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## Atmospheric Dispersion Analysis Method Using MACCS2

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The Nuclear Regulatory Commission (NRC) Regulatory Guide 1.145 requires an evaluation of the offsite atmospheric dispersion coefficient,  $\chi/Q$ , as a part of the acceptance criteria in the accident analysis. In it, it requires in sequence computations of (1) the overall site 95<sup>th</sup> percentile  $\chi/Q$ , (2) the maximum of the sixteen sector 99.5<sup>th</sup> percentile  $\chi/Q$ , and (3) comparison and selection of the worst of the two values for reporting in the safety analysis report (SAR). In all cases, the site-specific meteorology and sector-specific site boundary distances are employed in the evaluation. There are sixteen 22.5°-sectors, the nearest site boundary of which is determined within the 45°-arc centered on each of the sixteen compass directions.

Similarly, Appendix A to DOE-STD-3009-94 requires a dose consequence analysis in the accident analysis for the documented safety analysis (DSA) for Department of Energy (DOE) non-reactor nuclear facilities. Atmospheric dispersion analysis is entirely adopted from the analytical elements laid out in NRC Regulatory Guide 1.145. However, only the overall site 95<sup>th</sup> percentile  $\chi/Q$  is required for the dose consequence analysis.

The commonly accepted computational code for the 95<sup>th</sup> percentile dose consequence analysis in the DOE complex is MACCS2. In the past, it was a common practice to analyze the potential dose consequences using MACCS2 at the minimum site boundary distance, even though the dominant wind direction and the nearest site boundary do not coincide, and to report the 95<sup>th</sup> percentile results as the overall site 95<sup>th</sup> percentile result in compliance with Appendix A to DOE-STD-3009-94, i.e., Regulatory Position C.2 in NRC Regulatory Guide 1.145. This results in excessive conservatism.

This paper presents an analytical approach that satisfies Regulatory Position C.2 in Regulatory Guide 1.145 and, therefore, Appendix A to DOE-STD-3009-94, and the requisite mathematical proof to establish the validity of the approach.

Key words: Atmospheric Dispersion Analysis, Accident Analysis, Safety Analysis, MACCS

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## 1.0 Introduction

There are several waste management facilities that dispose of nuclear waste generated from a variety of activities related to stockpile stewardship at Lawrence Livermore National Laboratory (LLNL). These are nuclear facilities that are subject to the regulatory requirements in 10 CFR 830. Provisions in 10 CFR 830 require each nuclear facility in the Department of Energy (DOE) complex to demonstrate that the design and operations of the facility do not pose significant impact on the environment and health and safety of the public and the workers. This task is done in a documented safety analysis (DSA), which is analogous to a safety analysis report (SAR) required by the NRC in 10 CFR 50.34, "Contents of application; technical information," for commercial nuclear power plants.

One of the most significant tasks of demonstrating safety of a commercial nuclear power plant is done through the accident analysis in Chapter 15, "Accident Analysis," of a SAR. Results for a commercial nuclear power plant must show that, among many parameters such as departure from nucleate boiling ratio (DNBR) and the peak cladding temperature (PCT), the offsite dose consequences are less than the siting criterion of 25 rem in 10 CFR 100.

Similarly for a DOE nuclear facility, Chapter 3, "Hazard and Accident Analyses," in DOE-STD-3009-94 (Reference 1) requires that the offsite dose consequences from potential credible accidents are not significant. One of the requirements in the accident analysis is the calculation of the atmospheric dispersion coefficient,  $\chi/Q$ , the computational method of which is elaborated in the NRC Regulatory Guide 1.145, "Atmospheric Dispersion Models for Potential Accident Consequence Assessments at Nuclear Power Plants," (Reference 2). For waste management facilities at LLNL, the offsite dose consequences based on the atmospheric dispersion analysis is a measure for approval of the safety analysis.

The primary mission of a number of waste management facilities at LLNL is the safe keeping and processing of waste contaminated with transuranic materials, called "TRU waste", typically in 55-gal drums. While the operations associated with the mission of the waste management facilities at LLNL do not pose a significant health and safety impact on the public, there are several difficulties with satisfying the requirements. Some of the difficulties in satisfying the requirements are (1) extremely close site boundary, (2) lack of acceptance criteria, and (3) variations in interpretation of the guidance on the dose consequence analysis in the DOE complex. The distance to the nearest site boundary for one of the TRU waste storage facilities at LLNL is only 140 m.

The purpose of the discussion is to describe the technical analysis by which LLNL has satisfied the regulatory requirements despite these difficulties. Because so many of DOE regulatory requirements for the safety analysis are borrowed from the NRC, applicable guidance from the NRC is discussed to clarify the DOE guidance. In particular, Regulatory Guide 1.145 is discussed to the extent necessary.

A typical dose consequence analysis is performed using either MACCS2 (Reference 3) or HOTSPOT (Reference 4) at LLNL. Both computational codes employ the Gaussian dispersion model. Significant differences between the two codes are the correlations for the dispersion coefficients and the statistical analysis capability. HOTSPOT employs the Briggs correlation for the dispersion coefficients and does not have the statistical analysis package to compute 95<sup>th</sup> percentile results. On the other hand, MACCS2 is based on the Tadmor-Gur correlation for the

dispersion coefficients and is capable of computing the 95<sup>th</sup> percentile results. For the purpose of this discussion, use of MACCS2 is discussed because of its statistical package, which is used to determine the 95<sup>th</sup> percentile dose consequence results based on the site-specific meteorological data.

MACCS2 input parameters are not discussed in detail for the sake of brevity and because they are not within the scope of this discussion. Only analytical results from MACCS2 are discussed to illustrate the effect.

## 2.0 Regulatory Requirements

For a commercial nuclear power plant, RG 1.145 requires in sequence computation of (a) the overall site 95<sup>th</sup> percentile  $\chi/Q$ , (b) the worst sector 99.5<sup>th</sup> percentile  $\chi/Q$ , and (c) selection of the higher of the two values for reporting in the safety analysis report (SAR). In all cases, the site-specific meteorology and sector-specific site boundary distances are employed in the evaluation. There are sixteen 22.5°-sectors, the nearest site boundary of which is determined within the 45°-arc centered on each of the sixteen compass directions as required by Regulatory Position C.1.2 in RG 1.145.

In short, Regulatory Position C.2 requires construction of a single cumulative distribution function for all  $\chi/Q$  values to determine the overall site 95<sup>th</sup> percentile  $\chi/Q$  based on the sector-specific site boundaries as defined in Position C.1.2 in RG 1.145. Regulatory Position C.3 requires construction of sixteen cumulative distribution functions of  $\chi/Q$  values to determine the worst sector 99.5<sup>th</sup> percentile  $\chi/Q$  among sixteen sectors based on the same sector-specific site boundaries as defined in Position C.1.2 in RG 1.145. Based on comparison, the higher of the worst sector 99.5<sup>th</sup> percentile  $\chi/Q$  and the overall site 95<sup>th</sup> percentile  $\chi/Q$  is selected as the value to be reported in a SAR in accordance with Regulatory Position C.4.

The DOE guidance is contained in Appendix A to DOE-STD-3009-94, "Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Analysis Reports" (Reference 1). It simply requires the overall site 95<sup>th</sup> percentile  $\chi/Q$  and, hence, represents only a portion of the requirements in RG 1.1.45. An excerpt from Appendix A is provided below:

"The EG [Evaluation Guideline] is 25 rem total effective dose equivalent (TEDE). The dose estimates to be compared to it are those received by a hypothetical maximally exposed offsite individual (MOI) at the site boundary for an exposure duration of 2 hours. The nominal exposure duration of 2 hours may be extended to 8 hours for those release scenarios that are especially slow to develop...

The value of 25 rem TEDE is not to be used as a 'hard' pass/fail level. Unmitigated releases should be compared against the EG to determine whether *they challenge the EG*, rather than exceed it. This is because consequence calculations are highly assumption driven and uncertain.

...

The 95<sup>th</sup> percentile of the distribution of doses to the MOI, *accounting for variations in distance to the site boundary as a function of direction*, is the comparison point for assessment against the EG. The method used should be consistent with the statistical treatment of calculated  $\chi/Q$  values described in

regulatory position 3 of NRC Regulatory Guide 1.145 for the evaluation of consequences along the exclusion area boundary. The determination of distance to the site boundary should be made in accordance with the procedure outlined in position 1.2 of Regulatory Guide 1.145.” *[Italics added for emphasis]*

A typical atmospheric dispersion analysis using MACCS2 in a DOE nuclear facility would result in computing the overall site 95<sup>th</sup> percentile  $\chi/Q$  based on the distance to the nearest site boundary and the entire meteorological data in the same direction regardless of the wind direction. That is, the worst-case meteorology is assumed at the nearest site boundary even if the prevailing wind direction and the direction to the nearest site boundary do not coincide. Results tend to be conservative relative to the requirement in Appendix A to DOE-STD-3009-94 for nuclear facilities in the DOE complex. For most DOE nuclear facilities, such conservatism was not an issue because of the enormity and public support for the sites unlike LLNL.

### 3.0 Analytical Approach

For waste management facilities at LLNL, such a conservative approach presents a significant compliance burden because of the proximity to the public and the political sensitivity. Because of the public opposition to weapons related activities at LLNL, there is a significant reluctance thus far to exceed the worst-case dose consequence in the 1992 Environmental Impact Statement (EIS). The radiation dose consequence of 4.4 rem TEDE, which was the most severe dose consequence predicted from postulated accidents analyzed in the EIS, has become the *de facto* radiation dose consequence acceptance criterion for waste management facilities at LLNL. Furthermore, as alluded to previously as a difficulty, the predicted dose consequence of 1 rem for the maximally exposed offsite individual is construed to “challenge” the evaluation guideline of 25 rem, without formal or official declaration of definition of “challenging”, in certain circles within DOE.

In 2002, the typical conservative approach of piling the worst-case meteorological data on the shortest distance to the site boundary regardless of the prevailing wind direction in the atmospheric dispersion analysis was re-examined for waste management facilities at LLNL based on Appendix A to DOE-STD-3009-94 and the requirements in RG 1.145. The statement of interest in Appendix A to DOE-STD-3009-94 reads as follows: “The 95<sup>th</sup> percentile of the distribution of doses to the MOI, accounting for variations in distance to the site boundary as a function of direction, is the comparison point for assessment against the EG.”

The change in the analytical approach for the waste management facilities is comprised of calculating the nearest site boundary for each sector in accordance with Regulatory Position C.1.2 and computing the  $\chi/Q$  as a function of wind direction and the calculated sector-specific distances to the nearest site boundary. The significant difference is the reporting of the maximum 95<sup>th</sup> percentile sector  $\chi/Q$  as the overall site 95<sup>th</sup> percentile  $\chi/Q$ . The mathematical proof of this last point is discussed in the next section.

#### 4.0 Mathematical Proof

By employing a proof by contradiction, it can be shown that the maximum 95<sup>th</sup> percentile sector  $\chi/Q$  is greater than or equal to the 95<sup>th</sup> percentile overall site  $\chi/Q$ , which is required in Appendix A to DOE-STD-3009-94. The probability density function for the overall site  $\chi/Q$  can be expressed in terms of the corresponding sector densities, as follows:

$$f(x) = \sum_i p_i f_i(x) \quad (1)$$

where  $p_i$  is the probability, or the relative frequency, for sector  $i$  and  $f_i(x)$  is the density function of  $x$  for each sector  $i$ .  $x$  is the calculated atmospheric dispersion coefficient,  $\chi/Q$ , for each hourly data in the site-specific meteorological data file.

Since the sectors form a partition, the sum of the probability, or the relative frequency, over all sectors must be unity; therefore,

$$\sum_i p_i = 1 \quad (2)$$

Equation (1) has a counterpart in terms of cumulative distribution functions:

$$F(x) = \sum_i p_i F_i(x) \quad (3)$$

where, for example,  $F(x)$  is the cumulative distribution function for all values of  $x$ . The cumulative distribution function for  $x$  in sector  $i$  is:

$$F_i(x) = \int_0^x f_i(u) du \quad (4)$$

For any  $\alpha$ , the  $\alpha$ -quantile of  $F$ ,  $x_\alpha$ , is as follows:

$$\alpha = F(x_\alpha) \quad (5)$$

Similarly for each sector, the  $\alpha$ -quantile of  $F_i$ ,  $x_\alpha^{(i)}$ , is defined as follows:

$$\alpha = F_i(x_\alpha^{(i)}) \quad (6)$$

In this analysis, the value of  $\alpha$  of interest is 0.95, or the 95<sup>th</sup> percentile result.

It is posited that:

$$x_\alpha \leq \text{MAX}_i \{x_\alpha^{(i)}\} \quad (7)$$

In particular, the maximum sector 95<sup>th</sup> percentile  $\chi/Q$ , i.e.,  $\alpha = 0.95$ , is greater than or equal to the 95<sup>th</sup> percentile overall site  $\chi/Q$ .

In order to prove the inequality in Equation (7), assume for the moment that  $x_\alpha > x_\alpha^{(i)}$  for all  $i$ . Then, because  $F_i$  is a strictly increasing function for  $x$ , it follows from Equation (6) that:

$$F_i(x_\alpha) > F_i(x_\alpha^{(i)}) = \alpha \quad \forall i \quad (8)$$

Therefore, by substitution Equation (8) becomes:

$$\sum_i p_i F_i(x_\alpha) > \sum_i p_i \alpha \quad (9)$$

Simplifying the left side of the inequality in Equation (9) by combining Equations (3) and (5) yields:

$$\sum_i p_i F_i(x_\alpha) = F(x_\alpha) = \alpha \quad (10)$$

Simplifying the right side of the inequality in Equation (9) with Equation (2) yields:

$$\sum_i p_i \alpha = \alpha \sum_i p_i = \alpha \quad (11)$$

Putting them all together from Equations (10) and (11):

$$\sum_i p_i F_i(x_\alpha) > \sum_i p_i \alpha \Rightarrow \alpha > \alpha$$

It is shown that a value is less than itself. This cannot be true for any value. Therefore, it is proven by contradiction that the maximum sector 95<sup>th</sup> percentile  $\chi/Q$  among the sixteen sector results is greater than or equal to the overall site 95<sup>th</sup> percentile  $\chi/Q$ . This establishes the mathematical basis for selecting the maximum sector 95<sup>th</sup> percentile  $\chi/Q$  as the overall site 95<sup>th</sup> percentile  $\chi/Q$  in the analysis to satisfy the requirement in Appendix A to DOE-STD-3009-94 cited previously in Section 2.0, "Regulatory Requirements."

## 5.0 Results

The distance to the nearest site boundary for one of the waste management facilities, the Decontamination and Waste Treatment Facility (DWTF), is 140 m to north. The prevailing wind direction in the annual LLNL-specific meteorological data is to northeast. This is the direction that yields the maximum sector 95<sup>th</sup> percentile  $\chi/Q$ , which has been mathematically proven to be equal to or to exceed the overall site 95<sup>th</sup> percentile  $\chi/Q$ . One of the waste management facilities, with dimensions of 100×40×16-ft high, is located with 150 m from the nearest site boundary toward south and 240 m from the nearest site boundary toward the prevailing wind direction to northeast. Result from a postulated accident with a plume sensible heat of 5 MW are 0.26 rem per Pu<sup>239</sup> equivalent curie (PE Ci) released to the atmosphere in the south sector and 10.9 rem per PE Ci in the northeast sector at respective sector-specific nearest site boundaries.

For the same postulated large fire leading to an accidental release of radioactivity with a plume sensible heat of 5 MW from the DWTF, for example, the 95<sup>th</sup> percentile  $\chi/Q$  computed at the nearest site boundary of 140 m, independent of the wind direction, is 22.1 rem per PE Ci. This would be the result from the typical conservative approach of piling the worst-case meteorological data on the shortest distance to the site boundary.

Because the site boundary runs parallel to the building from east to west, the nearest site boundary distance in accordance with Regulatory Position C.1.2 is then 150 m to northeast. For the same case, the predicted dose consequence for the overall site 95<sup>th</sup> percentile  $\chi/Q$  at the nearest sector-specific site boundary of 150 m to northeast is 19.8 rem per Pu<sup>239</sup> equivalent curie

(PE Ci) released to the atmosphere reported in a documented safety analysis (DSA) for one of the waste management facilities at LLNL. This is a reduction of approximately 10%. While it may appear trivial in comparison to the effort, because of the *de facto* acceptance criterion of 4.4 rem in the EIS, the smallest of reduction in the dose consequence results contributes significantly to the compliance effort at LLNL.

## 6.0 Conclusion

The primary mission of waste management facilities at LLNL is the safe keeping and processing of TRU waste typically in 55-gal drums. Results of the safety analysis show that the operations associated with the mission of the waste management facilities at LLNL do not pose a significant health and safety impact on the public even though the extremely close site boundary and lack of clear guidance on the dose consequence acceptance criterion in DOE, as discussed in Section 1.0, "Introduction," present substantial technical challenges to satisfying the regulatory requirements. As stated previously, the distance to the nearest site boundary for one of the TRU waste storage facilities at LLNL is only 140 m.

Based on the regulatory analysis of RG 1.145, the analytical approach at LLNL was to report the maximum sector 95<sup>th</sup> percentile  $\chi/Q$  as the overall site 95<sup>th</sup> percentile  $\chi/Q$  in a documented safety analysis (DSA). It was proven mathematically that the maximum sector 95<sup>th</sup> percentile  $\chi/Q$ , is greater than or equal to the overall site 95<sup>th</sup> percentile  $\chi/Q$ ; therefore, the analytical approach in a documented safety analysis (DSA) for the waste management facilities at LLNL satisfies the requirement in Appendix A to DOE-STD-3009-94, which borrows heavily from regulatory positions outlined in the NRC Regulatory Guide 1.145 for commercial nuclear power plants. The mathematical basis was laid out in Section 4.0, "Mathematical Proof." In addition, the analytical approach assures compliance with the current *de facto* dose consequence criterion for the public established in the 1992 EIS.

In the continuing effort to quantify accurately the potential impact on the safety and health of the public and the workers, LLNL is adopting the latest information on the biological health effects of radiation in ICRP 72 (Reference 5), published by the U.S. Environmental Protection Agency as Federal Guidance Report No. 13 (Reference 6) dose conversion factors. Combined with the latest data in ICRP 72, results of the quantitative analysis in a DSA clearly demonstrate that the operations of the waste management facilities at LLNL do not pose a significant impact on the public health and safety.

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