07/2002	11:50a	104,960
n1ffl.xls	08/06/2002	01:41p	104,448
n21fl.xls	08/05/2002	09:33a	99,328
n22fl.xls	08/05/2002	11:15a	99,328
n23fl.xls	08/06/2002	01:11p	99,328
n24fl.xls	08/06/2002	01:29p	99,328
n2ffl.xls	08/06/2002	01:17p	99,328
n31fl.xls	08/06/2002	09:42a	99,840
n3ffl.xls	08/05/2002	04:56p	99,840
n41fl.xls	08/05/2002	08:41a	99,328
n4ffl.xls	08/05/2002	08:16a	99,328
Directory of CD-ROM :\near_field\outputs\Tab6_1			
f1nf.io	08/19/2002	05:17p	181,826
l1nf.io	08/19/2002	05:17p	182,542
m1nf.io	08/19/2002	05:17p	180,310
n1nf.io	08/19/2002	05:17p	181,015
n2nf.io	10/02/2002	02:35p	181,340
n3nf.io	10/07/2002	05:02p	181,403
r1nf.io	08/19/2002	05:17p	181,658
s1nf.io	08/19/2002	05:17p	181,340
t1nf.io	08/19/2002	05:17p	181,340
v1nf.io	08/19/2002	05:17p	181,340
Directory of CD-ROM :\near_field\outputs\Tab6_2			
fcnf.io	08/19/2002	05:17p	444,601
mcnf.io	10/01/2002	08:46a	331,639
ncnf.io	08/19/2002	05:17p	380,771
Directory of CD-ROM :\near_field\spreadsheets			
Tab6_1&2.xls	10/08/2002	04:16p	526,336