

United States Department of Energy

National Spent Nuclear Fuel Program

Review of Flow Models in GOTH_SNF for Spent Fuel MCO Calculations



September 2003

U.S. Department of Energy
Assistant Secretary for Environmental Management
Office of Nuclear Material and Spent Fuel

This document was developed and is controlled in accordance with NSNFP procedures.
Unless noted otherwise, information must be evaluated for adequacy relative to its specific
use if relied on to support design or decisions important to safety or waste isolation.

**DOE/SNF/REP-087
Rev. 0**

Review of Flow Models in GOTH_SNF for Spent Fuel MCO Calculations

September 2003

Work Breakdown Structure No. C.1.07.02.01.02.03

**Idaho National Engineering and Environmental Laboratory
Idaho Falls, Idaho 83415**

**Prepared for the
U.S. Department of Energy
Assistant Secretary for Environmental Management
Under DOE Idaho Operations Office
Contract DE-AC07-99ID13727**

REVISION LOG

Revision	DAR No.	Issue Date
0	NSNF-481	September 2003

Review of Flow Models in GOTH_SNF for Spent Fuel MCO Calculations

September 2003

John R. Kirkpatrick

Faxed signature on file with
report original

Date:

(Signature)

Oak Ridge National Laboratory
Document Preparer

Neal S. Mackay

(Signature)

Date:

National Spent Nuclear Fuel Program
Program Support Organization Quality Engineer

Philip D. Wheatley

(Signature)

Date:

National Spent Nuclear Fuel Program
Program Support Organization Manager

SUMMARY

The present report is one of a series of three. The series provides an independent technical review of certain aspects of the GOTH_SNF code that is used for accident analysis of the multicannister overpack (MCO) that is proposed for permanent storage of spent nuclear fuel in the planned repository at Yucca Mountain, Nevada. The work documented in the present report and its two companions was done under the auspices of the National Spent Nuclear Fuel Program. The other reports in the series are DOE/SNF/REP-088 and DOE/SNF/REP-089.

This report analyzes the model for flow through the fuel elements that is documented in the SNF report titled *MCO Work Book GOTH_SNF Input Data*.¹ Reference 1 combined the multiple parallel paths through which the hot gases flow vertically inside the MCO into simpler paths. This report examines the assumptions used to combine the paths and concludes that there are other ways to combine the paths than the one used by GOTH_SNF. Two alternatives are analyzed, and the results are compared to those from the model used in GOTH_SNF. Both alternatives produced a higher pressure drop from the top to the bottom of the flow channel for a given flow velocity than did the approximation used in GOTH_SNF. Therefore, for a given pressure drop, the flow velocity given by the GOTH_SNF approximation will be lower than that from either of the two alternatives.

The practical consequences of the differences in flow rate are not obvious. One way to evaluate the consequences is to repeat an important MCO calculation on GOTH_SNF using an altered hydraulic diameter (the one that produces the highest pressure drop for a given flow velocity) and see if the conclusions about the safety of the MCO are changed.

FOREWORD

This report was prepared as the product of a technical review of chemical reactivity modeling and analysis activities performed by the National Spent Nuclear Fuel Program (NSNFP). The scope of the review is contained within the "Task Management Agreement for Chemical Reactivity Modeling Technical Review Activities," DOE/SNF/TMA-003. The administrative leadership for this review work was provided by staff from the NSNFP. The author of the present report, J. R. Kirkpatrick, is a staff member of the Computational Sciences and Engineering Division at the Oak Ridge National Laboratory (ORNL) in Oak Ridge, Tennessee.

The NSNFP chemical reactivity analysis provides information about the performance of the Multi-Canister Overpack (MCO) loaded with N-Reactor spent fuel in the repository environment relative to the potential for intense chemical reactions on the corroded portions of the fuel elements. The review task was an independent review of the approach and reasonableness of results from the NSNFP chemical reactivity analysis. The chemical reactivity analysis performed by the NSNFP is not a part of the primary licensing strategy for U. S. Department of Energy spent nuclear fuel in the repository. An additional technical review is not required to meet NSNFP Quality Program requirements. The review discussed in this report was performed as a good technical practice to provide an independent evaluation of the technical adequacy of the NSNFP chemical reactivity analysis. To ensure the technical independence of the review, ORNL personnel conducted the assessment and review to technical standards defined by ORNL without intervention from the NSNFP. NSNFP involvement in the definition of standards and requirements was limited to ensuring that work by ORNL personnel was performed under NSNFP procedures, using ORNL personnel as augmented staff. Preliminary review and discussion of results of the evaluation were conducted during the evaluation. NSNFP formal response to recommendations in this report will be documented in a future engineering design file, EDF-NSNF-031 "NSNFP Plan for Response Activities to Chemical Reactivity Technical Review Recommendations."

CONTENTS

REVISION LOG	2
SUMMARY	5
FOREWORD	7
1. INTRODUCTION	11
2. ANALYSIS	11
3. CONCLUSIONS AND RECOMMENDATIONS	17
4. REFERENCES	18

FIGURES

1. Schematic showing location of fuel rings.....	12
2. Flow area (hatched area) formed by fuel triangular pitch arrangement	12
3. Flow area (hatched area) of triangular pitch flow cell in between the first and second ring of fuel elements	13
4. Comparison of pressure difference vs average flow velocity for the three different approaches for calculating flow.....	17
5. Comparison of flow area velocities in different flow areas vs average velocity for three different flow area flow calculations	18

Review of Flow Models in GOTH_SNF for Spent Fuel MCO Calculations

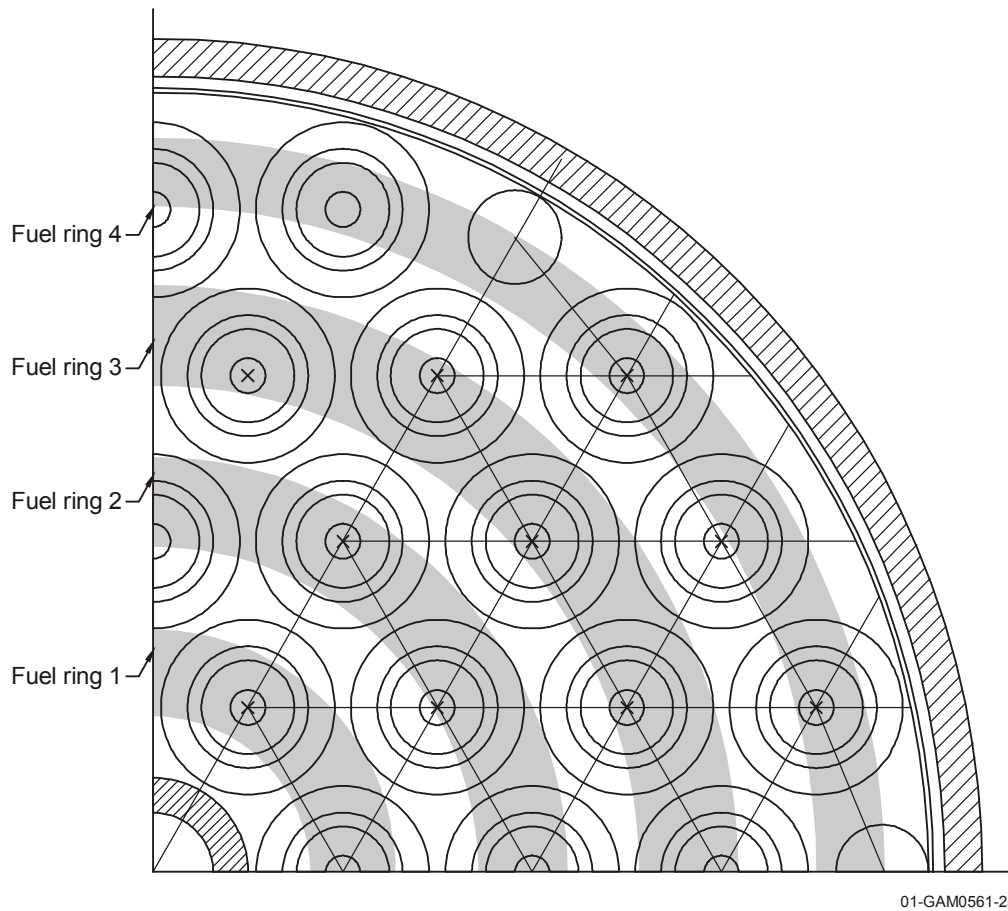
1. INTRODUCTION

This report studies the GOTH_SNF code and how it calculates the flow rates in the gas channels in the fuel baskets. In GOTH_SNF, the many different parallel physical flow areas are combined into a smaller set of computational gas channels. The input to GOTH_SNF uses a particular method for calculating the friction through the gas channels. The objective of the present analysis is to compare this method with some other methods for calculating flow rates in the gas channels to see how much difference might be found by the various methods.

2. ANALYSIS

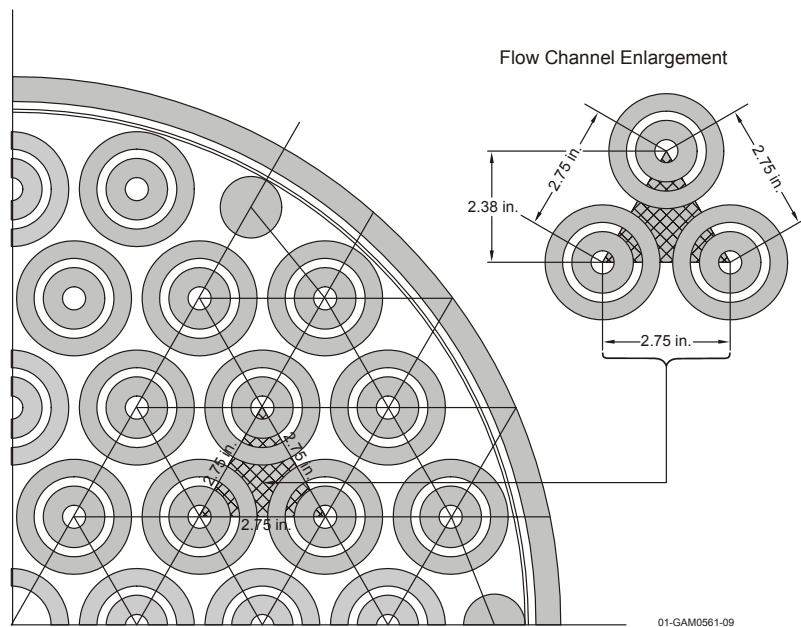
Figure 1 shows a schematic of the fuel elements in the basket. In GOTH_SNF, the solid metal is combined into a series of rings, which are shaded grey in the figure. The various flow areas are combined into annular gas channels represented by the portions that are not shaded in Figure 1. The unshaded area between fuel ring 1 and fuel ring 2 is called "Gas Channel 3." There are several different types of flow areas. Figure 2 shows a schematic of the three different types of flow areas that are present in Gas Channel 3 (the hatched area in this figure is actually in Gas Channel 4). These three types of flow areas also make up Gas Channels 2, 4, and 5. These flow areas are also important in Gas Channel 6. The largest of the three flow areas is the one between the fuel elements shaped like a trefoil. In Reference 1, it is called "triangular pitch" element. The other two flow areas are the annulus between the inner and outer fuel element and the central hole in the middle of the inner element.

Figure 2 is slightly misleading. It is supposed to show a set of flow areas that belong to Gas Channel 4. The figure seems to suggest that the 1/6 segments of the inner and annular flow areas of all three fuel elements bounding the triangular pitch flow area are combined with the triangular pitch flow area. This area creates a total flow area that is then multiplied by the number of triangular pitch areas in each ring to create the gas channel. This is not correct. Instead, the inner and annular flow areas for each fuel element are used in total. This can best be explained by examples starting from the inside and working out. Although Figure 1 and Figure 2 (for that matter, Figure 3) show the fuel elements in a quarter circle, a 1/6 circle segment has lines connecting the fuel elements. The arrangement of fuel elements in the fuel basket is composed of six identical segments, each 1/6 of the circle. In Figure 2, one can see that there are two fuel elements (actually two half fuel elements) in the 1/6 of a circle segment in the inner slant row almost touching the inner support pipe. These two half fuel elements are multiplied by 6 to produce six fuel elements in Gas Channel 2. In addition, there is a single triangular pitch flow area between the inner support pipe and these two half elements. Therefore, Gas Channel 2 also contains 6×1 triangular pitch elements. The next layer of fuel elements (the next slant row) in Figure 2 contains one complete fuel element and two half elements in the 1/6 of a circle segment. In addition, there are three triangular pitch areas in the 1/6 of a circle element between the first and second slant rows. Figure 3 shows a schematic that includes a triangular pitch flow area from Gas Channel 3. The combination of the fuel elements and triangular pitch areas multiplied by 6 is Gas Channel 3. Thus, Gas Channel 3 is composed of $6 \times 3 = 18$ triangular pitch elements plus $6 \times (1 + 1/2 + 1/2) = 12$ each of the fuel element inner and annular flow areas. The constitution of Gas Channels 4 and 5 can be calculated by the same method. Because the insides of the fuel elements are all allocated to Gas Channels 2–5, Gas Channel 6, which is between the outermost layer of fuel elements and the inside of the basket shroud, does not contain any contribution from flow inside the fuel elements.



01-GAM0561-25

Figure 1. Schematic showing location of fuel rings. (Figure 4-2, p. 4-4 of Reference 1.)



01-GAM0561-09

Figure 2. Flow area (hatched area) formed by fuel triangular pitch arrangement. (Figure 4-1, p. 4-2 of Reference 1.)

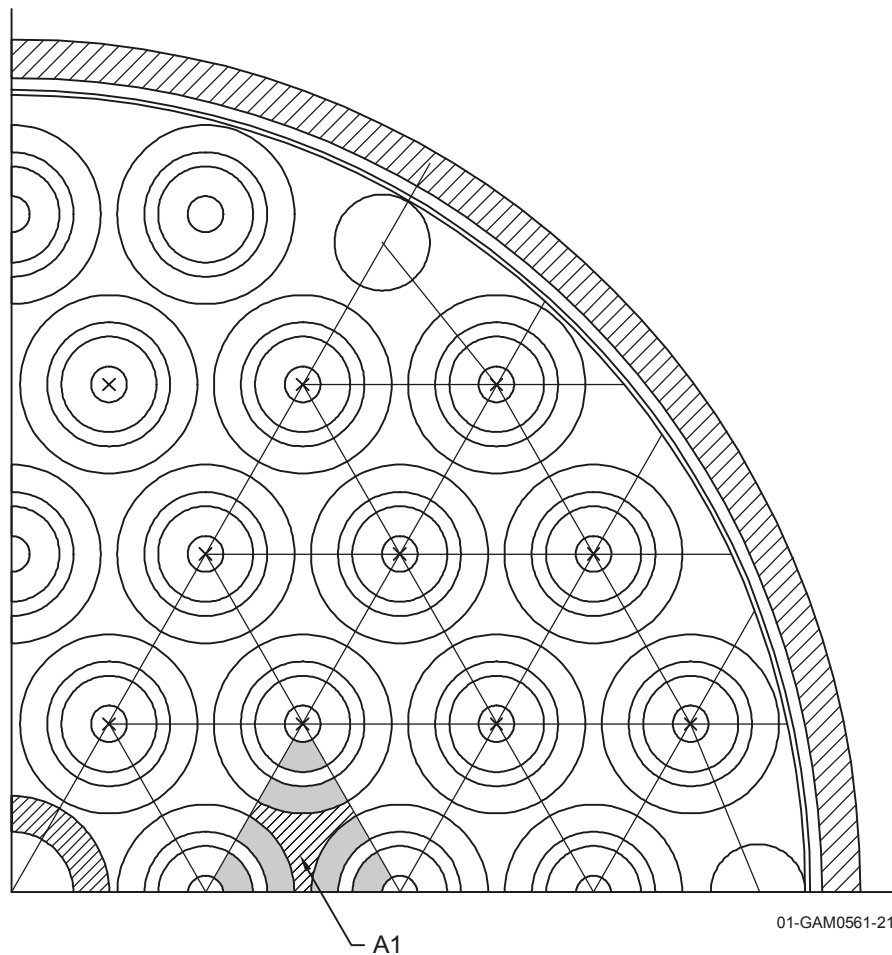


Figure 3. Flow area (hatched area) of triangular pitch flow cell in between the first and second ring of fuel elements. (Figure 4-4, p. 4-7 of Reference 1.)

The concept behind the combination of flow areas into gas channels as illustrated in GOTH_SNF is that all the flow areas of each gas channel have the same velocity. Of course, different gas channels have different velocities. For each gas channel, a total flow area is calculated. Then, approximations are made to calculate the velocity through each gas channel.

Consider Gas Channel 3. This channel is arbitrarily being chosen for analysis as an example. The flow areas are calculated in Reference 1 (pp. 4-1 through 4-7). From now on, all cited equation and page numbers are assumed to come from Reference 1 unless otherwise stated. The flow area of a triangular pitch flow area as given by Equation 4-2 on p. 4-1 is

$$\text{Triangle_area} = 3.2747 \text{ in.}^2 \quad \text{Eq (1)}$$

The sum of the flow areas of the inside of the fuel element and the annulus as given by Equation 4-4 on p. 4-1 is

$$\text{A_elem_fluid} = 1.1686 \text{ in.}^2 \quad \text{Eq (2)}$$

The outside perimeter of a fuel element as given by Equation 4-6 on p. 4-1 is

$$Pw_{elem} = 7.6184 \text{ in.}$$

The wetted perimeter for a triangular pitch flow area is calculated using the portion of the three fuel elements touching the triangular pitch area. From Equation 4-22 on p. 4-6, this is $3^{1/6}$ of the wetted perimeter of the outside of a fuel element or

$$Pw1 = 0.3174 \text{ ft} \quad \text{Eq (3)}$$

Note that the change in units is from inches to feet. At this point, Bratton proceeds to calculate the hydraulic diameter of the triangular pitch area (by the well-known definition, the hydraulic diameter is 4 times flow area divided by wetted perimeter—see for example, the Schaum's Outline Series²). From Equation 4-23 on p. 4-6, the result is

$$Dh_6 = 0.08448 \quad \text{Eq (4)}$$

Bratton then calculates the total flow area, which is 18 times the flow area of a triangular pitch element plus 12 times the flow area inside a fuel element. The result from eq. 4-24 on p. 4-7 is

$$A_6 = 0.2181 \text{ ft}^2 \quad \text{Eq (5)}$$

Bratton then defines the wetted perimeter of the entirety of Gas Channel 3 by dividing 4 times the entire flow area (that of the triangular pitch areas plus that of the areas within the fuel elements) in Equation 4-25 on p. 4-7 by the hydraulic diameter of the triangular flow area as follows:

$$PW_6 = 4 * A_6 / Dh_6 = 10.3252 \text{ ft} \quad \text{Eq (6)}$$

The reader may have noticed the following. The wetted perimeters were not calculated for the inside of the fuel element and the annulus. Instead, the wetted perimeter for the sum of the flow areas was calculated using the total flow area and the hydraulic diameter of the triangular pitch area. The rationale for this is unclear. The objective of the present report is to examine what happens if that calculation is not made. What happens to the flow if one calculates the actual wetted perimeter of the sum of the flow areas and calculates a hydraulic diameter based on the sum of the flow areas and the sum of the wetted perimeters? A second objective of this report is to examine the effect of one further relaxation in the level of approximation. That is, how does the flow behave if separate velocities are calculated for each of the individual flow areas in isolation and then how are the flow rates are summed to get a total flow area?

The terms necessary to approximate the flow are calculated using the actual sum of wetted perimeters divided into 4*the sum of flow areas. For identification purposes, let this approximation be called "Version 2" (the original GOTH_SNF calculation is Version 1). The sum of the wetted perimeters inside the fuel element is as follows:

$$Pw_{total_for_fuel_element} = \pi (1.701 + 1.279 + 0.480) = 10.870 \text{ in.} \quad \text{Eq (7)}$$

Therefore, the wetted perimeter for the total assemblage of flow areas in Gas Channel 3 is

$$Pw_{Gas_Channel_3_Version_2} = 12 * 10.870 \text{ in.} + 18 * 0.3174 \text{ ft} * (12 \text{ in./ft}) = 199.00 \text{ in.} = 16.583 \text{ ft} \quad \text{Eq (8)}$$

The resulting hydraulic diameter is

$$Dh_Gas_Channel_3_Version_2 = 4 * 0.2181 / 16.583 = 0.0526 \text{ ft} \quad \text{Eq (9)}$$

Next, the flow areas and hydraulic diameters for the annulus between the inner and outer fuel elements and also in the center of the inner fuel element are calculated. For the annulus, the results are as follows:

$$A_for_fuel_element_annulus = \pi/4 (1.701^2 - 1.279^2) = 0.9877 \text{ in.}^2 \quad \text{Eq (10)}$$

$$Pw_for_fuel_element_annulus = \pi (1.701 + 1.279) = 9.362 \text{ in.} \quad \text{Eq (11)}$$

$$Dh_for_fuel_element_annulus = 4 * 0.9877 \text{ in.}^2 / 9.362 \text{ in.} = 0.4220 \text{ in.} = 0.0352 \text{ ft} \quad \text{Eq (12)}$$

For the inside of the inner fuel element, the results are as follows:

$$A_for_inside_fuel_element = \pi/4 (0.480^2) = 0.1810 \text{ in.}^2 \quad \text{Eq (13)}$$

$$Pw_for_inside_fuel_element = \pi (0.480) = 1.508 \text{ in.} \quad \text{Eq (14)}$$

$$Dh_for_inside_fuel_element = 4 * 0.1810 \text{ in.}^2 / 1.508 \text{ in.} = 0.4800 \text{ in.} = 0.0400 \text{ ft} \quad \text{Eq (15)}$$

In almost any fluid flow text (see, for example, Reference 2), one will find the idea of using the hydraulic diameter to calculate the Reynolds number and friction factor for a noncircular duct. The geometry of the flow of the gas channels and the underlying flow areas suggests that each is connected to a plenum at the top and another at the bottom of the flow path. Thus, the pressure drop across each flow area of a gas channel is the same, and the flow in a gas channel is nominally that of a number of parallel flow areas of different shapes. (In the case of Gas Channel 3, there are three different kinds of flow area.) The most accurate method of calculating flow through the combination of flow areas would be to calculate the flow through each of the flow areas for a particular pressure drop and add the contributions from each of the sets of flow areas to get a total flow rate. As an alternative method, a total flow area for the sum of flow areas and a total wetted perimeter for the sum would be calculated and then use four times the ratio of flow area to perimeter to calculate a hydraulic diameter for Gas Channel 3. This alternative, one in which the flow areas are lumped together, contains the tacit assumption that the velocities in all the flow areas making up Gas Channel 3 are the same. This alternative is the model called "Version 2" in an earlier paragraph. As has already been noted, the same assumption of equal flow velocity through each of the different flow areas of a gas channel is used in GOTH_SNF. However, GOTH_SNF uses a different method for calculating the friction due to the flow through the combined set of flow areas.

The rationale for the way GOTH_SNF calculates the hydraulic diameter is still unclear. Apparently, the assumption is that the friction through the triangular pitch flow areas dominates the flow. Although the triangular pitch flow areas contain a slight majority of the flow area in Gas Channel 3 (55%), using the GOTH_SNF calculation of the hydraulic diameter of the combined set of flow areas understates the wetted perimeter by 38% compared to Version 2. Therefore, for a particular flow velocity, the Reynolds number using the GOTH_SNF calculation will be ~38% higher than that for Version 2, which translates into a ~38% lower friction factor (assuming flow is laminar). Therefore, for the GOTH_SNF calculation, the flow rate for a particular pressure difference will be higher than for Version 2.

The objective in this report is to compare the results from the three different ways of calculating the flow that have been described. In particular, the report will determine how much difference one gets in the flow velocities as a function of pressure drop. An Excel spreadsheet was set up to calculate pressure drops and flow rates. According to discussions with R. L. Bratton³ of the National Spent Nuclear Fuel Program, the flow velocities should not exceed 2 ft/s. Bratton recommended a temperature of 900°F. For the calculations, the molecular weight of air is

$$MW_{\text{air}} = 28.96443 \text{ g/mole} \quad \text{Eq (16)}$$

and a viscosity using Chapman-Enskog⁴ theory as follows:

$$\mu_{\text{air}} = 2.6693 \times 10^{-5} \sqrt{MW T} / \sigma^2 / \Omega_{\mu} \text{ (g/cm/s)} \quad \text{Eq (17)}$$

where

MW = the molecular weight in g/mole

T = the absolute temperature in K

σ and Ω_{μ} = Lennard-Jones constants for air.

The collision integral Ω_{μ} is a function of temperature. The fit for Ω_{μ} versus temperature is taken from the GOTHIC documentation,⁵ pp. 10-7 to 10-8, as is the value for σ . The Chapman-Enskog representation for viscosity and the value of σ shown in the GOTHIC documentation (see Reference 5) are taken directly from Reference 4. The fit for Ω_{μ} as a function of temperature is a fit of numbers from a table given in Reference 4. The air density was calculated using the ideal gas equation of state by assuming a pressure of 1 atm. The friction factor for the smooth pipe in the GOTH_SNF GOTHIC documentation was adopted for this analysis (see Reference 5, p. 8-18). Because the maximum velocity for any of the GOTH_SNF cases is less than that needed to initiate a transition from laminar to turbulent flow, the details of the friction factor in the transition region and the turbulent region are not relevant to the present discussion.

Figure 4 shows a comparison of the pressure differences generated by the three different approaches to calculating the flow as functions of the average velocity. In the figure, Version 2 is the line marked "corr perim" (which stands for "corrected wetted perimeter"), and the three different flow areas approach is the line marked "3 piece." In the laminar range, the pressure drop is proportional to the average velocity for each of the three approximations. If one does the algebra, it can be seen that the pressure difference for a given average flow velocity is inversely proportional to the square of the hydraulic diameter. The approach used by GOTH_SNF has the highest hydraulic diameter (0.084 ft) and, therefore, has the lowest pressure drop for a given average velocity. The Version 2 approach has the lowest hydraulic diameter (0.053 ft) and, therefore, has the highest pressure drop for a given velocity. The square of the ratio of the GOTH_SNF hydraulic diameter to that of Version 2 is ~2.6. This is the same as the ratio between the velocities at any given pressure drop as shown in Figure 4. The three separate flow areas approach creates a curve of pressure drop versus average velocity in the laminar range that corresponds to an apparent average hydraulic diameter of 0.0673 ft. Therefore, this approach gives results in the laminar range that are between the other two.

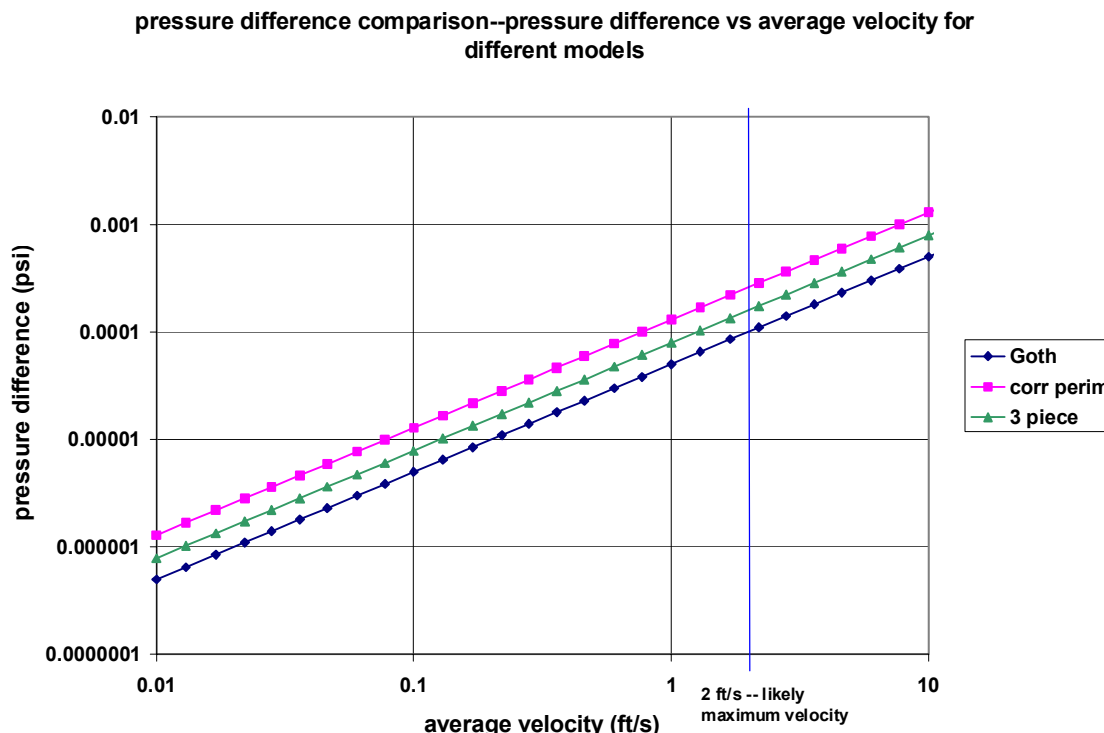


Figure 4. Comparison of pressure difference vs average flow velocity for the three different approaches for calculating flow.

Figure 5 shows the velocities in the three different flow areas for the three separate flow areas approach compared to the average velocity. The effect of the three different hydraulic diameters is obvious. The ratio of the velocity in the triangular pitch area to that in the annulus between the inner and outer elements is the largest. The combination of different hydraulic diameters and different flow area velocities leads to different locations for the beginning of the laminar to turbulent transition. However, none of the flow areas reaches turbulent transition before the maximum velocity of 2 ft/s. If one uses the apparent average hydraulic diameter inferred from analysis of the three separate flow areas model in the previous paragraph and calculates a curve of pressure drop versus velocity in the turbulent range, the pressure drop for a given average velocity is only ~12% lower than the value given by calculating the flow in the three different flow areas and adding them up.

3. CONCLUSIONS AND RECOMMENDATIONS

After analyzing the effect of the three different approaches on the curves of pressure difference versus the average velocity, the most important question is what difference does it make? To answer that question it is recommended that a test in GOTH_SNF be run doing the following:

Select a MCO case that represents an important decision point. Such a case would be one for which, if the results were to change in the “wrong” direction, the conclusions about the safety of the MCO would be different. For this case, change the hydraulic diameter from the GOTH_SNF value of 0.084 ft to the value that represents Version 2 (0.053 ft—the lowest of the three values) and run the MCO case again. Gas Channels 2–5 (and perhaps 6 as well) are all subject to corrections based on having this more complex geometry. Each of the gas channels will have a different correction factor for its hydraulic diameter. As a first cut, one could try multiplying the hydraulic diameters of all Channels 2–6 by the same factor (0.053/0.084). See if the results of the MCO case using the hydraulic diameters with this

modification change the conclusions. If the conclusions do change, one might consider redoing the calculation using the apparent hydraulic diameter from the three different flow areas model (0.0673 ft). In this author's opinion, that model is the most accurate. Also, one might consider calculating the modified hydraulic diameters for each of Channels 2–6 rather than using the same multiplier for all of them. The spreadsheet that the author used to calculate the results for Gas Channel 3 should be able to calculate the other channels with small modifications.

3.1 NSNFP Evaluation and Response to Review Recommendations

The author of this report consulted with the NSNFP during his evaluation of the computer modeling. Several items were resolved and clarified during these consultations. Preliminary review and discussion of results of the evaluation were also conducted during these consultations. This report contains recommendations for future action by the NSNFP. The NSNFP formal response to the recommendation in this report will be documented in a future engineering design file, EDF-NSNF-031, "NSNFP Plan for Response Activities to Chemical Reactivity Technical Review Recommendations."

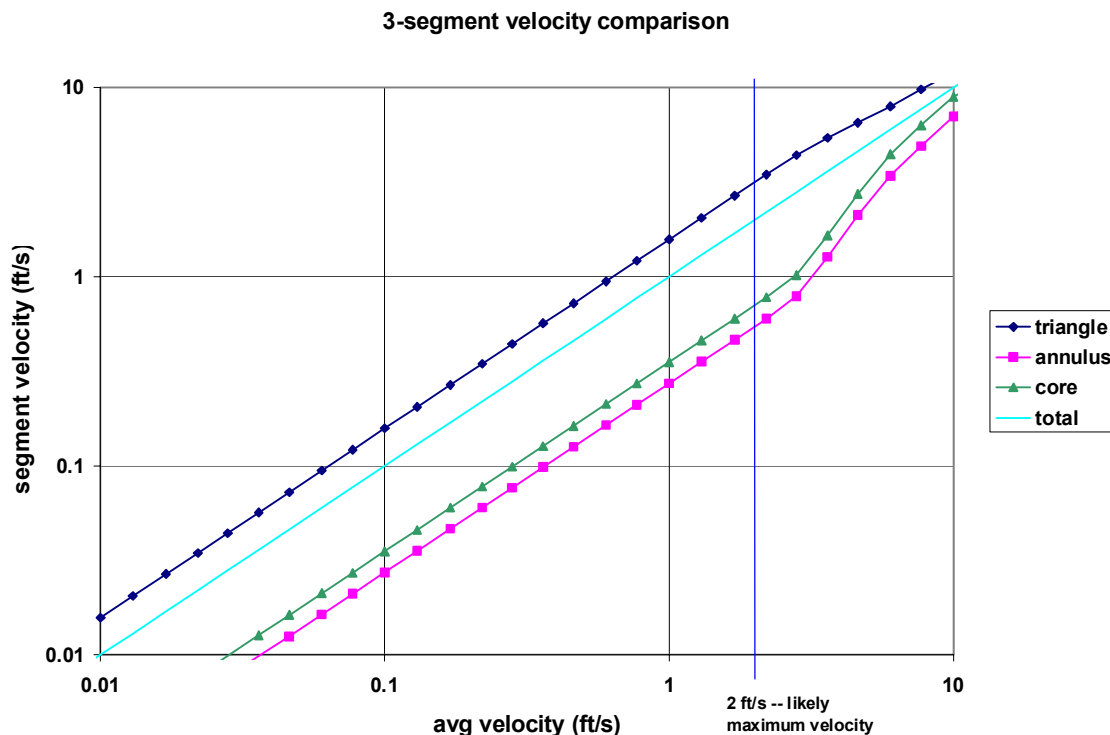


Figure 5. Comparison of flow area velocities in different flow areas vs average velocity for three different flow area flow calculations.

4. REFERENCES

1. R. L. Bratton, *MCO Work Book GOTH_SNF Input Data*, DOE/SNF/REP-071 Rev. 1, Idaho National Engineering and Environmental Laboratory, Idaho Falls, Idaho, August 2002.
2. R. V. Giles, *Schaum's Outline of Theory and Problems of Fluid Mechanics and Hydraulics*, second edition, McGraw-Hill, New York, 1962.

3. E-mail from R. L. Bratton (Idaho National Engineering and Environmental Laboratory) to J. R. Kirkpatrick (Oak Ridge National Laboratory) May 15, 2003.
4. R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, John Wiley and Sons, New York, 1960.
5. T. L. George, et al., *GOTHIC Containment Analysis Package Technical Manual*, Version 4.0, Report NAI 8907-06 Rev. 3, Numerical Applications, Inc., Richland, Washington, September 1993.