DOE/SNF/REP-076
Rev. 0

United States Department of Energy

National Spent Nuclear Fuel Program

Quick Look Report for Chemical Reactivity Modeling of Various Multi-Canister Overpack Breaches

April 2002

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

DOE/SNF/REP-076
Rev. 0

Quick Look Report for Chemical Reactivity Modeling of Various Multi-Canister Overpack Breaches

April 2002

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	New document	April 2002

Quick Look Report for Chemical Reactivity Modeling of Various Multi-Canister Overpack Breaches

April 2002

________________________________ **Date:** __________

National Spent Nuclear Fuel Program
Document Preparer

________________________________ **Date:** __________

National Spent Nuclear Fuel Program
Technical Lead

________________________________ **Date:** __________

National Spent Nuclear Fuel Program
Program Support Quality Engineer

________________________________ **Date:** __________

National Spent Nuclear Fuel Program
Program Support Manager

SUMMARY

This report makes observations or shows trends in the response and does not specifically provide conclusions or predict the onset of bulk uranium oxidation safety margins based on hole size. Comprehensive analysis will be provided in the future. The report should animate discussions about the results and what should be analyzed further in the final analysis. This report intends only to show the response of the breached multi-canister overpack (MCO) as a function of event time using the GOTH_SNF computer code. The response will be limited to physical quantities available on the exterior of the MCO. The GOTH_SNF model is approximate, because not all physical phenomenon was included in the model. Error estimates in the response are not possible at this time, because errors in the actual physical data are not known. Sensitivities in the results from variations in the physical data have not been pursued at this time, either.

This effort was undertaken by the National Spent Nuclear Fuel Program to evaluate potential chemical reactivity issues of a degraded uranium metal spent nuclear fuel using the MCO fully loaded with Mark IV N-reactor fuel as the evaluation model. This configuration is proposed for handling in the Yucca Mountain Project (YMP) surface facility. Hanford is loading N-reactor fuel elements into the MCO for interim storage at the Hanford site with permanent disposal proposed at YMP. A portion of the N-reactor fuel inventory has suffered corrosion, exposing the uranium metal under the zircaloy cladding. Because of the sealed MCO, the local radiation field, and decay heat of the fuel, hydrogen production cannot be ruled out from the metal hydrates on the surface of the zircaloy cladding and exposed fuel. Because of the much greater surface area, the oxyhydroxide composition, and water of hydration in the uranium metal corrosion product, the corrosion product will be a significant water source that may equal the absorbed water on the zircaloy cladding. A uranium oxide coating covers the exposed uranium metal, yet uranium hydride can still form under the protective oxide coating over the 40-year interim storage time span. The current treatment process at Hanford does not remove chemically bound water contained in the hydrates or in the waters of hydration. The chemically bound water is the source material for hydrogen production over the 40-year storage time. So, additional uranium hydride creates concerns that breaches of an MCO with the appropriate size openings could result in the onset of bulk uranium oxidation with the potential of a self-sustaining thermal excursion or pyrophoric event.

For this analysis, the worst-case scenario appears to be the match head configuration in a vertically standing MCO, where all the reactive surface area is placed on the tips of the fuel elements. This configuration concentrates the heat-producing chemical reaction at the tips of the fuel elements. Because no mechanistic drop analysis has been performed at this time to determine the MCO failure modes, parametric breach configurations were chosen in this analysis to determine the MCOs' external thermal response range. The first breach is a pair of holes that suddenly open in the MCO wall. This thermal excursion is controlled by the "thermal chimney effect" in the 4.27-m (14-ft) tall canisters caused by the multiple holes breach (one high and one low). A second breach where the MCO lid is suddenly removed and exposed to the ambient air environment is evaluated. This thermal excursion is controlled by the

countercurrent flow through the top of the MCO. Computer models for these breach configurations were constructed and executed.

Below is a table comparing the peak MCO exterior wall temperature, the peak exit gas temperature, and the elapse event time for each model.

Breach Configuration	Peak MCO Exterior Wall Temperature is °C (°F)	Peak Exit Gas Temperature is °C (°F)	Peak Exterior Wall Temperature at Gas Exit Temperature is ºC (ºF)	Elapsed Event Time (days)
Two 2-inch diameter holes	913 (1675)	788 (1450)	638 (1180)	3.5
Open top	782 (1440)	788 (1450)	NA	9
Two 1-inch diameter holes	460 (860)	496 (925)	386 (727)	15
Two 0.75-inch diameter holes	316 (600)	371 (700)	288 (550)	27
Two 0.5-inch diameter holes	182 (360)	254 (490)	182 (360)	>45

All values in the table have been rounded off and are approximate. The peak exterior wall temperature at the gas exit is the MCO wall temperature at the same computing node as the exit hole. The peak MCO exterior wall temperature is the hottest MCO wall temperature and may or may not be at the elevation of the exit hole.

CONTENTS

FIGURES

TABLES

ACRONYMS

NSNFP	National Spent Nuclear Fuel Program
MCO	multi-canister overpack
YMP	Yucca Mountain Project
GOTH_SNF	computer code developed by John Marvin, Inc.

Quick Look Report for Chemical Reactivity Modeling of Various Multi-Canister Overpack Breaches

1. INTRODUCTION

This report makes observations or shows trends in the response and does not specifically provide conclusions or predict the onset of bulk uranium oxidation safety margins based on hole size. Comprehensive analysis will be provided in the future. The report should animate discussions about the results and what should be analyzed further in the final analysis. This report intends only to show the response of the breached multi-canister overpack (MCO) as a function of event time using the GOTH_SNF computer code. The response will be limited to the exterior thermal response of the MCO. The GOTH_SNF model is approximate, because not all physical phenomenon was included in the model. Error estimates in the response are not possible at this time, because errors in the actual physical data are not known. Sensitivities in the results from variations in the physical data have not been pursued at this time, either.

This effort was undertaken by the National Spent Nuclear Fuel Program (NSNFP) to evaluate potential chemical reactivity issues of a degraded uranium metal spent nuclear fuel using MCO fully loaded with Mark IV N-reactor fuel as the evaluation model. This configuration is proposed for handling in the Yucca Mountain Project (YMP) surface facility. Hanford is loading N-reactor fuel elements into the MCO for interim storage at the Hanford site with permanent disposal proposed at YMP. A portion of the N-reactor fuel inventory has suffered corrosion, exposing the uranium metal under the zircaloy cladding. Because of the sealed MCO, the local radiation field, and decay heat of the fuel, hydrogen production cannot be ruled out from the metal hydrates present on the zircaloy cladding and exposed fuel. Because of the much greater surface area, the oxyhydroxide composition, and waters of hydration in the uranium metal corrosion product, corrosion product will be a significant water source that may equal the absorbed water on zircaloy. A uranium oxide coating covers the exposed uranium metal; yet uranium hydride formation can still form under the protective oxide coating over the 40-year interim storage time span. The current treatment process at Hanford does not remove these hydrates or waters of hydration, so additional uranium hydride creates concerns that breaches with the appropriate size openings could result in the onset of bulk uranium oxidation with the potential of a self-sustaining thermal excursion or pyrophoric event.

The effort of the NSNFP is to model the response of the MCO to various types of breaches and determine if a self-sustaining pyrophoric event is possible. To this end, dual analyses are being undertaken. The first analysis uses a computer model to analyze the MCO and its internal contents' response to a number of MCO breaches. The analysis goal is to determine the external MCO wall temperature and effluents up to the onset of bulk metallic uranium oxidation for various assumed MCO breaches. This report addresses the first approach. The second analysis is to construct a mechanistic model of the MCO to determine the size of the opening from potential accidental drops within the Yucca Mountain handling facilities. This analysis would take into account drop orientation, fracture mechanics, and nonlinear material behavior to determine the frequency and size of the opening in the MCO. The second analysis is beyond the scope of this report.

For this report, the worst-case scenario appears to be the match head configuration in a vertically standing MCO, where all the reactive surface area is placed on the tips of the fuel elements concentrating the chemical heats of reaction from uranium metal and hydride. Because the mechanistic drop analysis hasn't been performed at this time, the breach configurations chosen in this analysis are parametric scenarios used to determine the MCOs' external thermal response range. The first breach is a pair of holes that suddenly open in the MCO wall. This breach is controlled by the "thermal chimney effect" in the 4.27-m (14-ft) tall canisters caused by the multiple holes breach (one high and one low). Another breach that will be evaluated is the open top breach where the lid of the MCO is removed instantly. This breach is controlled by the countercurrent flow through the top of the MCO. Computer models were constructed of these MCO breaches and executed. This report is not intended to serve as a comprehensive analysis of the computer runs included in this report, but only to make observations from the data.

The GOTH_SNF version 5.3 computer code was developed by John Marvin Incorporated in West Richland, WA. Cognizant NSNFP personnel have reviewed the models and agreed on the approach as documented in DOE/SNF/REP-071, Rev 1, "MCO Work Book GOTH_SNF Input Data"; yet the code has not been independently reviewed at this time. Informal reviews of the derivation of the input deck have been completed; formal independent review of the input deck derivation is pending. A complete description of the MCO model is found in DOE/SNF/REP-071, *MCO Work Book GOTH-SNF Input Data*. All physical quantities and conclusions will be discussed in the future report, DOE/SNF/REP-077.

1.1 Problem Description

1.1.1 MCO Dimensions

The MCO is built for interim storage of conditioned N-reactor fuel elements at the Hanford site. The MCO is constructed from 304L stainless steel with a wall thickness of 1.27 cm (0.5 in.). The external diameter of the MCO is 61 cm (24 in.), while the upper portion of the MCO diameter increases to 64.3 cm (25.31 in.) to accommodate the top mechanical closure device. There is another 57.9 cm (22.80 in.) of shield plug length on top of the closure device. The bottom plate thickness is 5.01 cm (2.01 in.). The MCO is seal welded before being placed in interim storage. The maximum design pressure is approximately 3.1 Mpa (450 psia). Figure 1 shows the dimensions of the MCO.

1.1.2 Fuel Basket Description and Dimensions

The configuration being considered in this report is an MCO containing five baskets of Mark IV fuel. This configuration is divided into four fuel baskets positioned in the first four locations and one scrap basket located on top of the four fuel baskets. Other configurations will be used with the Mark IA fuel, but this Mark IV configuration has the largest uranium metal loading. Therefore, this configuration will be used as the bounding case in this report. There could be situations where other configurations outside of this bounding configuration would be necessary, yet these other configurations have been deemed unlikely at this time.

Each fuel basket contains 54 Mark IV N-reactor fuel elements with a uranium metal loading of 1269 kg (2798 lb) of metallic uranium per fuel basket. Each fuel basket has a base plate made of three pieces. The first piece is an aluminum plate with sockets for the N-reactor fuel elements resembling an egg carton (see Figure 2). This plate sits on a stainless steel grate. The grate is placed on top of a stainless steel 3.18-cm (1.25-in.)-thick plate with ninety-six 0.5-in. through holes. The sockets, grate, and 0.5-in. holes allow flow through the bottom of the basket, but restrict small material (greater than 0.32 cm [0.125 in.]) from migrating to the bottom of the MCO. The center support pipe is attached to the base plate by threads. The center support pipe extends beyond the top of the basket into the base plate and center support pipe of the next basket, thus locking together the stack of baskets. Six cylindrical rods are placed at equal positions around the inside perimeter of the base plate and are affixed by bolts through the base plate. The six rods extend the entire length of the basket. Together, the pipe and six rods support the weight of the above basket when stacked. The fuel basket has a skirt or shroud around the outside of the basket extending about halfway up the basket retaining the fuel elements. Figure 2 is a three-dimensional sectioned view of the Mark-IV MCO fuel basket, and Figure 3 provides dimensions of the basket.

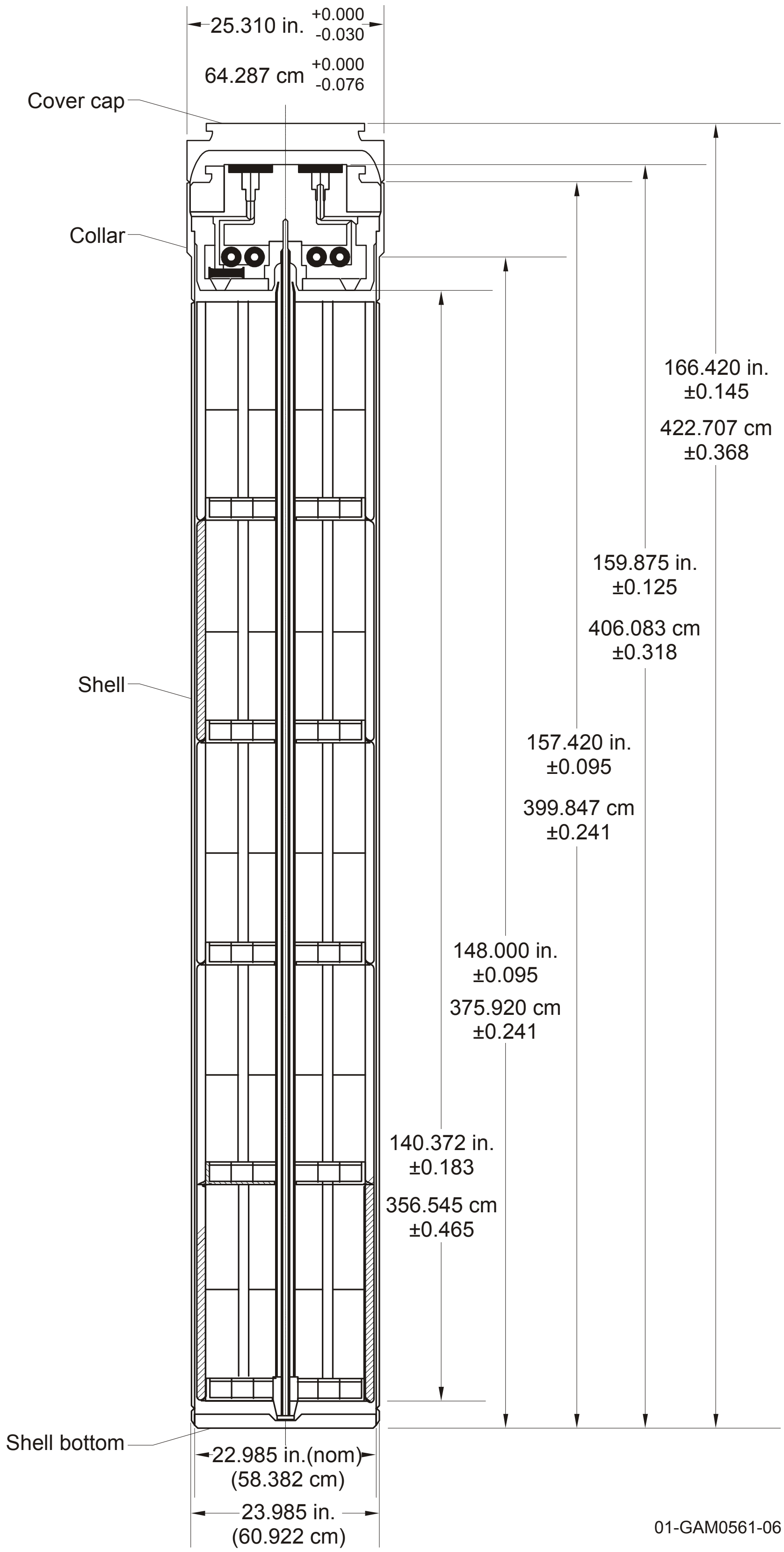

Figure 1. Dimension of the MCO.

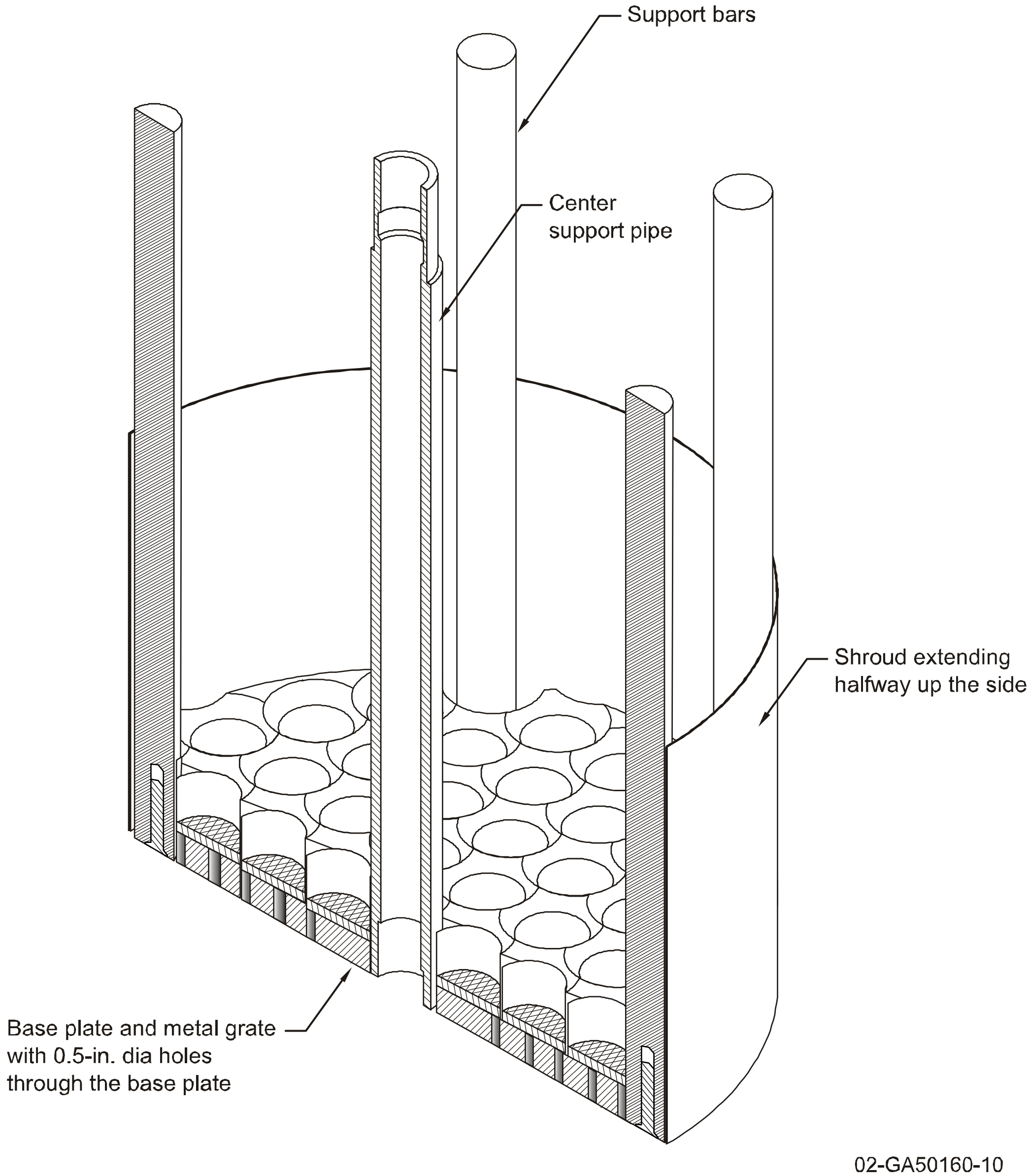

Figure 2. Cutaway of the MCO Mark-IV fuel basket.

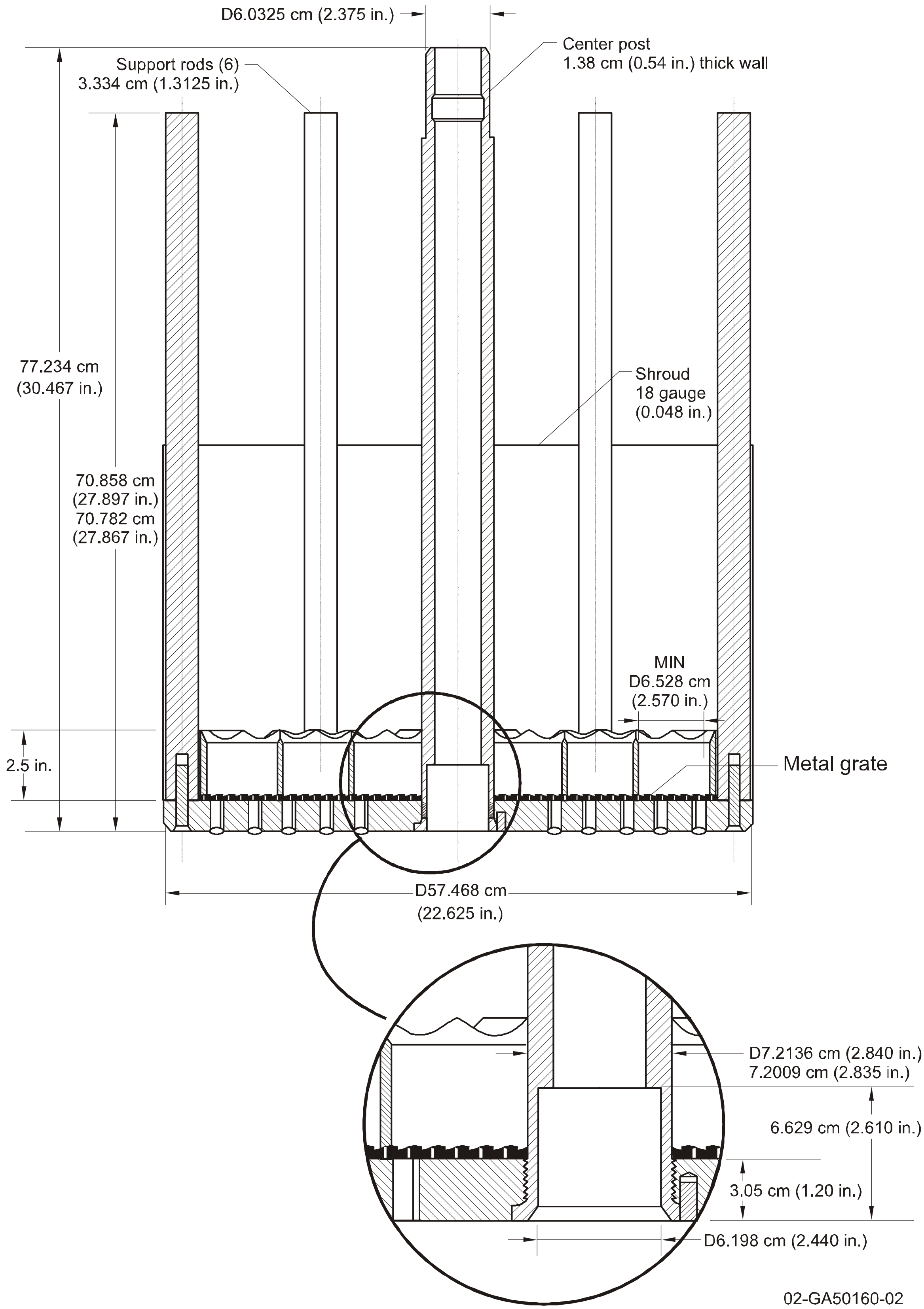

Figure 3. Dimensions of the fuel basket.

1.1.3 Scrap Basket Description and Dimensions

The scrap basket holds segregated scrap in two sizes: 3 to 1 in. (coarse) and 1 to 0.25 in. (fines). Total uranium mass in the scrap basket is limited to 980 kg (2161 lb). The scrap basket is similar except for the internal dividers that partition the scrap basket into six pie-shaped full-length channels on the periphery of the hexagonal channel around the center pipe. The shroud and internal dividers extend the full length of the basket. Both the internal dividers and shroud are made of copper to increase heat transfer away from the rubble fuel. The hexagon facets have a repeating pattern of slots distributed along the length of the basket to allow the exchange of gases between the two scrap sizes. Just below the top of the scrap basket a chevron seal attaches to the basket around the outside perimeter sealing the gap between the shroud and interior MCO wall. The seal has slits in the chevron allowing some movement of gases through the seal, but still offers a high flow resistance to the fluid and material flowing over the top of the scrap basket. The scrap basket base plate is similar to the fuel basket base plate except for the aluminum plate holding fuel. The coarse-sized scrap is placed in the six pie-shaped channels, while the fines-sized scrap is placed in the center hexagonal channel. Figure 4 is a three-dimensional sectioned view of the Mark-IV MCO scrap basket, and Figure 5 provides the dimensions. Figure 6 shows the location of the segmented scrap in the scrap basket.

1.1.4 Mark-IV N-Reactor Fuel Element

The 66-cm (26.1-in.) Mark-IV fuel elements contain the largest amount of uranium metal in the N-reactor fuel inventory, and thus their complete loading results in the largest uranium metal loading in the MCO. N-reactor fuel element uses two concentric tubes of uranium metal coextruded into Zircaloy-2 cladding. The tubes have Zircaloy-2 end caps permanently fixed and Zircaloy-2 spacers maintaining the concentric geometry of the fuel elements. Figure 7 shows the dimensions of the Mark-IV N-reactor fuel element.

1.2 GOTH_SNF MCO Model

1.2.1 Fuel and Scrap Basket

GOTH_SNF is a computer program that solves the equations for conservation of mass, momentum and energy for multicomponent, multiphase flows. The phase transformation equations are coupled by mechanistic models for interface mass, energy, and momentum transfer that cover the entire flow regime (bubbly flow to film/drop flow to single phase). The interface models allow for thermal nonequilibrium between phases and unequal phase velocities. GOTH_SNF includes a full treatment of momentum transport terms in multidimensional models with an optional one-dimensional turbulence model for turbulent shear and turbulent mass and energy diffusion. The code has been modified to model metallic uranium spent nuclear fuel thermal behavior during transportation, vacuum drying, and storage. Models for the oxidation of uranium metal and uranium hydride with water vapor and oxygen have been incorporated into the model. Uranium hydride decomposition models have also been incorporated.

This description of the MCO model is a summary only. A full description of the model is found in the report DOE/SNF/REP-071, Rev. 1, “MCO Work Book GOTH_SNF Input Data.” The heat transfer surfaces representing the metal components (stainless steel, uranium and copper) are represented by axisymetric rings see Figure 8. These will be referred to as the metal rings. The first fuel ring contains six fuel elements. The second fuel ring contains 12 fuel elements. The third and fourth fuel rings contain 18 fuel elements each. The rings have been sized to represent the same uranium metal mass as contained in the fuel elements. This geometry allows the model to use simplified axisymetric geometry, not a three-dimensional nodalization. Each ring in the basket is divided into five vertical segments or a single column of nodes; see Figure 9. The single column of nodes represents the axisymetric ring. The fifth

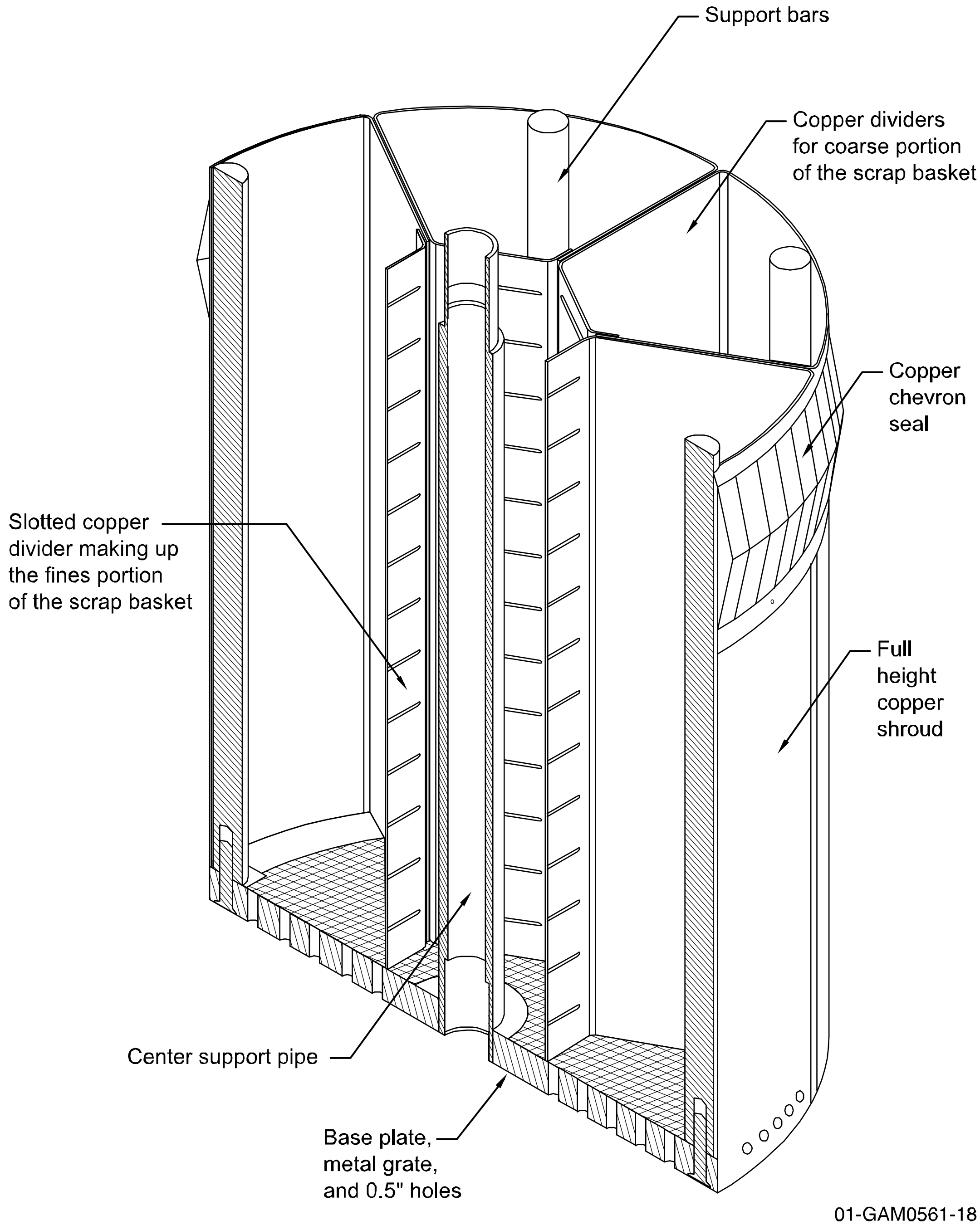

Figure 4. Cutaway of the Mark-IV MCO scrap basket.

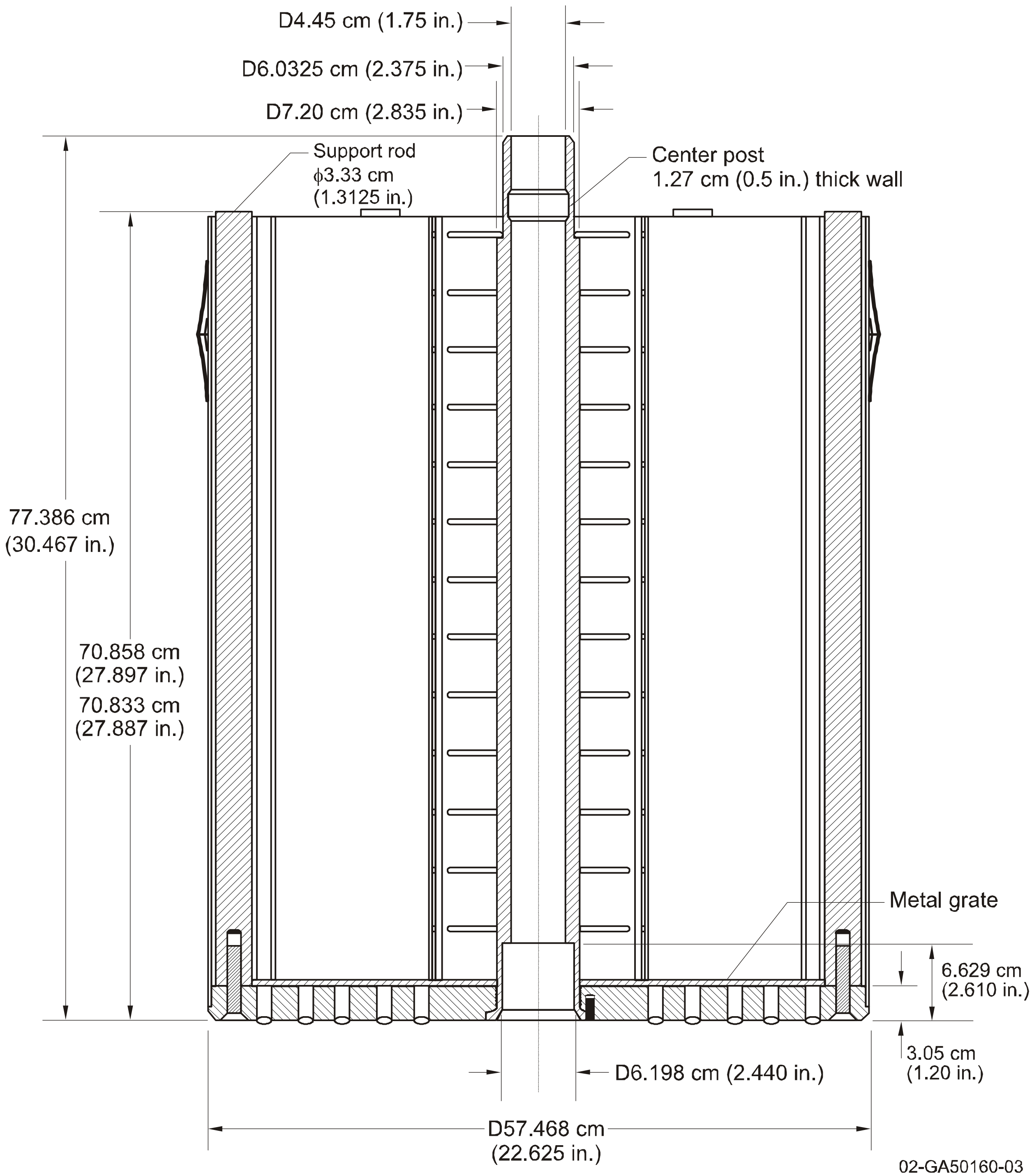

Figure 5. Dimensions of the Mark-IV MCO scrap basket.

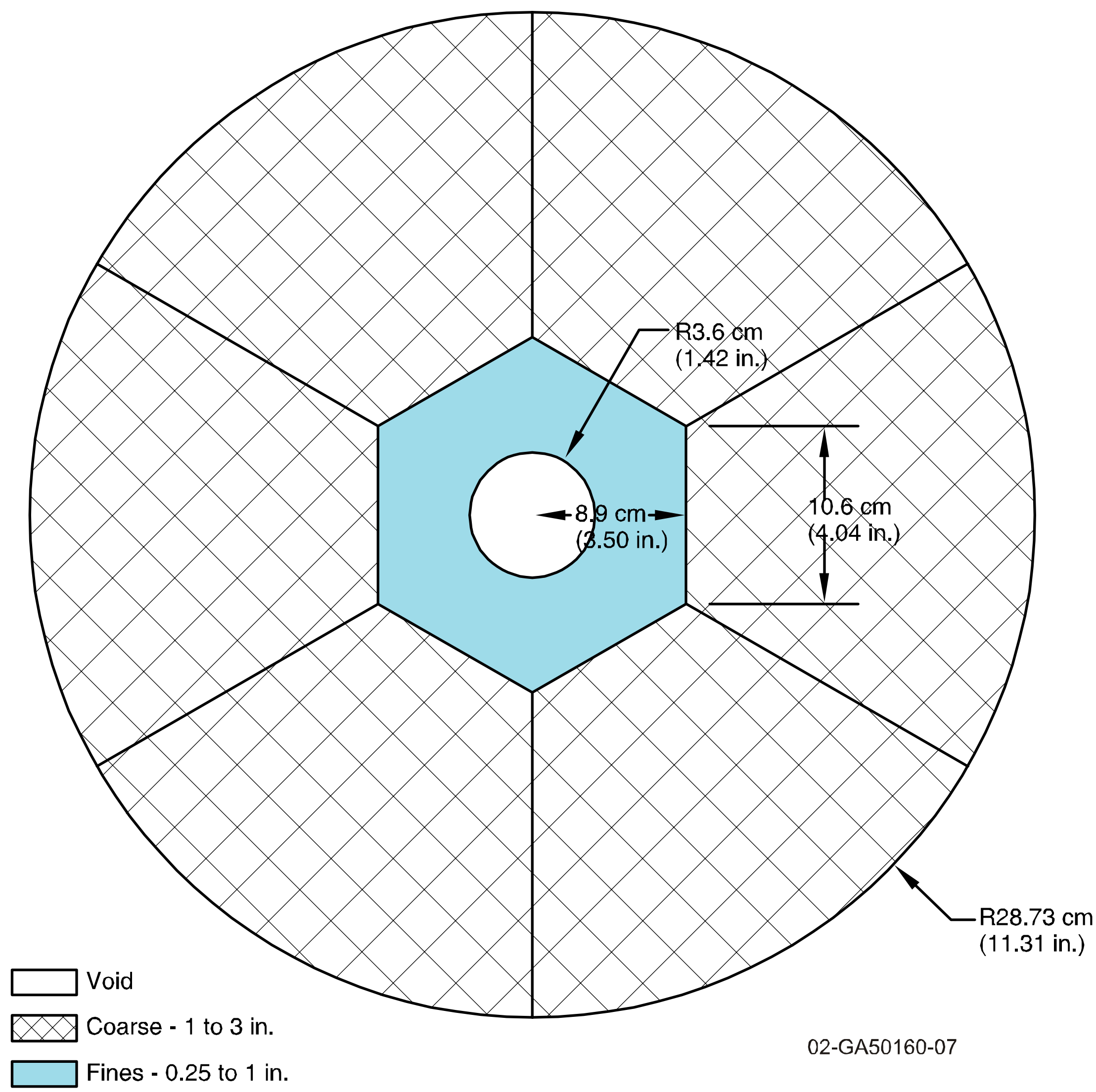

Figure 6. Locations of coarse (1 to 3 in.) and fine (0.25 in. to 1 in.) pieces in the scrap basket.

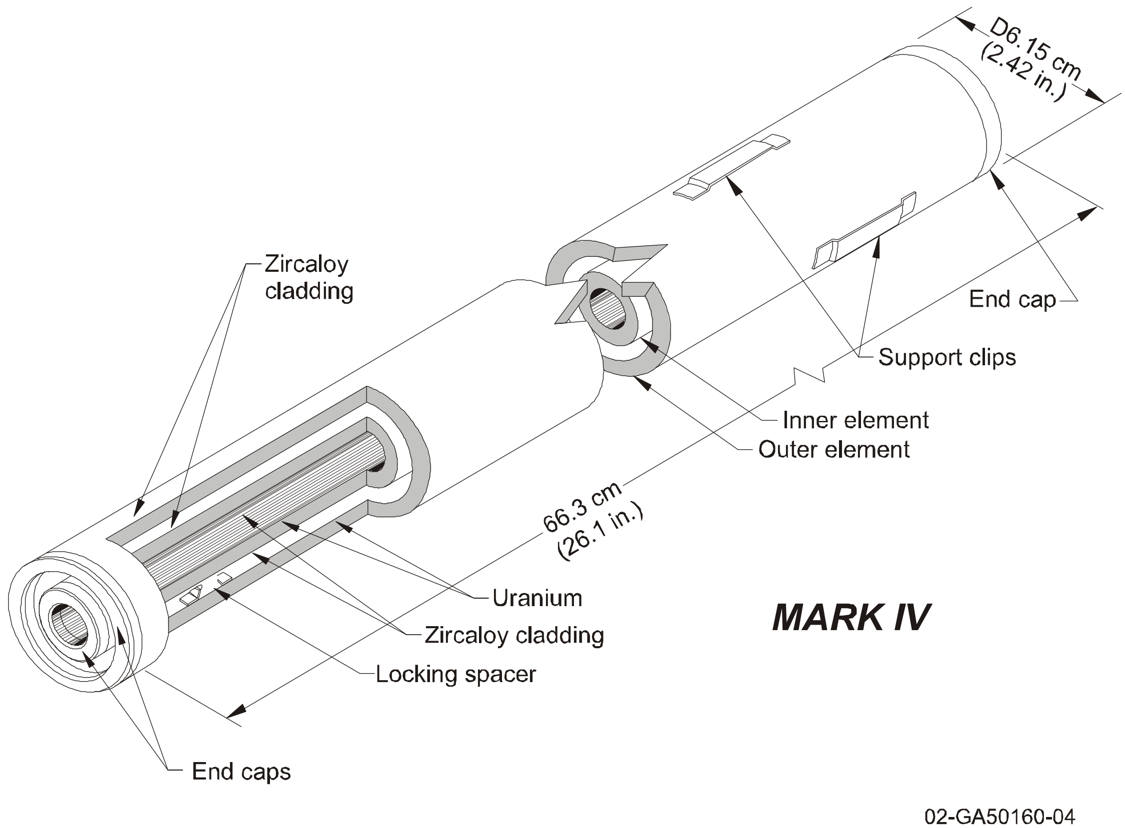

Figure 7. Mark-IV N-reactor fuel element dimensions.

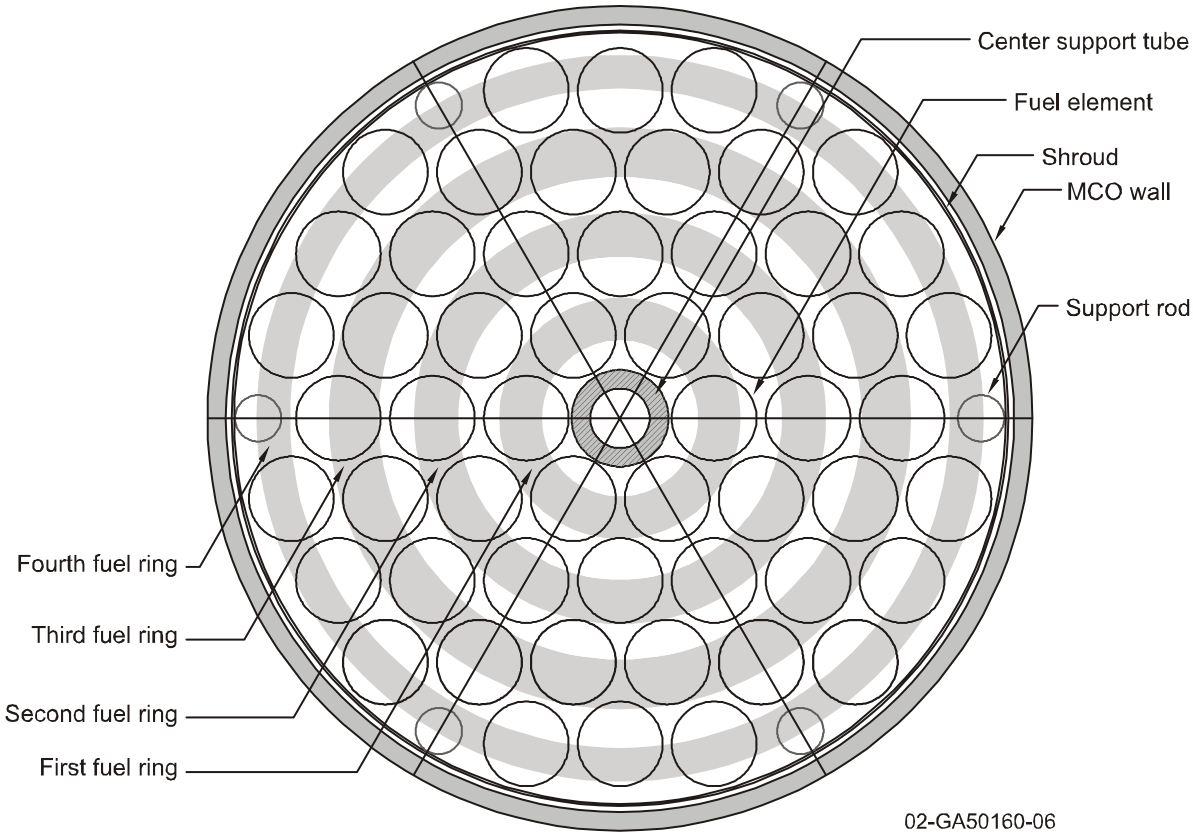

Figure 8. Layout of the ring model approximation in the MCO.

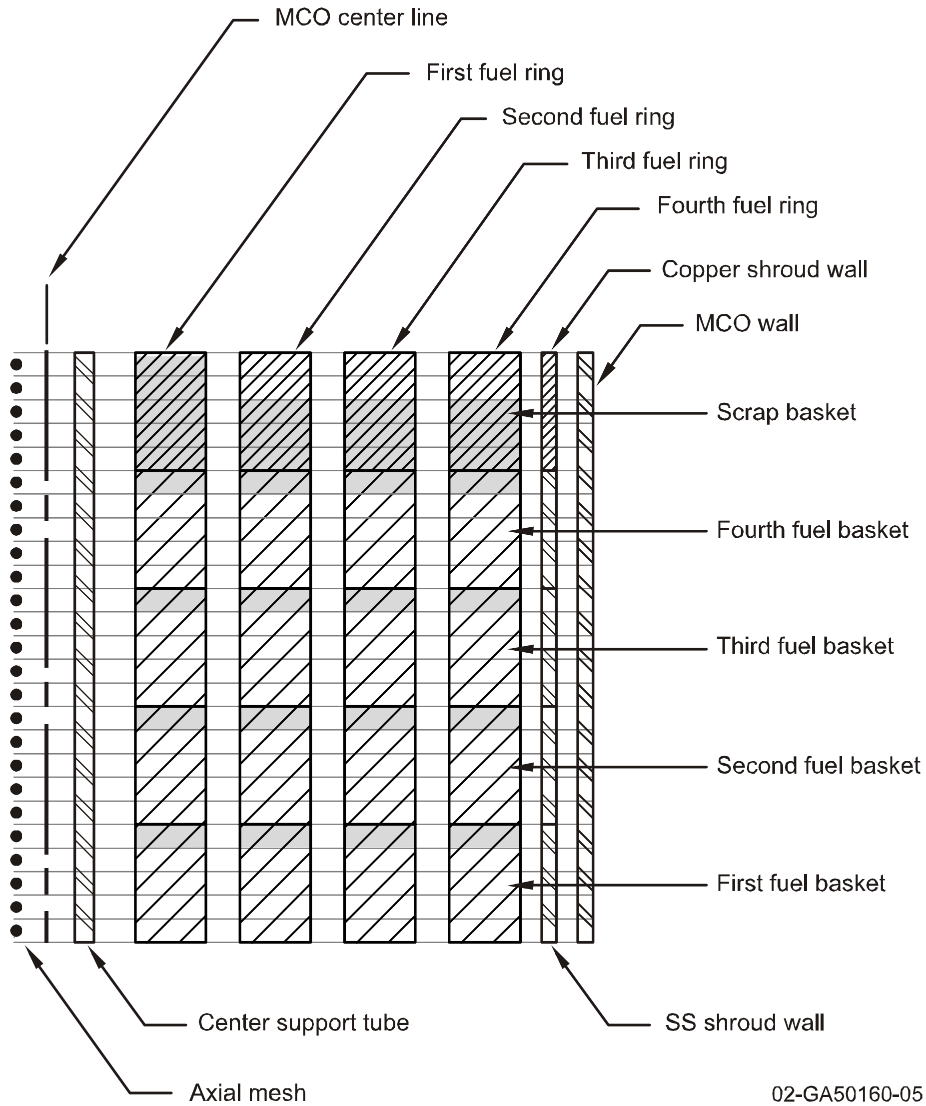

Figure 9. Nodal discretization of the metal conductors.

nodes in the four fuel baskets are the tips of the fuel elements where all the reactive surface areas are located. Once all the reactive material is consumed at the tip, no other material can react in nodes below the tip. The reason for this is that all the reactive surface area was assumed to be located at the tip and not below.

In the scrap basket, all the uranium mass has a surface area that is higher than the fuel reactive surface area. The first fuel ring represents the uranium mass in the fines portion of the scrap basket, which has the reactive surface area applied to all five of the vertical nodes. The second, third, and fourth fuel rings have uranium metal and reactive surface area applied to the first three nodes in order to achieve the correct void fraction in the coarse portion of the scrap basket. In both the fuel baskets and the scrap basket when all the reactive surface area has been consumed at the node, all the uranium metal has been consumed at that node as well. Each fuel ring in the five fuel baskets is modeled without the Zircaloy-2 cladding because the thermal mass of the cladding is negligible compared to the uranium metal. All three forms of heat transfer (conduction, convection, and radiation) are permitted on the uranium and metal surfaces.

The worst-case uranium loading is achieved using 66-cm (26.1-in.) long Mark IV fuel elements containing 23.5 kg (51.7 lb) of uranium metal. There are 54 fuel elements in each fuel basket, which amounts to 1,269 kg (2,792 lb) of uranium metal in each fuel basket. The worst-case uranium metal loading of the scrap basket is 980 kg (2,161 lb). This is based on the volume of the inner and outer chambers and expected porosity in the scrap basket. The scrap pieces can be cladding, spacers, and uranium metal; but for this worst-case analysis, the entire mass will be assumed uranium metal. The total uranium metal in the MCO with the worst-case configuration is 6,056 kg (13,228 lb).

The metal rings are called conductors in terms of the GOTH_SNF code vernacular. Heat transfer from the conductors, the uranium metal fuel elements, the MCO wall, shroud walls, copper dividers, and the center support pipe are modeled as conducting and radiating surfaces. Convection heat transfer occurs on all conductor surfaces. The fuel conductor thicknesses are sized to conserve the mass and surface area of the number of elements included in the ring. Thermal energy from chemical reactions (oxidation, heats of formation, etc.) is only present at locations where reactive surfaces have been defined on the node. Gas properties are defined at the local conditions allowing the density, specific heat C_p, conductivities, partial pressure, and sound velocity to vary according to the local conditions. Flow restrictions due to the 0.5-in. holes, mesh size of the screen in the fuel and scrap basket, slits in the chevron seal, and slits in the faceted sides of the divider between the fines and coarse portion in the scrap basket are included in the model. Approximating the fuel rings as solid uranium prevents radial gas flow to the perimeter of the basket. This flow around the elements and through the gaps has been artificially added to the conductors. This allows gas and fluid to migrate radially toward the periphery of the basket. The shrouds on the fuel baskets are modeled as a solid ring or conductors but have gaps added to them to account for their less than full height. The outside surface of the MCO wall sees a constant ambient temperature and has all three modes of heat transfer associated with the geometric surface area.

2. BREACHED CONFIGURATIONS

Because the mechanistic drop analysis hasn't been performed at this time, the breach configurations chosen in this analysis are parametric scenarios used to determine the MCOs' external thermal response range. This analysis has chosen two configurations to investigate the consequences of potential breaches in the MCO. This analysis will not determine location, size, or quantity of these hypothetical breaches, but will use a range of hole sizes to encompass the degree of consequences. The first configuration is an MCO with two holes in the wall, and the second is an open top.

2.1 Two-Hole Configuration

The two-hole configuration is composed of two holes with the same diameter. The bottom hole is located in the wall of the MCO at an elevation level of approximately 61 cm (2.0 ft) from the bottom. The top hole is located approximately 15 cm (6 in.) from the top. The two holes are opened simultaneously to the environment. A sketch of this configuration is seen in Figure 10.

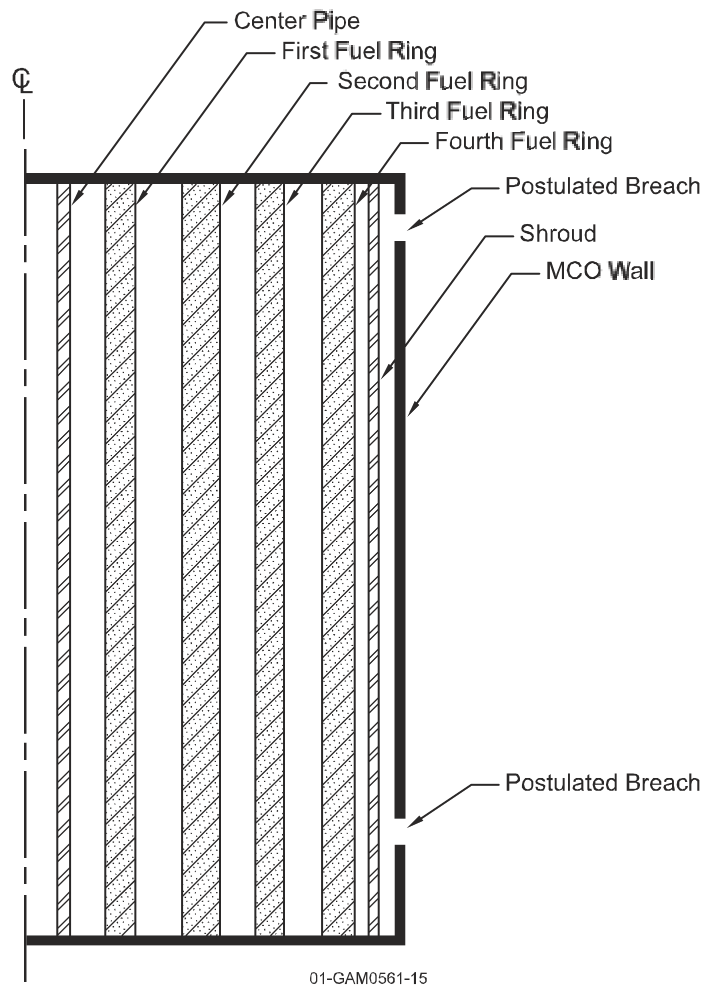

Figure 10. Configuration of the two-hole breach.

2.1.1 Description of Plots for Each Two-hole Configuration

Below is a description of the plots in Sections 2.1.2 (two 0.5-inch holes), 2.1.3 (two 0.75-inch holes), 2.1.4 (two 1.0-inch holes), and 2.1.5 (two 2.0-inch holes). Below each bullet is a table matching the plot that it describes.

- External MCO wall temperature vs. event time—The external MCO wall temperature plots are data taken at the nodes that represent the vertical exterior face of the wall. Each basket has five vertical nodes, where each node is vertically spaced 13.2 cm (5.2 in.) from the previous node. The bottom basket or Basket 1 is represented by nodes 1–5; Basket 2 uses nodes 6–10; Basket 3 uses nodes 11–15; and Basket 4 uses nodes 16–20. The scrap basket uses nodes 21–25. The temperature is in degrees Fahrenheit, and the event time is in days.

Two-Hole Configuration	Basket 1 Nodes 1–5	Basket 2 Nodes 6–10	Basket 3 Nodes 11–15	Basket 4 Nodes 16–20	Basket 5 Nodes 21–25
Two 0.5-in. Section 2.1.2	Figure 11	Figure 12	Figure 13	Figure 14	Figure 15
Two 0.75-in. Section 2.1.3	Figure 28	Figure 29	Figure 30	Figure 31	Figure 32
Two 1.0-in. Section 2.1.4	Figure 45	Figure 46	Figure 47	Figure 48	Figure 49
Two 2.0-in. Section 2.1.5	Figure 62	Figure 63	Figure 64	Figure 65	Figure 66

- External MCO wall heat flux vs. event time—The external MCO wall heat flux plots are data taken at the nodes that represent the vertical exterior face of the wall. Each basket has five vertical nodes, where each node is vertically spaced 13.2 cm (5.2 in.) from the previous node. The bottom basket or Basket 1 is represented by nodes 1–5; Basket 2 uses nodes 6–10; Basket 3 uses nodes 11–15; and Basket 4 uses nodes 16–20. The scrap basket uses nodes 21–25. The heat flux is in BTU/hr-ft^2 at each of the nodes, and the event time in days.

Two-Hole Configuration	Basket 1 Nodes 1–5	Basket 2 Nodes 6–10	Basket 3 Nodes 11–15	Basket 4 Nodes 16–20	Basket 5 Nodes 21–25
Two 0.5-in. Section 2.1.2	Figure 16	Figure 17	Figure 18	Figure 19	Figure 20
Two 0.75-in. Section 2.1.3	Figure 33	Figure 34	Figure 35	Figure 36	Figure 37
Two 1.0-in. Section 2.1.4	Figure 50	Figure 51	Figure 52	Figure 53	Figure 54
Two 2.0-in. Section 2.1.5	Figure 67	Figure 68	Figure 69	Figure 70	Figure 71

- Exiting gas temperature vs. event time—The exiting gas temperature from the upper hole is plotted versus the event time.

Exiting gas temperature	Two 0.5-in. Section 2.1.2	Two 0.75-in. Section 2.1.3	Two 1.0-in. Section 2.1.4	Two 2.0-in. Section 2.1.5
	Figure 21	Figure 38	Figure 55	Figure 72

- Relative concentration of gas species exiting the upper hole vs. event time—The mass fractions are the relative components of the mass flow rate that corresponds to the gas species hydrogen, nitrogen, oxygen, and water vapor in the mass flow. This plot shows the gas species concentrations leaving the MCO.

Exiting gas mass fractions	Two 0.5-in. Section 2.1.2	Two 0.75-in. Section 2.1.3	Two 1.0-in. Section 2.1.4	Two 2.0-in. Section 2.1.5
	Figure 22	Figure 39	Figure 56	Figure 73

- Mass flow at the inlet and outlet vs. event time—The plots show the flow rate (lbm/s) of the inlet flow and outlet flow. Negative flow rate means flow going into the MCO, and positive flow means flow leaving the MCO.

Mass flow	Two 0.5-in. Section 2.1.2	Two 0.75-in. Section 2.1.3	Two 1.0-in. Section 2.1.4	Two 2.0-in. Section 2.1.5
	Figure 23	Figure 40	Figure 57	Figure 74

- Flow velocity at the inlet and outlet vs. event time—The plots show the velocity (ft/s) of the inlet velocity and outlet velocity. Negative flow rate means flow going into the MCO, and positive flow means flow leaving the MCO.

Flow velocity	Two 0.5-in. Section 2.1.2	Two 0.75-in. Section 2.1.3	Two 1.0-in. Section 2.1.4	Two 2.0-in. Section 2.1.5
	Figure 24	Figure 41	Figure 58	Figure 75

- Oxygen, hydrogen, and water vapor consumption or production vs. event time—The plots show the consumption of oxygen and hydrogen as negative mass and production of water vapor as positive mass. As all the reactive metal is consumed, consumption and production goes to zero, and therefore, the lines become straight after the event.

Gas production or consumption	Two 0.5-in. Section 2.1.2	Two 0.75-in. Section 2.1.3	Two 1.0-in. Section 2.1.4	Two 2.0-in. Section 2.1.5
	Figure 25	Figure 42	Figure 59	Figure 76

- Uranium metal, uranium dioxide, and fine uranium metal consumption or production vs. event time—The plots show the consumption by negative mass and production by positive mass. As all the reactive metal is consumed, consumption and production goes to zero, and therefore, the lines become straight after the event.

Metal/oxide consumption or production	Two 0.5-in. Section 2.1.2	Two 0.75-in. Section 2.1.3	Two 1.0-in. Section 2.1.4	Two 2.0-in. Section 2.1.5
	Figure 26	Figure 43	Figure 60	Figure 77

- Total chemical energy output vs. event time—The plots show all energy generated from oxidation, disassociation, and formation of reactants.

Chemical energy output	Two 0.5-in. Section 2.1.2	Two 0.75-in. Section 2.1.3	Two 1.0-in. Section 2.1.4	Two 2.0-in. Section 2.1.5
	Figure 27	Figure 44	Figure 61	Figure 78

All the figures in this report have been scaled to the same length in elapsed event time and the peak values for each of the responses described above. This has been done to facilitate comparison of the different responses.

2.1.2 Two 0.5-inch Holes

This breach event did not finish in 45 days of elapsed event modeling time. Judging from the ratio of the uranium metal consumed to the amount available, at least 4 to 6 more days of event modeling would be needed for complete consumption of the uranium metal with reactive surface area. Upon the total consumption of reactive surface area, the event would terminate.

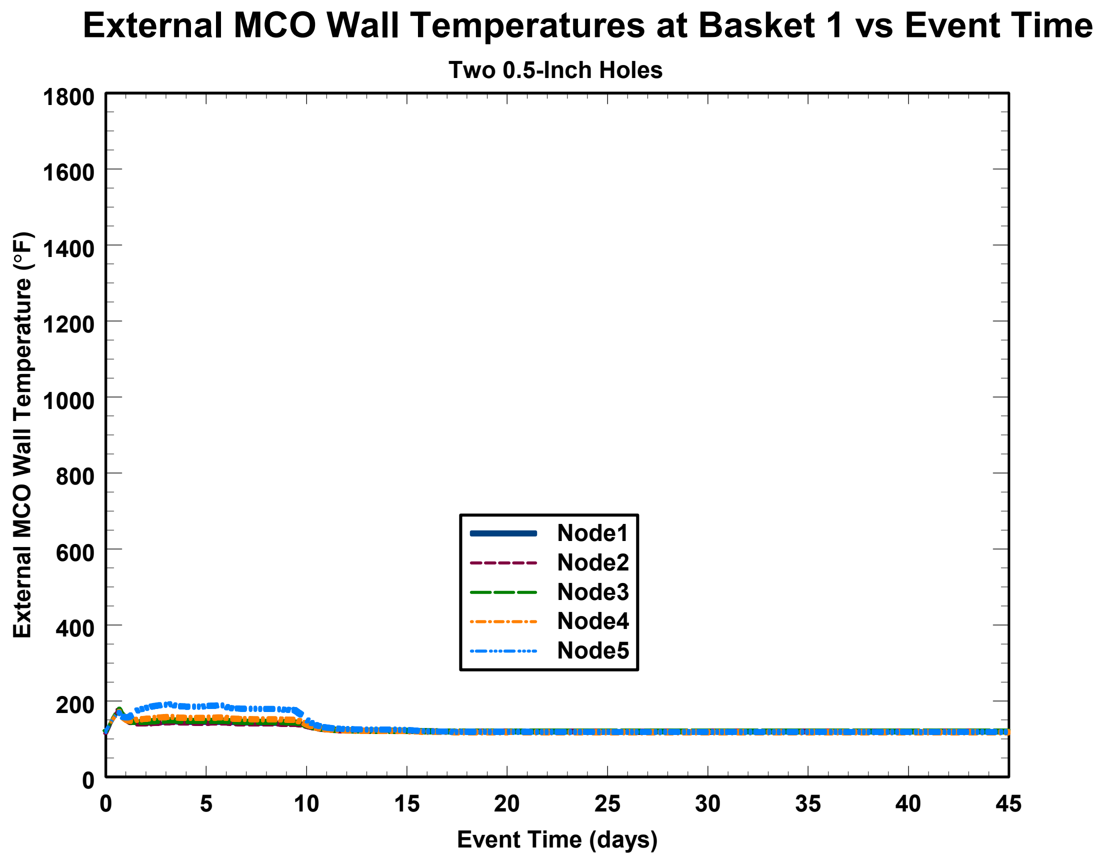

Figure 11. External MCO wall temperatures at nodes in Basket 1 for two 0.5-inch hole breach.

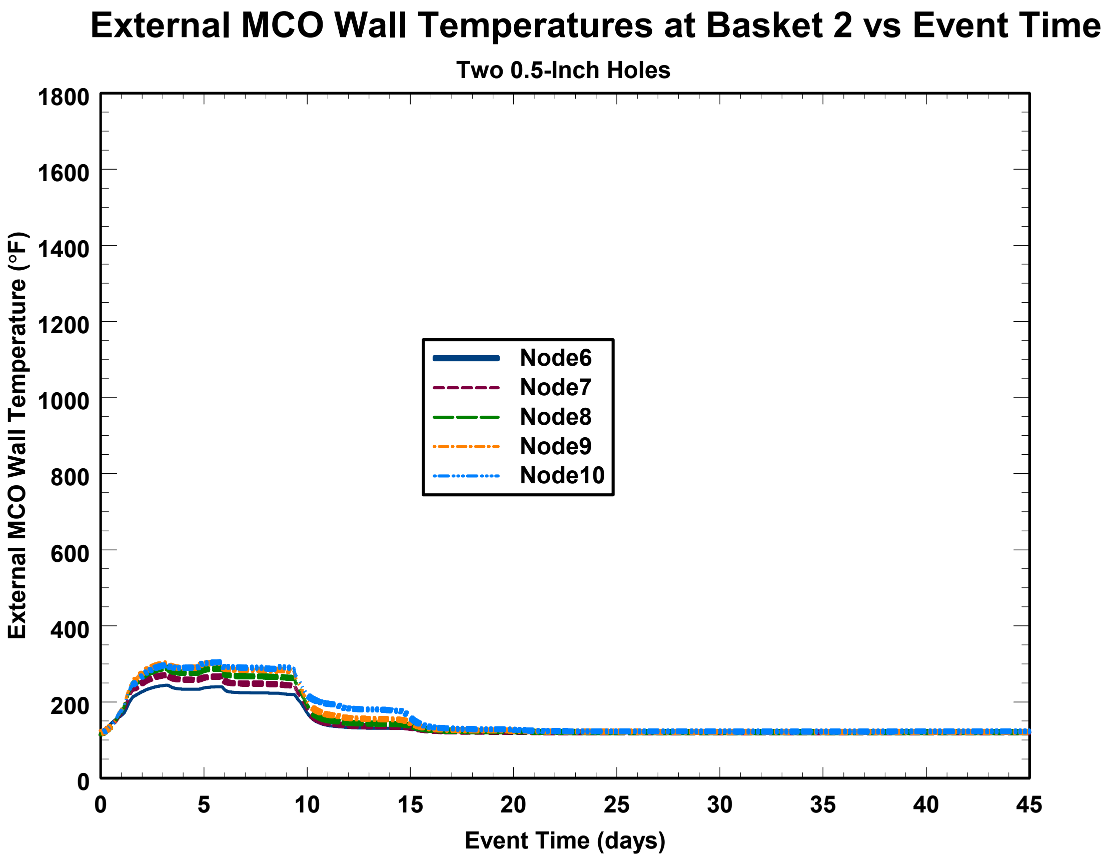

Figure 12. External MCO wall temperatures at nodes in Basket 2 for two 0.5-inch hole breach.

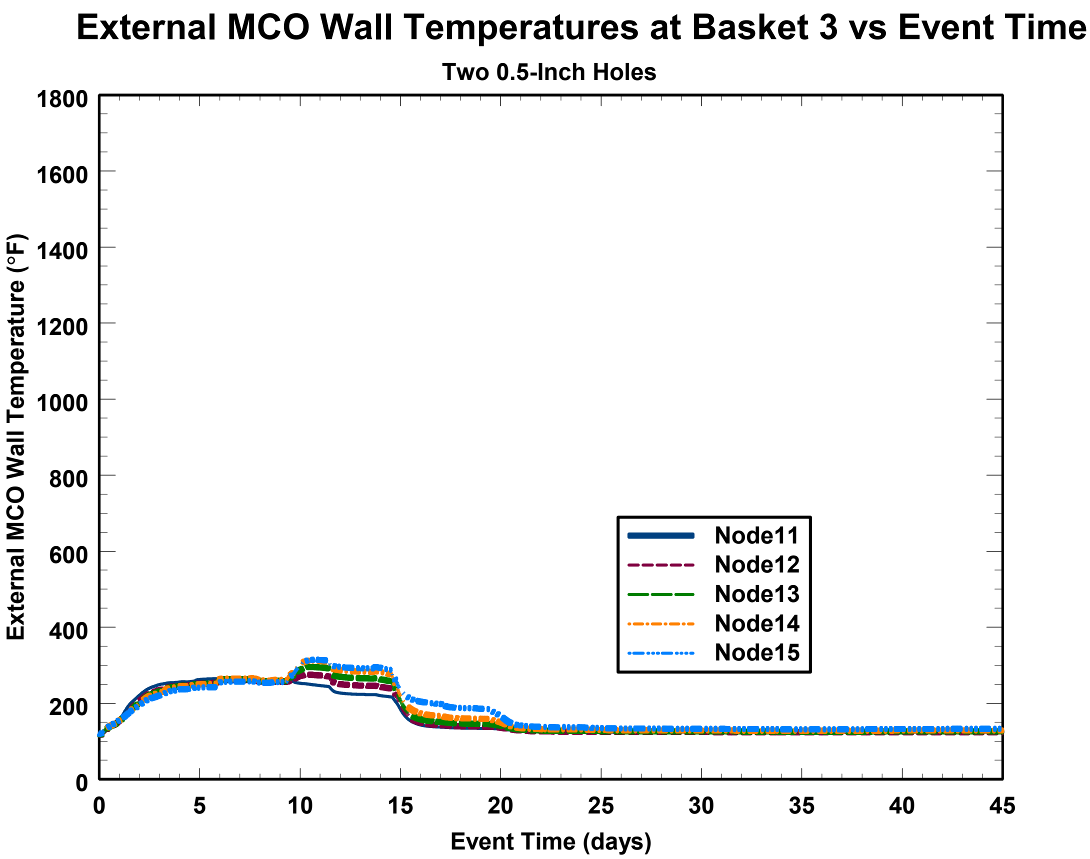

Figure 13. External MCO wall temperatures at nodes in Basket 3 for two 0.5-inch hole breach.

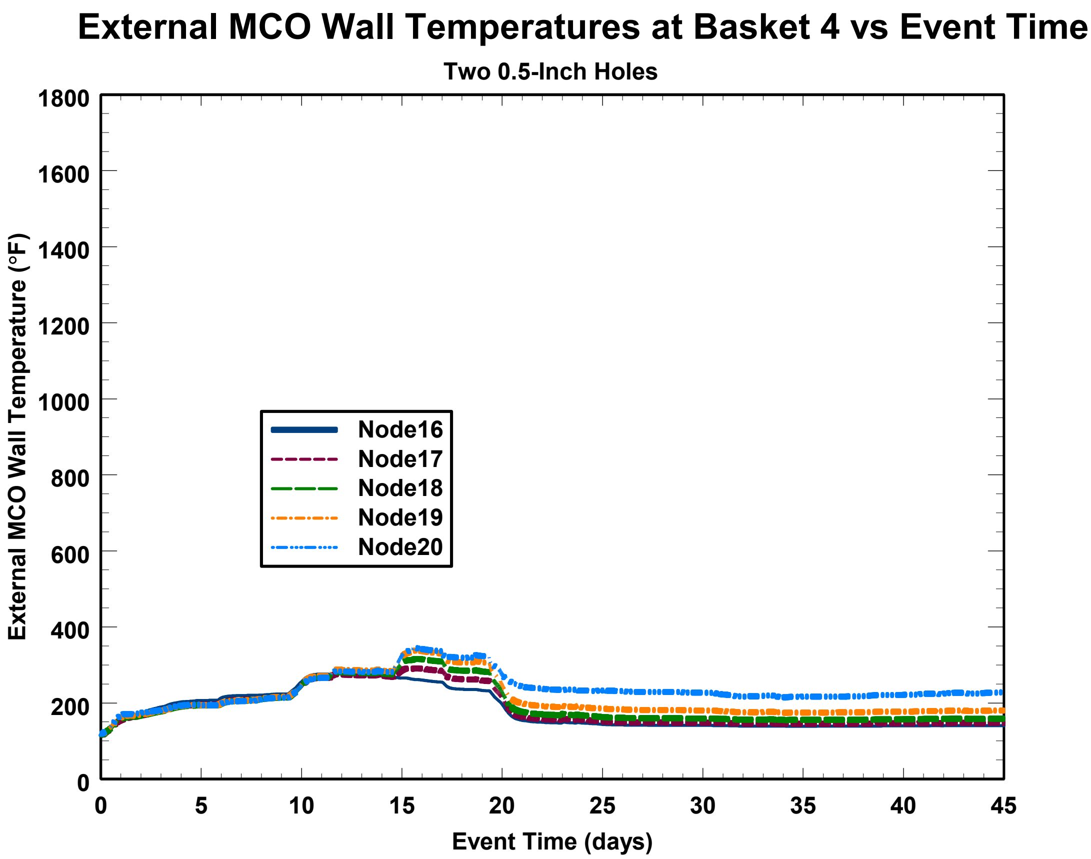

Figure 14. External MCO wall temperatures at nodes in Basket 4 for two 0.5-inch hole breach.

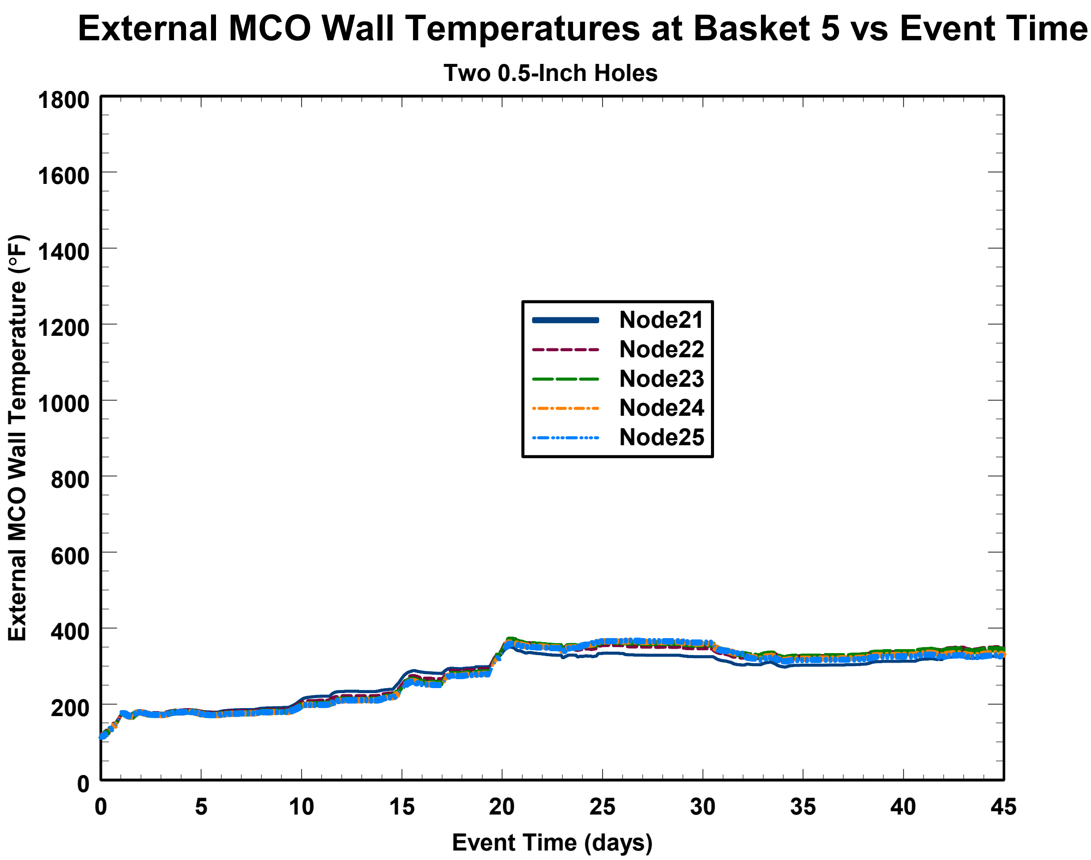

Figure 15. External MCO wall temperatures at nodes in Basket 5 for two 0.5-inch hole breach.

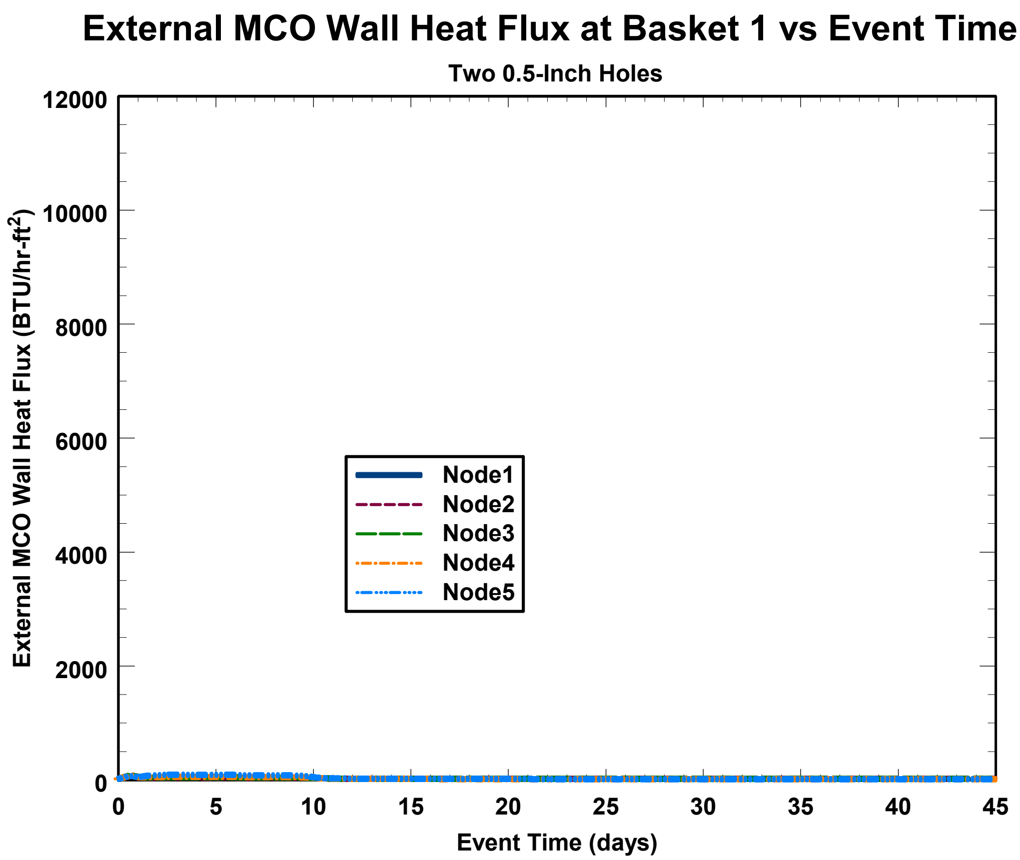

Figure 16. External MCO wall heat flux at nodes in Basket 1 for two 0.5-inch hole breach.

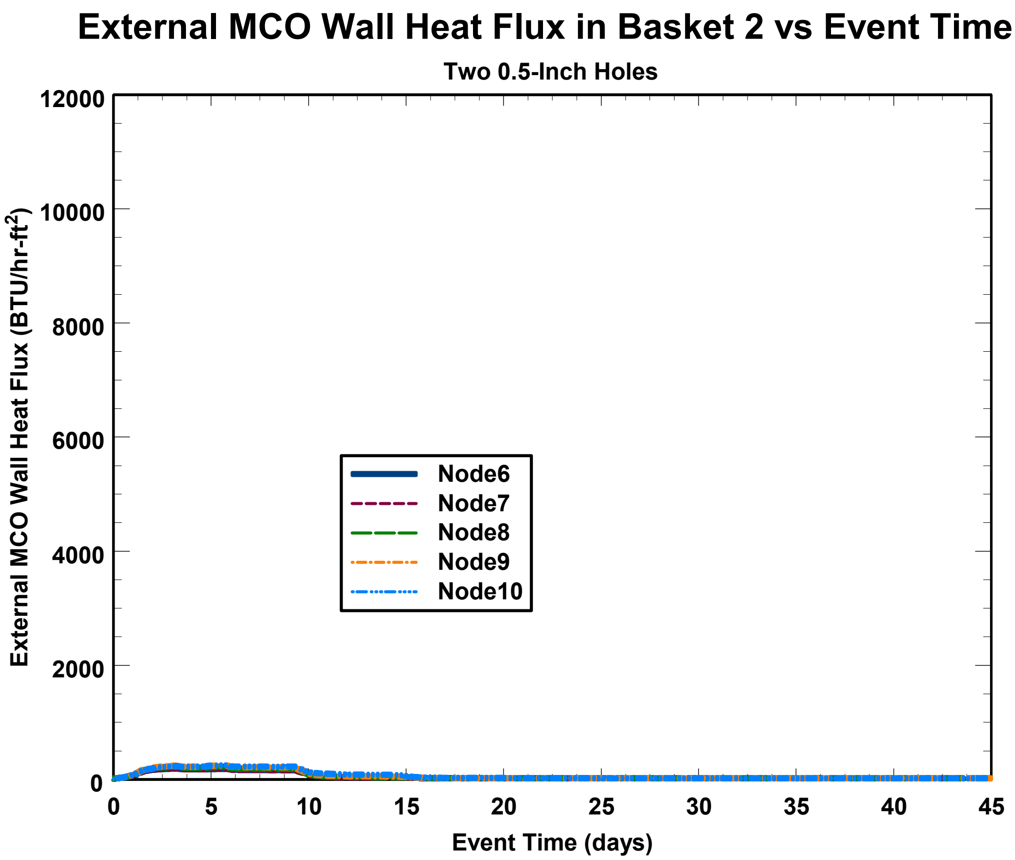

Figure 17. External MCO wall heat flux at nodes in Basket 2 for two 0.5-inch hole breach.

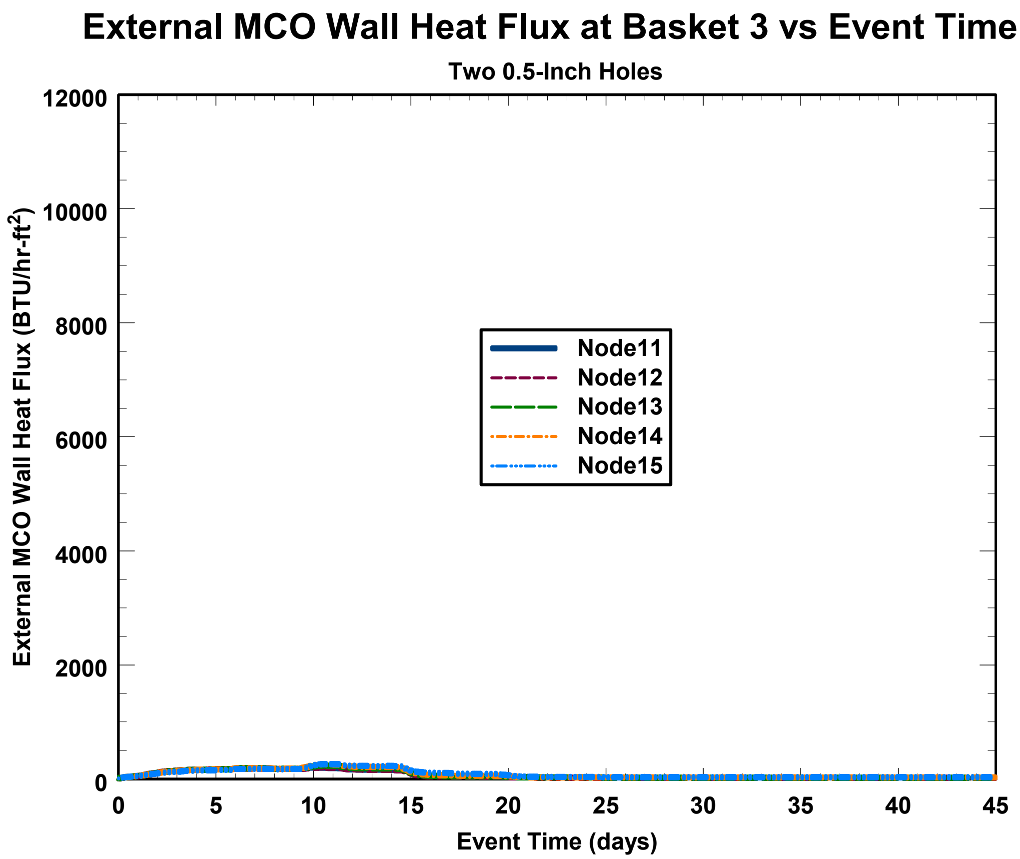

Figure 18. External MCO wall heat flux at nodes in Basket 3 for two 0.5-inch hole breach.

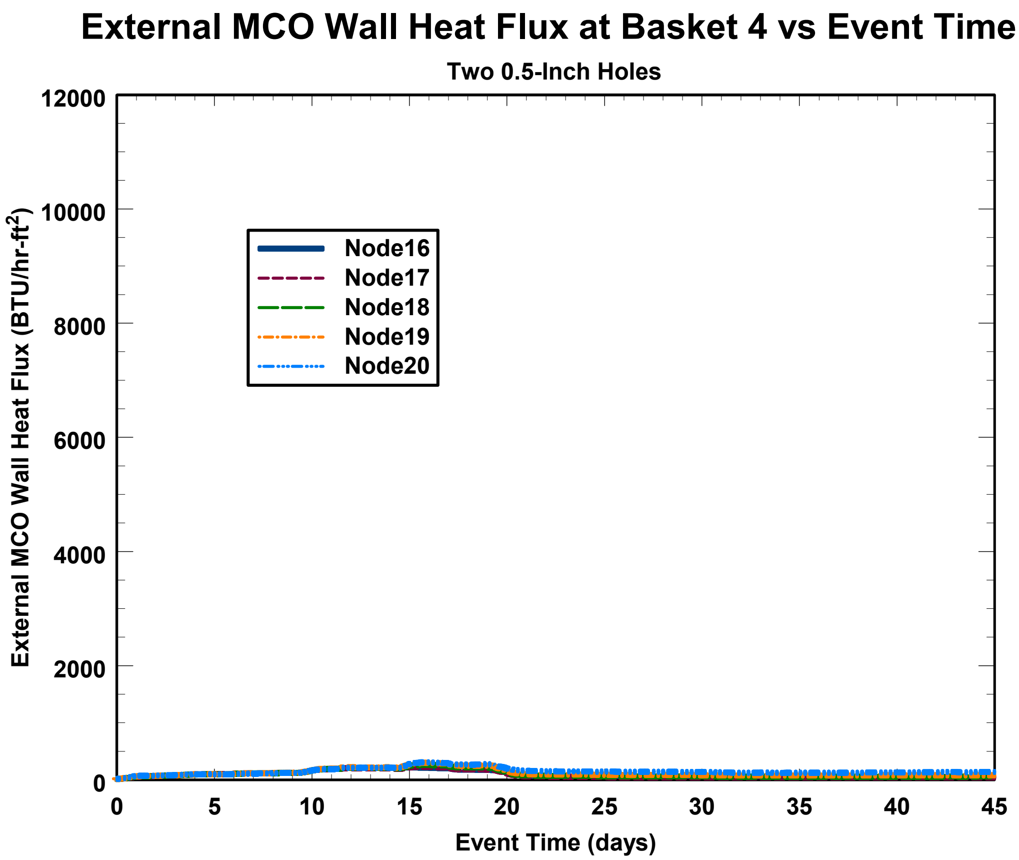

Figure 19. External MCO wall heat flux at nodes in Basket 4 for two 0.5-inch hole breach.

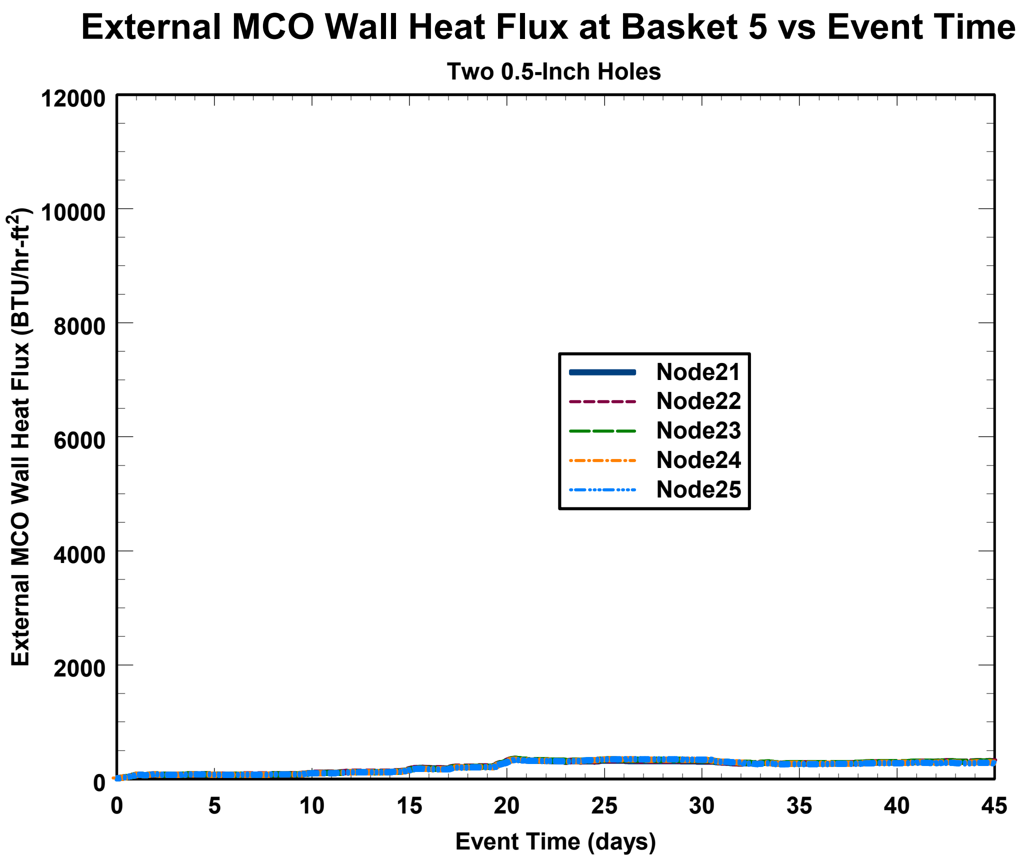

Figure 20. External MCO wall heat flux at nodes in Basket 5 for two 0.5-inch hole breach.

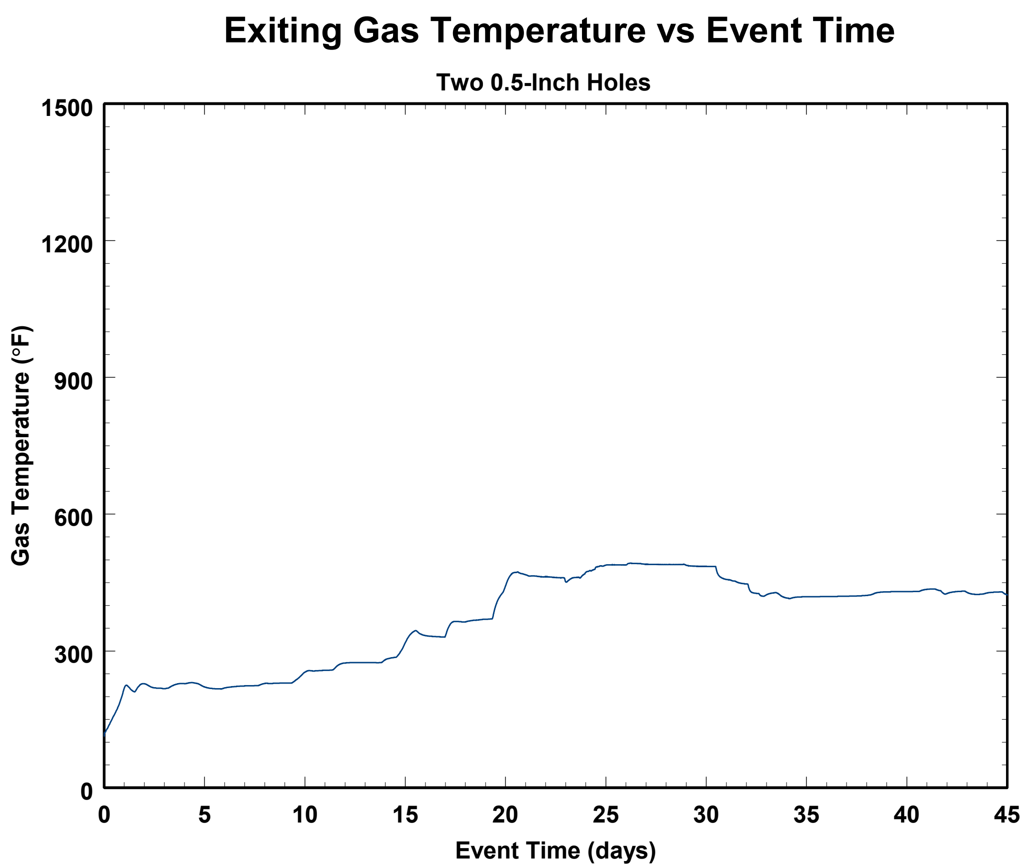

Figure 21. Exiting gas temperature from upper hole for two 0.5-inch hole breach.

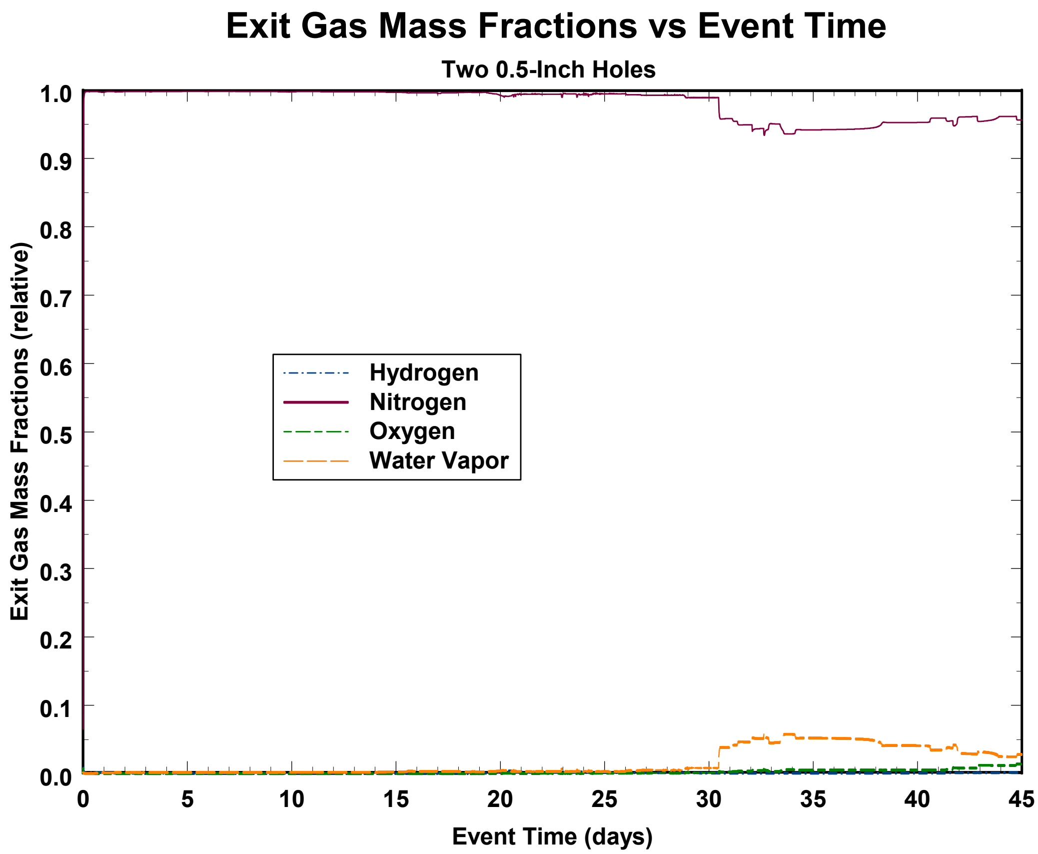

Figure 22. Relative concentration of gas species exiting upper hole for two 0.5-inch hole breach.

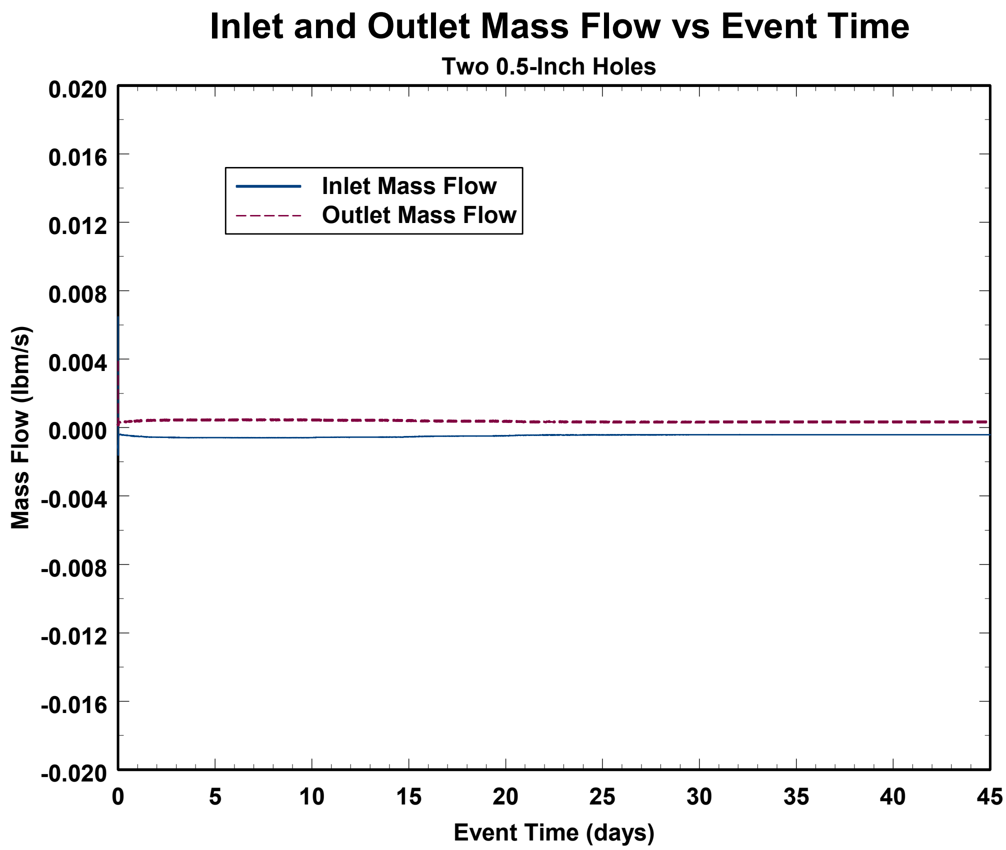

Figure 23. Mass flow at the inlet and outlet for two 0.5-inch hole breach.

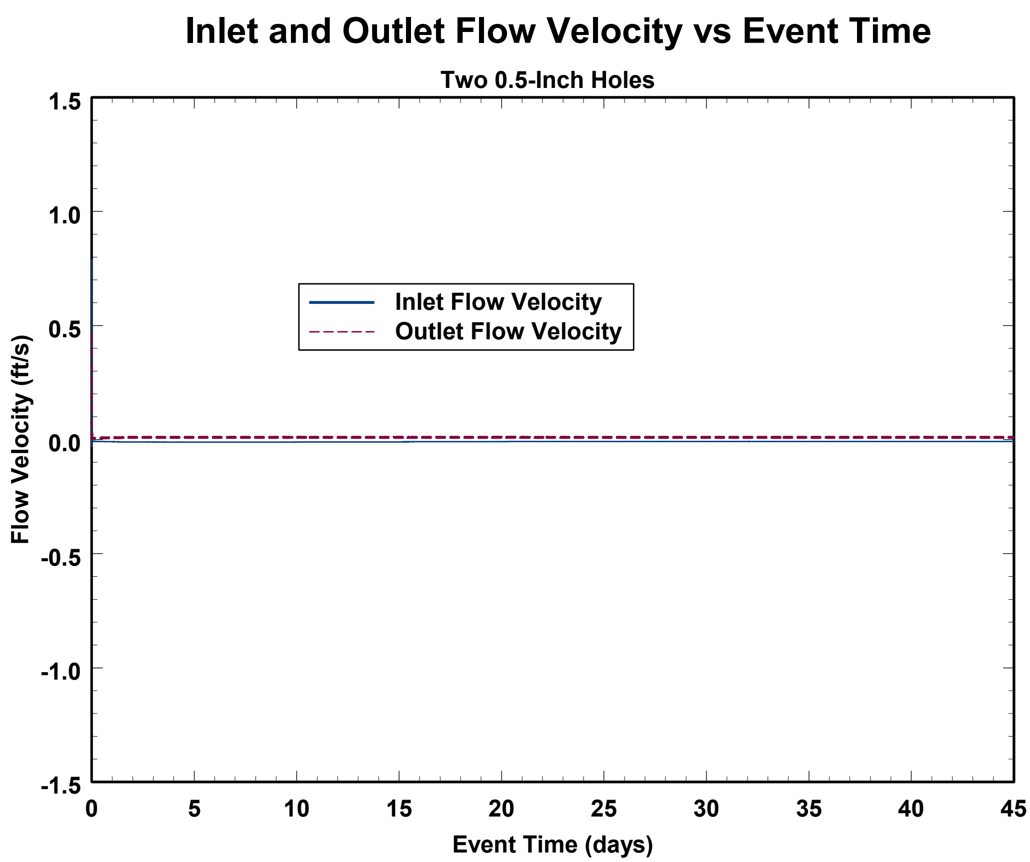

Figure 24. Flow velocity at the inlet and outlet for two 0.5-inch hole breach.

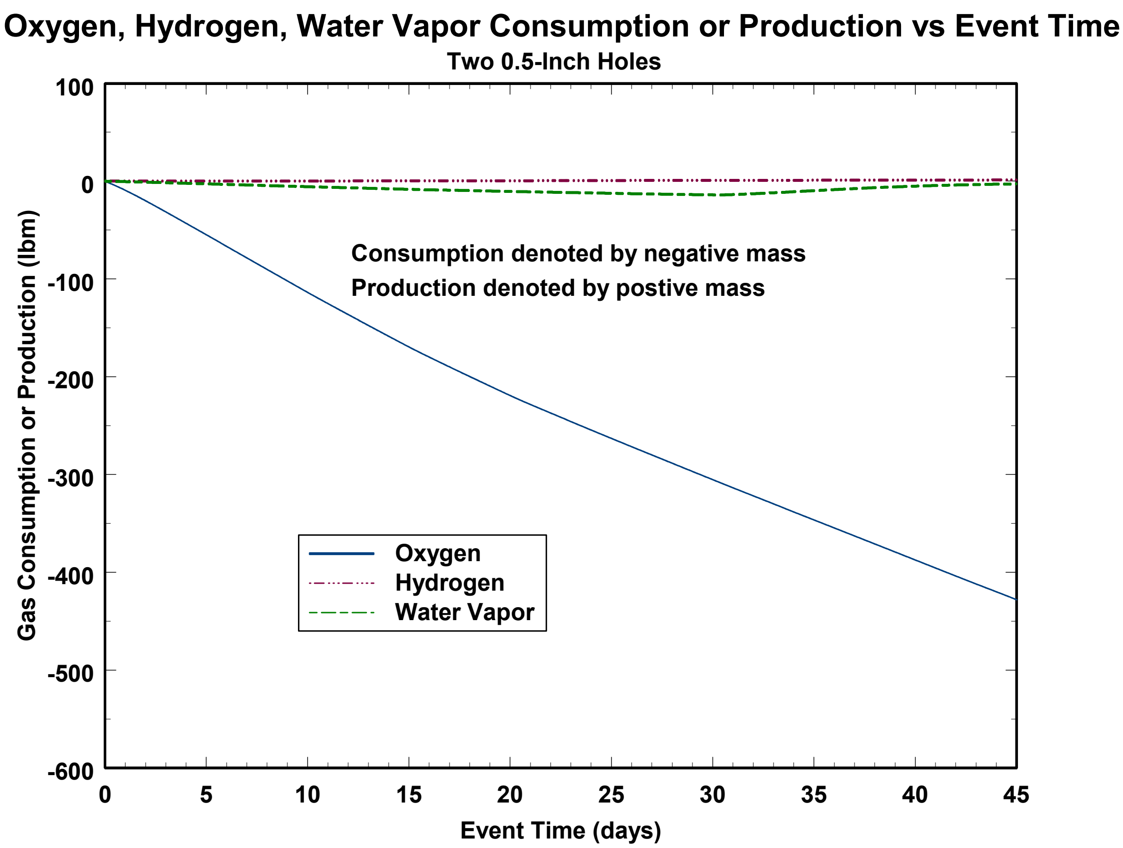

Figure 25. Oxygen, hydrogen, and water vapor consumption or production for two 0.5-inch hole breach.

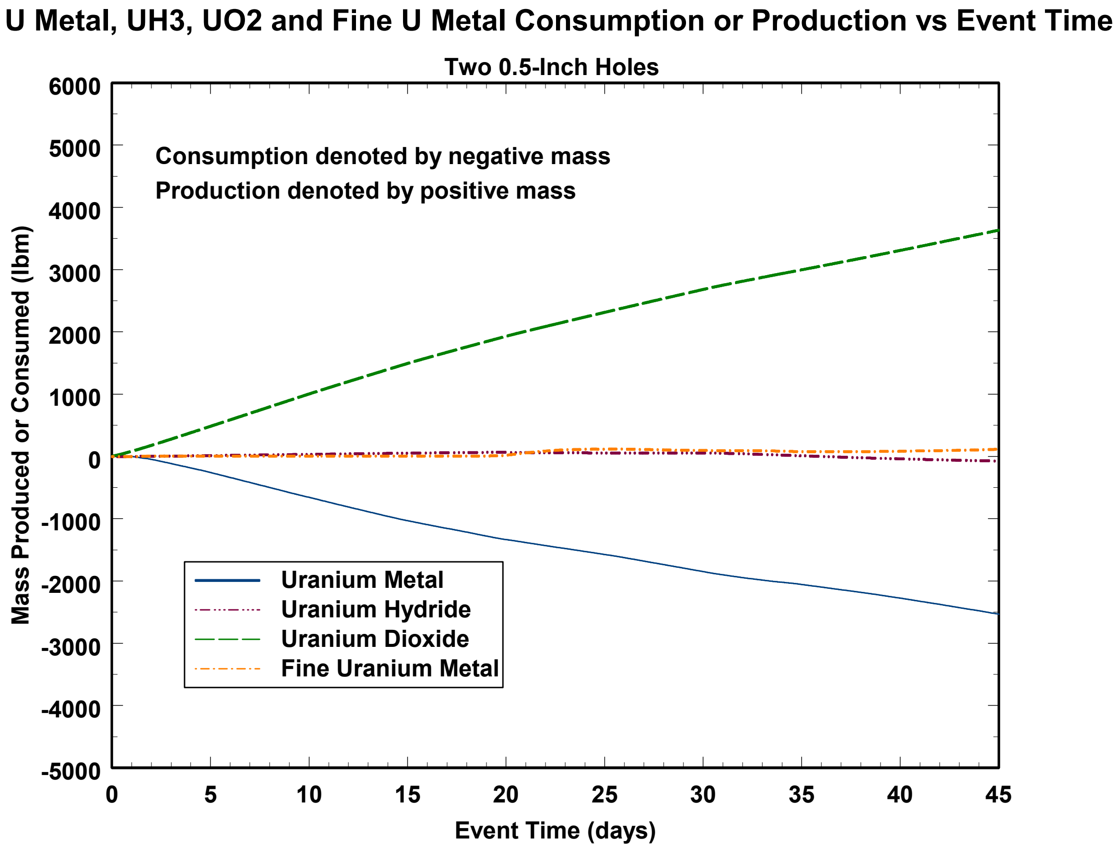

Figure 26. Uranium, uranium dioxide, uranium hydride, and fine uranium metal consumption or production for two 0.5-inch hole breach.

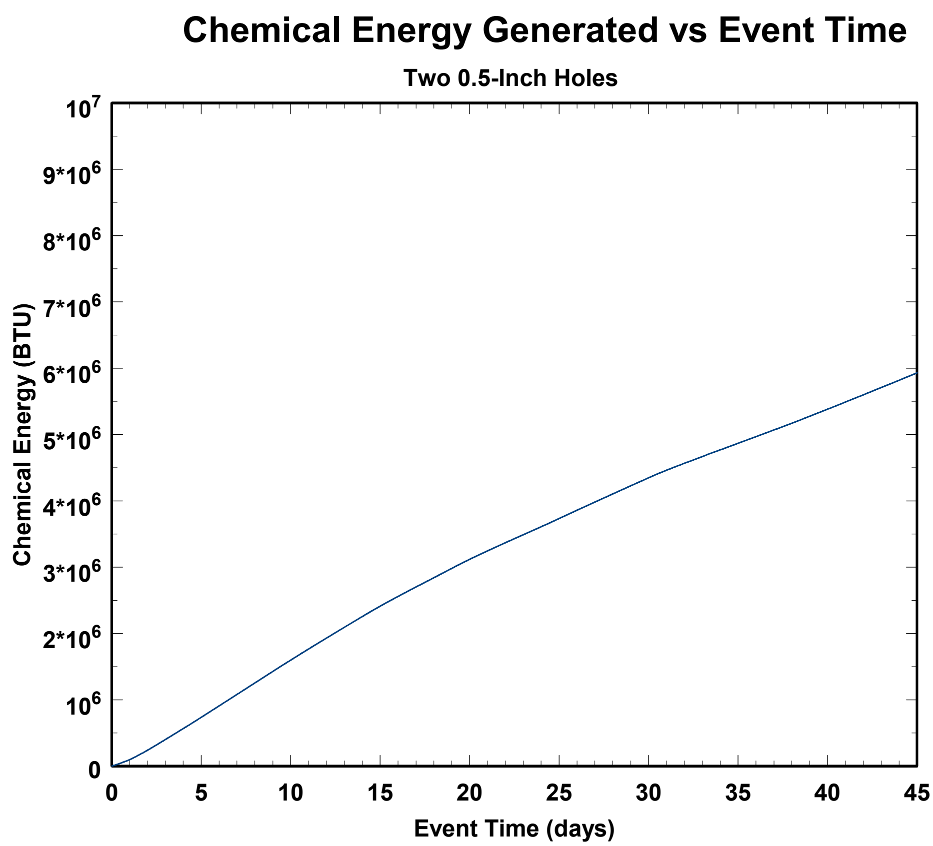

Figure 27. Chemical energy output for two 0.5-inch hole breach.

2.1.3 Two 0.75-inch Holes

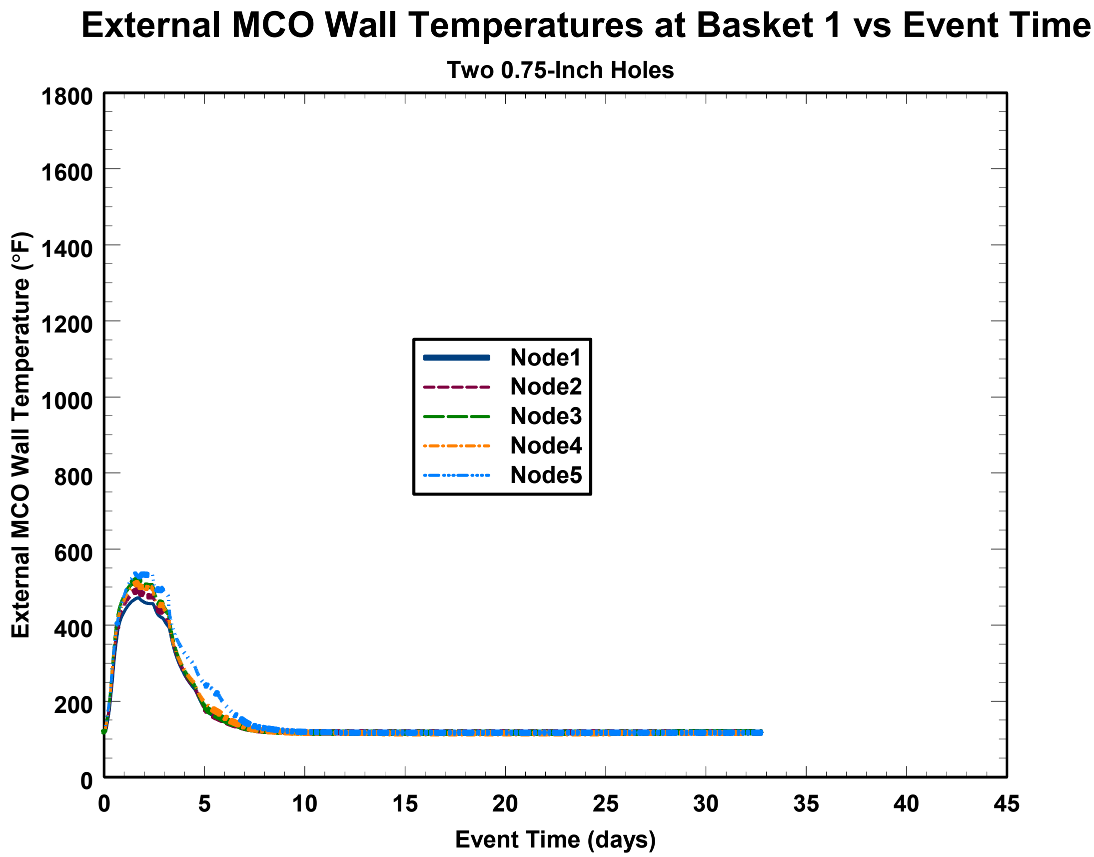

Figure 28. External MCO wall temperatures at nodes in Basket 1 for two 0.75-inch hole breach.

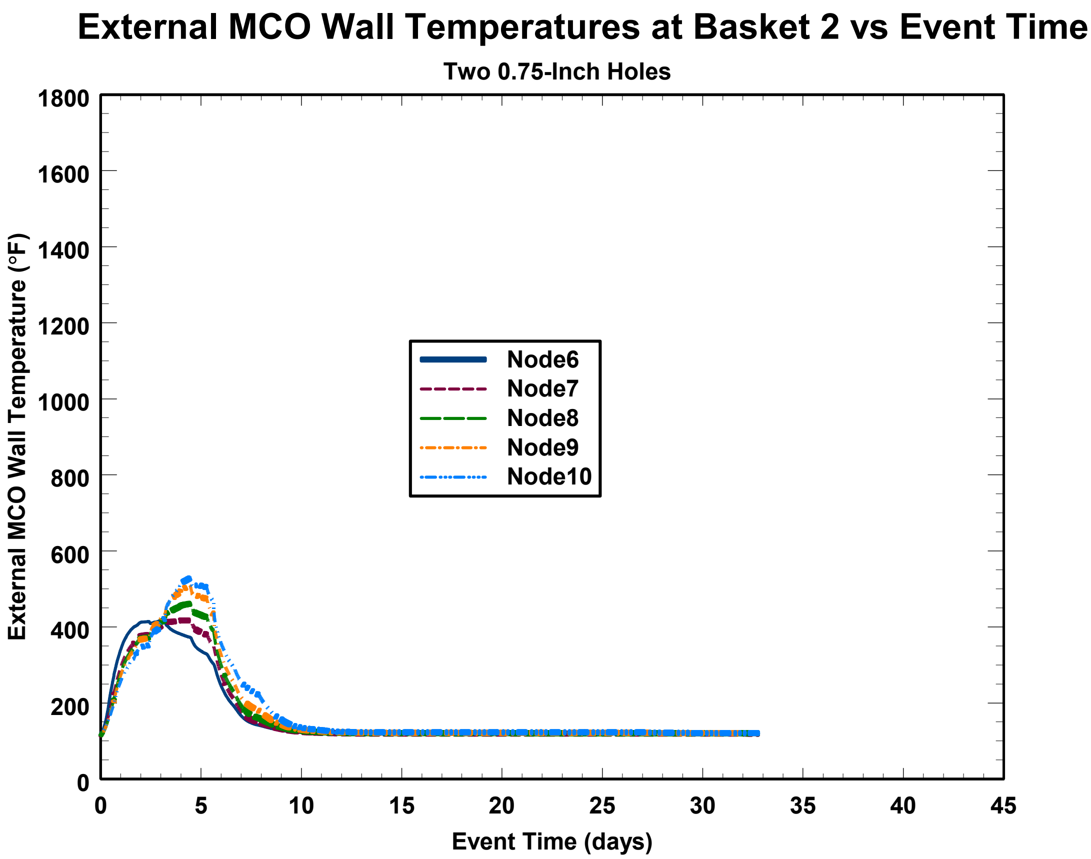

Figure 29. External MCO wall temperatures at nodes in Basket 2 for two 0.75-inch hole breach.

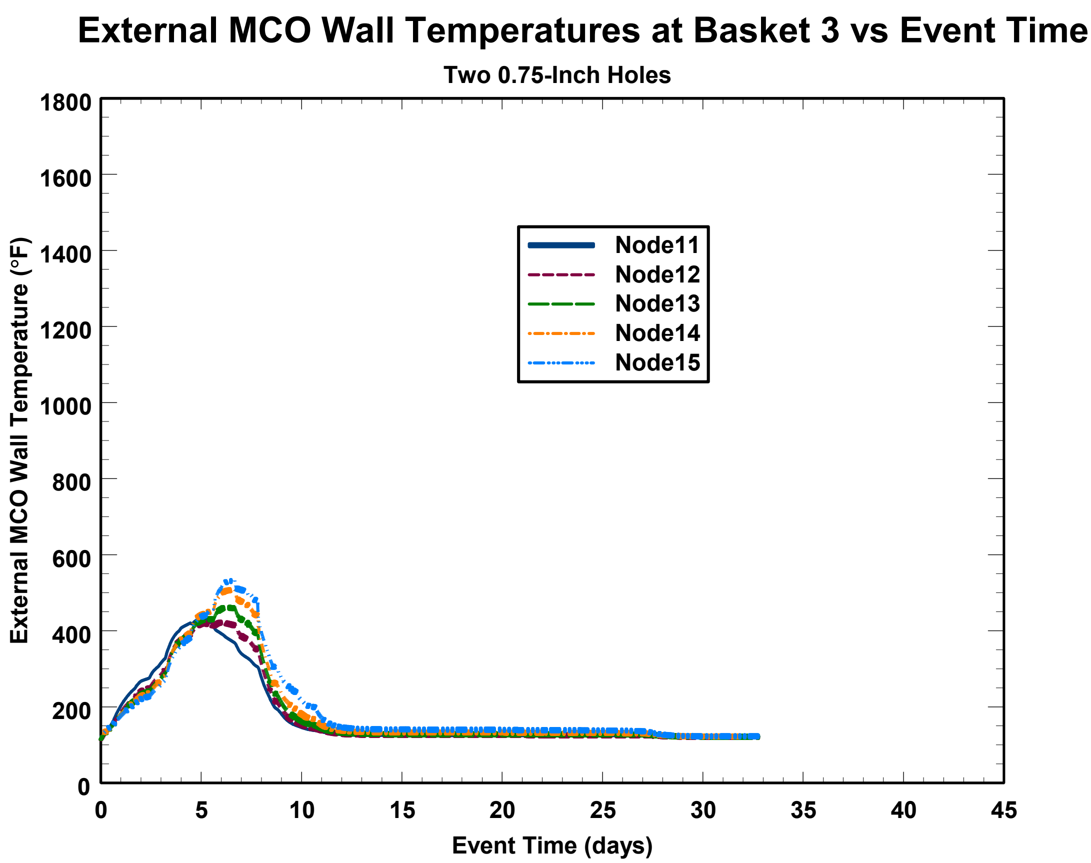

Figure 30. External MCO wall temperatures at nodes in Basket 3 for two 0.75-inch hole breach.

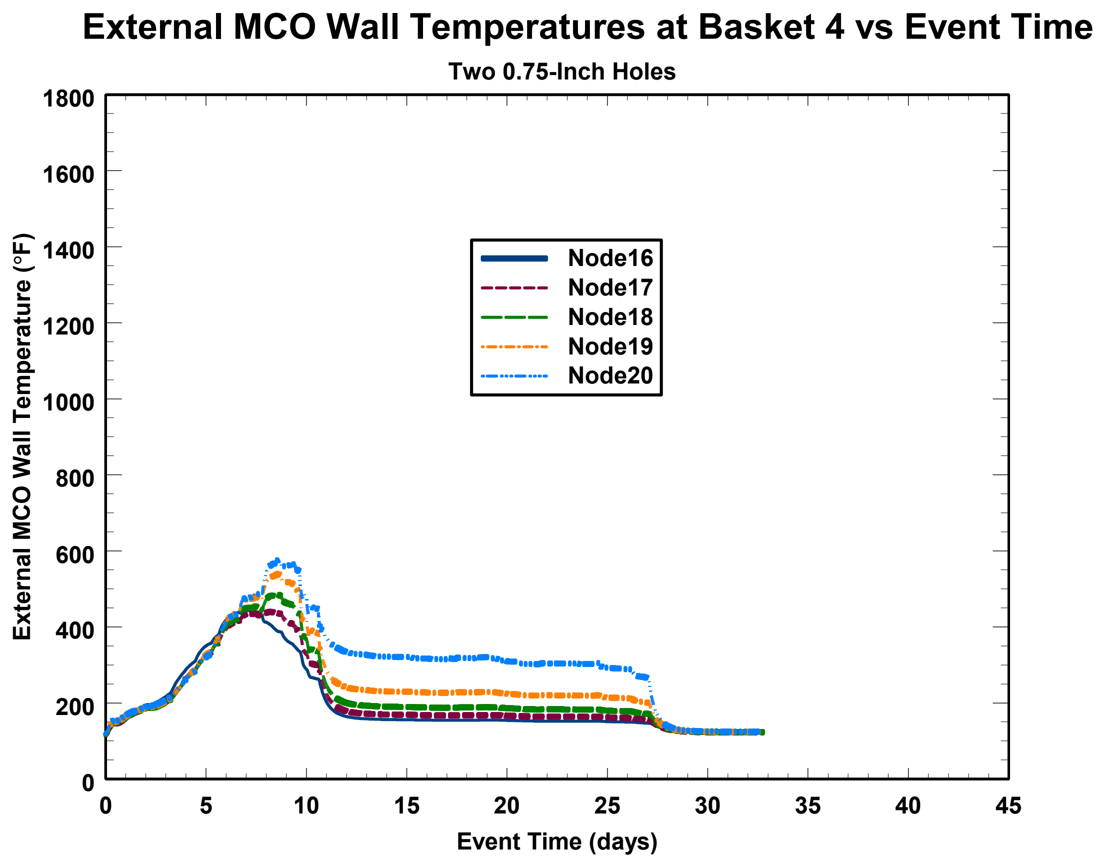

Figure 31. External MCO wall temperatures at nodes in Basket 4 for two 0.75-inch hole breach.

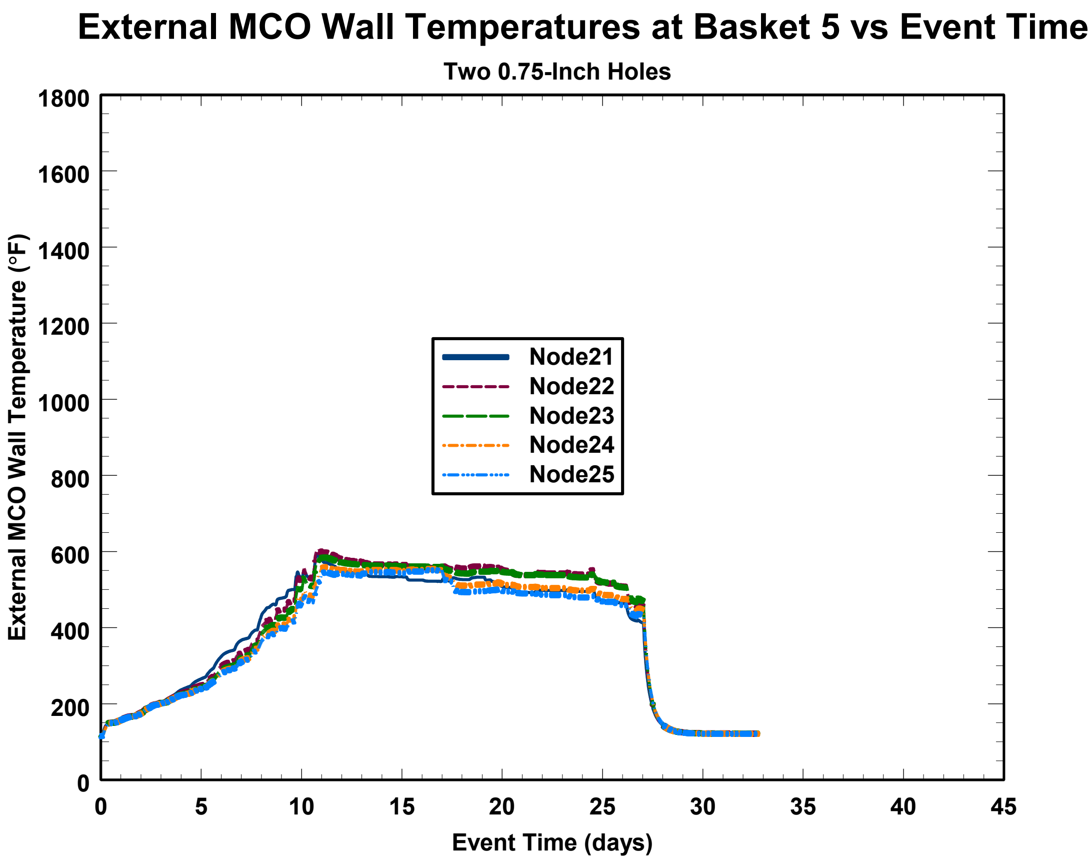

Figure 32. External MCO wall temperatures at nodes in Basket 5 for two 0.75-inch hole breach.

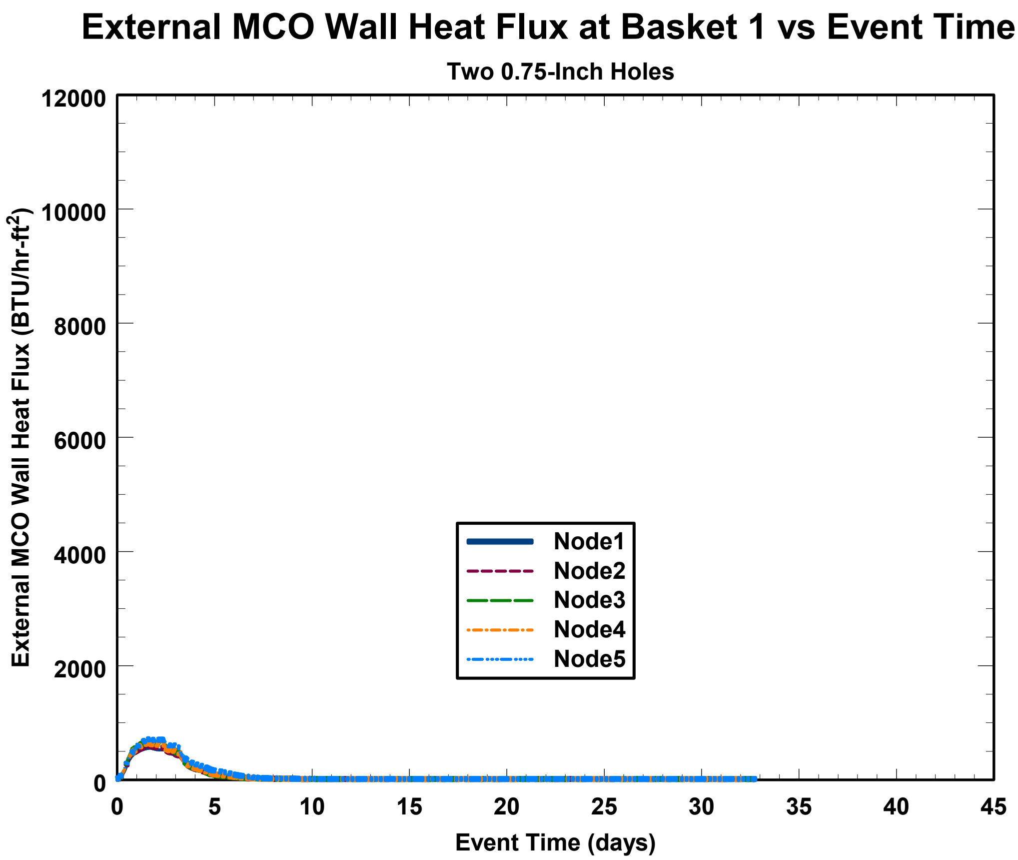

Figure 33. External MCO wall heat flux at nodes in Basket 1 for two 0.75-inch hole breach.

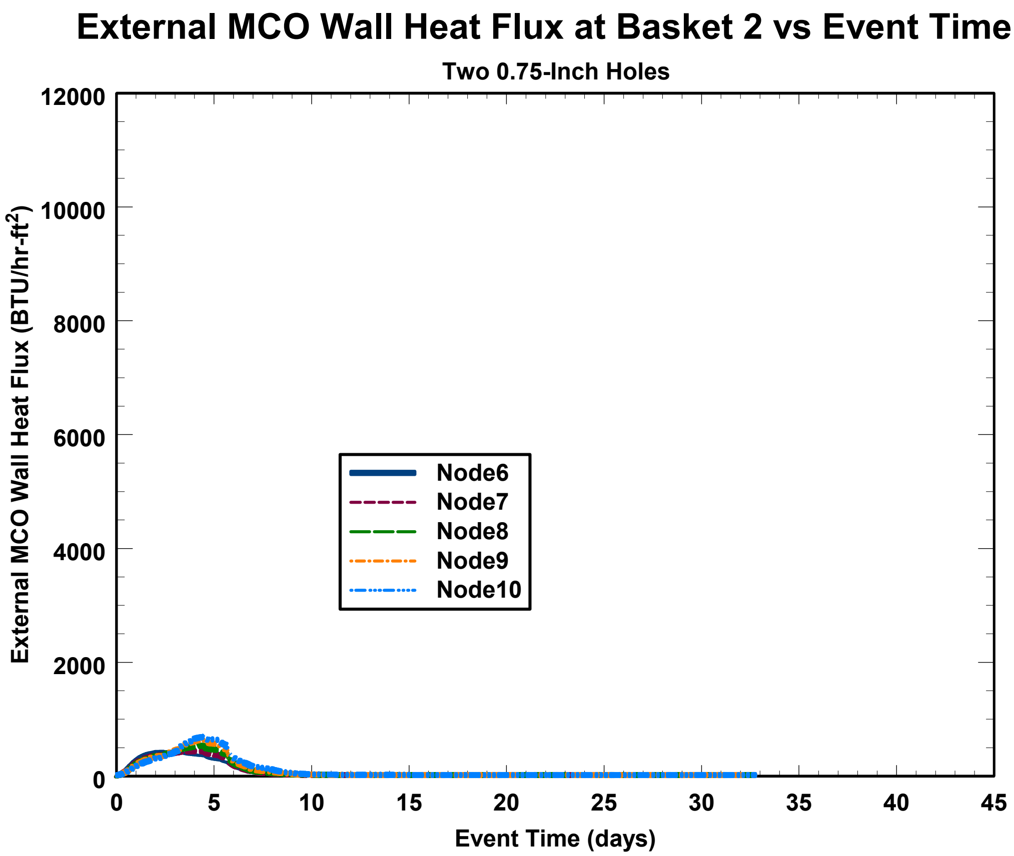

Figure 34. External MCO wall heat flux at nodes in Basket 2 for two 0.75-inch hole breach.

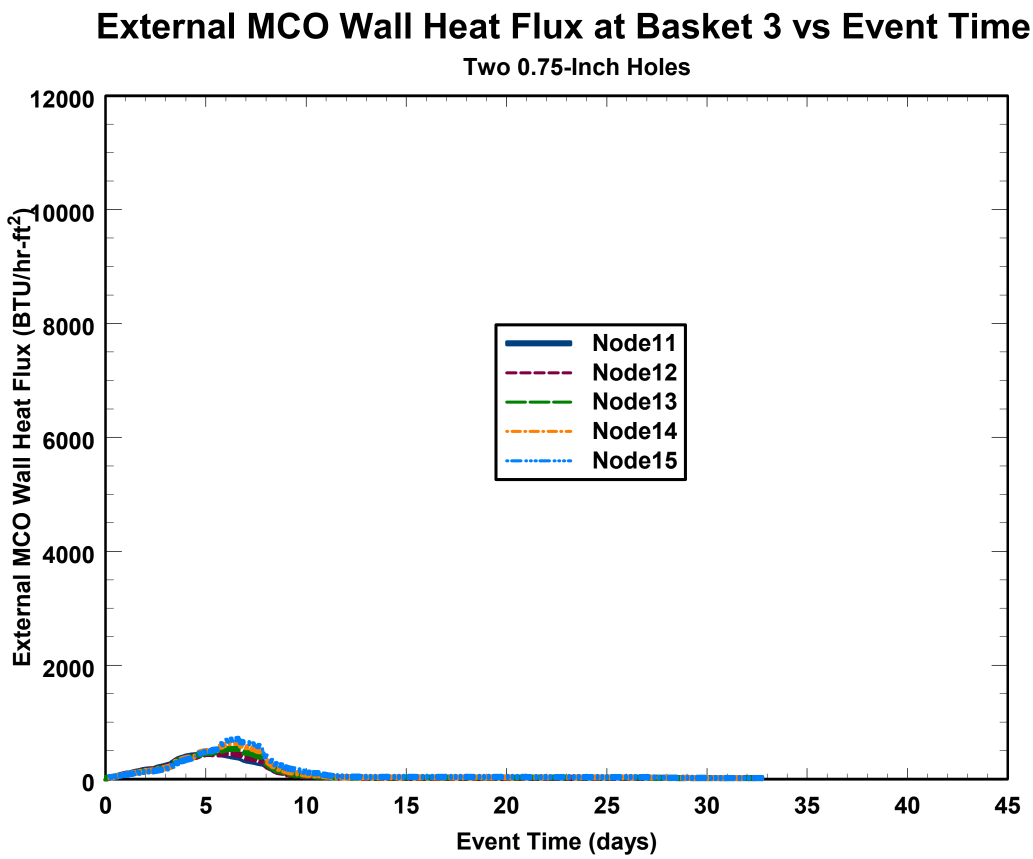

Figure 35. External MCO wall heat flux at nodes in Basket 3 for two 0.75-inch hole breach.

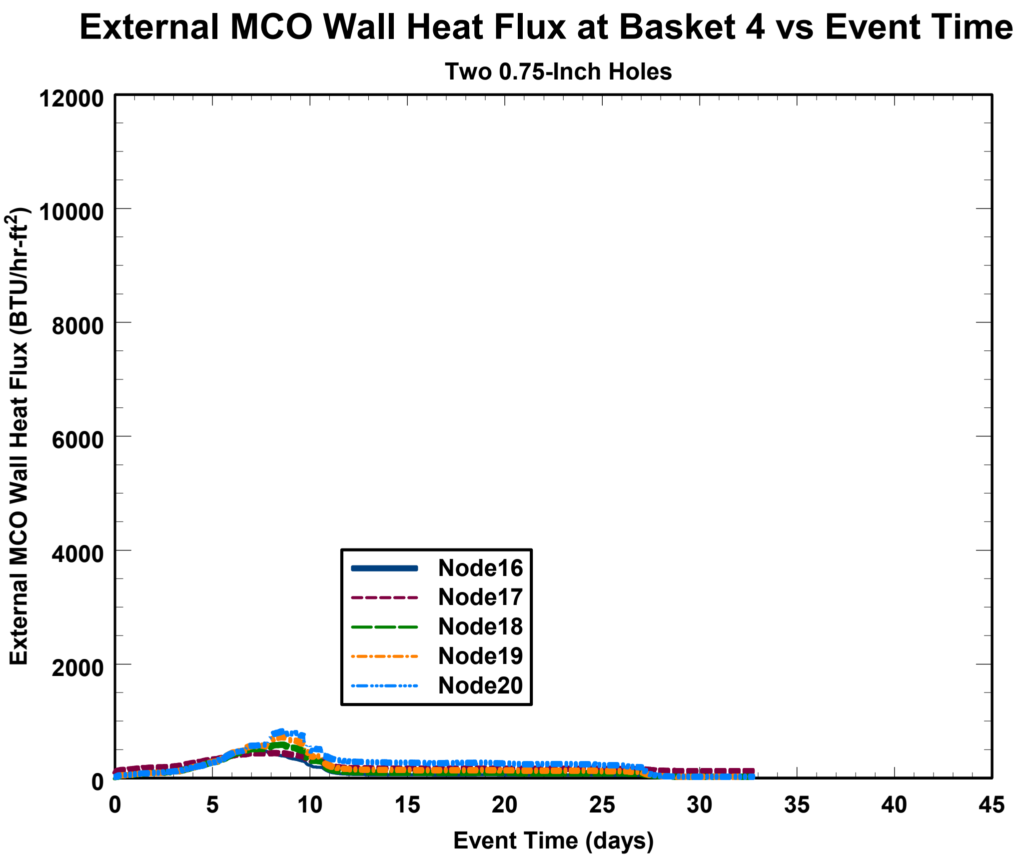

Figure 36. External MCO wall heat flux at nodes in Basket 4 for two 0.75-inch hole breach.

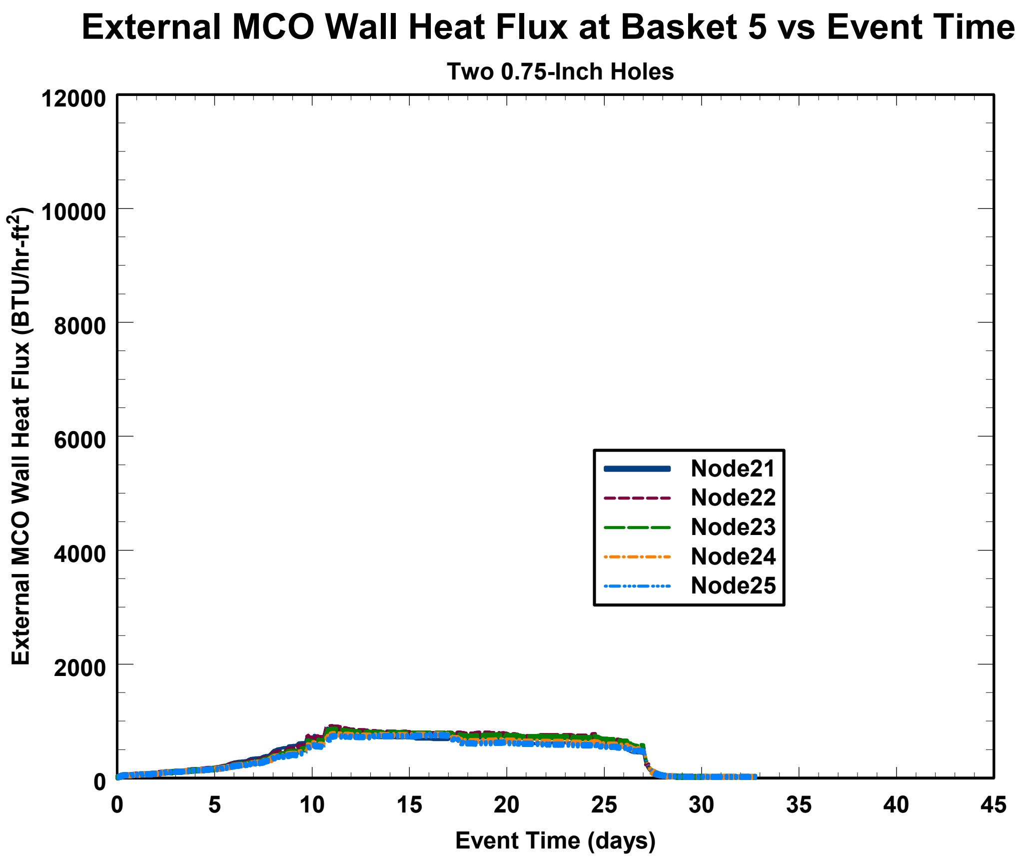

Figure 37. External MCO wall heat flux at nodes in Basket 5 for two 0.75-inch hole breach.

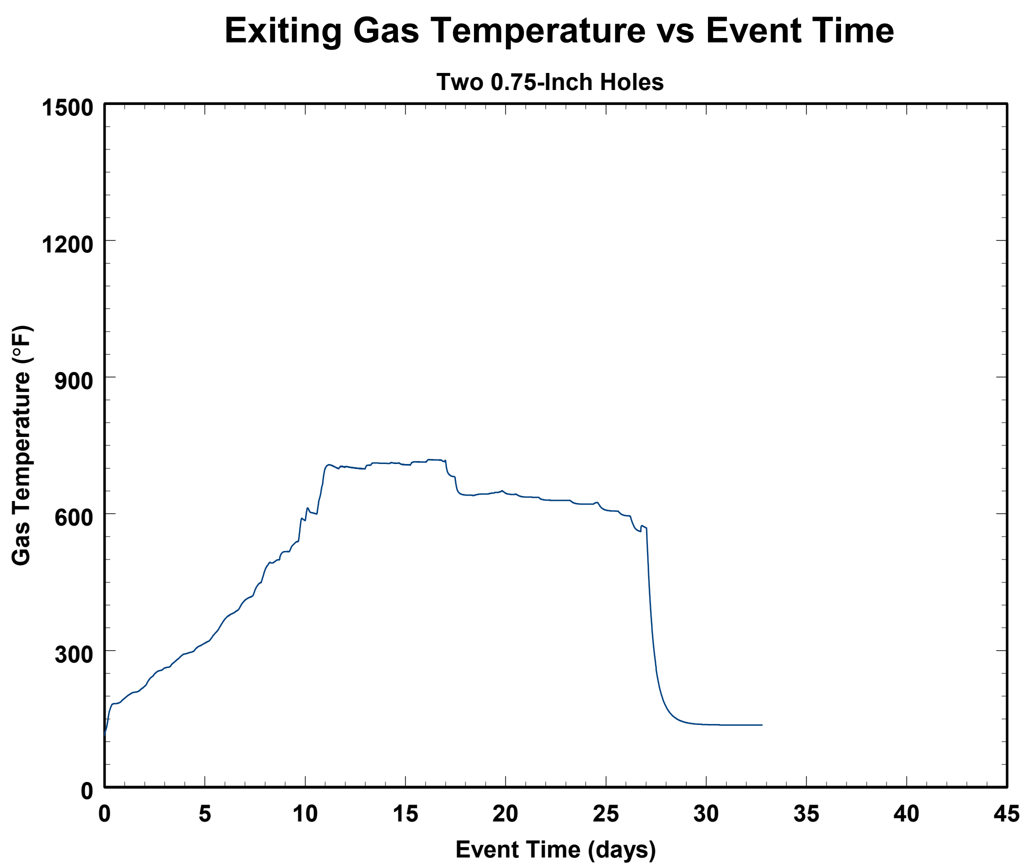

Figure 38. Exiting gas temperature from upper hole for two 0.75-inch hole breach.

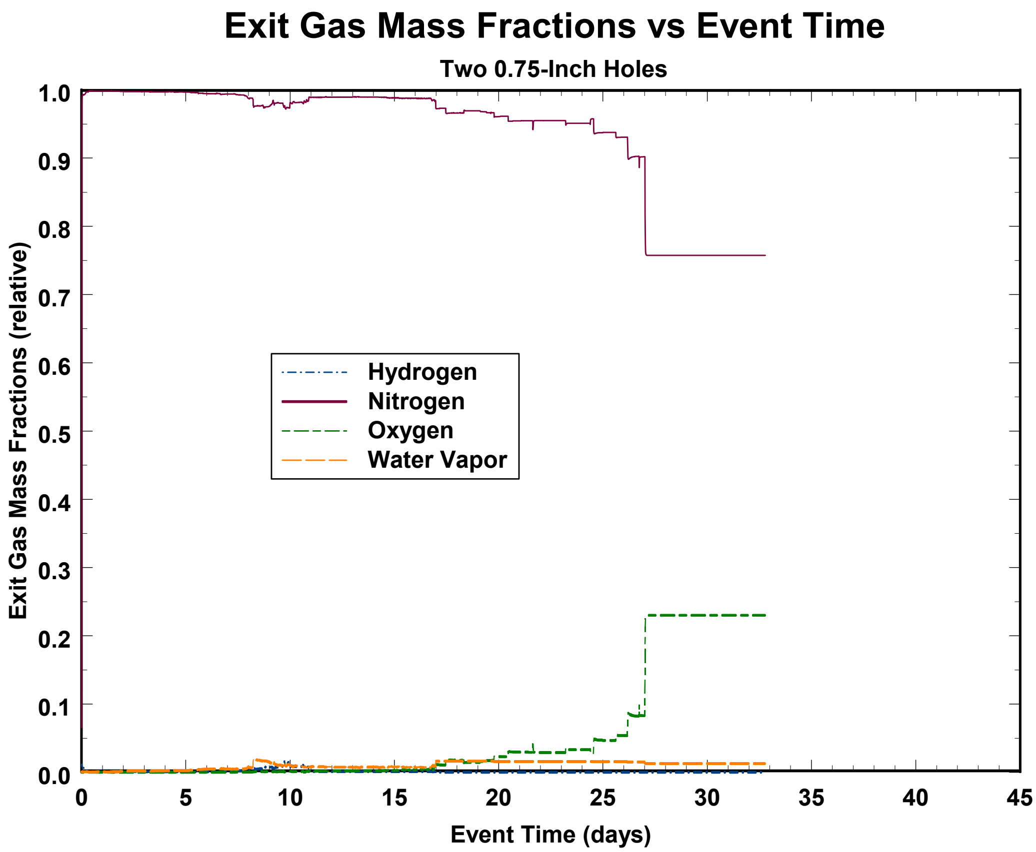

Figure 39. Relative concentration of gas species exiting upper hole for two 0.75-inch hole breach.

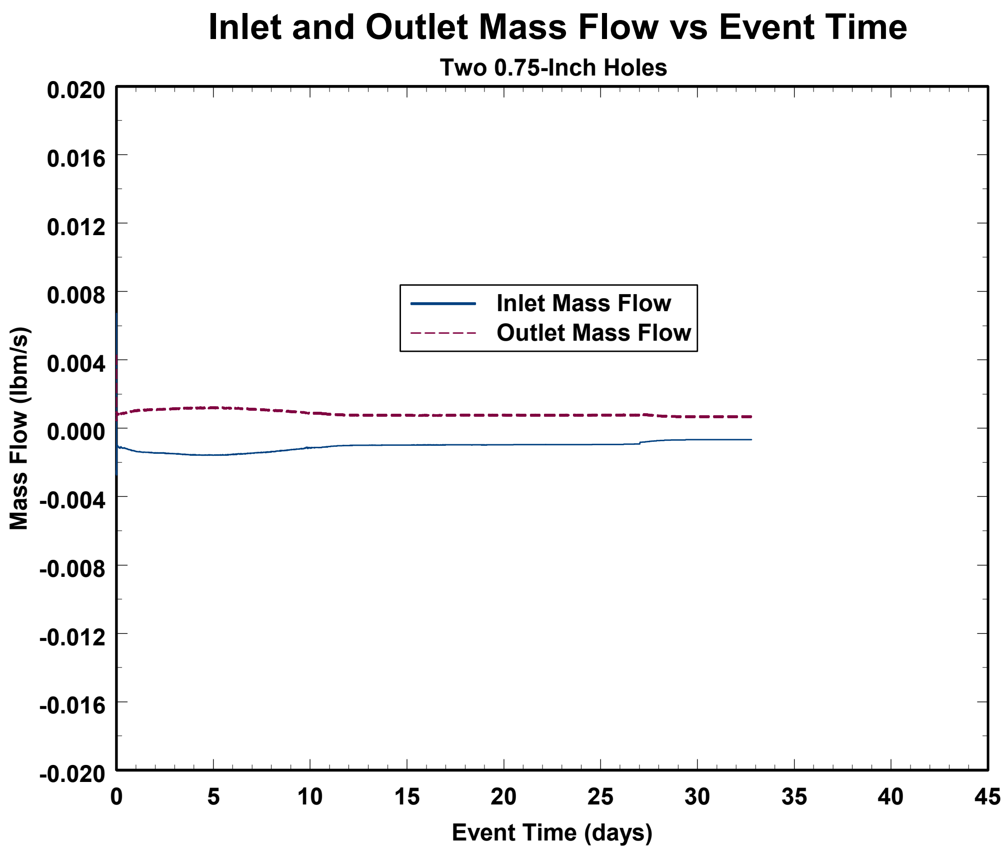

Figure 40. Mass flow at the inlet and outlet for two 0.75-inch hole breach.

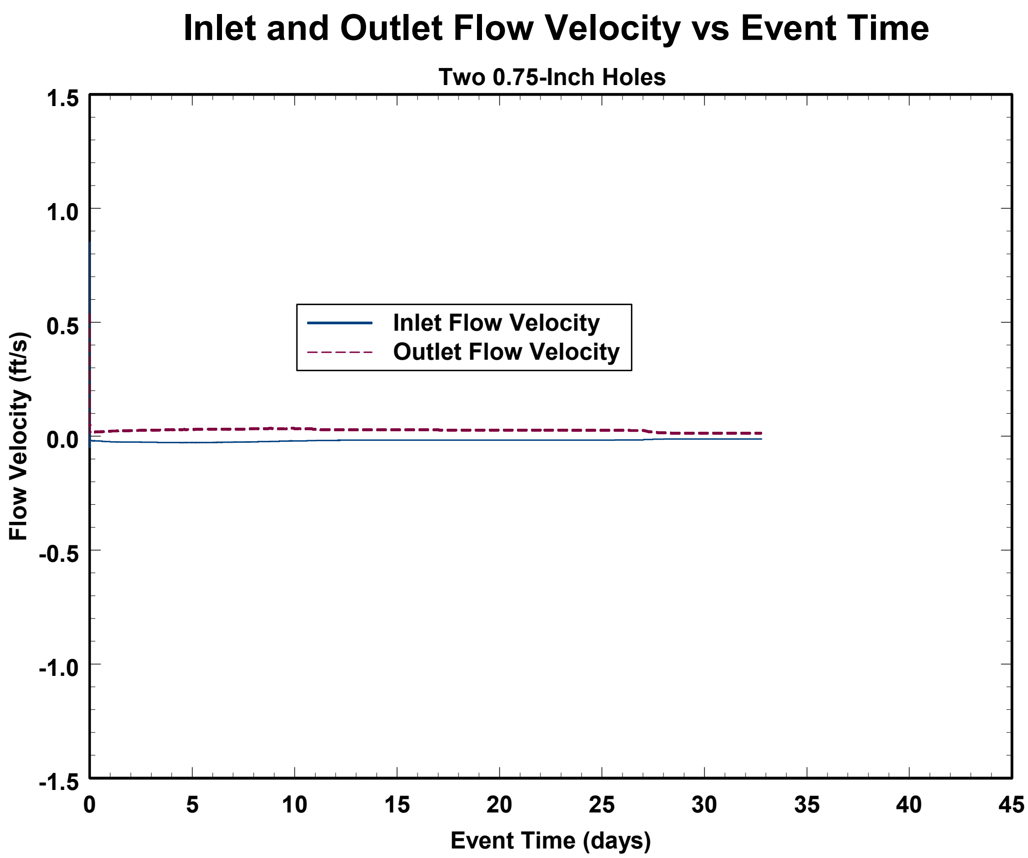

Figure 41. Flow velocity at the inlet and outlet for two 0.75-inch hole breach.

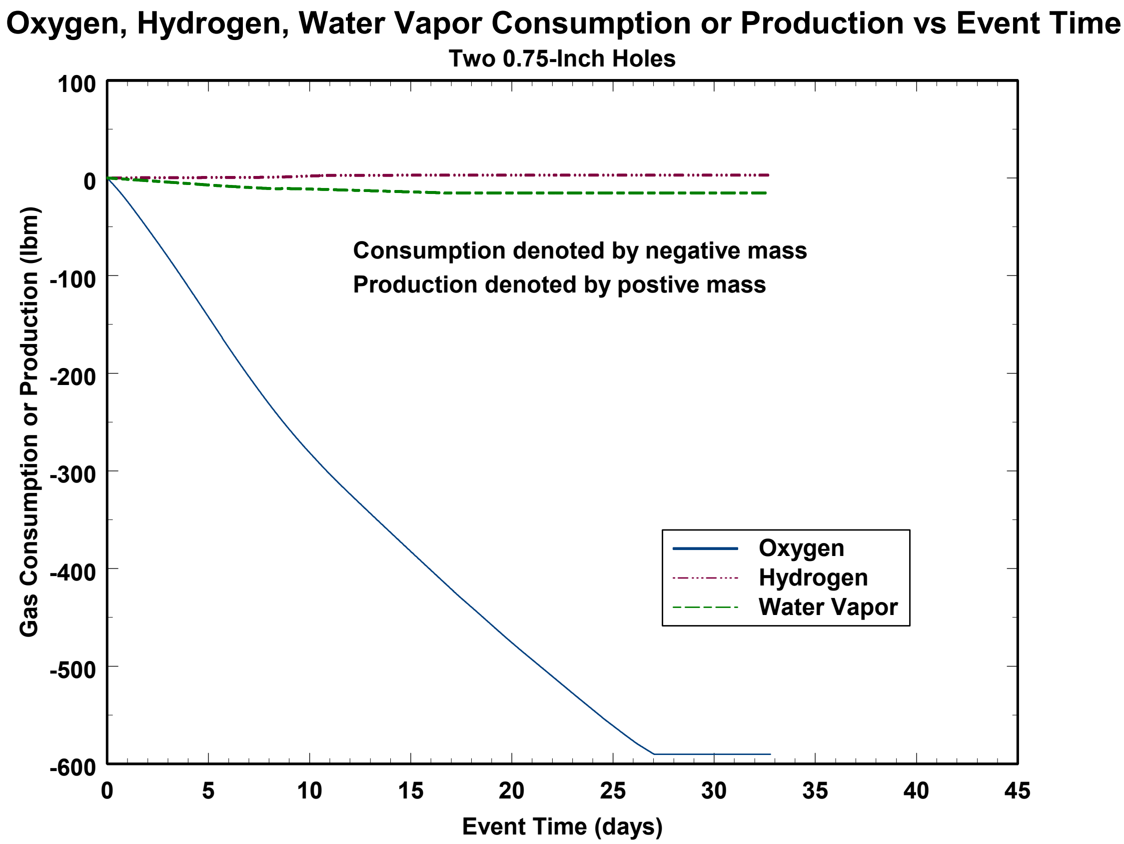

Figure 42. Oxygen, hydrogen, and water vapor consumption or production for two 0.75-inch hole breach.

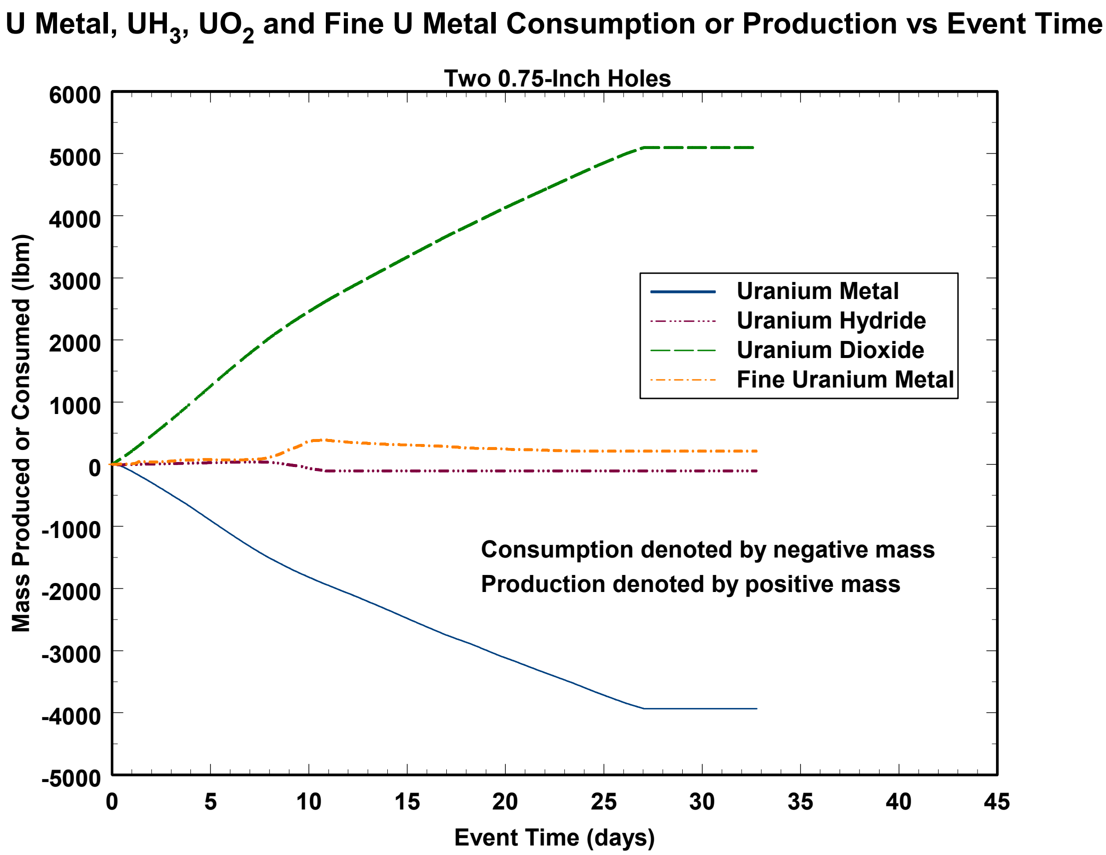

Figure 43. Uranium, uranium dioxide, uranium hydride, and fine uranium metal consumption or production for two 0.75-inch hole breach.

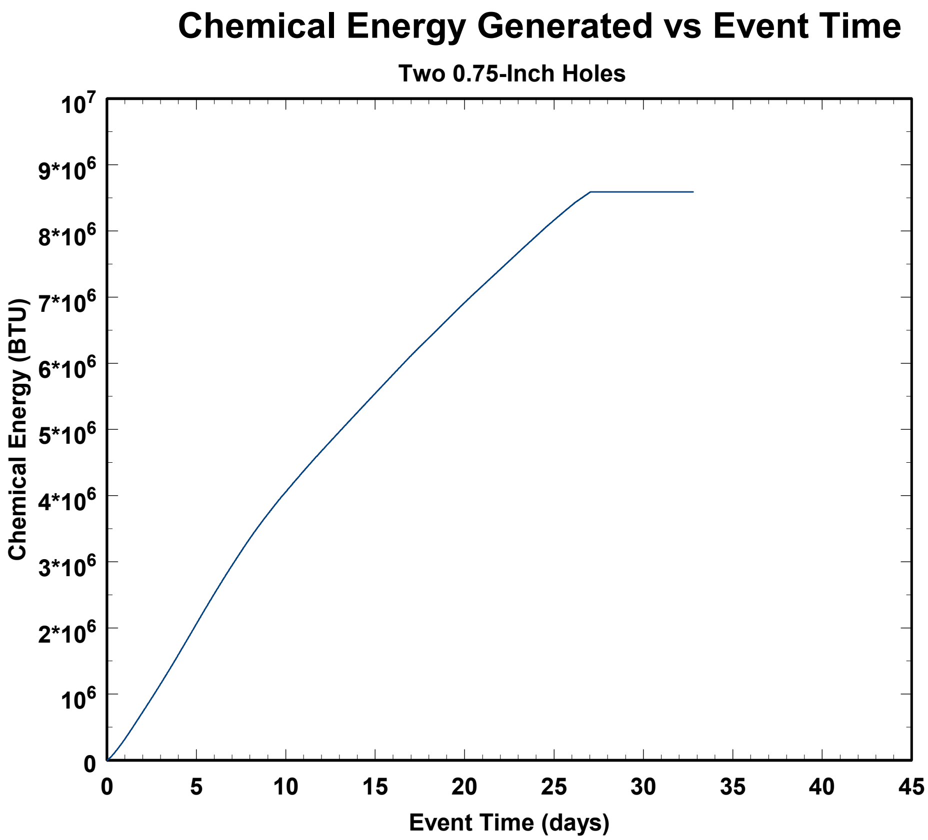

Figure 44. Chemical energy output for two 0.75-inch hole breach.

2.1.4 Two 1.0-inch Holes

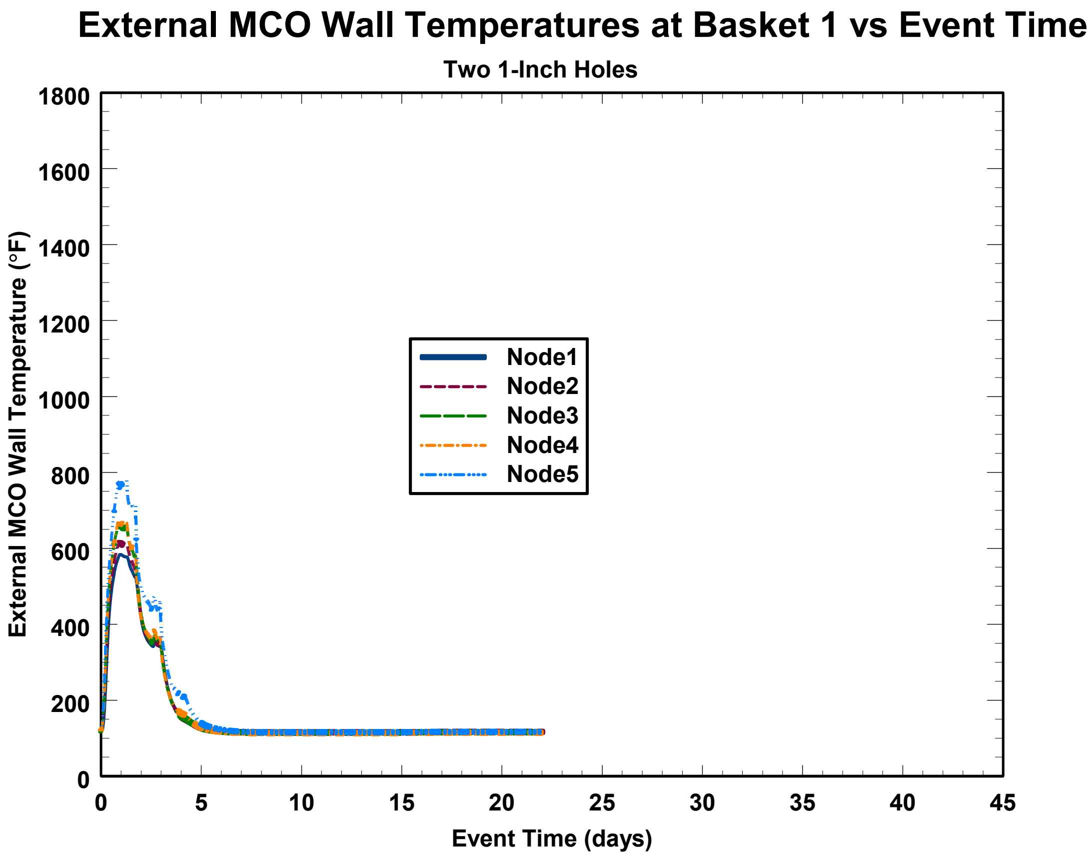

Figure 45. External MCO wall temperatures at nodes in Basket 1 for two 1.0-inch hole breach.

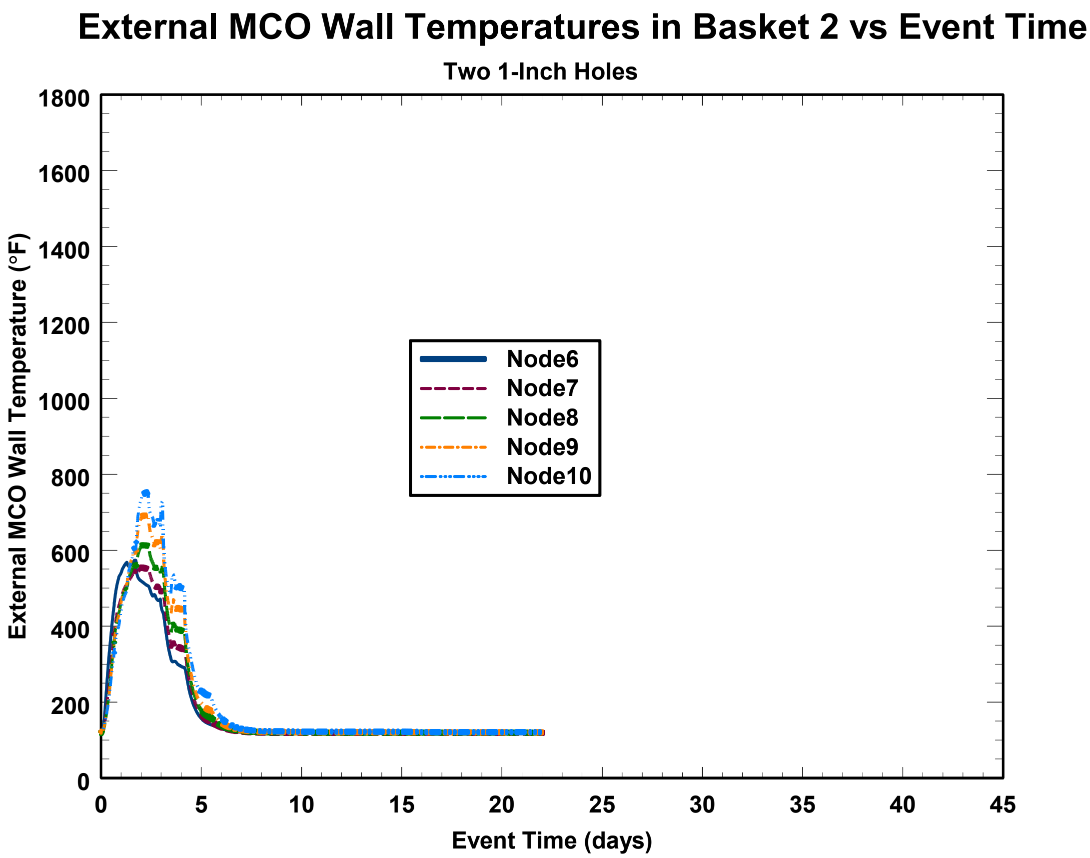

Figure 46. External MCO wall temperatures at nodes in Basket 2 for two 1.0-inch hole breach.

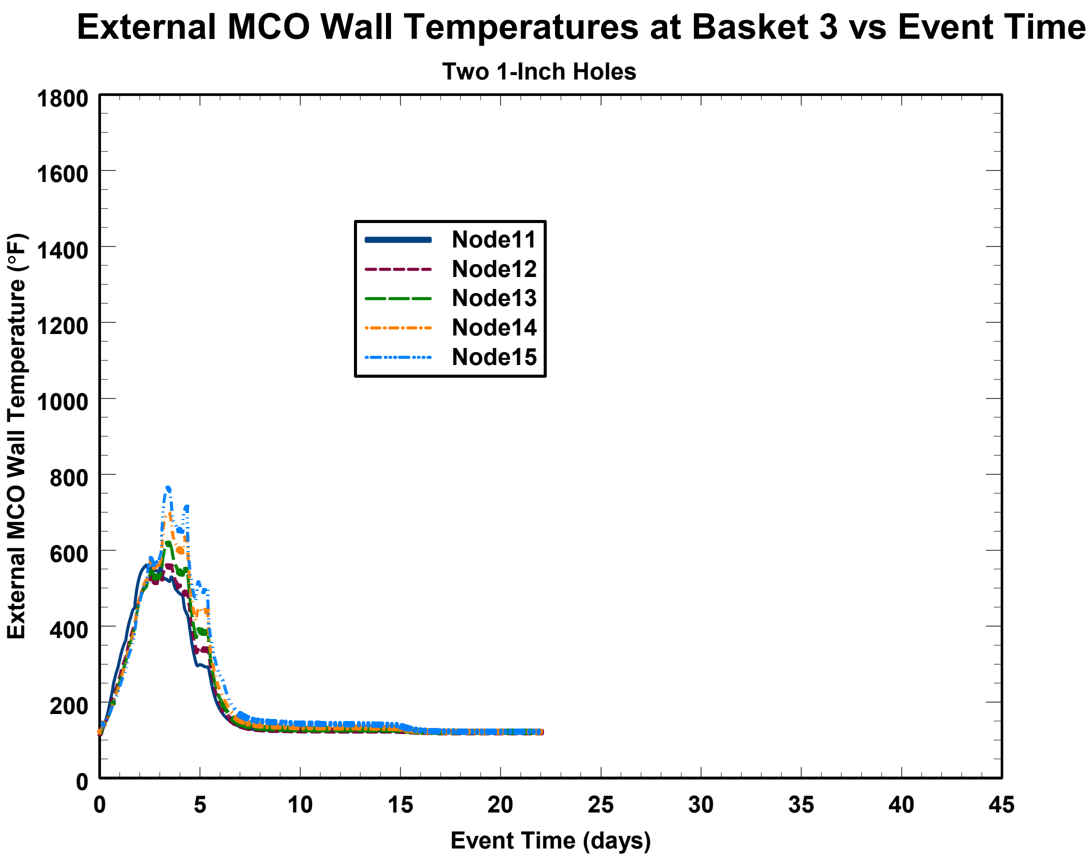

Figure 47. External MCO wall temperatures at nodes in Basket 3 for two 1.0-inch hole breach.

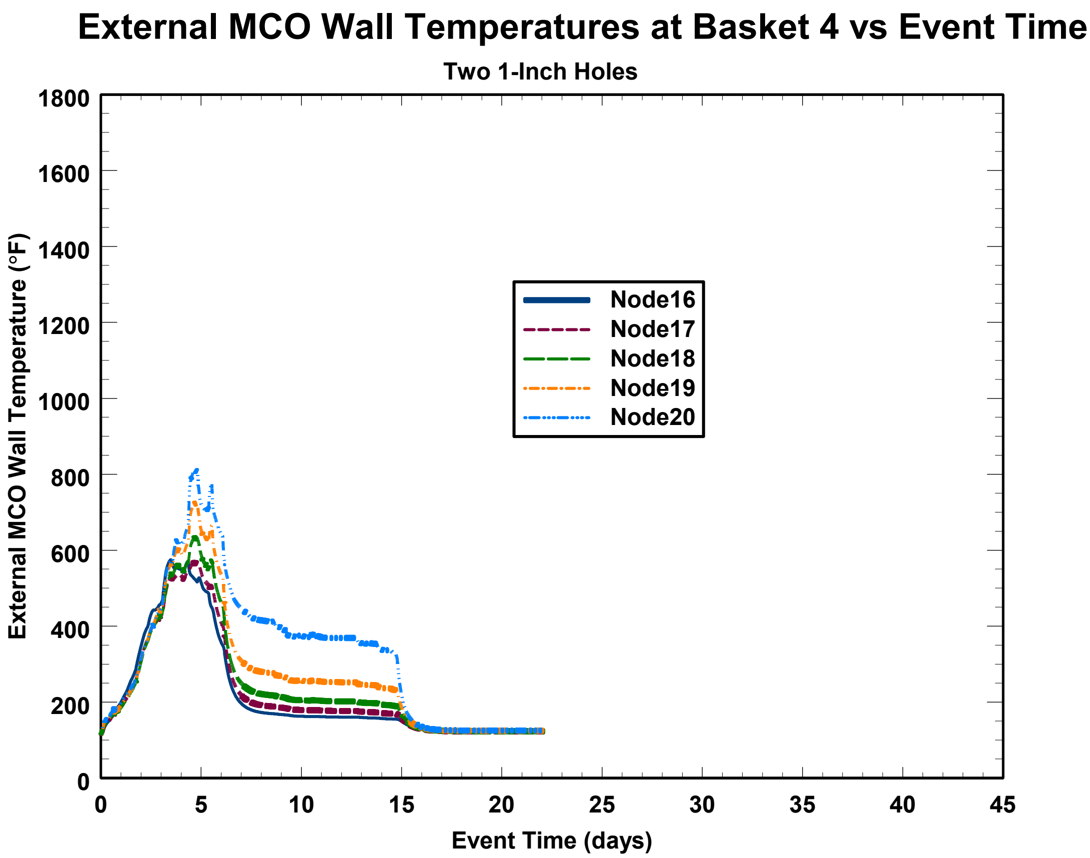

Figure 48. External MCO wall temperatures at nodes in Basket 4 for two 1.0-inch hole breach.

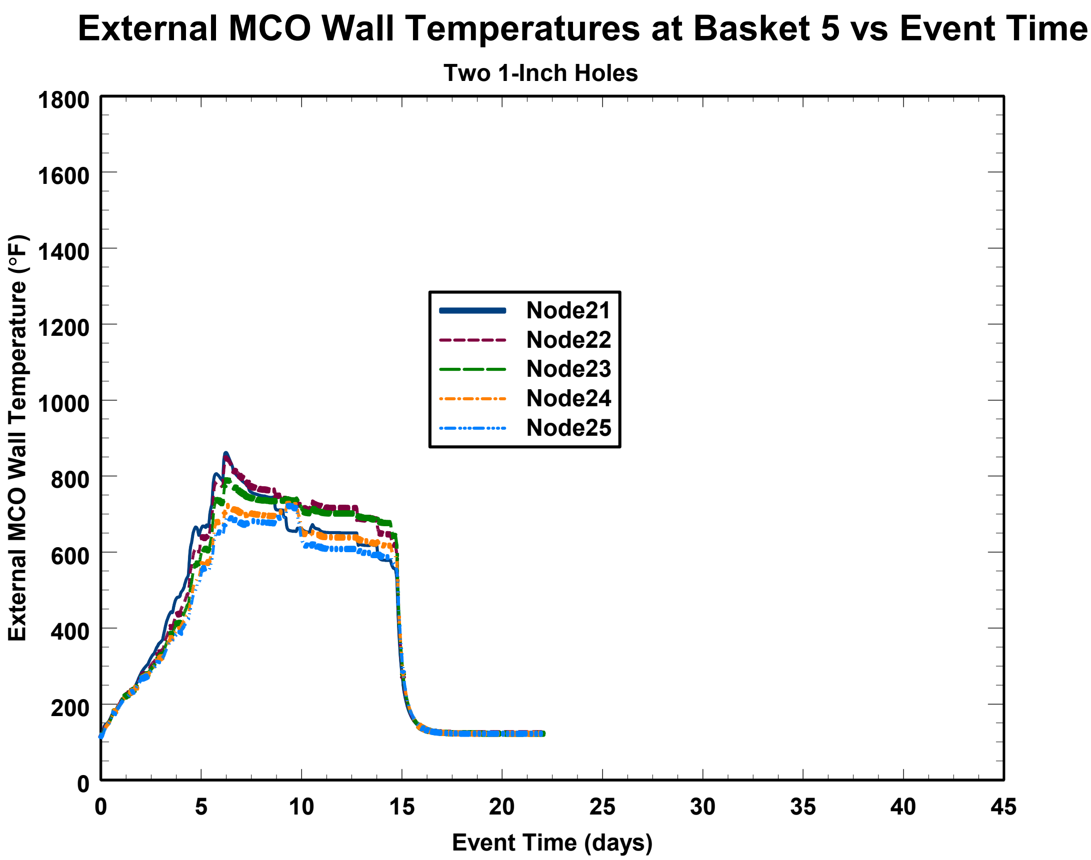

Figure 49. External MCO wall temperatures at nodes in Basket 5 for two 1.0-inch hole breach.

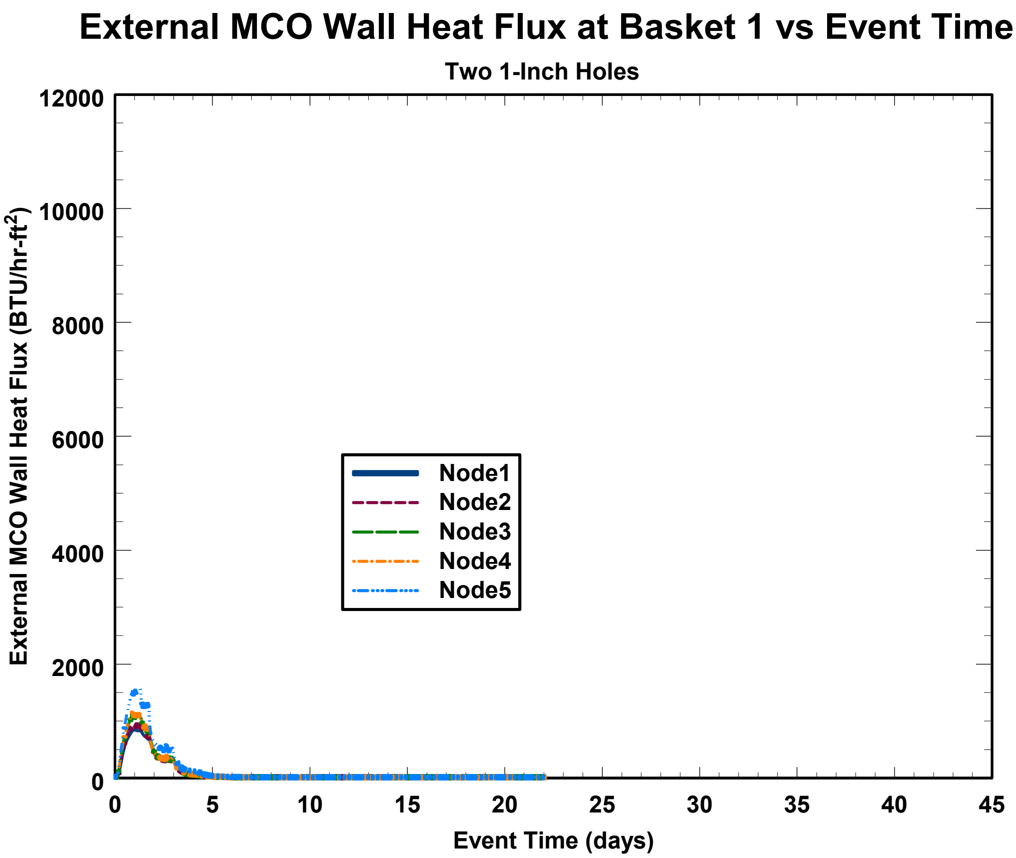

Figure 50. External MCO wall heat flux at nodes in Basket 1 for two 1.0-inch hole breach.

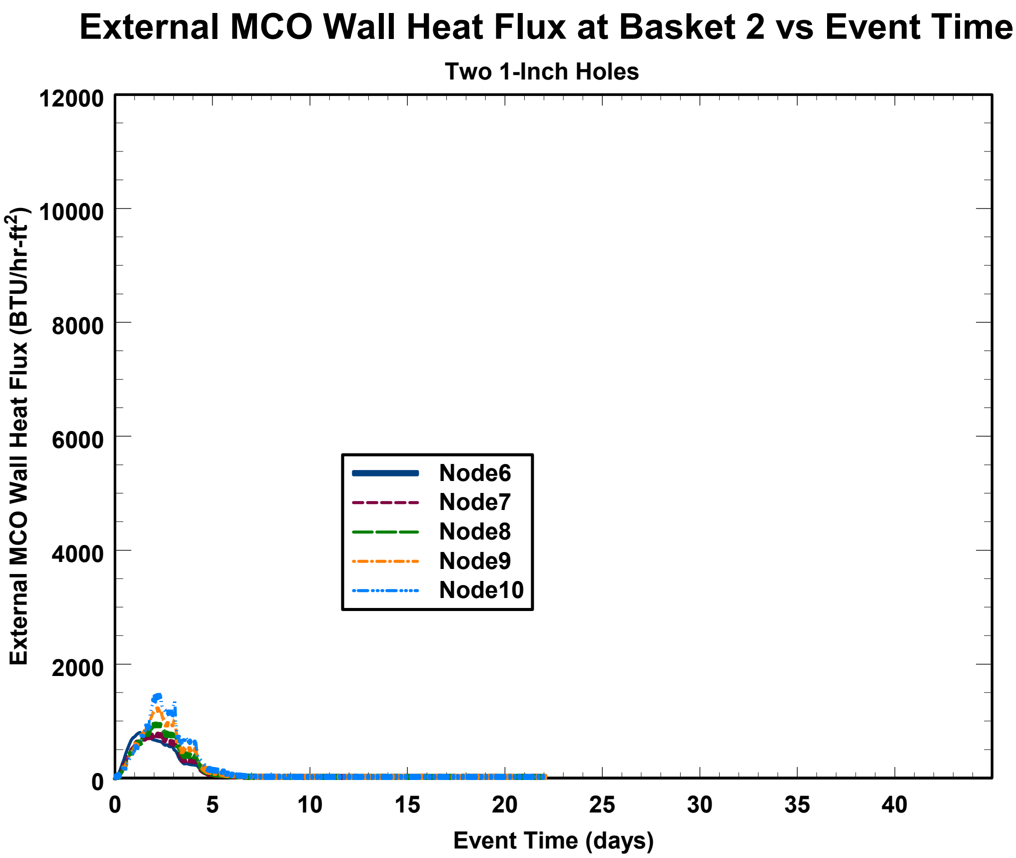

Figure 51. External MCO wall heat flux at nodes in Basket 2 for two 1.0-inch hole breach.

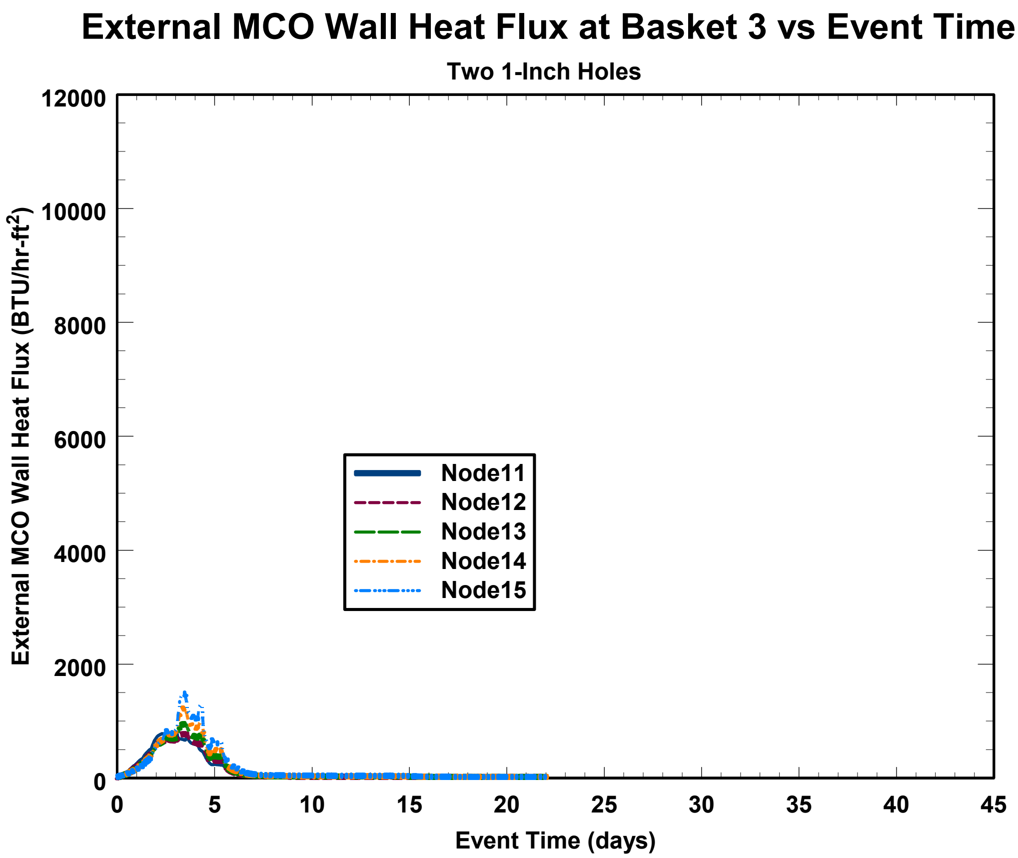

Figure 52. External MCO wall heat flux at nodes in Basket 3 for two 1.0-inch hole breach.

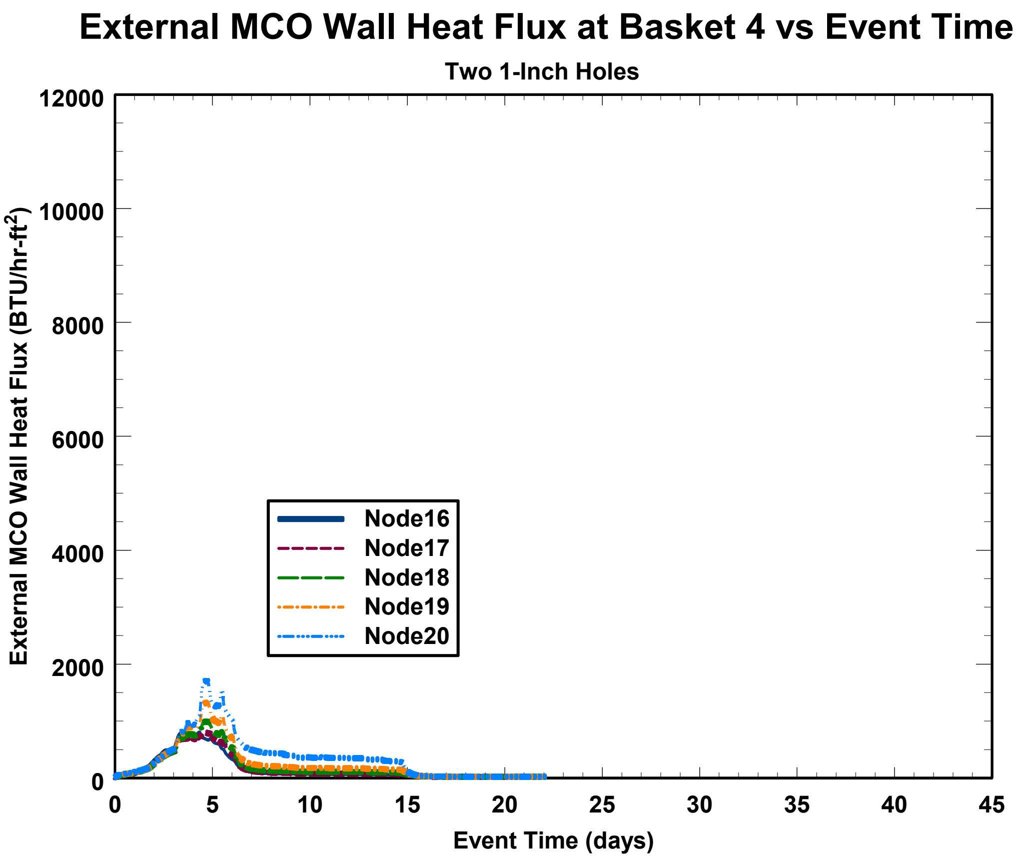

Figure 53. External MCO wall heat flux at nodes in Basket 4 for two 1.0-inch hole breach.

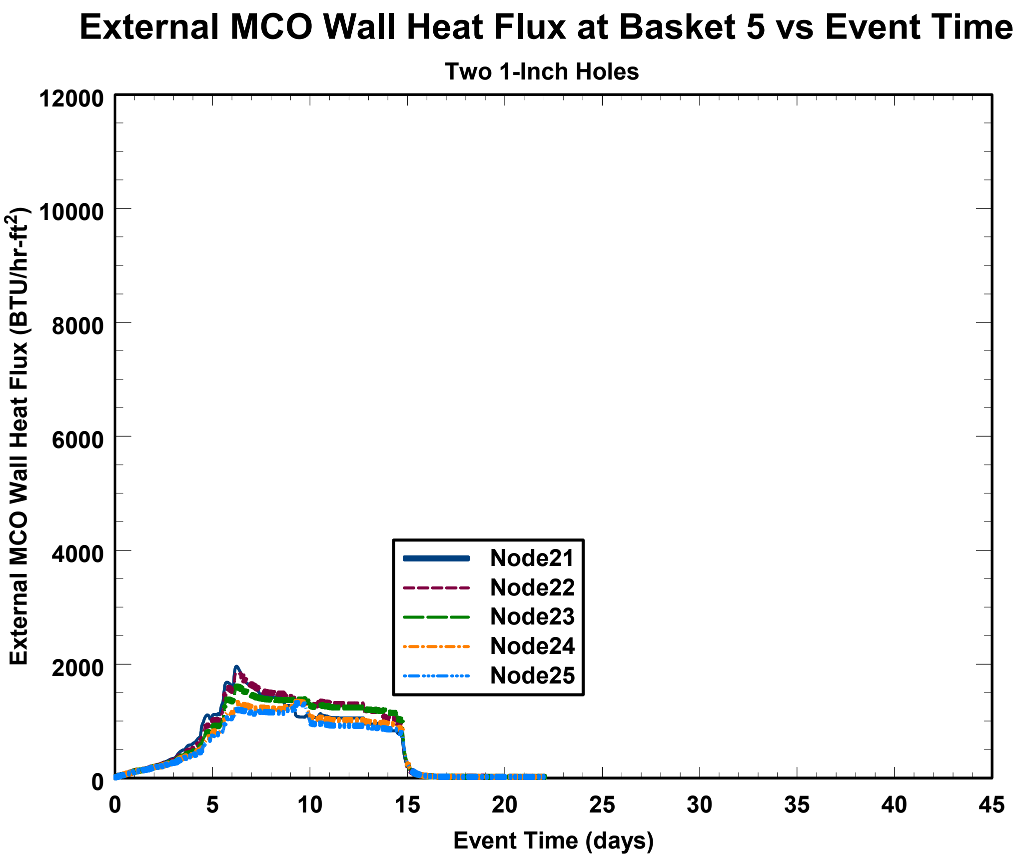

Figure 54. External MCO wall heat flux at nodes in Basket 5 for two 1.0-inch hole breach.

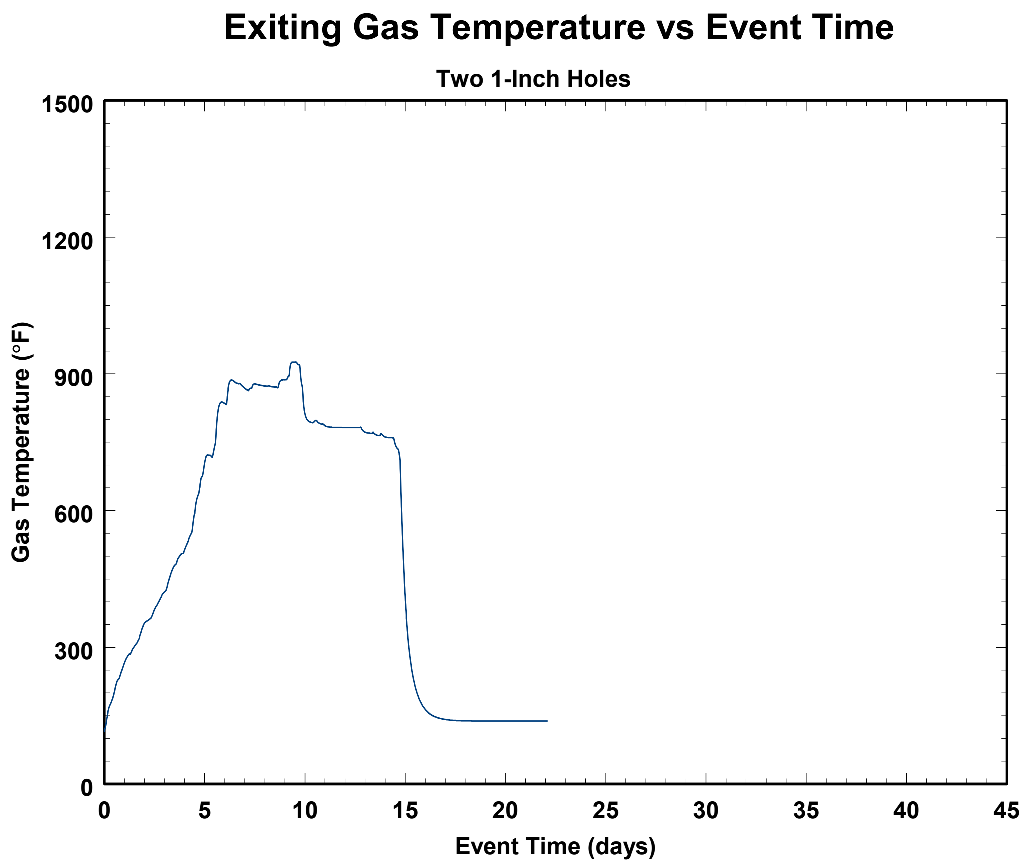

Figure 55. Exiting gas temperature from upper hole for two 1.0-inch hole breach.

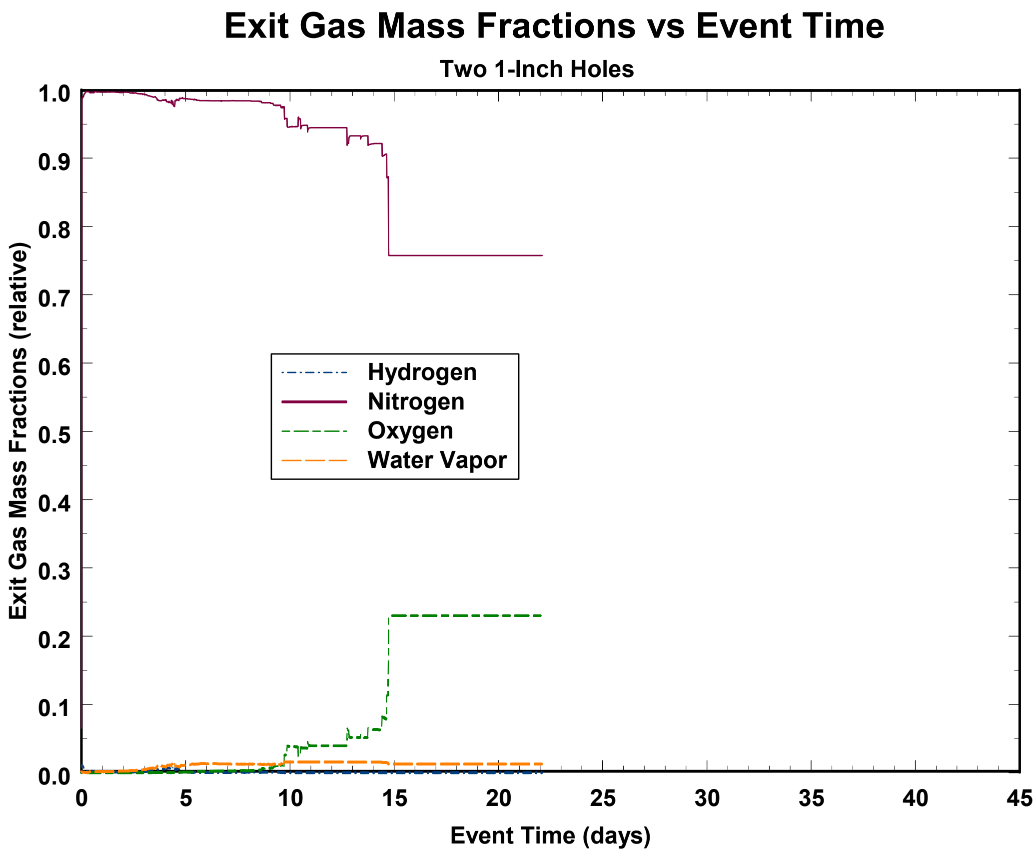

Figure 56. Relative concentration of gas species exiting upper hole for two 1.0-inch hole breach.

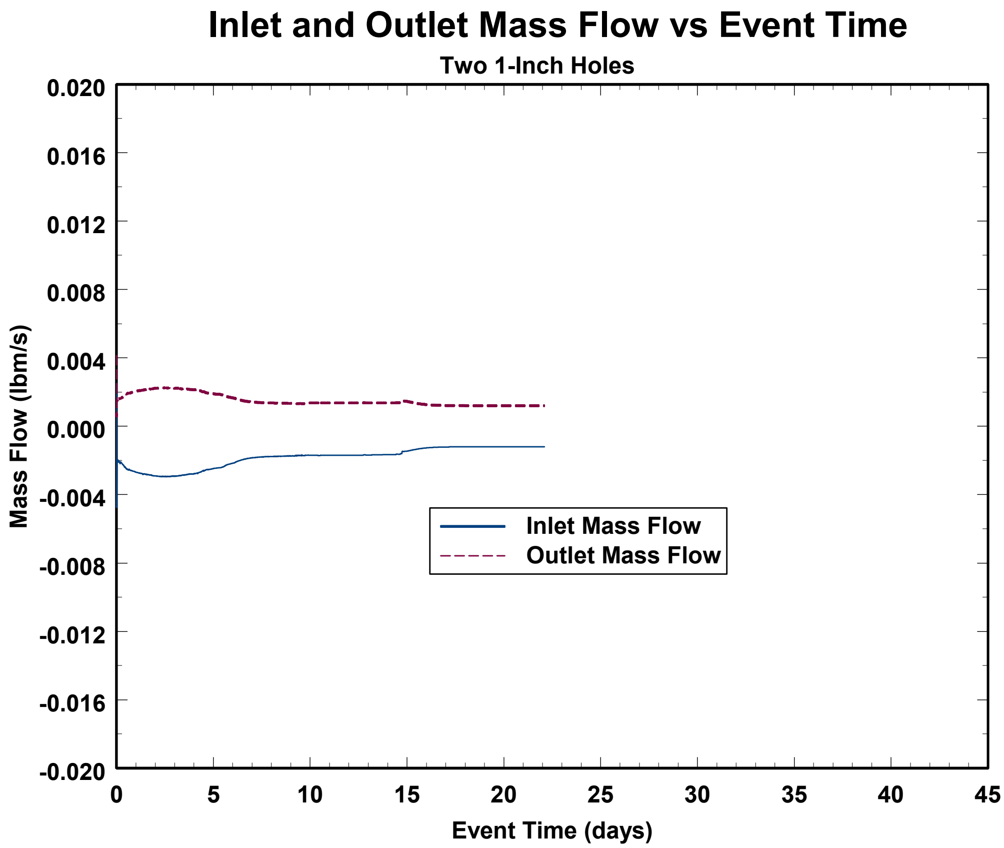

Figure 57. Mass flow at the inlet and outlet for two 1.0-inch hole breach.

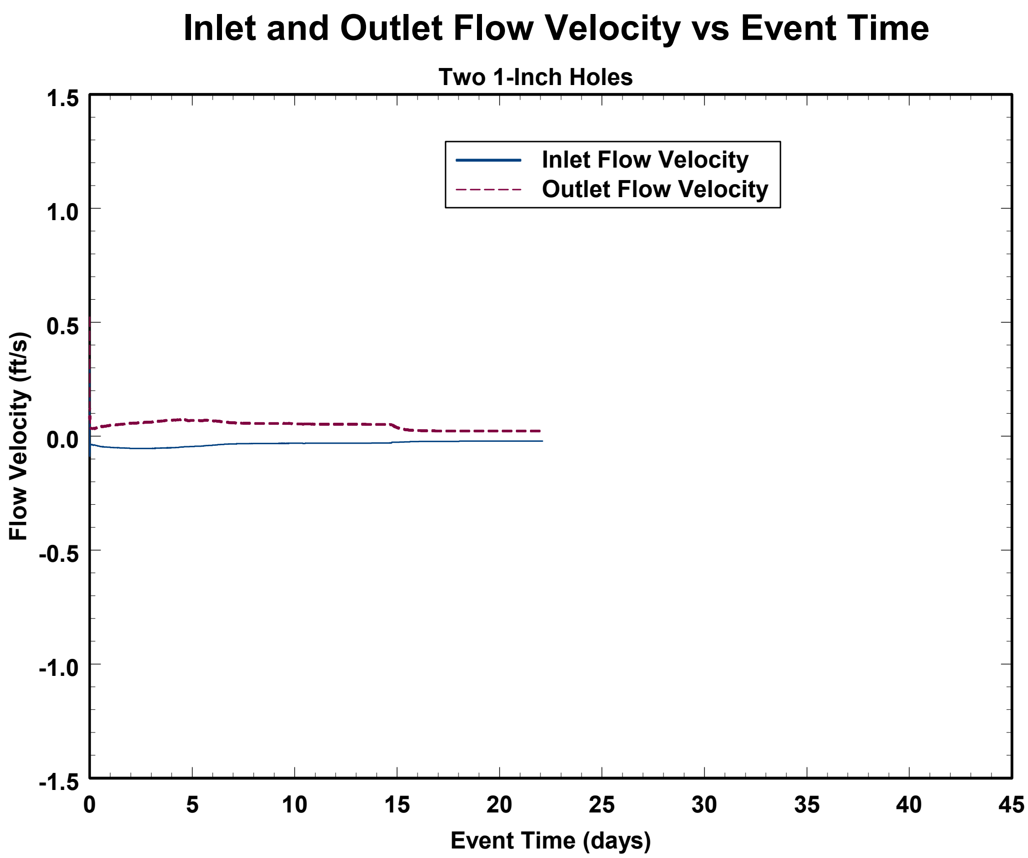

Figure 58. Flow velocity at the inlet and outlet for two 1.0-inch hole breach.

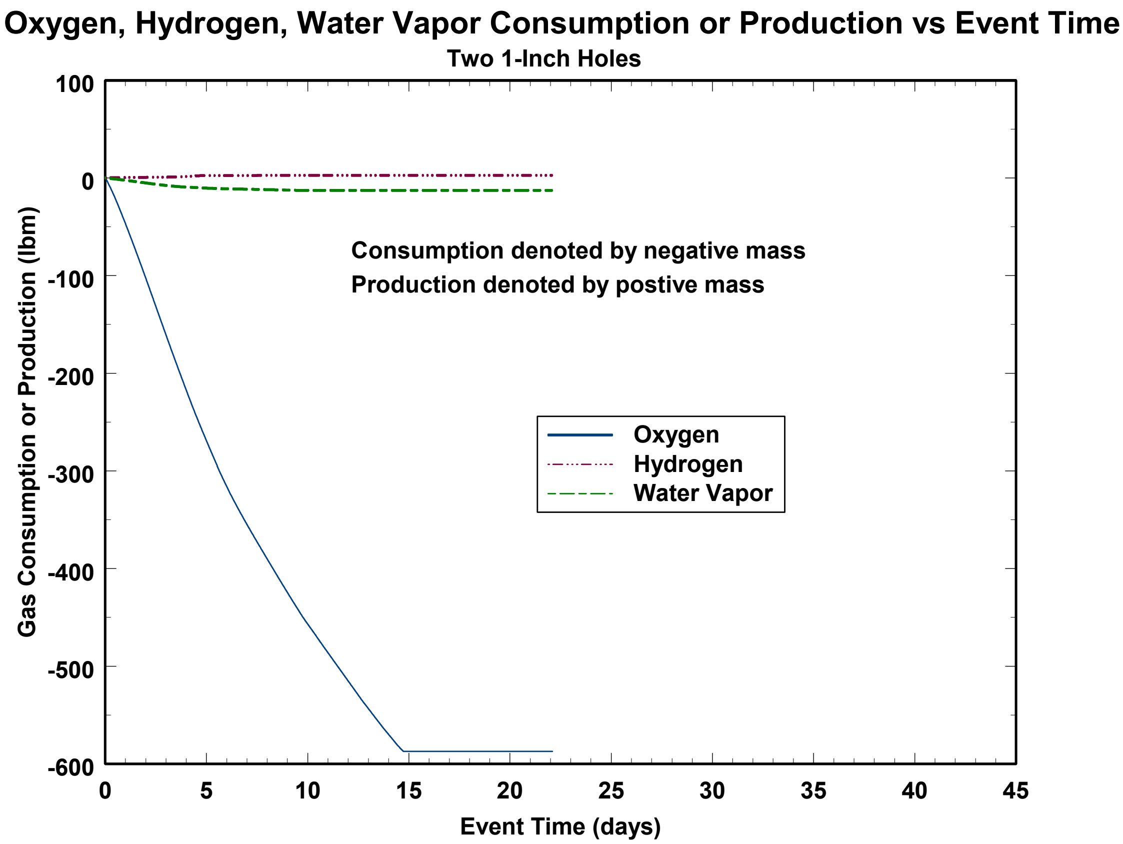

Figure 59. Oxygen, hydrogen, and water vapor consumption or production for two 1.0-inch hole breach.

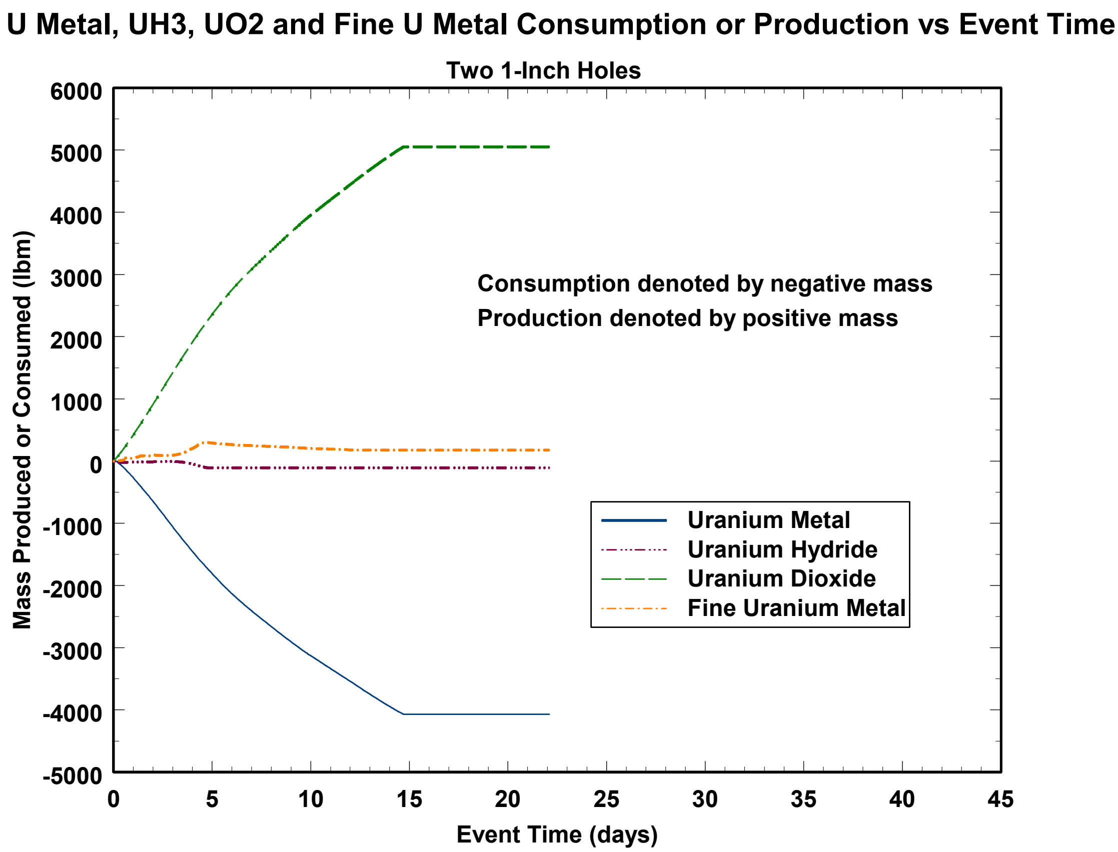

Figure 60. Uranium, uranium dioxide, uranium hydride, and fine uranium metal consumption or production for two 1.0-inch hole breach.

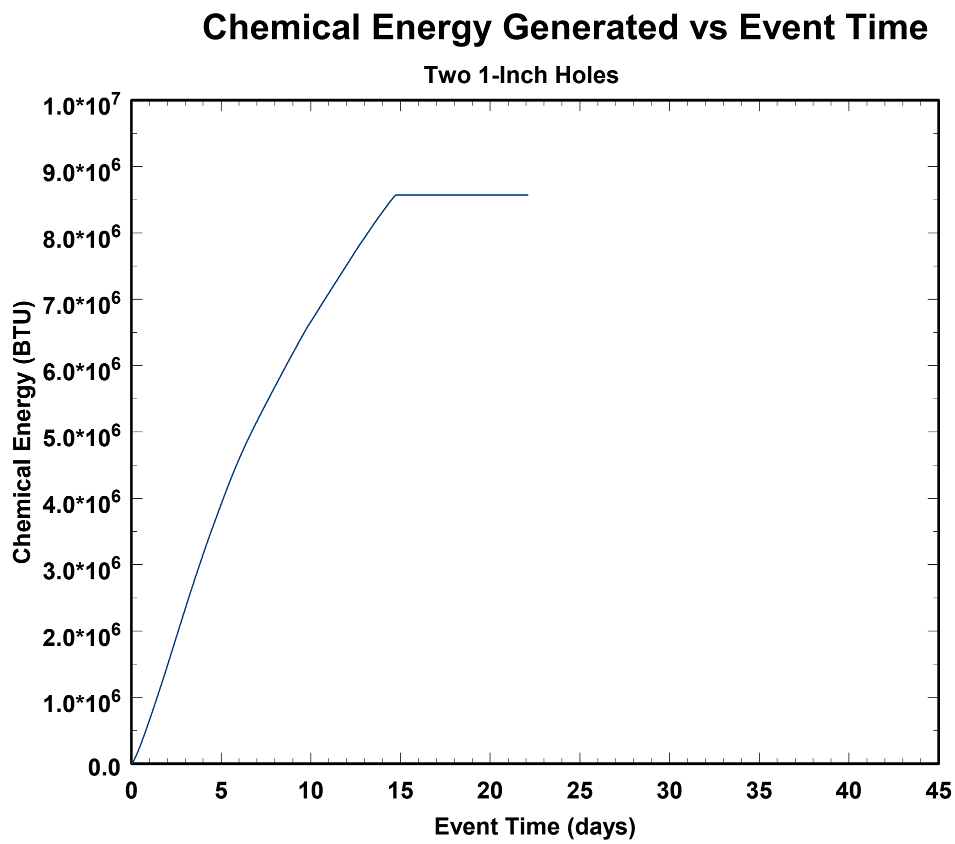

Figure 61. Chemical energy output for two 1.0-inch hole breach.

2.1.5 Two 2.0-inch Holes

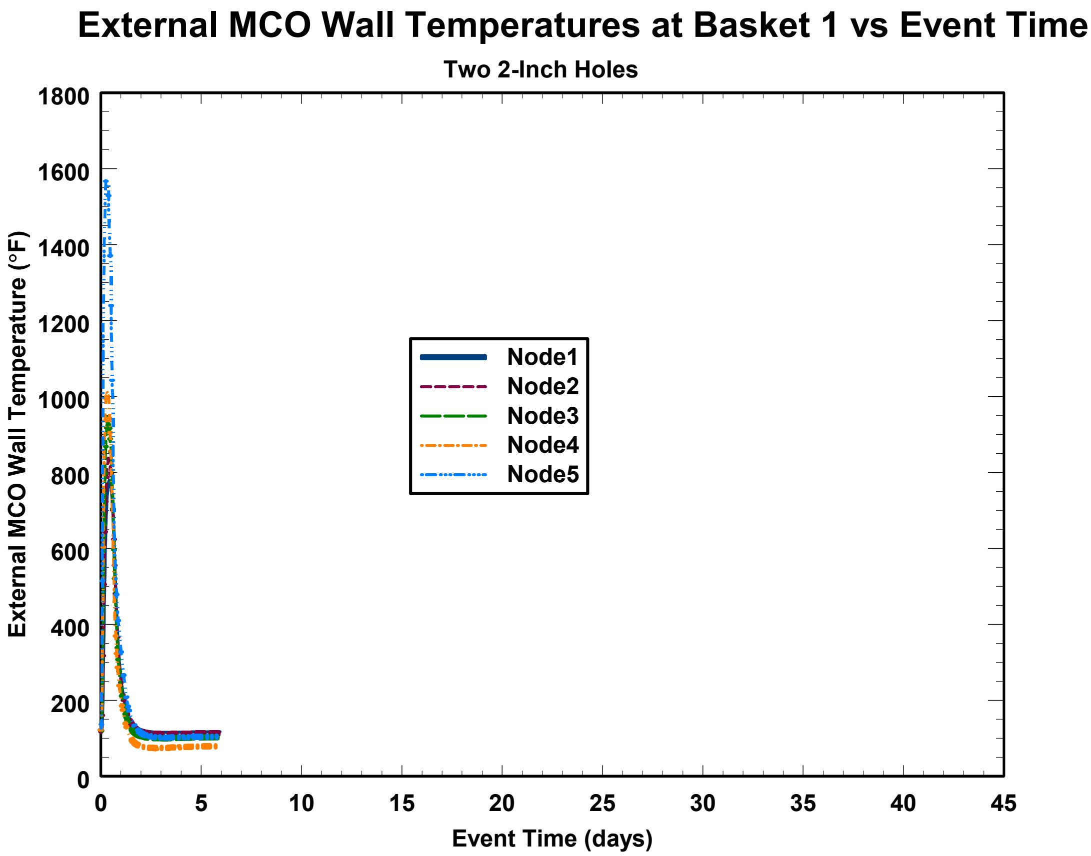

Figure 62. External MCO wall temperatures at nodes in Basket 1 for two 2.0-inch hole breach.

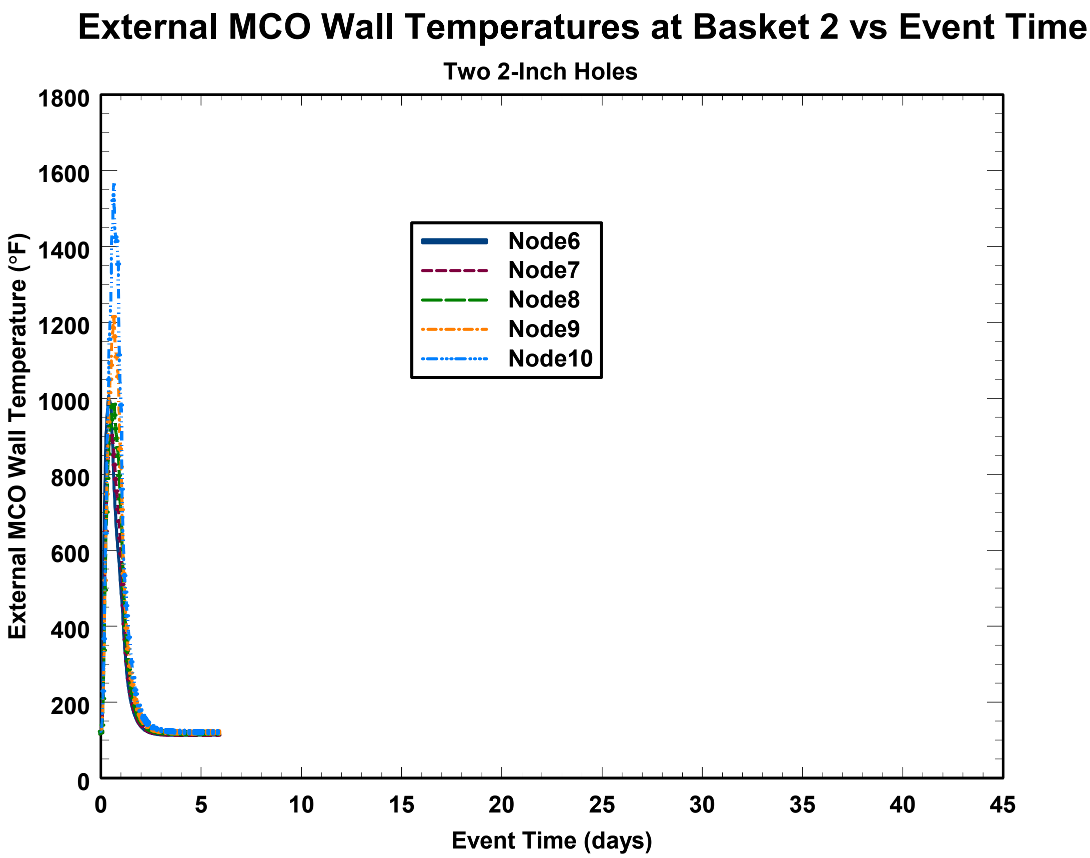

Figure 63. External MCO wall temperatures at nodes in Basket 2 for two 2.0-inch hole breach.

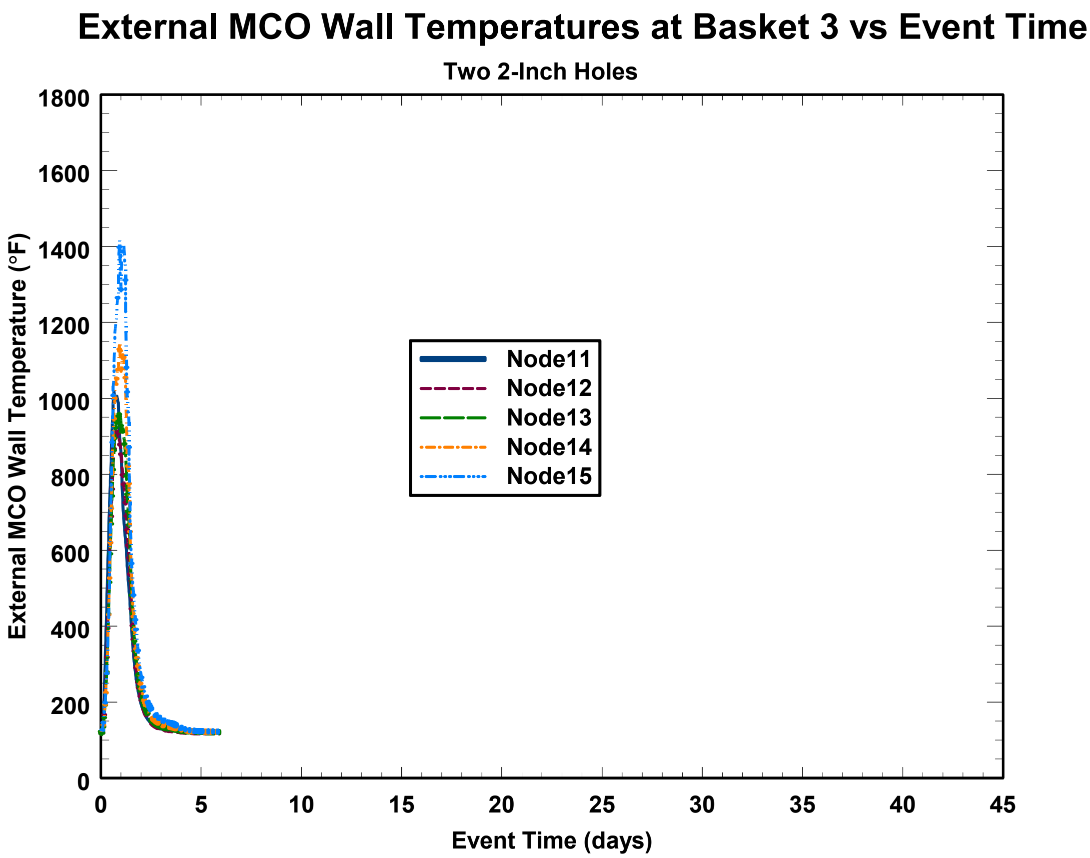

Figure 64. External MCO wall temperatures at nodes in Basket 3 for two 2.0-inch hole breach.

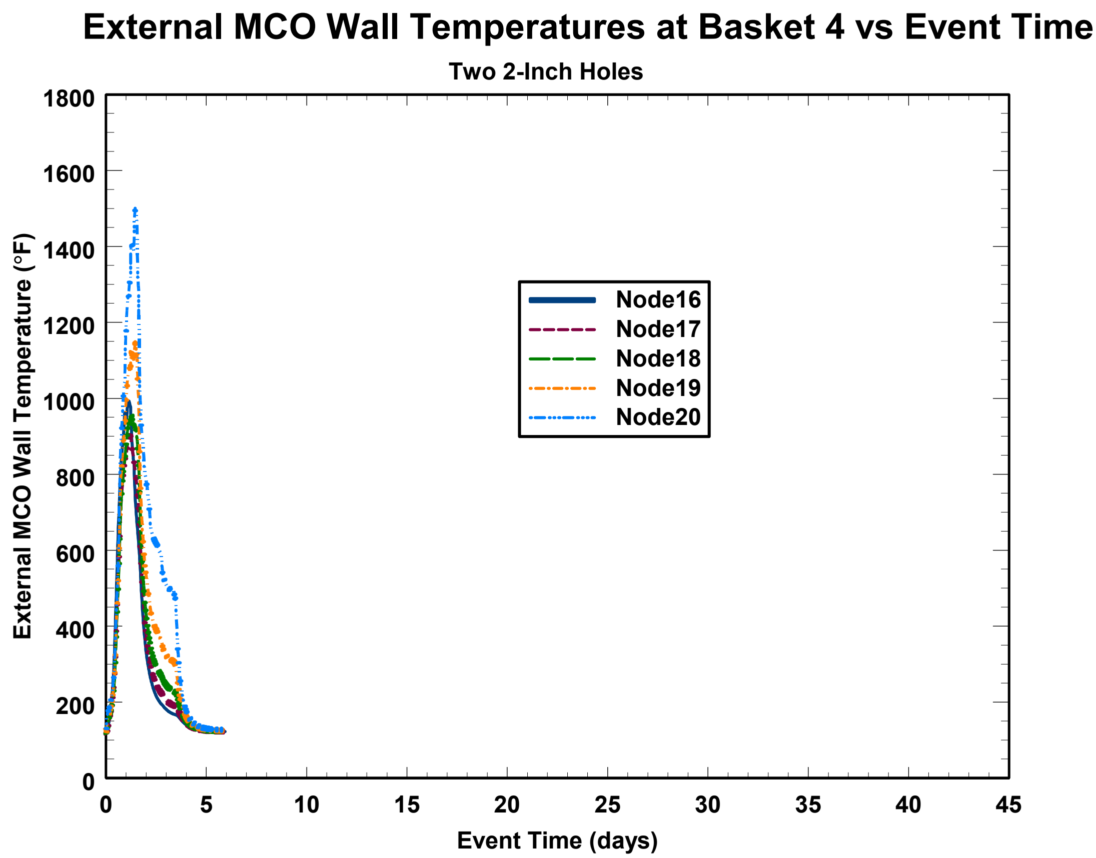

Figure 65. External MCO wall temperatures at nodes in Basket 4 for two 2.0-inch hole breach.

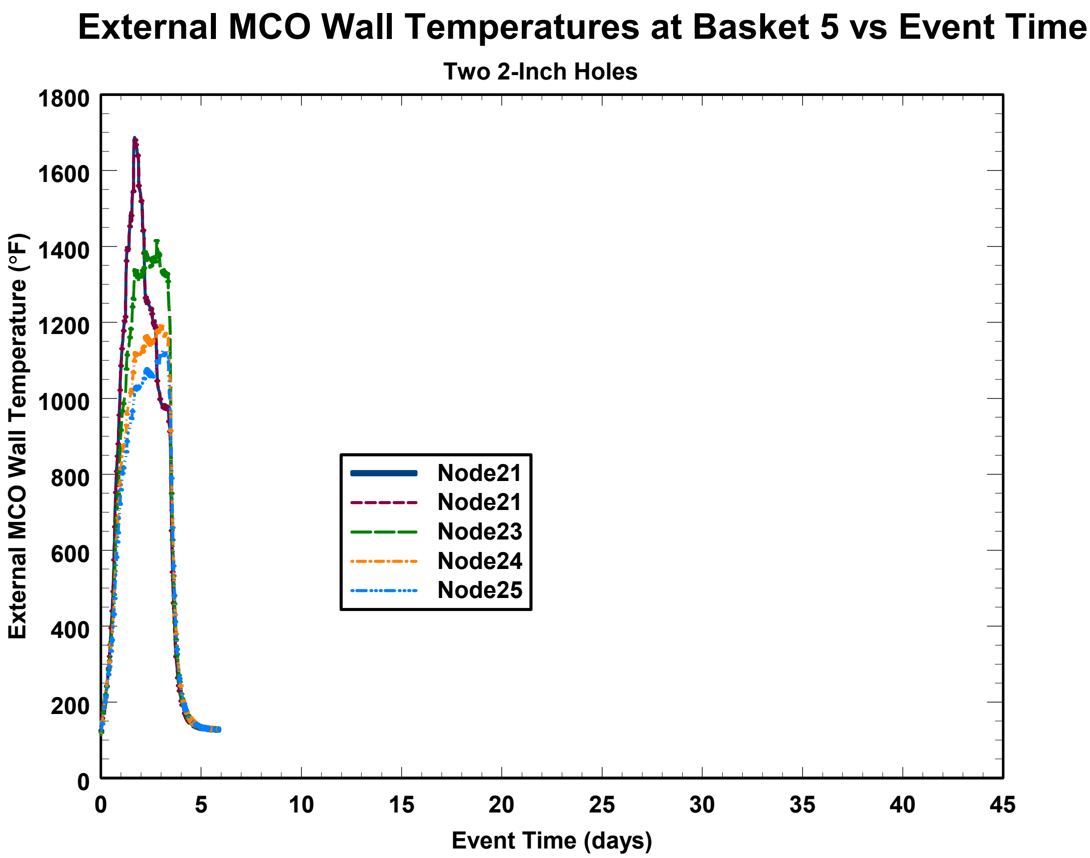

Figure 66. External MCO wall temperatures at nodes in Basket 5 for two 2.0-inch hole breach.

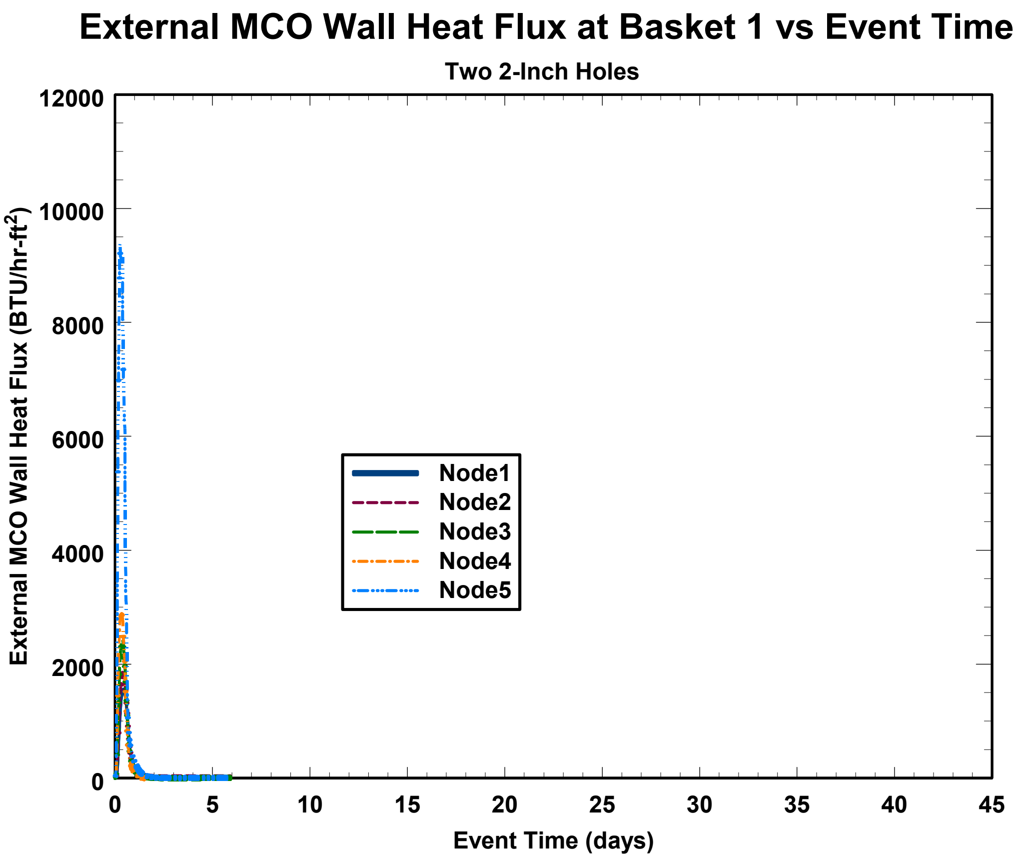

Figure 67. External MCO wall heat flux at nodes in Basket 1 for two 2.0-inch hole breach.

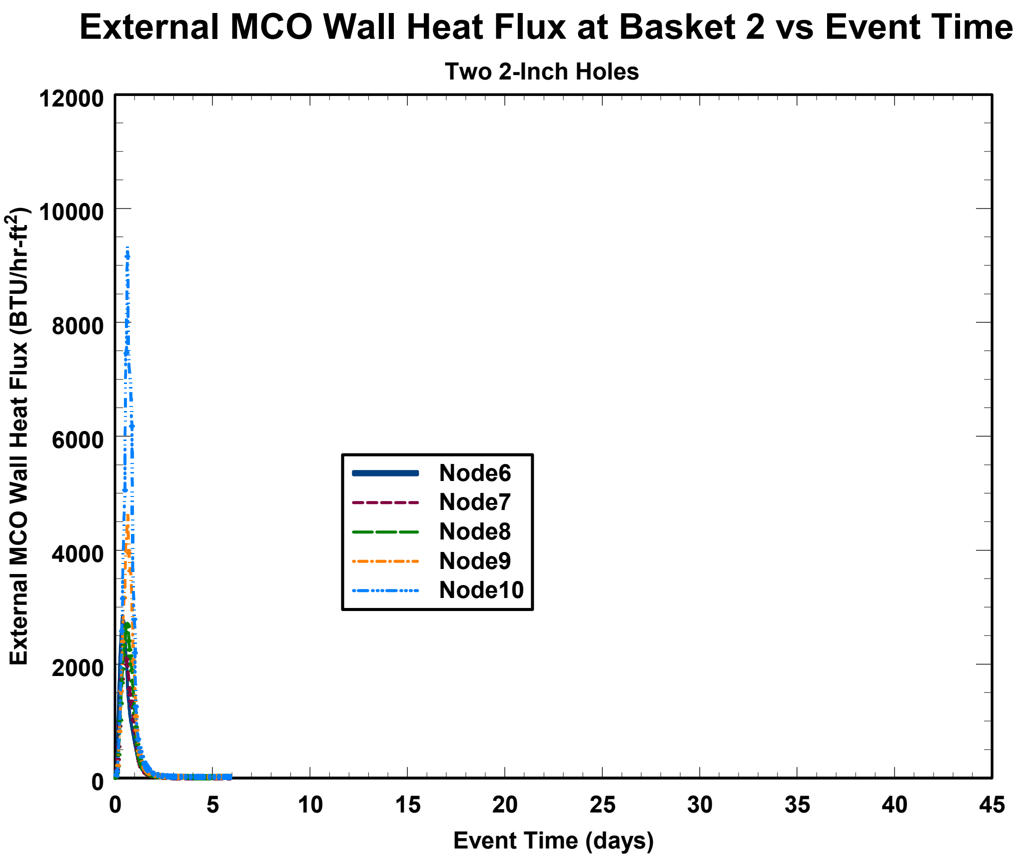

Figure 68. External MCO wall heat flux at nodes in Basket 2 for two 2.0-inch hole breach.

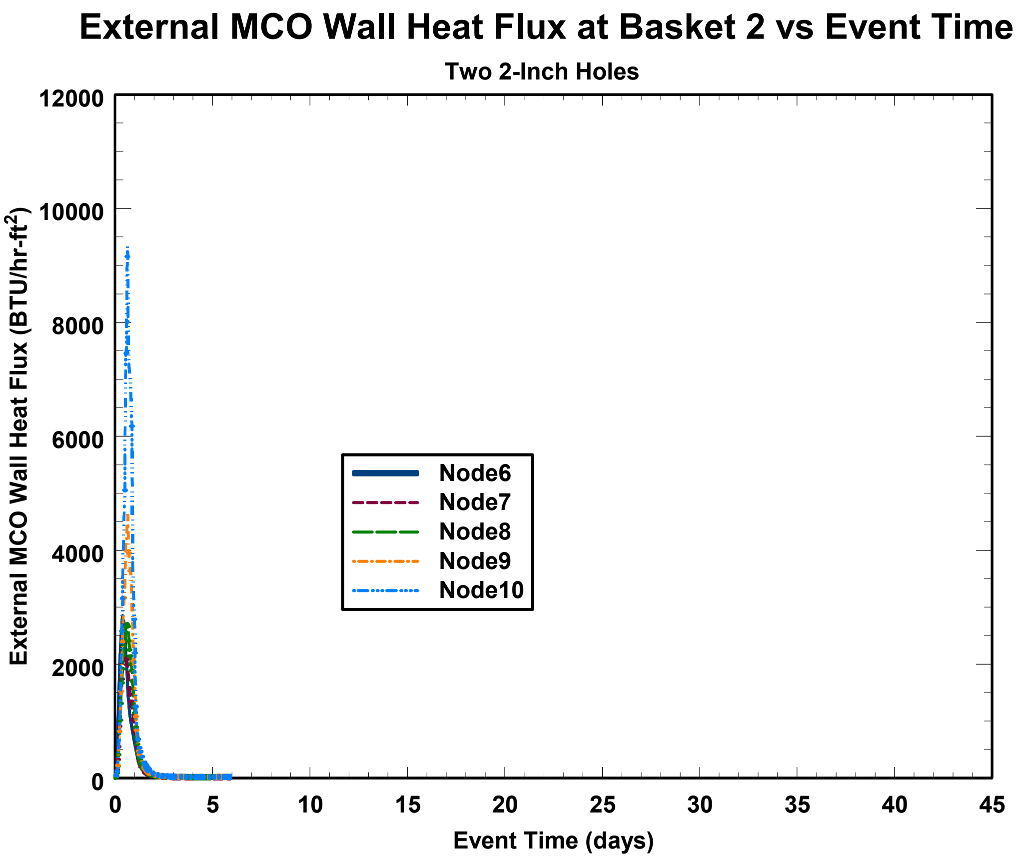

Figure 69. External MCO wall heat flux at nodes in Basket 3 for two 2.0-inch hole breach.

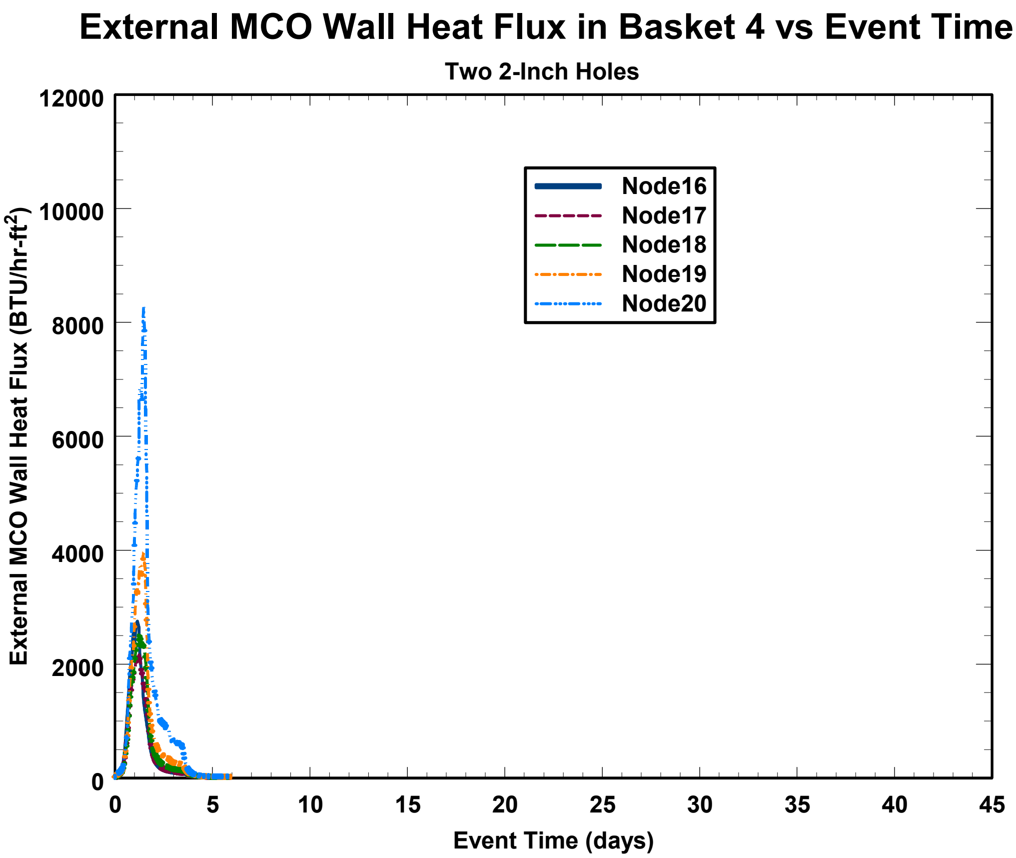

Figure 70. External MCO wall heat flux at nodes in Basket 4 for two 2.0-inch hole breach.

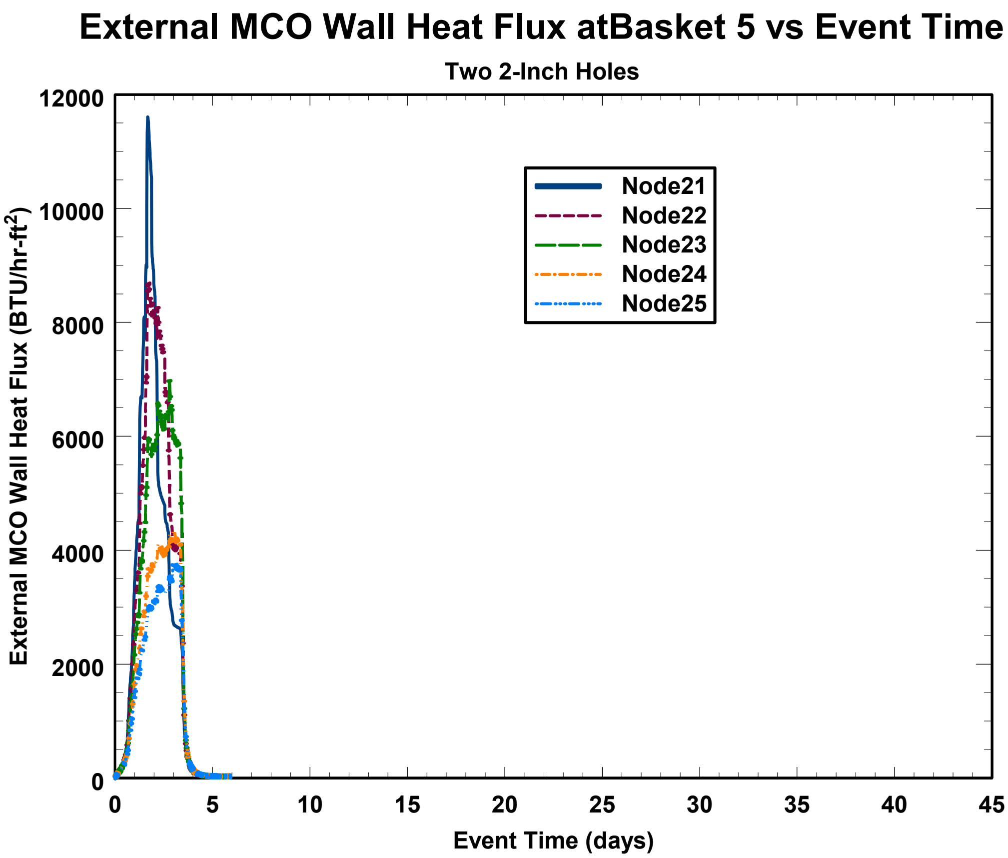

Figure 71. External MCO wall heat flux at nodes in Basket 5 for two 2.0-inch hole breach.

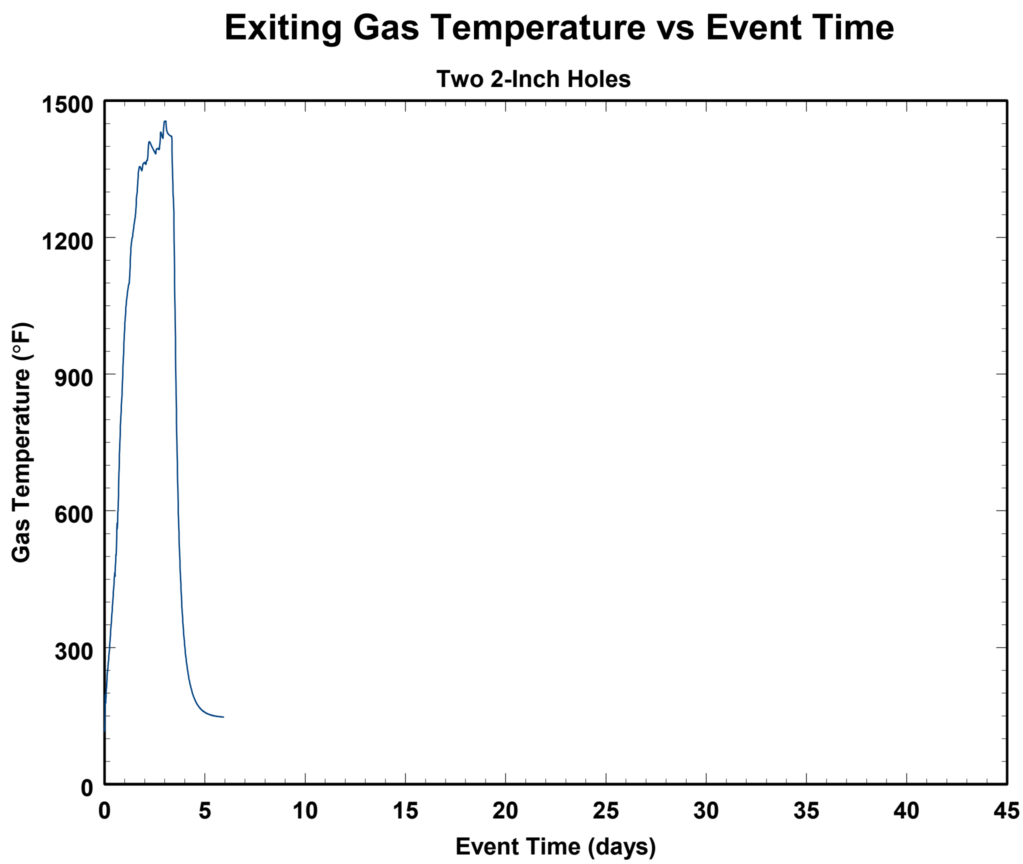

Figure 72. Exiting gas temperature from upper hole for two 2.0-inch hole breach.

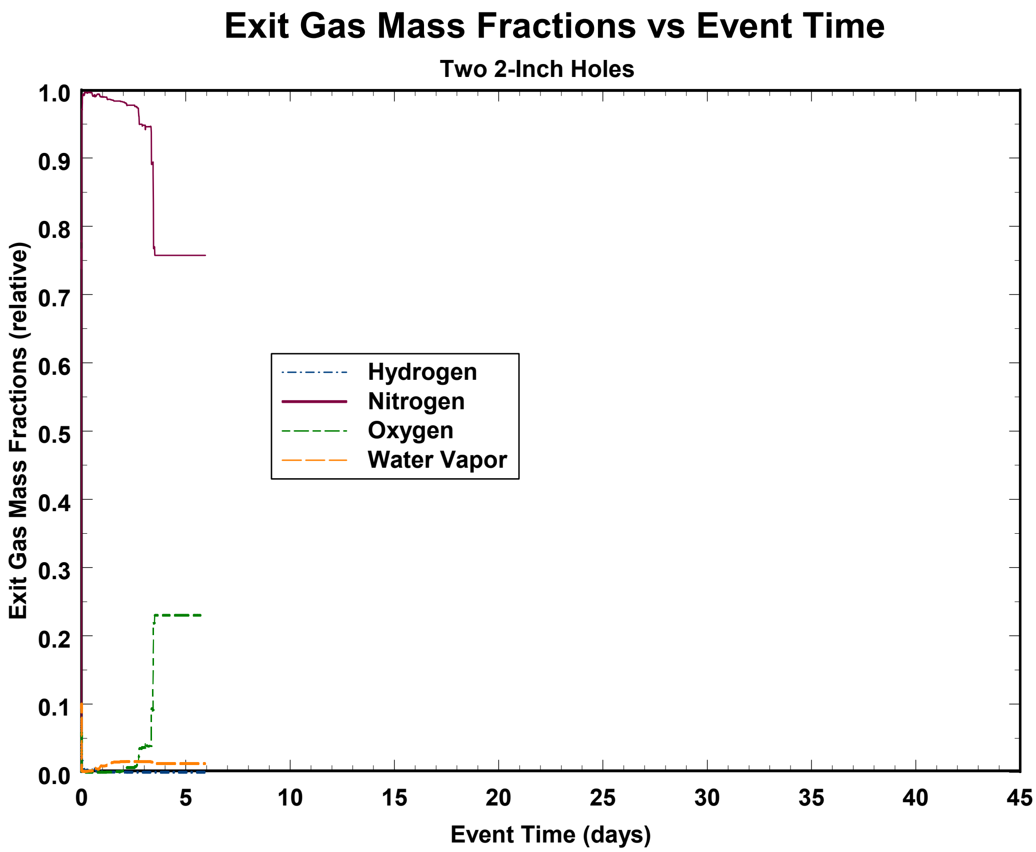

Figure 73. Relative concentration of gas species exiting upper hole for two 2.0-inch hole breach.

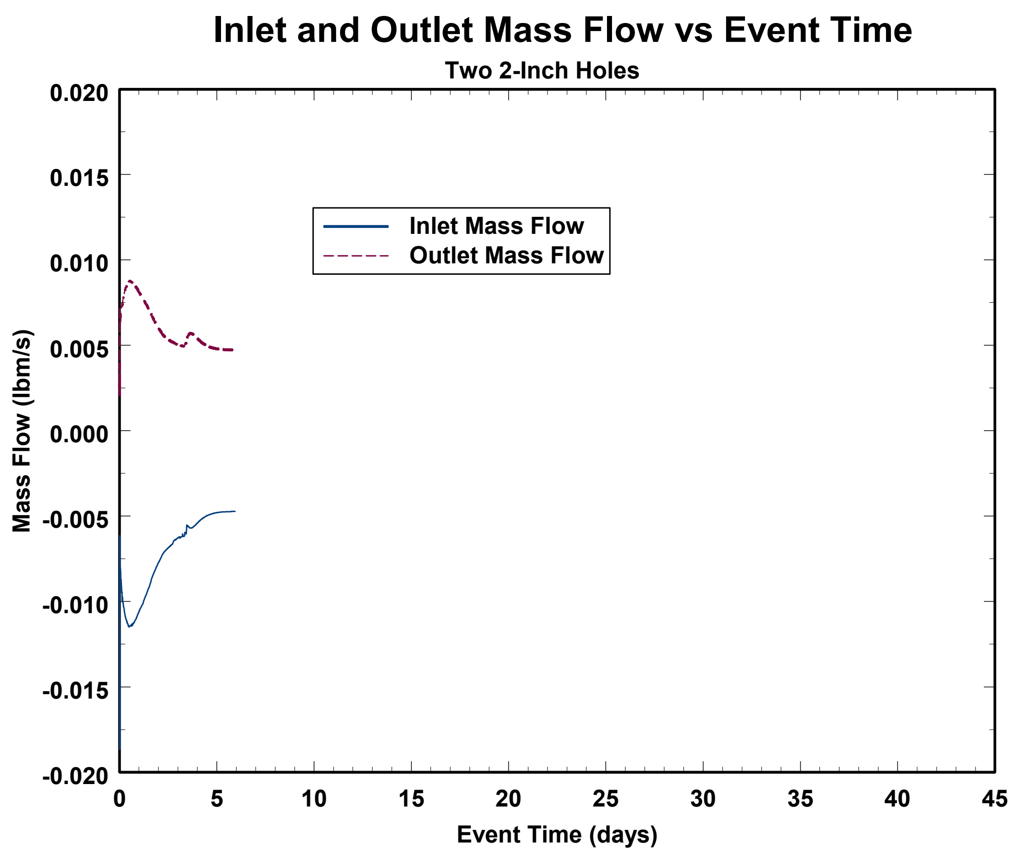

Figure 74. Mass flow at the inlet and outlet for two 2.0-inch hole breach.

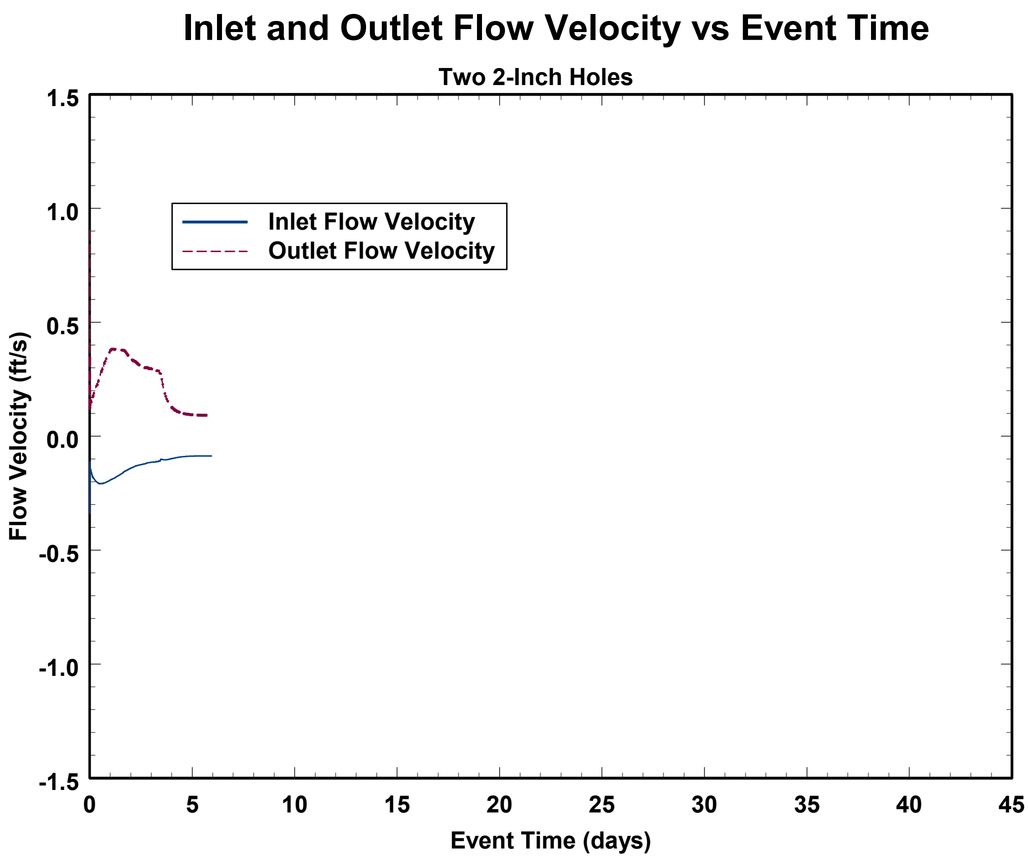

Figure 75. Flow velocity at the inlet and outlet for two 2.0-inch hole breach.

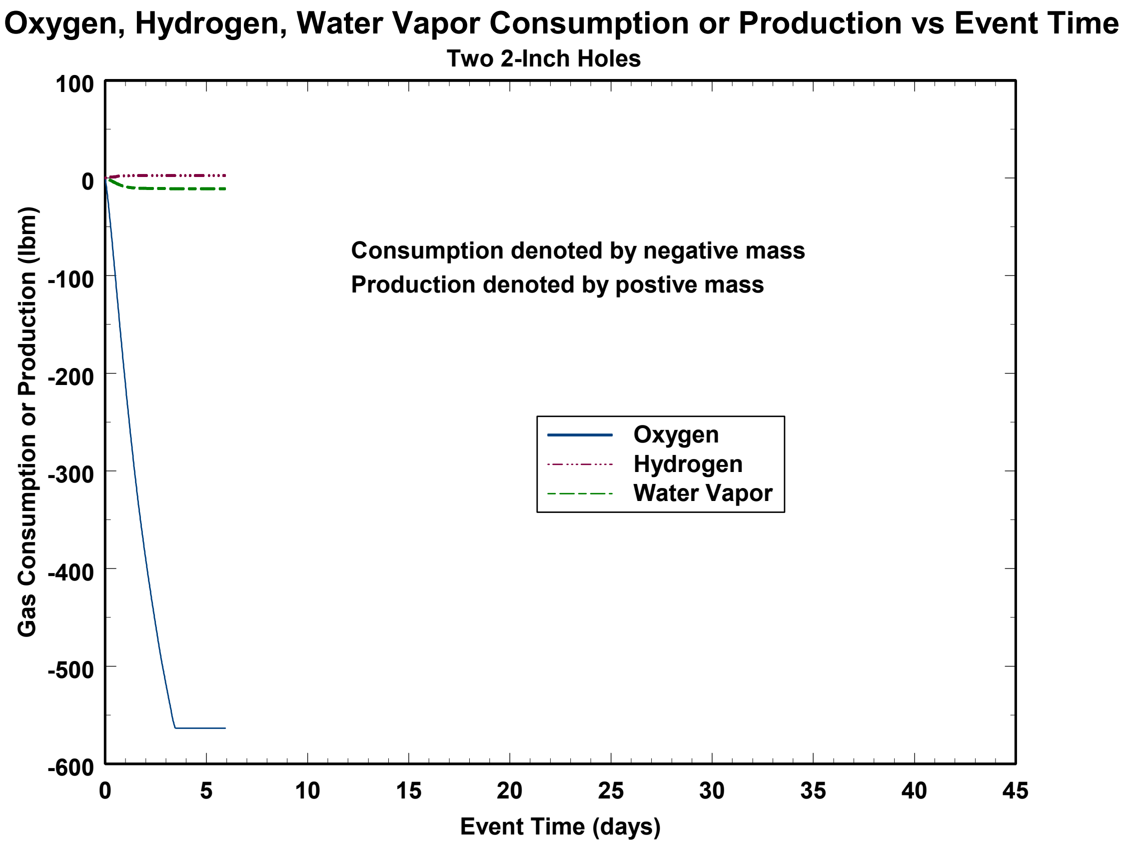

Figure 76. Oxygen, hydrogen, and water vapor consumption or production for two 2.0-inch hole breach.

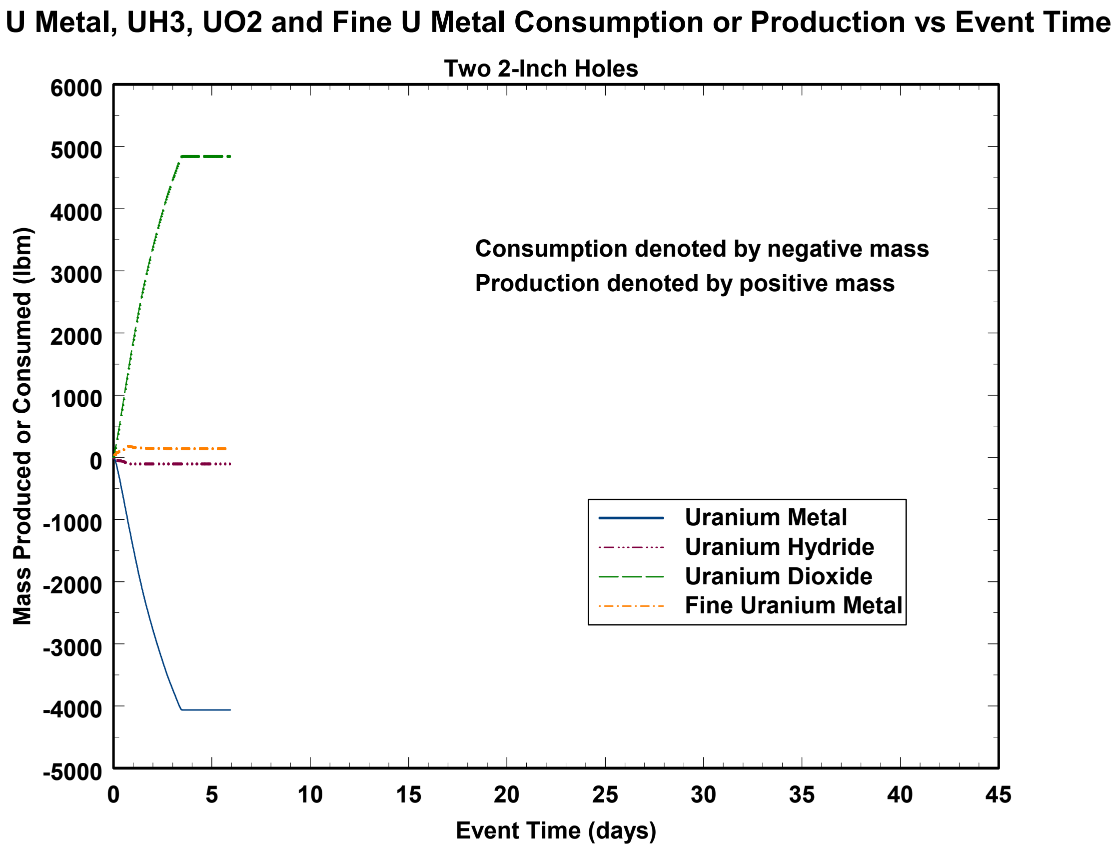

Figure 77. Uranium, uranium dioxide, uranium hydride, and fine uranium metal consumption or production for two 2.0-inch hole breach.

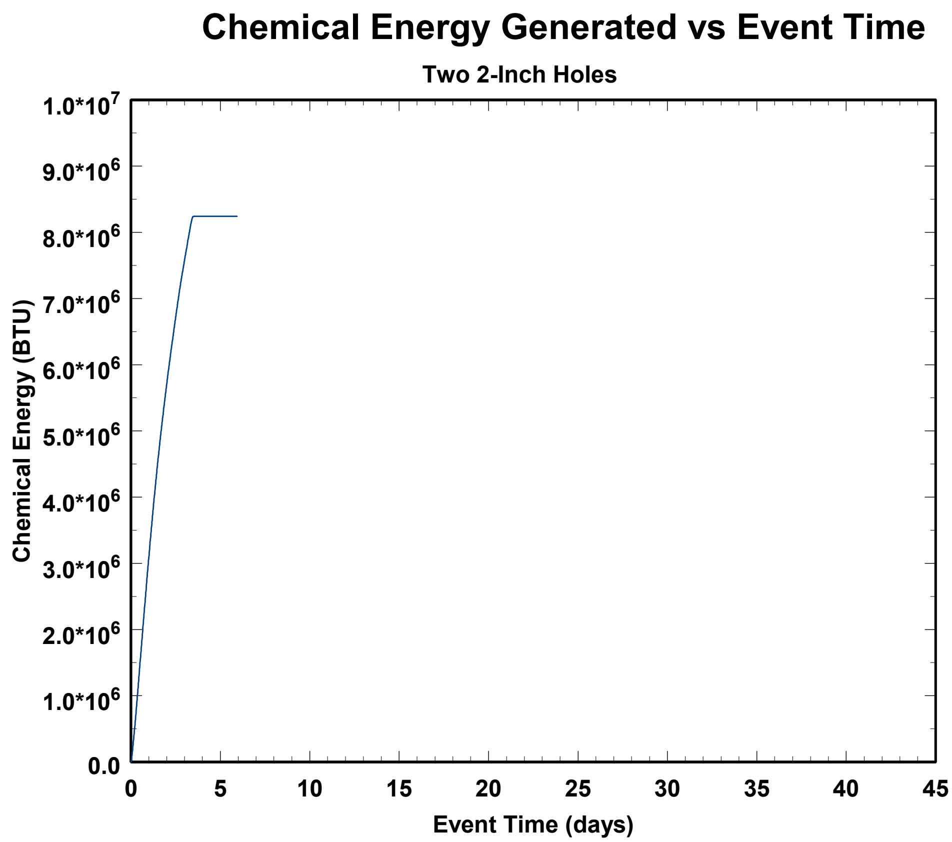

Figure 78. Chemical energy output for two 2.0-inch hole breach.

2.2 Open Top Configuration

This configuration simulates the sudden exposure of the scrap basket to the environment. This allows the gas channels between the rings to vent directly to and draw in air from the ambient atmosphere. The scrap basket reactions will cause a high degree of gas mixing within the basket resulting in heat generation in the scrap basket and additional heat generation at the tips in each of the lower fuel baskets. A sketch of this configuration is seen in Figure 79.

2.2.1 Description of Plots for the Open Top Configuration

Below is a description of the plots in Section 2.2.2 for a suddenly opened MCO top breach. Each bullet describes the information being presented in the plot and the associated figure numbers.

- External MCO wall temperature vs. event time—The external MCO wall temperature plots are data taken at the nodes that represent the vertical exterior face of the wall. Each basket has five vertical nodes, where each node is vertically spaced 13.2 cm (5.2 in.) from the previous node. The bottom basket or Basket 1 is represented by nodes 1–5; Basket 2 uses nodes 6–10; Basket 3 uses nodes 11–15; and Basket 4 uses nodes 16–20. The scrap basket uses nodes 21–25. The temperature is in degrees Fahrenheit.

Basket 1 Nodes 1–5	Basket 2 Nodes 6–10	Basket 3 Nodes 11–15	Basket 4 Nodes 16–20	Basket 5 Nodes 21–25
Figure 80	Figure 81	Figure 82	Figure 83	Figure 84

- External MCO wall heat flux vs. event time—The external MCO wall heat flux plots are data taken at the nodes that represent the vertical exterior face of the wall. Each basket has five vertical nodes, where each node is vertically spaced 13.2 cm (5.2 in.) from the previous node. The bottom basket or Basket 1 is represented by nodes 1–5; Basket 2 uses nodes 6–10; Basket 3 uses nodes 11–15; and Basket 4 uses nodes 16–20. The scrap basket uses nodes 21–25. The heat flux is in BTU/hr-ft^2 at each of the nodes.

Basket 1 Nodes 1-5	Basket 2 Nodes 6-10	Basket 3 Nodes 11-15	Basket 4 Nodes 16-20	Basket 5 Nodes 21-25
Figure 85	Figure 86	Figure 87	Figure 88	Figure 89

- Exiting gas temperature vs. event time—The exiting gas temperature is shown in Figure 90. Only four of the six channels are shown, because the other two channels are drawing in air. The fourth channel TV1s173 starts out exhausting, but switches to drawing in air after 2 days into the event.

  - TV1s170—Gas channel between the center support pipe and the first fuel ring
  - TV1s171—Gas channel between the first and second fuel ring
  - TV1s172—Gas channel between the second and third fuel ring
  - TV1s173—Gas channel between the third and fourth fuel ring.

- Exiting gas mass fractions vs. event time—The mass fractions are the relative components of the mass flow rate that corresponds to the gas species hydrogen, nitrogen, oxygen, and water vapor in the mass flow. This plot shows the gas species concentrations leaving the MCO.
  - TV1s170—Gas channel between the center support pipe and the first fuel ring
  - TV1s171—Gas channel between the first and second fuel ring
  - TV1s172—Gas channel between the second and third fuel ring
  - TV1s173—Gas channel between the third and fourth fuel ring
  - TV1s174—Gas channel between the fourth fuel ring and the shroud
  - TV1s175—Gas channel between the shroud and the interior MCO wall.

TV1s170	TV1s171	TV1s172	TV1s173	TV1s174	TV1s175
Figure 91	Figure 92	Figure 93	Figure 94	Figure 95	Figure 96

- Mass flow at the inlet and outlet vs. event time—Figure 97 shows the flow rate (lbm/s) of the inlet flow and outlet flow at the top of the MCO. Negative flow rate means flow going into the MCO, and positive flow means flow leaving the MCO.
  - FV3—Mass flow between the center support pipe and the first fuel ring
  - FV4—Mass flow between the first and second fuel ring
  - FV5—Mass flow between the second and third fuel ring
  - FV6—Mass flow between the third and fourth fuel ring
  - FV7—Mass flow between the fourth fuel ring and the shroud
  - FV8—Mass flow between the shroud and the interior MCO wall.
- Flow velocity at the inlet and outlet vs. event time—Figure 98 shows the velocity (ft/s) of the inlet and outlet flow at the top of the MCO. Negative flow rate means flow going into the MCO, and positive flow means flow leaving the MCO.
  - VV3—Mass flow between the center support pipe and the first fuel ring
  - VV4—Mass flow between the first and second fuel ring
  - VV5—Mass flow between the second and third fuel ring
  - VV6—Mass flow between the third and fourth fuel ring
  - VV7—Mass flow between the fourth fuel ring and the shroud
  - VV8—Mass flow between the shroud and the interior MCO wall.

- Oxygen, hydrogen, and water vapor consumption or production vs. event time—Figure 99 shows the consumption of oxygen and hydrogen as negative mass and production of water vapor as positive mass. As all the reactive metal is consumed, consumption and production goes to zero, and therefore, the lines become straight after the event.

- Uranium metal, uranium dioxide, and fine uranium metal consumption or production vs. event time—Figure 100 denotes mass consumption by negative mass and production by positive mass. As all the reactive metal is consumed, consumption and production goes to zero, and therefore, the lines become straight after the event.

- Total chemical energy output vs. event time—Figure 101 shows all energy generated from oxidation, disassociation, and formation of reactants.

2.2.2 Open Top Plots

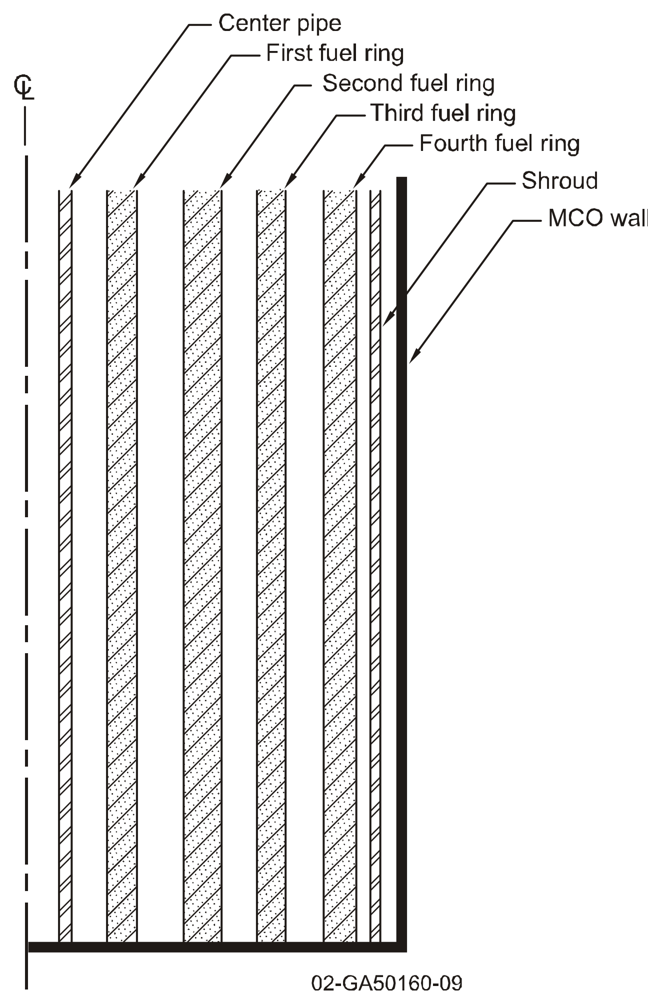

Figure 79. Configuration of an open top breach.

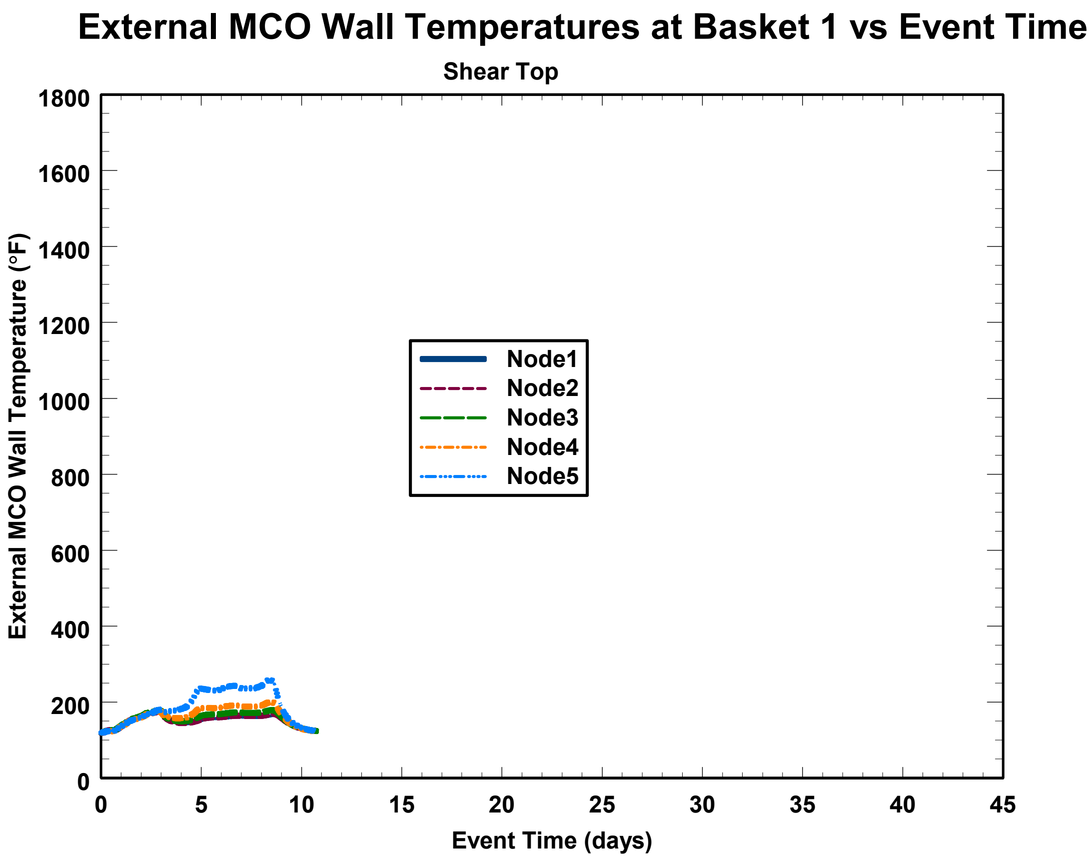

Figure 80. External MCO wall temperatures at nodes in Basket 1 for open top breach.

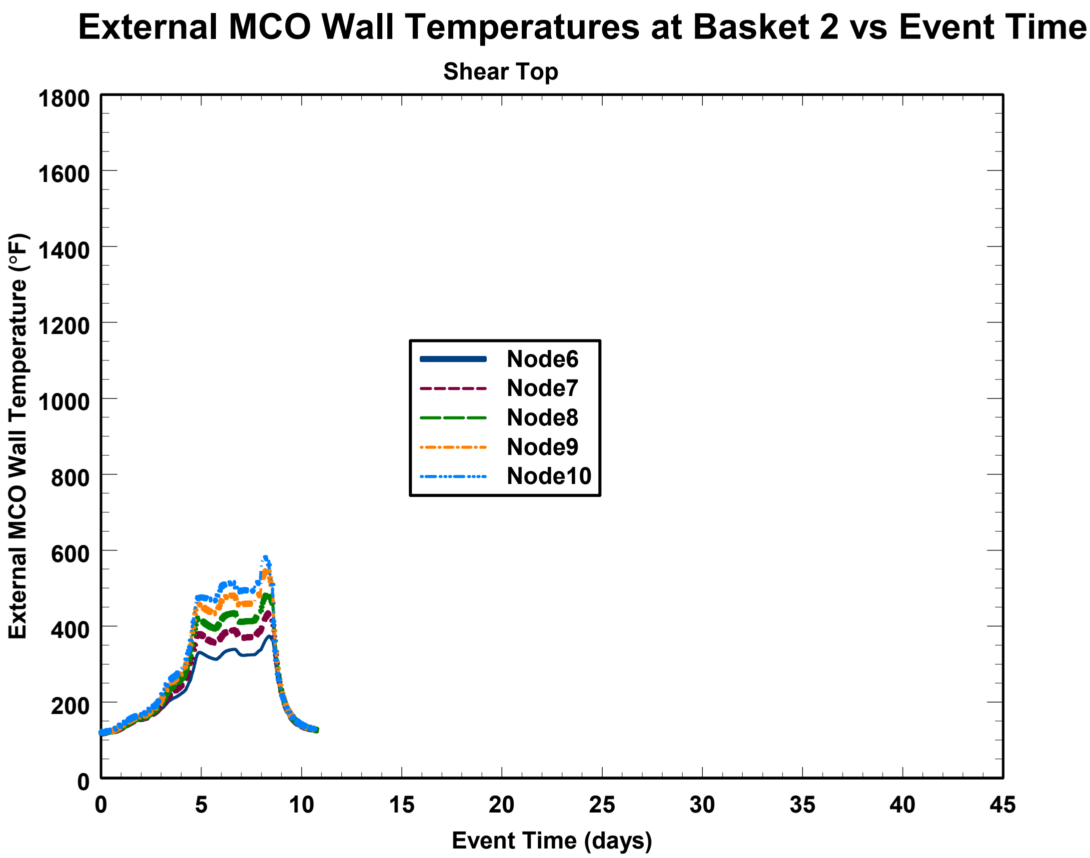

Figure 81. External MCO wall temperatures at nodes in Basket 2 for open top breach.

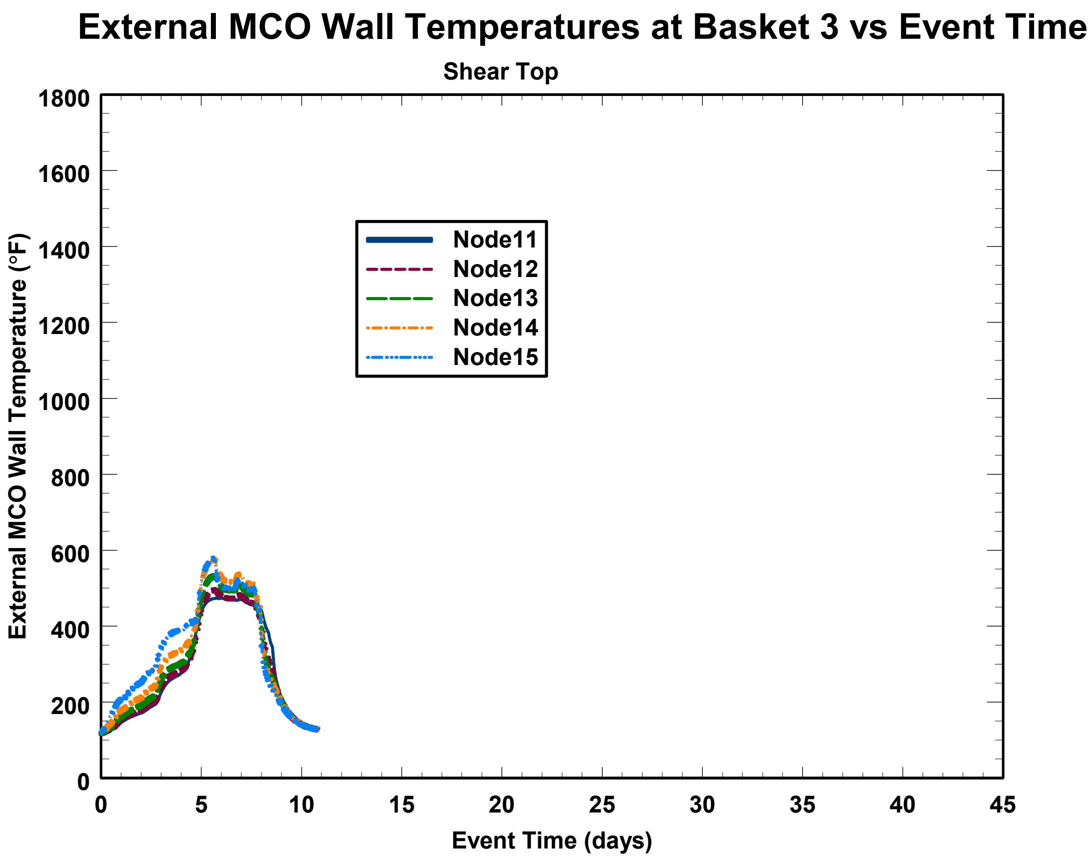

Figure 82. External MCO wall temperatures at nodes in Basket 3 for open top breach.

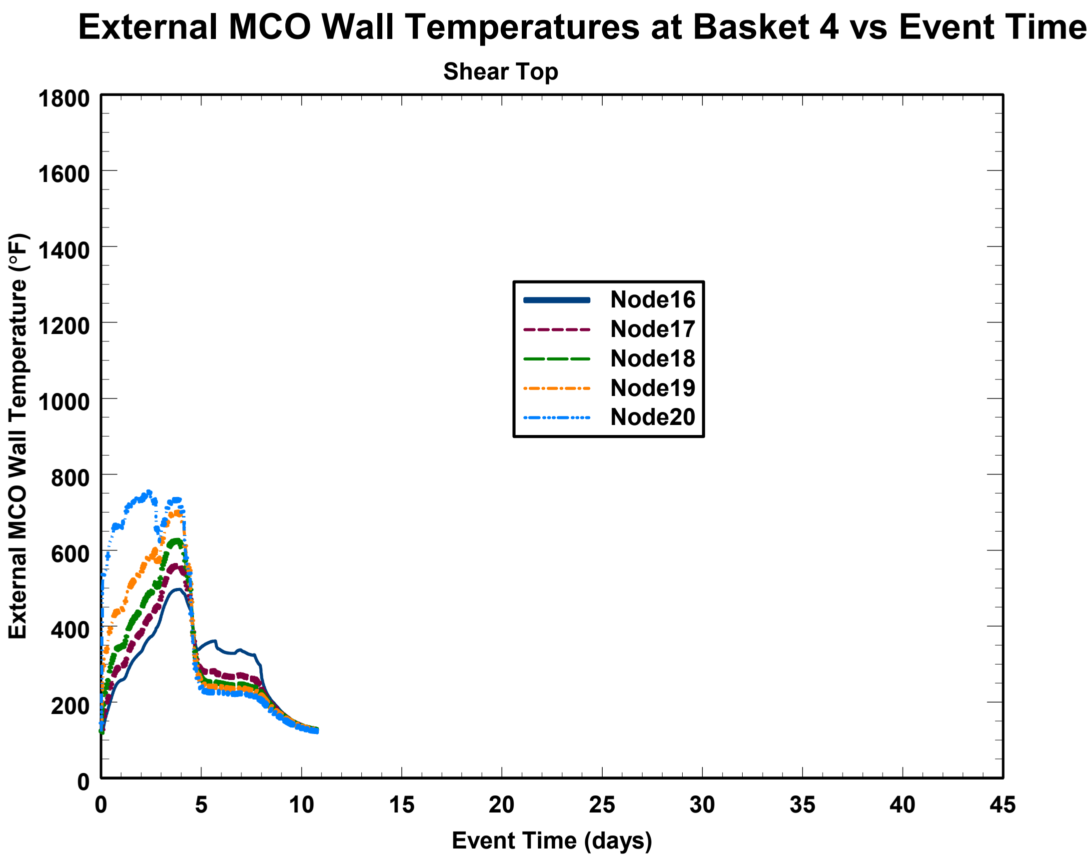

Figure 83. External MCO wall temperatures at nodes in Basket 4 for open top breach.

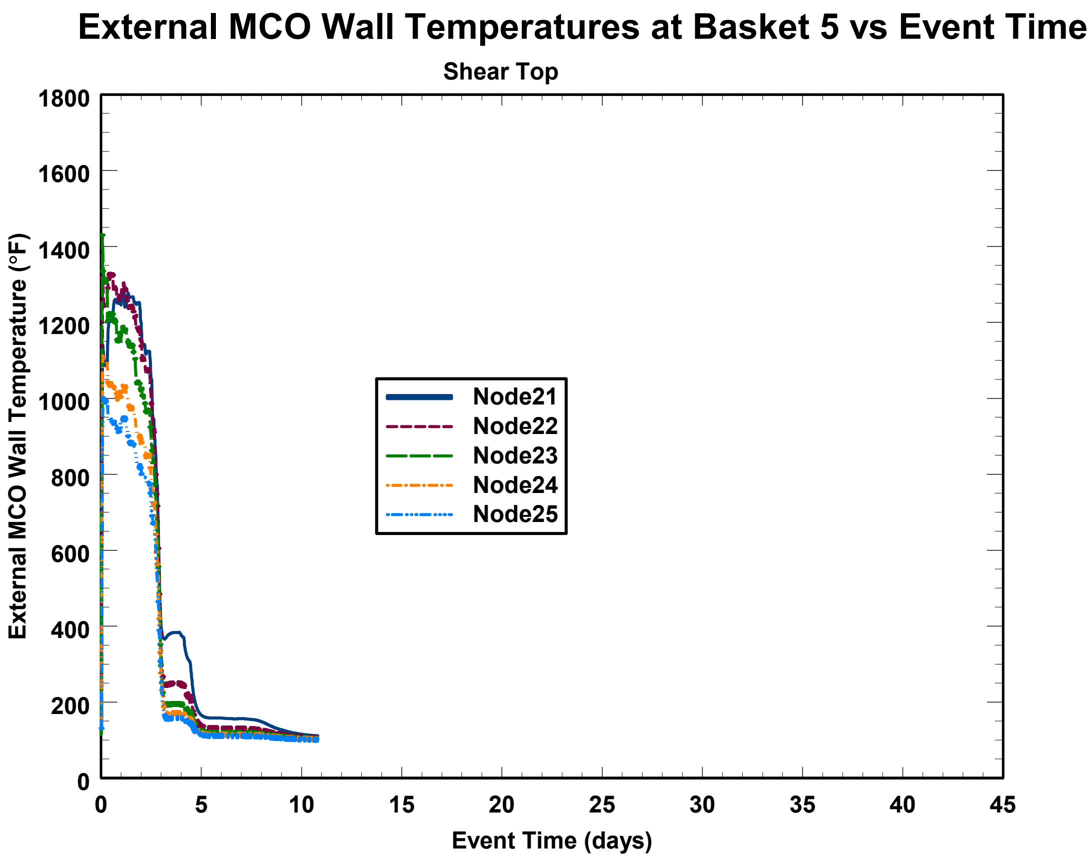

Figure 84. External MCO wall temperatures at nodes in Basket 5 for open top breach.

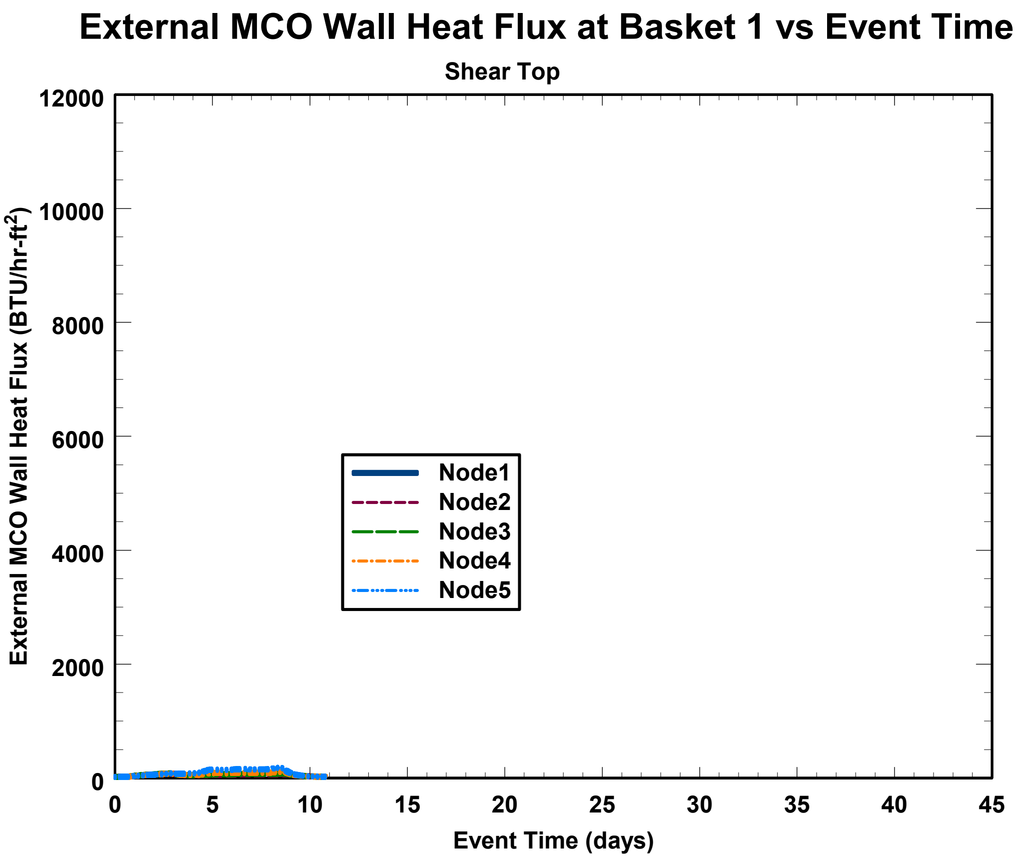

Figure 85. External MCO wall heat flux at nodes in Basket 1 for open top breach.

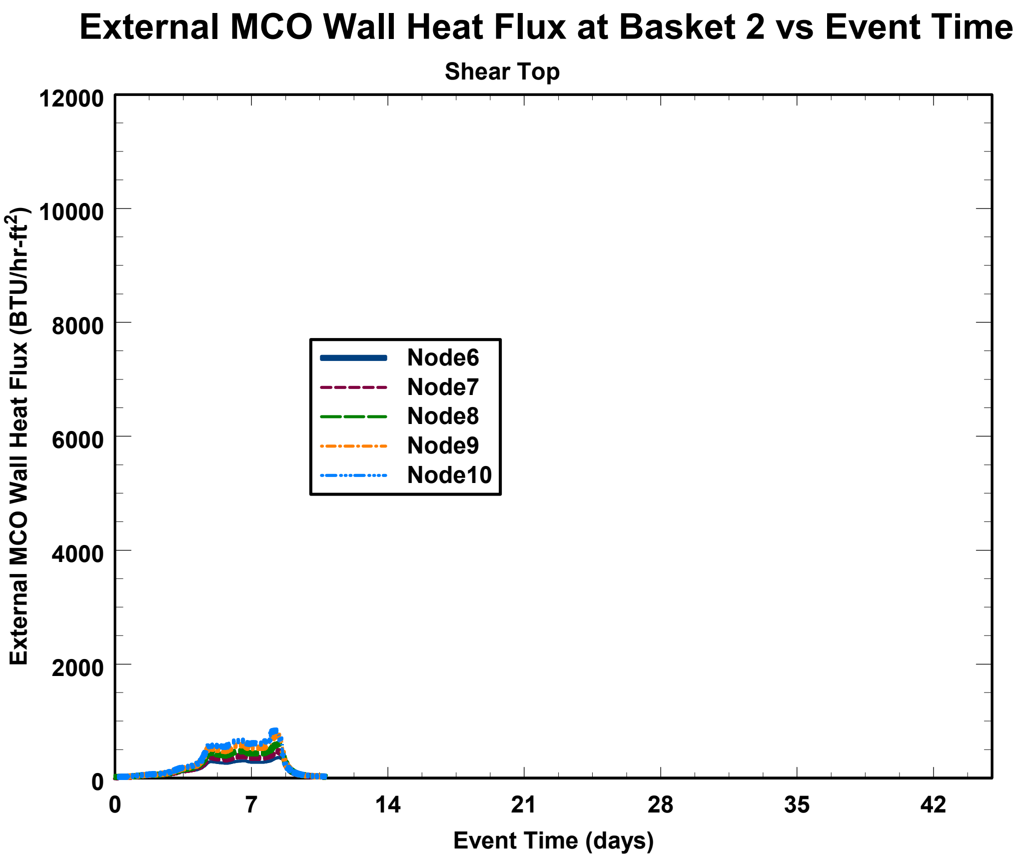

Figure 86. External MCO wall heat flux at nodes in Basket 2 for open top breach.

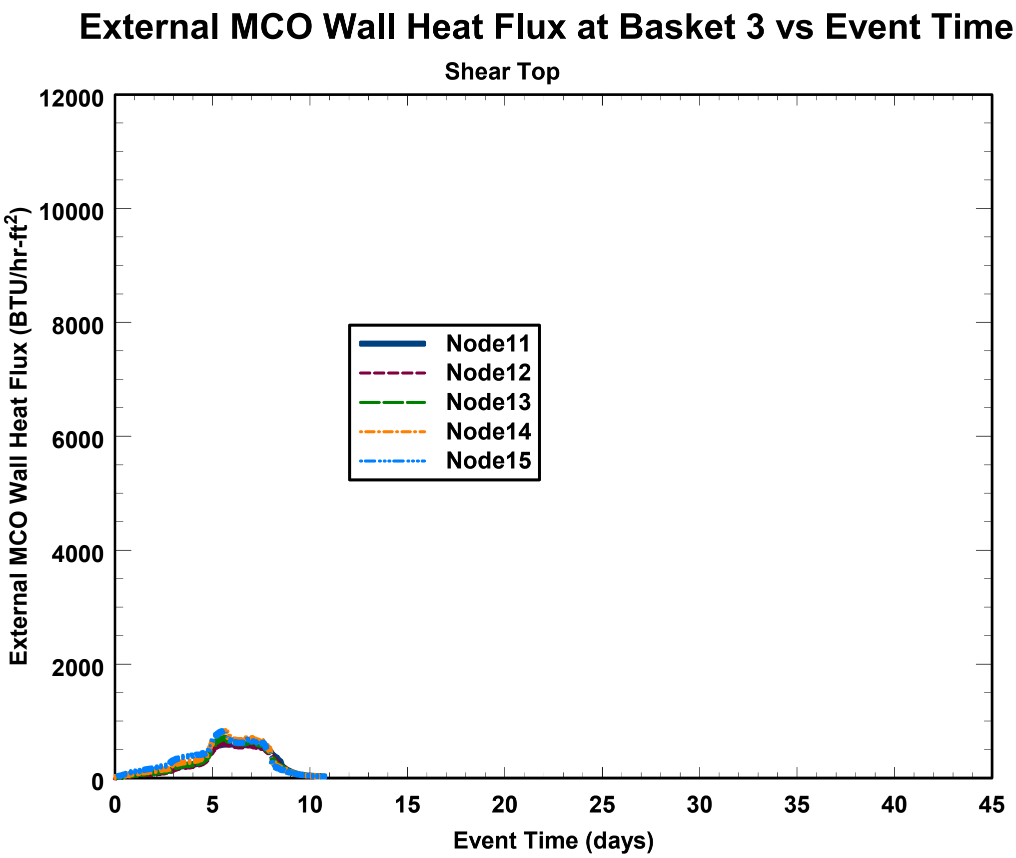

Figure 87. External MCO wall heat flux at nodes in Basket 3 for open top breach.

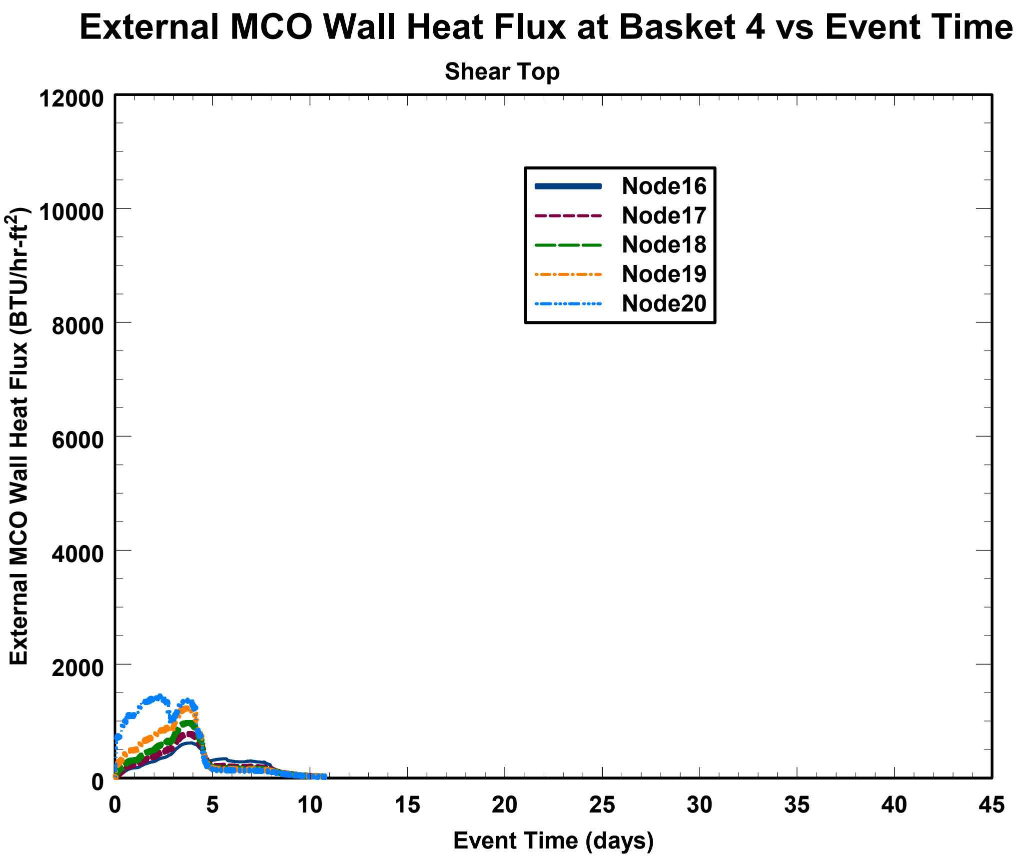

Figure 88. External MCO wall heat flux at nodes in Basket 4 for open top breach.

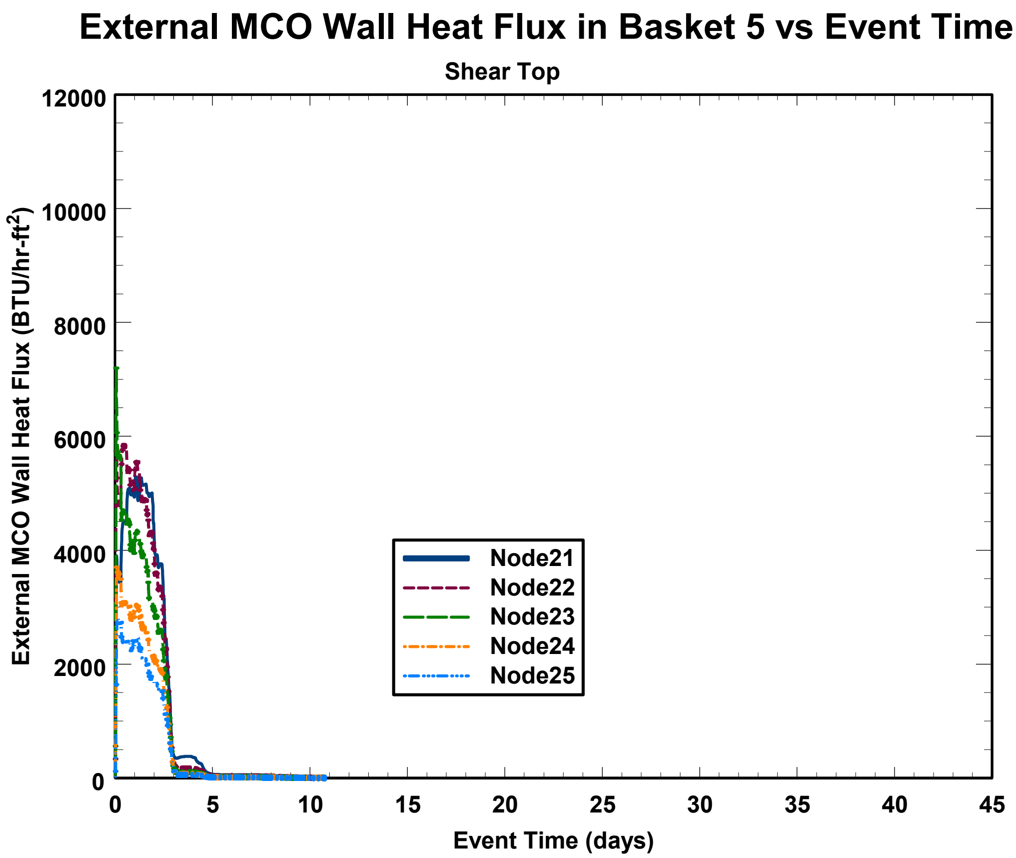

Figure 89. External MCO wall heat flux at nodes in Basket 5 for open top breach.

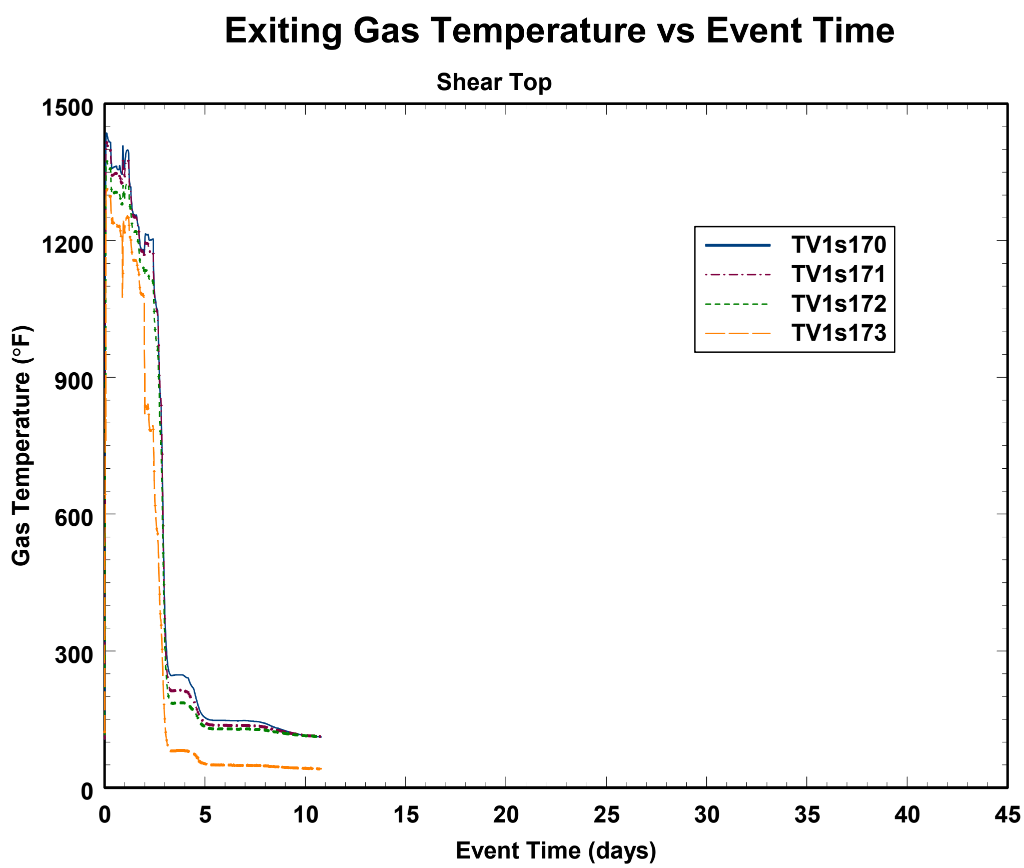

Figure 90. Exiting gas temperatures from open gas channels for open top breach.

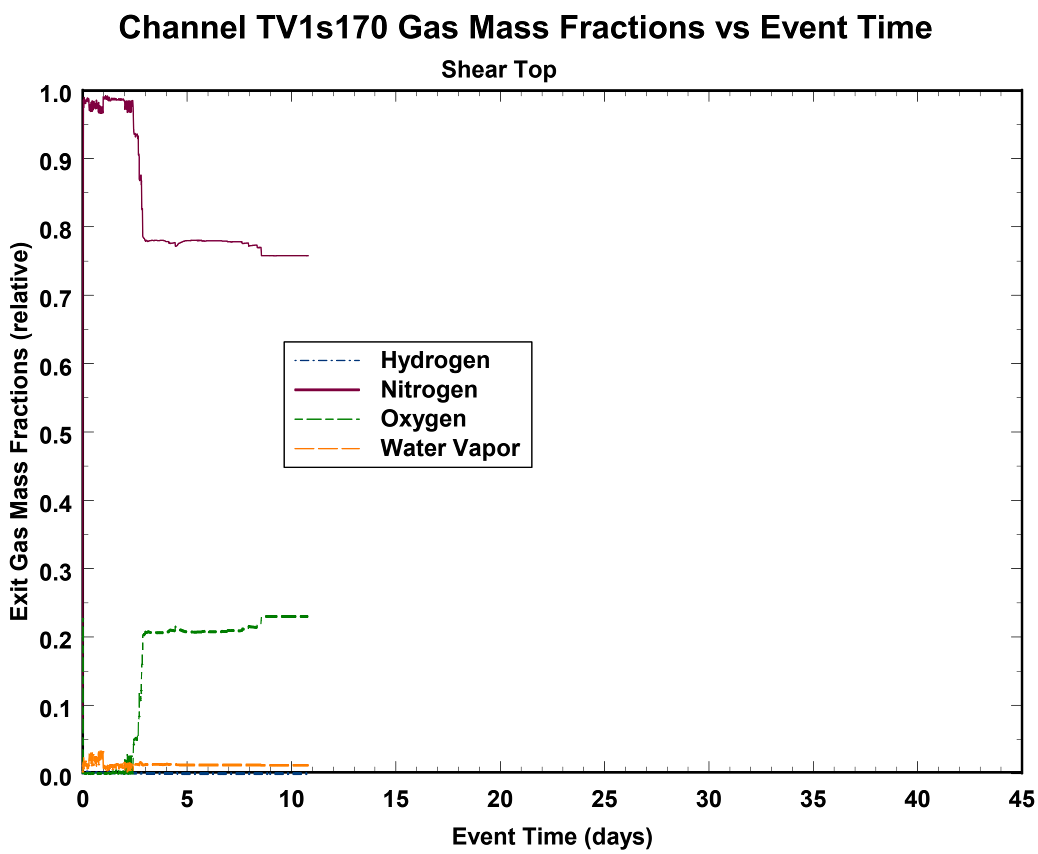

Figure 91. Relative concentration of gas species exiting gas channel TV1s170 for open top breach.

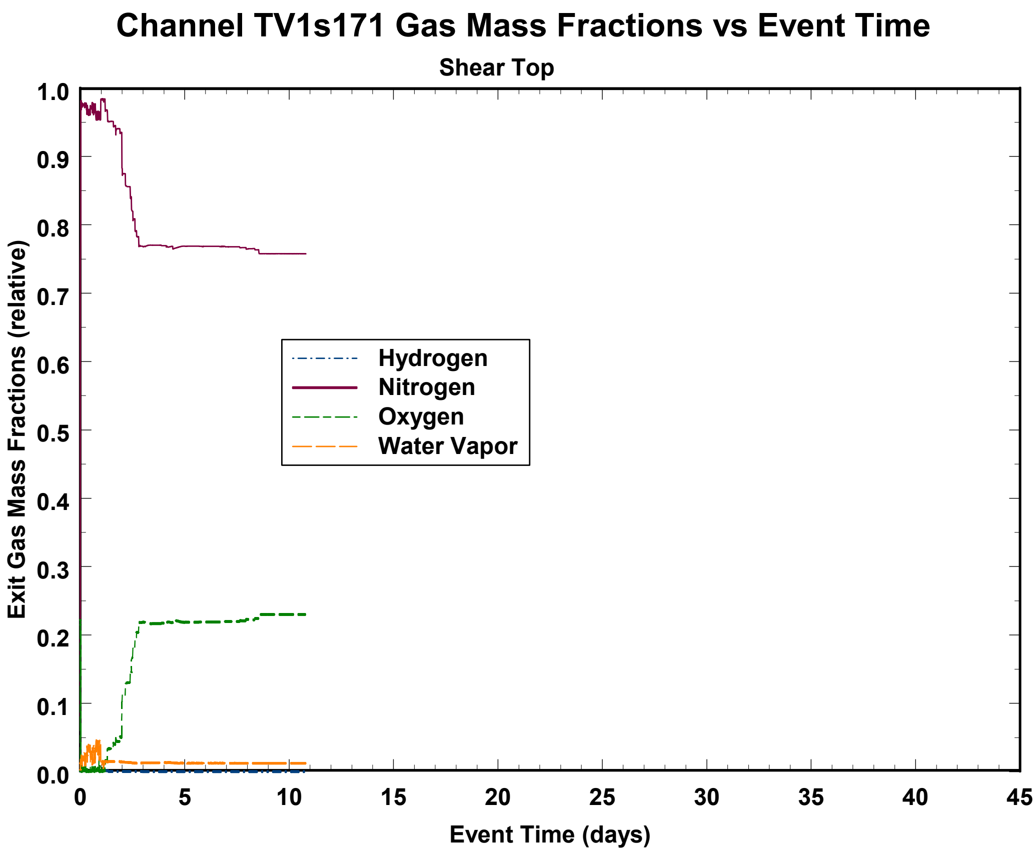

Figure 92. Relative concentration of gas species exiting gas channel TV1s171 for open top breach.

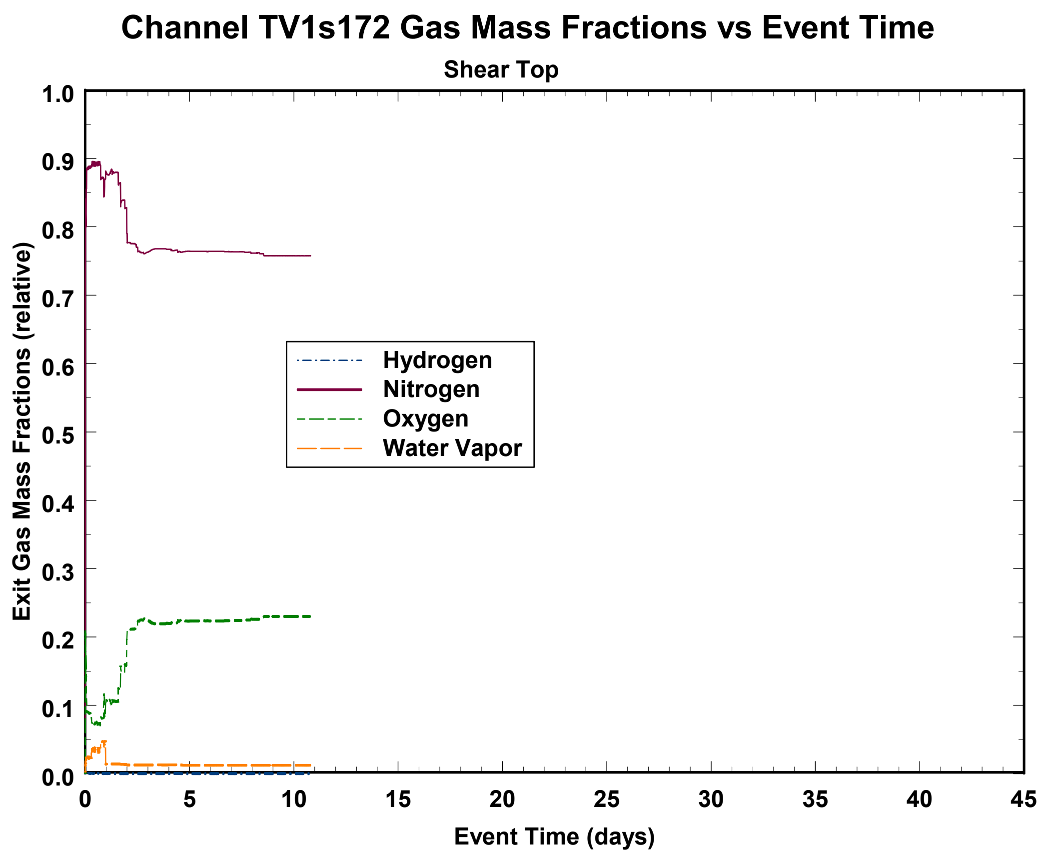

Figure 93. Relative concentration of gas species exiting gas channel TV1s172 for open top breach.

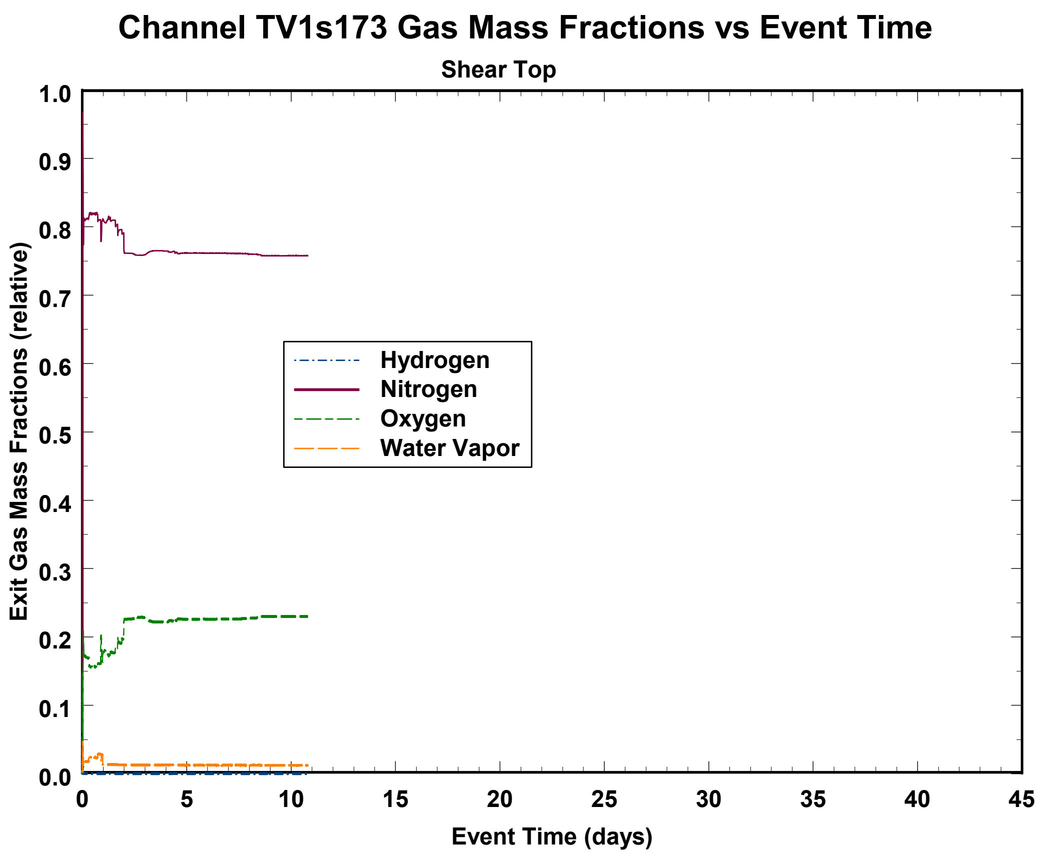

Figure 94. Relative concentration of gas species exiting gas channel TV1s173 for open top breach.

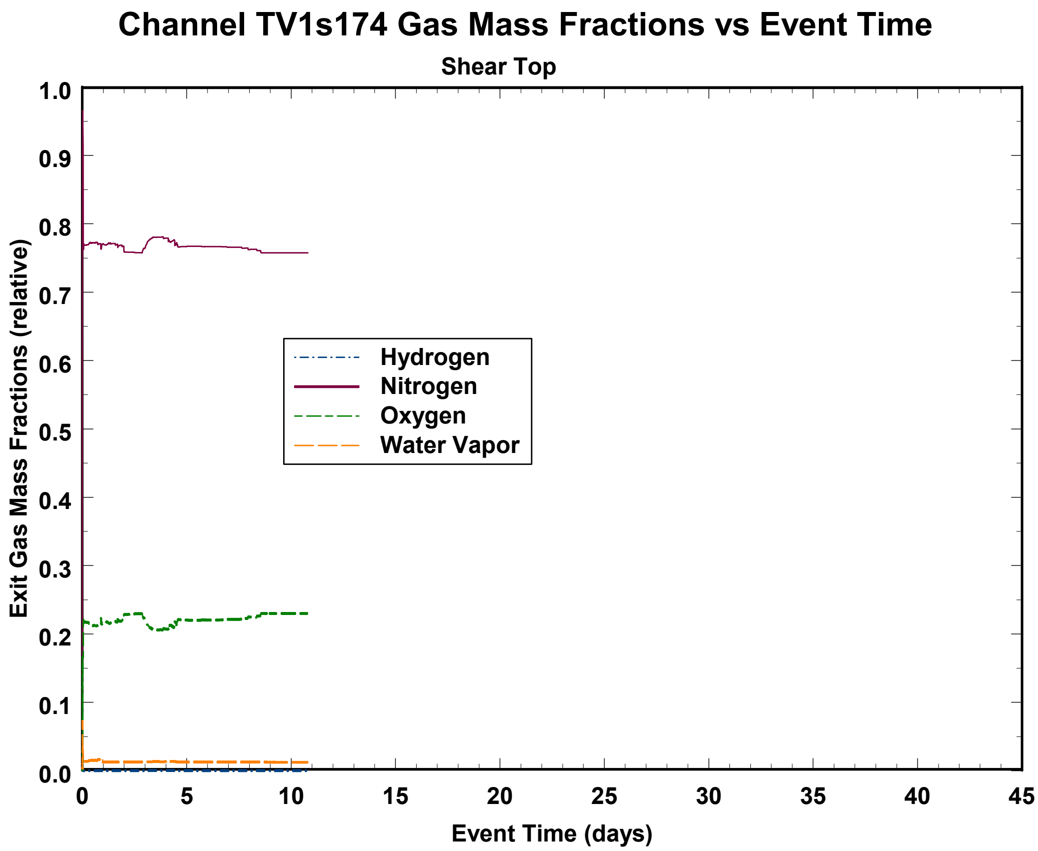

Figure 95. Relative concentration of gas species exiting gas channel TV1s174 for open top breach.

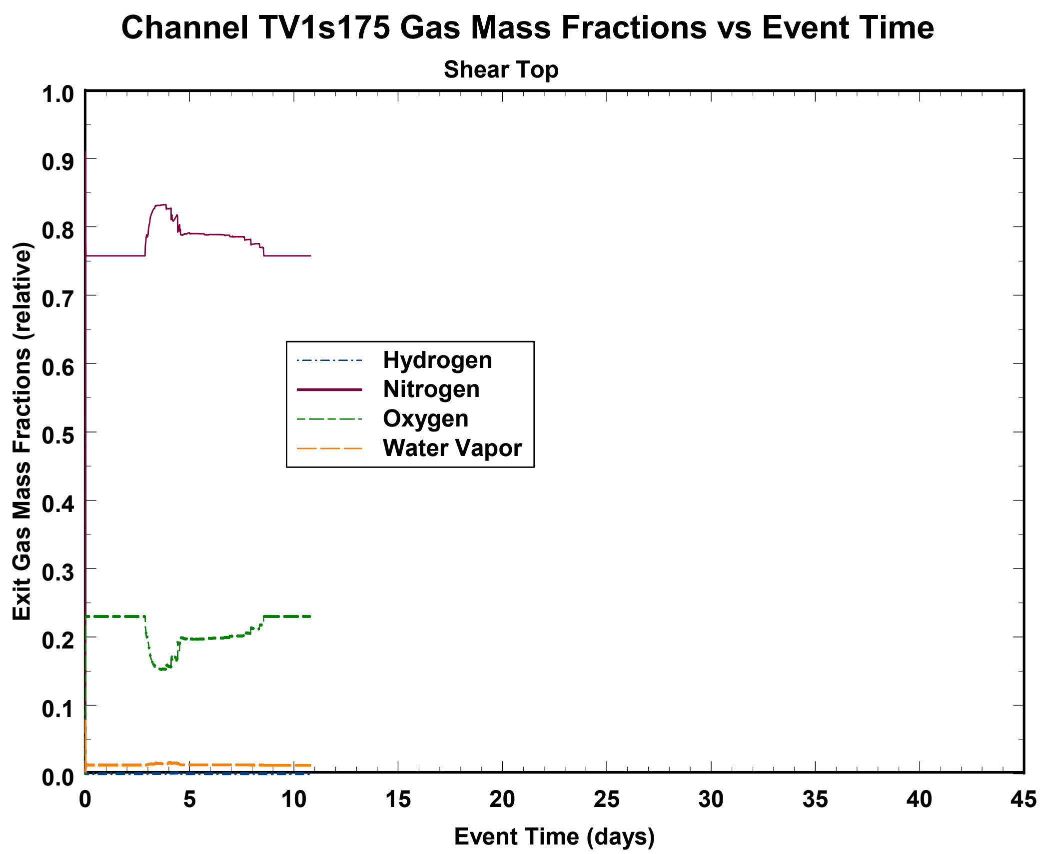

Figure 96. Relative concentration of gas species exiting gas channel TV1s175 for open top breach.

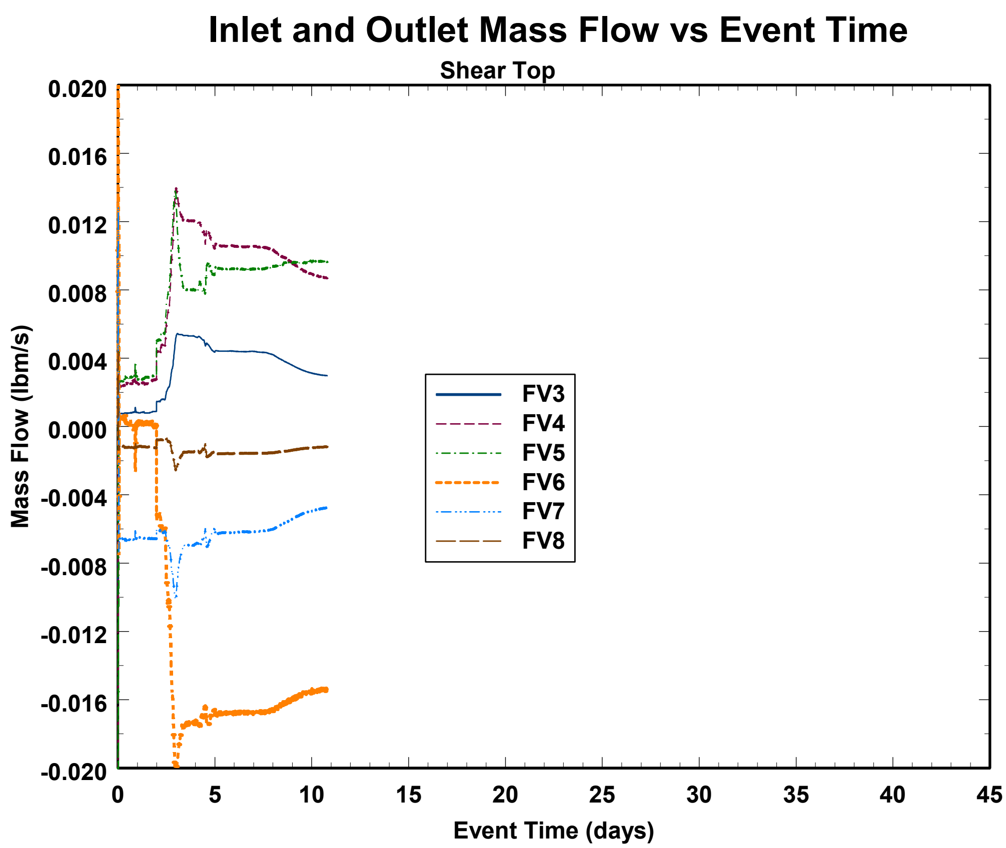

Figure 97. Mass flow at open gas channels for open top breach.

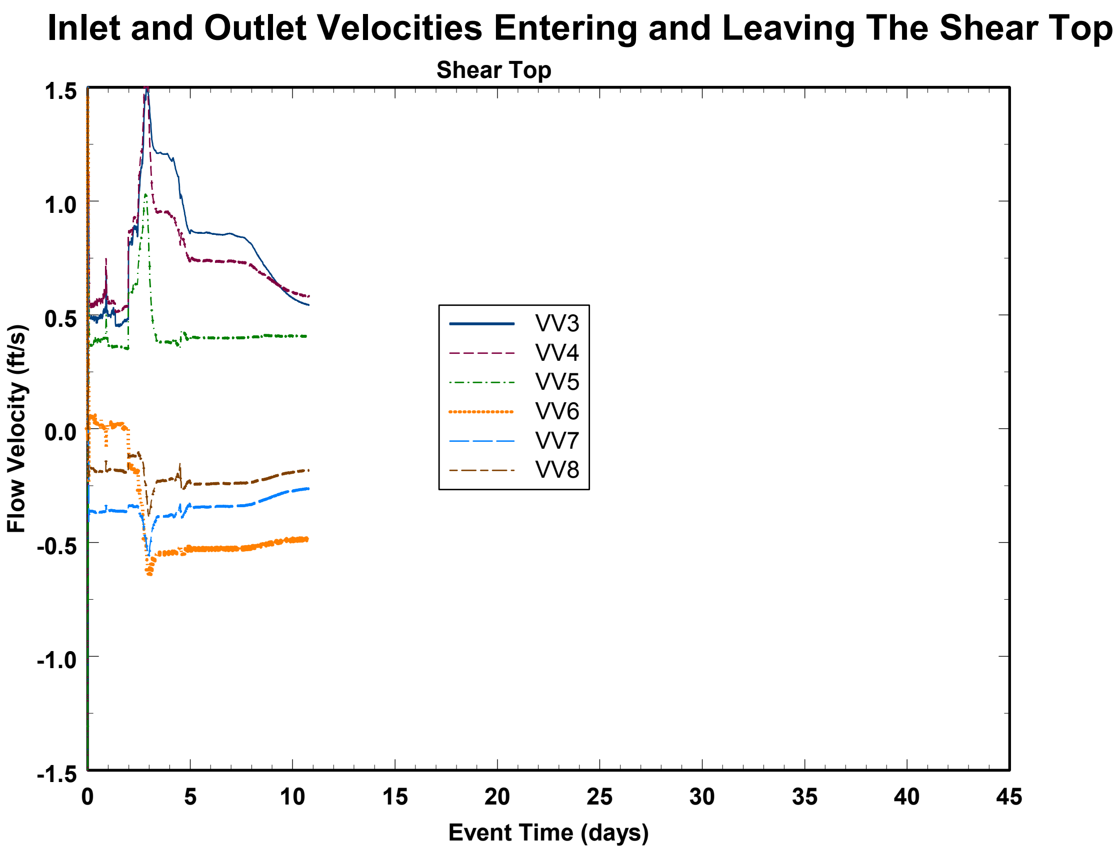

Figure 98. Flow velocity at open gas channels for open top breach.

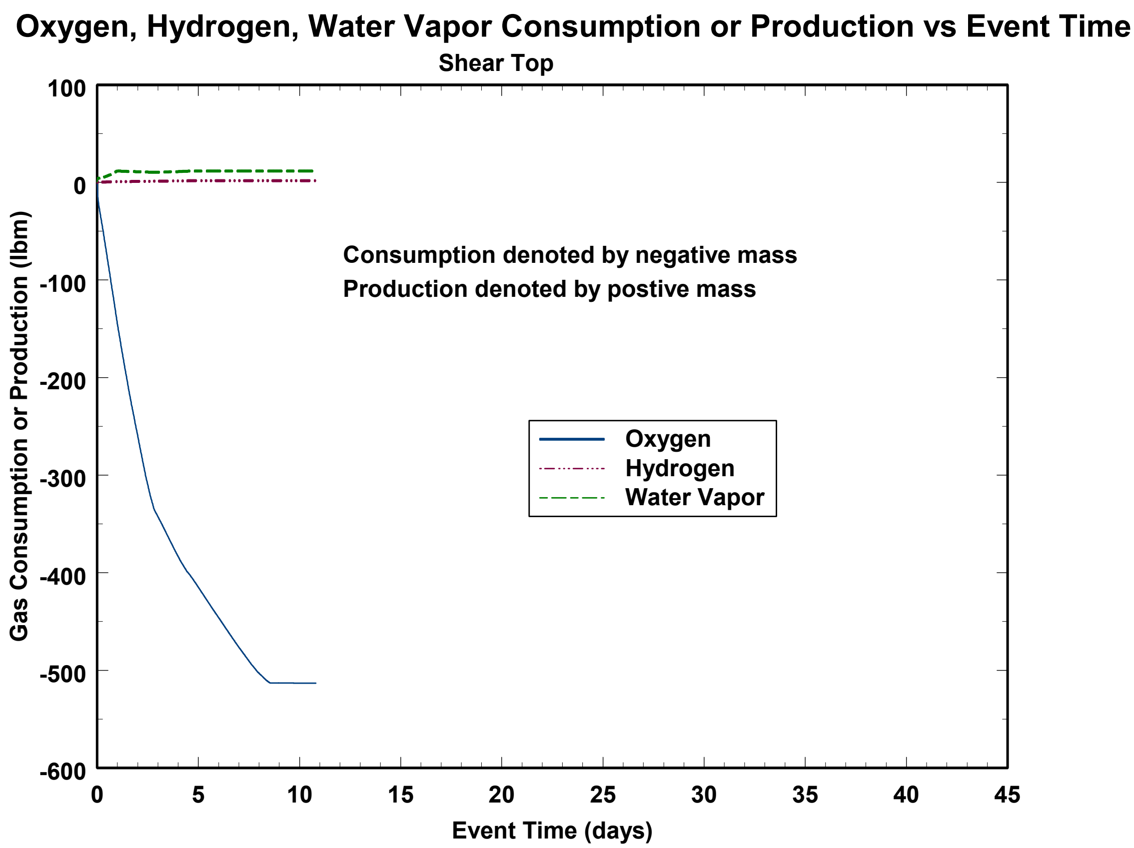

Figure 99. Oxygen, hydrogen, and water vapor consumption or production for open top breach.

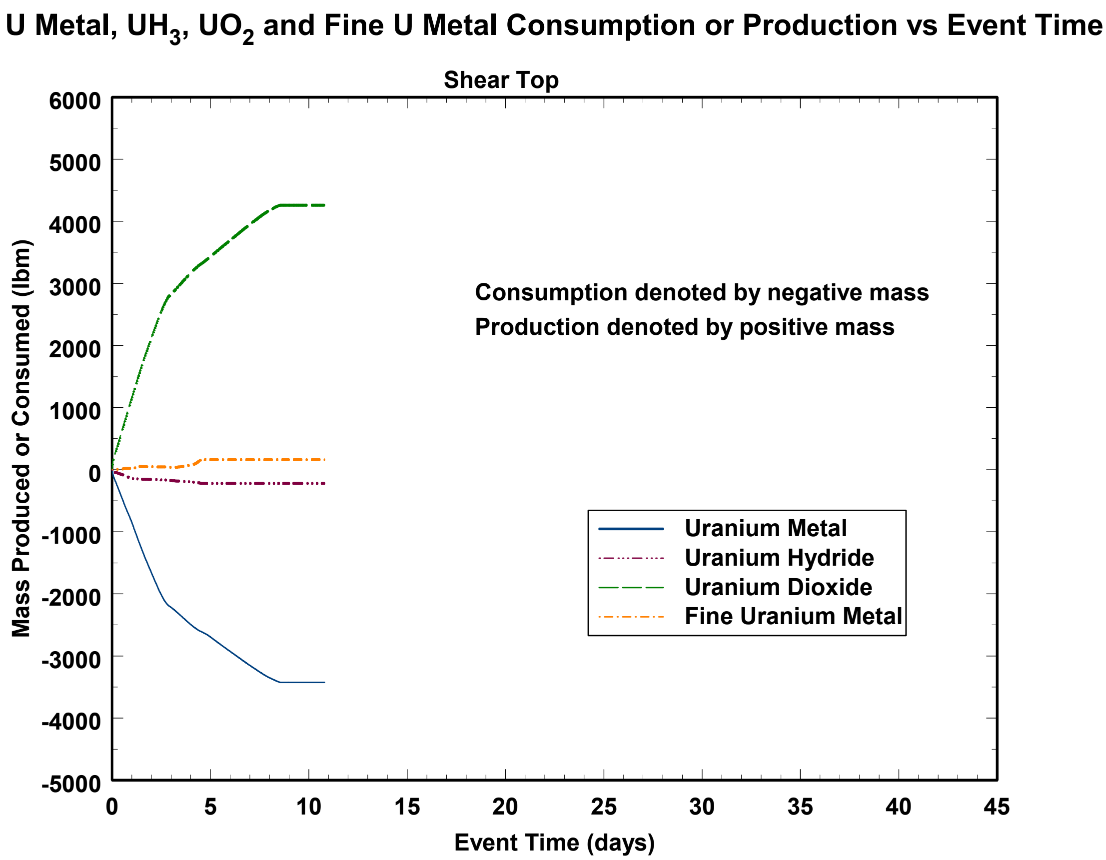

Figure 100. Uranium, uranium dioxide, uranium hydride, and fine uranium metal consumption or production for open top breach.

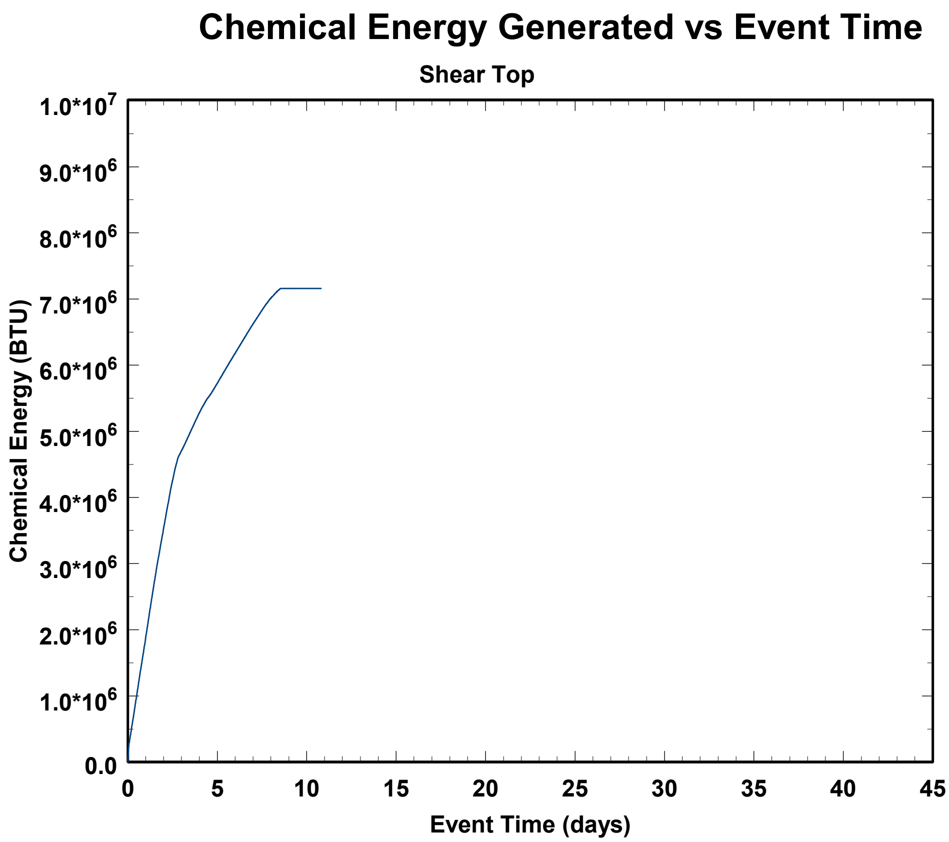

Figure 101. Chemical energy output for open top breach.

3. SUMMARY OF OBSERVATIONS

The main trend seen in the GOTH_SNF computer model is the influence of hole size used in the **two-hole breach models**. As the hole size increases, the following increases except for the elapsed event time, which decreases:

- Peak MCO exterior wall temperatures
- Peak MCO exterior heat flux
- Peak inlet and outlet mass flows
- Peak inlet and outlet flow velocities
- Peak exit gas temperatures
- Uranium metal consumption rates
- Uranium dioxide production rates
- Oxygen consumption rates.

Other two-hole breach model key observations are:

- During the event the exiting gas is entirely composed of nitrogen since oxygen is consumed
- After the event both nitrogen and oxygen flow out because the oxygen is no longer reacting with the uranium
- Hydrogen is released in nonflammable quantities
- Peak MCO exterior wall temperatures and heat fluxes occur in the top portion of the MCO wall occupied by the scrap basket
- Outlet velocities are not life threatening or injurious high velocity jets.

Observations for the open top breach:

- Countercurrent flow in the open top breach
- Peak values, elapsed event time, and chemical energy output bounded by similar values in the 1-in. and 2-in. two-hole breaches
- Highest mass flow and flow velocities of all breaches
- Hydrogen is released in nonflammable quantities.

Below is a comparison table for peak MCO exterior wall temperatures, peak exit gas temperature, peak exterior wall temperature at gas exit, and elapsed event time output for all breach configurations.

Table 1. Comparison of peak external MCO wall temperature, peak exit gas temperature, peak exterior wall temperature at gas exit, and elapsed event time with breach configuration.

Breach Configuration	MCO Exterior Wall Peak Temperature in °C (°F)	Peak Exit Gas Temperature in °C (°F)	Peak Exterior Wall Temperature at Gas Exit Temperature is ºC (ºF)	Elapsed Event Time (days)
Two 2-inch holes	913 (1675)	788 (1450)	638 (1180)	3.5
Open top	782 (1440)	788 (1450)	NA	9
Two 1-inch holes	460 (860)	496 (925)	386 (727	15
Two 0.75-inch holes	316 (600)	371 (700)	288 (550)	27
Two 0.5-inch holes	182 (360)	254 (490)	182 (360)	>45

All values in the table have been rounded off and are approximate. The peak exterior wall temperature at the gas exit is the MCO wall temperature at the same computing node as the exit hole. The peak MCO exterior wall temperature is the hottest MCO wall temperature and may or may not be at the elevation of the exit hole.