

Butene and Carbon Monoxide Flammable Clouds in a Glovebox with Two Hotplates

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management
Project Hanford Management Contractor for the
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Richland, Washington

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M. G. Piepho
Fluor Federal Services, Inc.

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Key Words: Butene, carbon monoxide, hydrocarbon, magnesium hydroxide, flammable gas

Abstract: Two flammable gases in a glovebox (HC-230C-3) at the Plutonium Finishing Plant (PFP) were modeled to quantify the amount of flammable gas and its spatial location. The two flammable gases are butene (C_4H_8) and carbon monoxide (CO). Butene is a hydrocarbon (C_4H_8) gas that is released from magnesium hydroxide precipitate containing dibutyl-phosphate when sufficiently heated. Carbon monoxide is a flammable gas that is released from precipitate containing oxalic acid when sufficiently heated. The model for calculating butene and carbon monoxide gas concentrations is described in Section 2.0. The scenarios of release with the specific model and parameters are described in Section 3.0. The results of calculations are described in Section 4.0 with the summary and conclusions appearing in Section 5.0.

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IN A GLOVEBOX WITH TWO HOTPLATES**

By

M. G. Piepho
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BUTENE AND CARBON MONOXIDE FLAMMABLE CLOUDS IN A GLOVEBOX WITH TWO HOTPLATES

1.0 INTRODUCTION

Two flammable gases in a glovebox (HC-230C-3) at the Plutonium Finishing Plant (PFP) were modeled to quantify the amount of flammable gas and its spatial location. The two flammable gases are butene (C₄H₈) and carbon monoxide (CO). Butene is a hydrocarbon (C₄H₈) gas that is released from a precipitate obtained from solutions containing dibutyl-phosphate when sufficiently heated. Carbon monoxide is a flammable gas that is released from precipitate containing oxalic acid when sufficiently heated. Plutonium nitrate solutions are processed as part of the stabilization campaign. Some of these solutions contain miscellaneous organic compounds at 1%vol or less. Flammability concerns must be address to insure plant safety during this campaign. Two scenarios are examined:

- 1) Low-Exhaust-Rate Scenario – the exhaust or vent rate is lowered to 75 ft³/min instead of the normal rate of 150 ft³/min.
- 2) Loss-of-Ventilation Scenario – the electric power to the exhaust fan is lost after the hotplates have become hot; the hotplate power is on or off (2 cases) for 15 minutes after ventilation is lost.

The model for calculating butene and carbon monoxide gas concentrations is described in Section 2.0. The scenarios of release with the specific model and parameters are described in Section 3.0. The results of calculations are described in Section 4.0 with the summary and conclusions appearing in Section 5.0.

2.0 GENERAL MODEL AND CODE

The time-dependent C₄H₈ and CO concentrations are calculated by using the FLUENT code, which also calculates the gas velocities and temperatures in the glovebox. The FLUENT code is a commercially available computational fluid dynamics code that was developed by Fluent Incorporated (10 Cavendish Court, Centerra Resource Park, Lebanon, New Hampshire 03766, telephone 603-643-2600) under the ANSI software quality assurance standard ISO-9001. The code was first used at Hanford for calculating leak path factors in the K-Basin facilities, which was documented in the K-Basin Safety Analysis Report's supporting calculation note, HNF-1777, *K West Basin Integrated Water Treatment System Annular Filter Vessel Accident Calculations and Derivation of Leak Path Factors*.

Since its first applications, FLUENT has been used for calculating Leak Path Factors of respirable particles with thermal effects for vented tanks, receiver tanks, and the 204-AR unloading facility (*Stochastic Consequence Analysis for Waste Leaks*, RPP-5667), and the T-Plant facility (*Calculation of Leak Path Factors for T-Plant Accident Scenarios*, CO-2001-SNF-00019). It has also been used to calculate the thermal natural circulation effects in the Canister Storage Building (CSB) due to different heat loads from vitrified high-level waste in canisters. The code also was used to model sodium spray combustion (CO-2001-FFTF-024).

FLUENT was used to calculate butene gas concentrations in a PFP glovebox, releases from two boats on one hotplate (*Butene Release from Magnesium Hydroxide Precipitation Process Precipitates Containing Dibutyl Phosphate*, HNF-8091). It also was used to calculate carbon monoxide gas concentrations in the glovebox, released from two boats on one hotplate (Appendix 2B of *Attachment 1 – Supplemental Hazards Analysis for the PFP Oxalate Precipitation Process*, HNF-5389).

In this report, the FLUENT code was used to calculate both butene and carbon monoxide gas concentration, released from precipitate in 4 boats placed on two hot plates in Glovebox HC-230C-3 at the PFP. Hence, the model for this analysis is different from previous analyses in that two flammable gases are being released from two hotplates. The second hotplate will add more heat to the glovebox in addition to twice the gas masses as a single hotplate. Also, in the previous models (HNF-5389 and HNF-8091), the single hotplate was flush against the glovebox corner walls, which allowed no air to flow between the hotplate and glovebox walls. Since it is not realistic to have the hotplate flush against the glovebox walls, it was moved away from the walls (6 inches from left end and 3 inches from front). The second hotplate was placed in a more central location about ¼ ft from the first hotplate, as shown in Figure 1 to 3. For this analysis, FLUENT solved ten coupled partial differential equations, in a three-dimensional domain representing the glovebox, which are itemized below:

1. Mass Continuity
2. X Velocity (horizontal)
3. Y Velocity (horizontal)
4. Z Velocity (vertical)
5. Energy (Temperature)
6. Turbulence Kinetic Energy
7. Turbulence Dissipation Rate
8. Mass Balance of Butene (C_4H_8)
9. Mass Balance of Carbon Monoxide (CO)
10. Mass Balance of Carbon Dioxide (CO_2)

The mass balance of air is not calculated directly by FLUENT, but is calculated indirectly by subtracting the calculated sum of C_4H_8 , CO, and CO_2 mole fractions from one, which is always the value of the sum of all four gas mole fractions. The gas properties in the glovebox are calculated in FLUENT from a mixture of air, CO and CO_2 properties, weighted by the volume of each gas, for each of the 55,000 computational cells. The ideal gas law was used to estimate the pressure in each cell with the effects of temperature and forced convection included.

Also, for turbulent flow conditions, which occur in this analysis due to large velocities and corresponding large Reynolds numbers near the exhaust vent and inlet port, the RNG (Re-Normalized Groups) k-epsilon option in FLUENT code was chosen for the viscosity model.

3.0 DESCRIPTION OF MODEL, SCENARIOS AND CASES

The magnesium hydroxide precipitation process involves plutonium nitrate solutions, and both the heated wet oxalate precipitates and magnesium hydroxide precipitates contain organics. The solutions contain less than 1%vol organics.

Plutonium nitrate solutions containing organics at concentrations of less than 1%vol do not pose an increase in hazards for the Magnesium Hydroxide Precipitation Process (MHPP) accidents previously documented (ECN 658096). Most of the organics in the solutions are tributyl phosphate (TBP) or degradation products of TBP such as dibutyl phosphate (DBP), monobutyl phosphate (MBP) and phosphoric acid (HNF-6254). The TBP, DBP, and MBP react with plutonium to form insoluble precipitates. If other organics are present and have a vapor pressure significantly greater than water, they will have vaporized and have been swept away from the cans during air exchanges over the past 25 years. Any remaining organics do not present a fire hazard because of their low concentrations and high solubility in plutonium nitrate solutions, and their formation of compounds with plutonium. Therefore, none of the organics at concentrations less than 1%vol in these solutions are flammable. However, organics in the heated precipitates can be released as a flammable gas upon decomposition of the precipitates.

A supplemental hazards analysis was performed to identify and evaluate hazards associated with changing the solutions stabilization process from precipitation with magnesium hydroxide to precipitation using oxalic acid (HNF-5389). The hazards posed by the solutions are the same as described above. However, this supplemental analysis identified issues associated with heating oxalate precipitates due to the generation of flammable gases. The additional accident that needs to be analyzed is "Deflagration in the Glovebox" because the oxalate precipitation process generates both CO and C₄H₈ flammable gases when the precipitate containing organic is dried in boats on hotplates. This analysis addresses the deflagration accident and issues.

Butene (C₄H₈) and carbon monoxide (CO) concentrations were calculated for Glovebox HC-230C-3 from two hotplates at PFP for two scenarios. The first scenario used bounding release rates per two boats per hot plate for both butene and carbon monoxide, and a low exhaust (ventilation) rate of 75 ft³/min, instead of the normal 150 ft³/min. The second scenario includes the loss of ventilation for glovebox, due to electric power loss, with hotplate power on or off. The second scenario also covers loss of ventilation for glovebox due to fire damper closing, but the exhaust fan stays on. Having the fire damper closing and the exhaust fan going off are two independent events, each with a very low frequency, making the combined frequency beyond extremely unlikely.

3.1 GRID OF MODEL DOMAIN OF GLOVEBOX

The key features of the grid for the model domain of glovebox are shown in Figures 1 to 3. The overall dimensions of the glovebox were **45** in. wide by 168 in. long by **75** in. high. The **3D** grid of glovebox interior has 55,000 computational cells. In other words, values of all ten variables, listed in Section 2 above, are computed in each of the 55,000 cells for each time step, which varied from 1 to 10 seconds.

The inlet port is a rectangle in the model (**9** in. wide by **12** in. high) that was placed on the backside of the glovebox about **3** in. from left side of glovebox and about **9** in. above the glovebox floor. The exhaust vent is modeled as a 5 in. by 5 in. square with an area of **25** in². The volumetric exhaust rate is **75** ft³/min in the model, which represents a lower bound of the possible, exhaust rates, and is equivalent to an exit velocity of about **2.2** m/s.

In order to include the effects of flow resistance of the pipes, filter, tanks, etc., which are located in the approximate middle (Y-direction) and right side (X-direction) of the glovebox away from the inlet and hotplate, the porous-media option in the FLUENT code was chosen. This option is generalized enough to include flow through holes and around obstacles, for example, and not restricted to just porous media like soils. The porous media or flow-resistance region is shown in Figure 2; there are two regions with the smaller region's bottom touching the glovebox floor and the upper larger region is located on top (about **7.5** inches above the glovebox floor) of the smaller one. There is a free-flow region about **5** inches on each side of the larger porous region and about **7.5** inches above the top of it (just below the glovebox top). These free-flow channels will have faster gas velocities than the porous/resistive regions.

The flow resistance given to the porous regions was $10,000 \text{ m}^{-2}$, which represents the inverse of the permeability; hence, the equivalent permeability of the porous regions is 10^{-4} m^2 . Sensitivity cases were run with 10 times larger resistance and 100 times smaller resistance than base case's to determine that the horizontal velocity magnitude increases near the top of glovebox as the flow resistance increases. This did not affect the flammable clouds very much. For comparison, an open pea-sized gravel with no fine media imbedded has a permeability around 10^{-9} m^2 , and, thus has a much higher flow resistance than the porous regions in the glovebox. The porous/resistive modeling approach for the glovebox is more realistic, in regards to accuracy around the boat, and more conservative, in regards to total butene and CO masses in glovebox, than just having open regions throughout the glovebox with little or no flow resistance. However, the porous/resistive region would not be adequate for detailed accurate gas concentrations in the region around pipes or tanks. Fortunately, based on previous simulations (HNF-8091 and HNF-5389), the high flammable gas concentrations occur just above the boat. Hence, high accuracy is desired in and near the boats, as expected. The flow resistance farther away adds realism to the model, in regards to the flow around many obstacles in the glovebox and its effect on concentrations near the boats.

The top of the Belhaven hotplate was modeled as square that is **12** in. by **12** in. with a vertical height of about **2** in. It was placed 6 in. from the lower left corner of the glovebox on the opposite side of the inlet vent, and **3** in. from the front of glovebox. The second hotplate was placed **3** in. back and **3** in. to the right of the first hotplate (see Figures 2 and 3). Even though it may be more conservative to place the first hotplate in the corner touching the sides of glovebox,

it is not realistic or practical to place it so tight against the glovebox. If it touches the glovebox, much heat would be lost to the glovebox and it is not easy to reach or work around in a corner.

The walls of the glovebox are fixed at a temperature of 300 K (27 °C) in the model. Since the exhaust rate brings in fresh air (assumed to be 27 °C or -80 °F), the glovebox is also air-cooled.

3.2 CARBON MONOXIDE AND DIOXIDE SOURCE AND PROPERTIES

The source location of the butene, CO and CO₂ in the model is the surface located one inch below the top of the boats, representing the effects of a shrinking precipitate due to decomposition and emission of gases. It was of interest to see the effects of the boat sides on the gas concentrations. Only one boat boundary in the model is used to represent the two boats side by side and was given the dimensions of 12 in. by 12 in. by 2 in. high, even though the real boats together are little smaller. The boat sides and top precipitate surface were given a fixed temperature of 200 °C, which is lower than expected with the hotplate and precipitate reaching temperatures above 250 °C in experiments. A lower temperature causes less natural circulation and is conservative in regards to flammable concentrations. The receded surface below the top of boats conservatively represents the precipitate's upper surface after it has shrunk or decomposed down from the top boat level. The CO gas was released at a temperature of 200 °C in the model, which is lower than the major CO release shown in HNF-5389, and is conservative because lower temperatures will cause less gas buoyancy and expansion, resulting in higher concentrations. Even though the decomposition temperature of 150 to 187 °C is listed for the decomposition of CH₂O₂ to CO + H₂O (HNF-5389), the more rapid releases occur at higher temperatures, and the decomposition is exothermic, which will also heat up the CO and the surrounding precipitate. The temperature increases of a cerium precipitate in a boat on a new Bellhaven hotplate is described in HNF-9339, which indicates a long time (> 1 hr) to heat the entire boat's contents above 200 °C with the center part getting heated last. This indicates that the early CO release will be from a corner, then from the sides, and then the center part, which takes more than an hour, with the exothermic effects of decomposition sequentially staged over the entire boat.

The gas space located in the top inch of the interior of the boat was included in the model with the CO release rate specified at the surface one inch deep. The release of 1.14 gmole/min, which was a rate derived in HNF-5389 for two boats, is based on a bounding fractional release of 5%/min measure from a 130-g sample of precipitate. The peak fractional release rate observed in 130 g of cerium oxalate slurry containing 0.5 M free oxalic acid was less than 5%/min when stirred and less than 1.2% when not stirred (HNF-5389), which is 4.2 times lower ($4.2 = 5.0/1.2$) than when stirred. Also, there was evidence from the experiments that as the sample size gets larger, the fractional release rate gets smaller, which is expected since a larger sample will not heat up as fast as a smaller one and the decomposition will be sequentially staged and slower. Since the amount of precipitate in a boat is much larger than 130 grams, the fractional release rate, including measurements uncertainties, will be bounded by 5%/min when stirred. Previously, in HNF-5389, a CO mass release rate was based on a 10%/min fractional release rate, yielding 2.27 gmole/min, which included margin. However, this high rate of

2.27 gmole/min, with a margin of at least two, is now considered overly conservative for the following reasons:

- 1) the entire boat, with much greater precipitate than 130 grams, does not heat up fast enough to support such a large release rate ($> 5\%/min$), especially with the new Bellhaven hotplate (HNF-9339),
- 2) the volume of the wet filtercake in a hatch (36 L) with 2500 g of Pu was 6.578 L (HNF-5389), which will not fit into two boats (per hotplate). If three or four boats were needed to hold the 6.578 L, then this alone would lower the mass release rate, independent of the lower rate of temperature rise resulting from the new hotplate.

However, to be somewhat conservative, the same bounding mass of CO (-635 g per hotplate or two boats) is assumed in this analysis. However, it is released at $5\%/min$ in the model, the bounding peak percentage release rate for a small sample, or 31.75 g/min in terms of mass per unit time for the large boat, which is about 1.14 gmole/min, for 20 minutes ($20 \times 31.75 = 635$ grams/2boats). Keeping the same peak release rate constant for the entire release period is also very conservative, since even the very small 130-g cerium precipitate had a release period of more than 40 minutes (HNF-5389). The larger amount of precipitate in boats, which lowers the fractional release rate, is used as margin to cover any uncertainties associated with the CO fractional-release-rate measurements from the smaller 130-g cerium precipitate and to cover any potential differences of precipitate with plutonium, instead of cerium. Other conservative assumptions in the release model are 1) both CO and butene are released at the same time, and 2) both pairs of boats on two hotplates in the glovebox heat up at the same rate.

The CO maximum release rate of 1.14 gmole/min, which represents about 48% of the total composite gas release (includes CO_2 and butene) from each hotplate, was held constant for the entire simulation time of 20 minutes. The diffusion coefficient for CO gas in air was set to a low value of 1.81×10^{-5} m^2/s , which is the normal diffusion coefficient value of air molecules at $0^\circ C$. At higher gas temperatures around $300^\circ C$, the diffusion coefficient value for CO (and air) would be larger by about a factor of 3, so at a temperature of $200^\circ C$ or so, the diffusion coefficient would still be somewhat larger than used here. Low diffusion coefficient values, such as used here, tend to minimize the spread of high concentrations, which is conservative in regards to peak concentration and flammability concerns. The diffusion coefficients are the key input parameters for the turbulent diffusion model in the FLUENT code.

CO has a molecular weight of about 28 g/gmole, and at room temperature, has a viscosity value of 1.84×10^{-5} kg/m-s, a thermal conductivity value of 0.026 w/m-K, and a specific heat value of 1040 J/kg-K. Each of these properties, except for molecular weight, increase in value at higher temperature, which was included in the FLUENT simulations.

In addition to CO release (see Section 3.3 for butene release), the release of carbon dioxide (CO_2) was also included in the FLUENT simulations. The main effect of the CO_2 gas is to dilute the mole concentration of the CO at the release surface and throughout the glovebox. The CO_2 release rate in model is 0.62 gmole/min based on the ratio of CO to CO_2 of about 1.84 due to not all CO_2 being released during decomposition (HNF-5389). This represents about 41% of the total mass release rate from boat surface. Water vapor was conservatively excluded from

the model. The water vapor, which is also released from precipitate decomposition, would dilute the flammable source term, resulting in lower flammable gas volumes. The model is conservative because it does not include water vapor in the source term, although, in reality most of the water vapor is released before CO is.

3.3 BUTENE SOURCE AND PROPERTIES

Previously (HNF-8091), the maximum butene release rate into a glovebox was specified at 2 grams/minute for magnesium hydroxide precipitate for 29 minutes, for a total inventory of 58 grams of butene. However, for oxalate precipitate with 1% organic, or 0.12 L of dibutyl phosphate (DBP) per boat, the total inventory of DBP per two boats is about 255.6 g ($2 \times 0.12 \text{ L} \times 1065 \text{ g/L}$, where 1065 g/L is the mass density of DBP). The 255.6 grams of DBP represent about 1.216 gmole of DBP, which contains two gmole of butene per gmole of DBP for a total of 2.43 gmole of butene. Since one gmole of butene is 56 g, there are about 136 g of butene (2.43×56) per two boats on one hotplate. The butene release rate was held constant at 6.96 g/min (-7 g/min) for 20 minutes, resulting in a total butene mass of 139 grams released from the precipitate per hotplate or a total of 258 g for two hotplates. The butene release is much higher (-3.5 times) than the previous bounding number of 2 g/min in HNF-8091 for magnesium hydroxide, partly because of the shorter release time of 20 minutes instead of 29 minutes in HNF-8091, and because the precipitate fits into smaller number of boats than did the magnesium hydroxide. For example, the bounding 139 grams of butene in two boats of oxalate used here is about 2.4 times ($139 \text{ g}/58 \text{ g} = 2.4$) larger than the 58 grams of butene mass used in HNF-8091 for magnesium hydroxide, which would increase the peak 2-g/min rate in HNF-8091 to 4.8 g/min. The peak rate used here, -7 g/min is about 50% higher than the 4.8 g/min, which adds margin to account for potential differences of butene release from oxalate instead of magnesium hydroxide. **Also**, to be conservative, this analysis assumed the release time periods of CO and butene to be identical.

The butene mass release of 7 g/min per hotplate, which is about 10.5% of the total composite gas release (which includes CO and CO₂) from each hotplate, was held constant for the entire simulation time of 20 minutes. The butene gas was released at a temperature of 200 °C, the same as the CO release temperature, as the most rapid butene release is above 200 °C, peaking around 252 °C (HNF-6254). The diffusion coefficient for butene in air was set to a low value of $1 \times 10^{-5} \text{ m}^2/\text{s}$, which is conservative. A low diffusion coefficient value was used for butene because exact data was not found. Thus, in order to minimize the mitigating effects of the diffusion rate, a low value was used in order to slow down the spread of butene, which is conservative in regards to peak concentration and flammability concerns.

Butene has a molecular weight of about 56 g/gmole, a viscosity value of $7 \times 10^{-6} \text{ kg/m-s}$, a thermal conductivity value of 0.016 W/m-K, and a specific heat value of 2620 J/kg-K. The temperature dependence of these properties for butene was not included in the model, because the butene mole fractions of gas mixture are smaller than the other gases, and the mixture properties are dominated by the other gases on a volumetric basis. As mentioned above, the diffusion rate coefficient value was $1 \times 10^{-5} \text{ m}^2/\text{s}$, which is small and conservative in regards to peak concentration.

3.4 SUMMARY OF GAS PROPERTIES

Since there are many gas properties, which are described above, used in the model, they are summarized in Table 1.

Table 1. Gas Properties of Four Gases in Model

Gas Property	CO	C₄H₈	CO₂	Air
Grams/gmole	28	56	44	29
Release Rate per Hotplate or 2 boats	31.8 g/min, 1.14 gmole/min	7.0 g/min, 0.036 gmole/min	27.1 g/min, 0.62 gmole/min	NA
Total Release in 20 minutes for 2 hotplates	-1270 grams	-280 grams	1082 grams	NA
Viscosity (kg/m-s) @ 300 K (800 K)	1.84 x 10 ⁻⁵ (3.77 x 10 ⁻⁵)	7.0 x	1.49 x (3.64 x 10 ⁻⁵)	1.84 x (3.7 x 10 ⁻⁵)
Specific Heat (J/kg-K) @ 300 K (800 K)	1040 (1136)	2620	846 (1155)	1012 (1110)
Thermal Cond (W/m-K) @ 300 K (800 K)	0.026 (0.057)	0.016	0.026 (0.057)	0.026 (0.057)
Diffusion Coef. (m ² /s) with respect to Air	1.81 x 10 ⁻⁵	1 x 10 ⁻⁵	1.31 x 10 ⁻⁵	NA

3.5 SCENARIOS

Two scenarios or cases, which were simulated, are defined as follows:

3.5.1 Low Exhaust Rate Scenario

The low exhaust rate scenario consists of the bounding release rates for all of the gases (Sections 3.2 and 3.3), and the exhaust vent rate is decreased to 75 ft³/min, instead of the normal 150 ft³/min. The bounding release rates take 20 minutes to release 100% of the CO and butene inventory in the precipitate.

3.5.2 Loss of Ventilation Scenario

The loss of ventilation scenario starts out the same as the first scenario for the first 15 minutes, which provides the "worst-case" initial conditions for the loss-of-ventilation case. The initial conditions are conservative because the exhaust rate is only 75 ft³/min, instead of the

normal $150 \text{ ft}^3/\text{min}$ and a lower exhaust rate results in higher CO and butene concentrations. Then the electric power is lost to the exhaust fan and, perhaps, the hotplates. The rate of decomposition slows down because there is no stirring due to evacuation of operators from the room (see Section 4.2). During the time that ventilation is off, there can be no stirring of precipitate because the operators are gone, which causes a lower release rate of gas by as much as a factor of four (see Section 3.2), based on experiment for CO (FF-5389). The factor of four is assumed to be true for butene as well, because the stirring increases the permeability of the precipitate and creates new gas flow paths, which would have the same effect on butene release rate.

The scenario has the remaining CO and butene inventory, that is left after 15 minutes of bounding release rates and a low exhaust fan rate, released over the following 15 minutes (at $1/3$ the bounding rates) for a total time period of release of 30 minutes. To be conservative and to cover other similar cases, 100% of the CO and butene is released from precipitate over the entire 30 minutes with 75% released during the first 15 minutes and 25% released during the last 15 minutes. The release rates over the last 15 minutes are one third of the bounding release rates. The 15-minute release period is for the case when the hotplate power is on.

For the case with the hotplate power off, when the ventilation is lost, then the decomposition of precipitate would stop within minutes with some CO and butene remaining in the precipitate, due to less heat being added to the precipitate. Therefore, the one-third release rate bounds the release rate when the hotplate power is on or off, and the 15-minute time period of release bounds the case with hotplate power off. Note that even with the smaller release rates, releases lasting longer than 15 minutes start to build a flammable cloud that is getting sizable and may stay benign for only another 10 minutes, as shown by sensitivity cases. Therefore, the hotplates must be turned off within the 15 minutes (the safety envelope) after a loss of glovebox ventilation.

4.0 RESULTS OF CALCULATIONS

4.1 LOW-EXHAUST-RATE SCENARIO

4.1.1 Carbon Monoxide Concentrations, Flammability Conditions

The bounding CO release rate is $1.14 \text{ gmole}/\text{min}$ ($31.8 \text{ g}/\text{min}$) and a CO_2 release rate of $0.62 \text{ gmole}/\text{min}$ ($-27 \text{ g}/\text{min}$) from the boat surface. This corresponds to a fractional release rate of $5\%/\text{min}$ of the CO initial mass inventory.

The CO mole fraction contours are shown in Figures 4 to 5. Figure 4 shows the front side view of the CO flammable cloud (mole fraction $> 12.5\%$) in and above the boat. Much of the flammable cloud has a CO mole percentage just above 12.5% and below 14% . The sides of the boat and hotplate together are 4 inches high, which run together in all of the figures. The full flammable plume extends just a fraction above the boat top rim surface. Figure 5 shows the CO half-flammable cloud, which is defined as the cloud or spatial region with CO mole percentages above $1/2$ of its LFL or 6.25% .

The half-flammable cloud is of interest because of Le Chatelier's principle (Crowl and Louvar 1990), which essentially states that the flammability conditions of a mixture of flammable gases over a region is determined by the sum of each gas's fraction of LFL. A modified form of Le Chatelier's principle is written in equation form as follows:

$$C_{\text{mix}}/\text{LFL}_{\text{mix}} = C_{\text{co}}/\text{LFL}_{\text{co}} + C_{\text{butene}}/\text{LFL}_{\text{butene}} \quad (1)$$

where C_i = Concentration (mole fraction) of species i (mixture, CO, butene) at a location,
 LFL_i = Lower Flammability Limit (mole fraction) of species i (mixture, CO, butene)

Equation (1) holds for all species concentrations and many different combinations of CO and butene concentrations can cause the mixture to be flammable, which happens whenever the right hand side of equation becomes greater than or equal to one. In other words, if CO and butene concentrations (mole fractions or percentages) are at $\frac{1}{2}$ of their respective LFLs, then the mixture is flammable; or if CO is at $\frac{7}{8}$ LFL_{co} and butene is at $\frac{1}{8}$ $\text{LFL}_{\text{butene}}$, then the mixture's mole fraction is also at its LFL. In general, if two flammable gases are added together with each gas's mole fraction (concentration) having a value greater than $\frac{1}{2}$ of its LFL ($C_i > \frac{1}{2} \text{LFL}$), then the mixture will be flammable ($C_{\text{mix}} > \text{LFL}_{\text{mix}}$) even though each individual gas by itself is not. In other words, the sum of two half-flammable clouds (same size) will equal a flammable cloud for the mixture. Note that LFL_{mix} and C_{mix} need not be calculated individually, as only their ratio is needed, because the primary focus is on the spatial region where this ratio is greater than or equal to 1, which indicates the mixture is flammable there. In other words, the spatial size of mixture's flammable cloud is determined from the following equation (inequality):

$$C_{\text{co}}/\text{LFL}_{\text{co}} + C_{\text{butene}}/\text{LFL}_{\text{butene}} = 1 \text{ (or } > 1) \quad (2)$$

where each specie's concentration is calculated over space and time by the FLUENT code. The mixture's flammable cloud is the spatial region where Equation (2) is true. Le Chatelier's principle may not be true for such different gases as CO, which has a high LFL of 12.5%, and butene, which has a low LFL of 1.6%. However, to be conservative, the principle is assumed here to be true for CO and butene, even though they are vastly different.

Also, Equation (2) states that the region at the edge (or outside) of the larger half-flammable cloud is **not** flammable. The half-flammable cloud, as previously defined, of a gas species is the spatial region where the species' mole fraction (or percentage) is greater than or equal to $\frac{1}{2}$ of its LFL. Inside or on the edge of the smaller half-flammable cloud, the sum of partial LFL fractions is greater than one, and the mixture is flammable. The edge of the mixture's flammable cloud is in between the edges of the two half-flammable clouds.

In this report, the mixture's flammable cloud size is determined by first observing the visual size of the half-flammable cloud for each gas species to see how their sizes compare. For the simulations here, the CO half-flammable cloud is larger than the butene half-flammable cloud (see Figures 5 and 7). To be conservative, the volume of the butene half-flammable clouds (one over each hotplate or pair of boats) is assumed to be equal to the volume of the CO clouds.

The CO mass concentrations range from 0.057 to 0.10 kg/m³ in the CO half-flammable cloud ($C_{co} > 6.25\%$) above the boat (Figure 5). The CO mass in this region is estimated to be about 0.37 gram, based on the concentrations and the volume of CO half-flammable clouds as shown below. The half-flammable cloud is about 6 inches high above the second hotplate with an average cylinder diameter of 6 inches, which has a volume of 170 in³ or 0.0028 m³ with an average CO concentration of about 0.08 kg/m³. This half-flammable cylinder has about 0.22 gram (0.0028 x 0.08) of CO. The half-flammable cloud above the first hotplate is about 4 inches with an average diameter slightly larger than 6 inches for an equivalent volume of about 2/3 of the cloud over second hot plate. The estimated mass in the cloud above first hotplate is about 0.15 grams. The CO mass above both hotplates in the half-flammable clouds is about 0.37 gram (0.22 + 0.15).

Also, there is about 0.42 gram in the boat interiors (based on FLUENT output, 0.2 gram and 0.22 gram of CO in boat interiors on first and second hotplate). Adding the CO mass above the boats in half-flammable clouds and in the boat interiors gives a total CO flammable mass of 0.79 gram. This is less than the 1 gram of CO estimated in HNF-5389, which showed that the impulse from a burn of 1 gram of CO was benign (did not break glovebox window or gloves). HNF-9339 showed that a burn of 2 grams of CO produced an impulse of 22 Pa-sec, which is also benign.

The total amount of CO mass in the glovebox is about 265 grams after 20 minutes with an exhaust rate of only 75 ft³/min, which is about 1/2 of the design exhaust rate. Since the volume of the glovebox is about 9.2m³, the average CO mass concentration after 20 minutes is about 0.05-kg/m³ (mole percentage < 2.7 %). The average mole percentage of CO in glovebox is less than 21% of its LFL. Only the small region above the hotplates has a mixture that is above LFL_{mix} as described in the preceding paragraph for CO (note that the butene concentration has to be factored into the equation to determine mixture's flammability, which is shown in next section).

4.1.2 Butene Concentrations, Flammability Conditions

The bounding butene release rate is about 0.125 gmole/min (-7 g/min) from the boat surface. This corresponds to a fractional release rate of 5%/min of butene's initial mass inventory. This section uses the CO flammable conditions determined in preceding section to obtain the flammability conditions of the mixture.

Figure 6 shows the butene mole fraction contours, with the maximum mole percentage being 3.1% in the interior of boat. This small butene volume is flammable because the butene LFL is only 1.6%. However, basically none of the butene gas, by itself, is flammable outside of the boat, because the maximum mole percentage is only 1.5% out of the boat. However, the

half-flammable butene clouds, shown in Figure 7, is about two thirds of the CO half-flammable clouds (see Figure 5), with the cloud over the first and second hotplate being about 3 and 4.5 inches tall, respectively. Since the butene cloud is smaller than the CO cloud, the mixture's flammable cloud is smaller than the CO half-flammable cloud and larger than the butene flammable cloud. However, there is not much difference, so the butene clouds were conservatively assumed to have the same volume as CO half-flammable clouds.

There is very little butene mass in the half-flammable clouds, as calculated below. The butene half-flammable cloud ($C > 0.8\%$) volume is smaller than the CO cloud volume (0.0047 m^3) above both hotplates combined. Multiplying butene's average mass density in clouds of about 0.015 kg/m^3 (range is 0.011 to 0.02 kg/m^3) by 0.0047 m^3 , the butene mass in its half-flammable clouds is only about 0.07 gram above the boats. This butene mass would release less than 3500 joules ($0.07 \text{ g} \times 50,000 \text{ J/g}$, [Crowl and Louvar 1990]). The burning of this small amount of butene would not add significantly to the CO burn. There also is about 0.09 grams in the boat interiors (based on FLUENT output) for a total of about 0.15 gram of butene in the half-flammable clouds. It is expected that the butene mass would be smaller than the CO mass because the butene mole fraction release rate per hotplate (0.125 gmole/min) is about 9 times ($1.14/0.125$) smaller than the CO release rate (1.14 gmole/min), and its higher mole mass (factor of 2) is not enough to make up the factor of 9 mole fraction difference.

The total amount of butene mass in the glovebox is about 58 grams after 20 minutes with the low exhaust rate of $75 \text{ ft}^3/\text{min}$, which is about $\frac{1}{2}$ of the design exhaust rate. Since the volume of the glovebox is about 9.2 m^3 , the average butene mass concentration after 20 minutes is about 0.01-kg/m^3 (mole percentage $< 0.29\%$, calculated by FLUENT code). The average butene mole percentage in entire glovebox is about 18% of its LFL.

The mixture's average flammability conditions are calculated by Equation (1) using a butene concentration (mole fraction) of $0.18 \text{ LFL}_{\text{butene}}$ and a CO mole concentration of 0.21 LFL , (Section 4.1.1). The mixture's average flammable mole percentage is less than 40% of its LFL, based on Equation (1). However, the most important result is the size and location of the mixture's flammable clouds (region where the mixture's concentration exceeds its LFL), which are just above the boats, smaller than the CO half-flammable clouds (Figure 5) and larger than the butene half-flammable clouds (Figure 7).

4.1.3 Velocities and Temperature in Glovebox

The velocity vectors are shown in a plane located 25 cm from the front of the glovebox in Figure 8. This plane cuts through the first hotplate and boats. The swirling flow pattern is visible with the maximum gas velocity located on top, above the porous/resistance region, near the exhaust outlet on the right side of glovebox. Just below the highest velocities, the resistive porous region is located, which clearly is slowing down the gas flow there. The higher density or number of arrows on the left side of glovebox indicates that the mesh or grid is much finer near the hotplates than in the porous/resistance region. Figure 9 shows the velocity vectors in the plane located 50 cm from the glovebox front. This plane cuts through the second hotplate and boats, where the velocities are much more vertical than velocities located by first hotplate and

boats. It is this strong vertical velocity that causes the gas clouds to be so straight above the second hotplate.

The temperature contours from 27 °C (300 K) to 52 °C (325 K) in the glovebox are shown in Figure 10. The very hot temperatures near the hotplates (200 °C) are not shown explicitly, so that better resolution of the lower temperatures in the majority of the glovebox is shown. The glovebox is warmest (not counting hotplate region, which is obviously the hottest region) in the upper region just inside the resistive flow region.

4.2 LOSS-OF-VENTILATION SCENARIO

The loss-of-ventilation scenario covers several cases. One case has the exhaust fan off with the hotplates on, and another has the hotplates off. Another case has the fire damper closed with the exhaust fan on. **All** of these cases will be addressed. Also, a case with only CO and CO₂ released with no butene is discussed.

The release rates for the loss-of-ventilation scenario (exhaust rates off and hotplates on) are 1/3 of their bounding values (Section 4.1) because there can be no stirring when evacuation takes place, which happens when ventilation to glovebox is lost. Furthermore, Section 4.12 of PFP Operating Procedure ZO-190-605 (*Operating Procedure of the Magnesium Hydroxide Precipitation Process System*) states that one or more emergency stop switches are to be pressed during an evacuation when ventilation in the glovebox is lost. This means that the hotplate power should be turned off during an evacuation, but no credit is taken for this defense-in-depth procedure. In any case, the stirring of the precipitate, based on experiments, increases the release rates by a factor of 4 or more (HNF-5389), which is assumed to hold for CO and butene releases. **Also**, the simulation results for the loss-of-ventilation scenario, which are presented next, bound both cases (hotplate power on and off). When the hotplate power is turned off, the boats will cool and decomposition of the precipitate will stop along with the gas release within minutes. Most of the regions in boats that have not yet reached high decomposition temperatures (> 187 °C), when the hotplate power goes off, are not expected to reach high temperatures after several minutes with no hotplate power.

4.2.1 Concentrations, Flammability Conditions

The half-flammable cloud of CO is shown in Figure 11 and the half-flammable cloud of butene is shown in Figure 12. The clouds are smaller than those shown in Figures 5 and 7 for low-exhaust-rate scenario, except for the half-flammable cloud of CO above the first hotplate, which is slightly larger than in Figure 5. The butene half-flammable clouds in Figure 12 are a lot smaller than in Figure 7. The flammable mixture cloud has a size in between the CO half-flammable cloud and the butene cloud, which means the mixture flammable cloud, is smaller than the CO half-flammable cloud (Figure 11), and smaller than the mixture cloud for the first scenario. The mixture's flammable cloud is shown in Figures 13 (CO part) and 14 (butene part), where the CO cloud is at 54% of its LFL, and the butene cloud is at 46% of its LFL on the outer edges. Note that the 54%-flammable cloud of CO and the 46%-flammable cloud of butene are the same size, which is the size of the mixture's flammable cloud. By Equation (2), all of the volume inside the mixture's flammable cloud has a sum of partial LFLs larger than 1 and is

equal to 1 on the edge. The flammable mass of CO and butene in the mixture cloud is slightly less than in the preceding low-exhaust-rate scenario. Thus, the CO and butene flammable masses are still less than 0.8 gram and 0.14 gram, respectively, as calculated in Section 4.1 for the preceding scenario. These mass values include the mass that is in the boat interior (calculated by FLUENT code directly), which is 0.31 gram of CO and 0.07 gram of butene, which are less than the preceding scenario's. About half of the flammable mass in the glovebox is in the boat interiors.

However, the CO and butene masses in the entire glovebox are higher than the preceding scenario's. This is because with the exhaust fan off, the gas masses have to pressurize first, and the pressure increase rate is small, causing a much lower convection rate out of the glovebox than when the exhaust fan is working. Hence, the total CO mass in the glovebox increases from 260 grams at 15 minutes to 508 grams at 30 minutes with the CO mole percentage in entire glovebox increasing from 2.6% to about 4.9%. The total butene mass in the glovebox increases from 58 grams at 15 minutes to about 111 grams at 30 minutes with the butene mole percentage in entire glovebox increasing from 0.29% to about 0.54%. The average CO mole percentage in entire glovebox is less than 40% of its LFL, and the average butene mole percentage in entire glovebox is about 33% of its LFL. Using Equation (1), the mixture's average flammable mole percentage is less than 75% of the mixture's LFL.

The most important result, however, is the size of the mixture's flammable clouds, which is the only part in glovebox that is flammable. Even if the mixture's average mole fraction reaches 100% of its LFL, a large portion (at least half) of the glovebox is below flammable conditions. The mixture's flammable clouds (Figure 13 or 14) are localized above the boats for 15 minutes after glovebox ventilation (exhaust) is lost. This analysis only simulated the loss-of-ventilation (exhaust) and hotplate-on conditions for 15 minutes, which produced benign results. However, for time periods longer than 15 minutes, the flammability conditions get worse and may not be benign after another 10 minutes. Hence, the hotplate power should be turned off within 15 minutes after ventilation is lost or the glovebox ventilation has to be restored within 15 minutes in order to avoid potential flammability conditions. Workers should not return to the room until after the glovebox ventilation has been restored for some time period.

Another case related to the loss-of-ventilation scenario is the loss of inlet air, which can be caused by the fire damper, located before the inlet vent, closing when it's not supposed to. The accidental closing of the fire damper is only possible if the fusible link, which holds the fire damper open, fails to keep the damper lifted. The fusible link has high reliability and the duration of stabilization campaign is short (3 months). Furthermore, the hotplate heat will not cause a failure of the fusible link because air flows into the glovebox, convecting the heat away from fusible link, and the hotplates are not in view of fusible link for any thermal radiation heating. The consequences of a closed inlet are expected to be benign, primarily because of the alternate inlet with HEPA filter on top of glovebox. With 1) the alternate inlet of air, 2) an operating exhaust fan, and 3) the natural gas circulation by hotplate, which is enhanced by the hot gas releases from the boats, the flammable conditions of this case are expected to be bounded by the results from the preceding two scenarios. The loss-of-ventilation scenario clearly bounds the total CO and butene masses in entire glovebox, because the exhaust fan is off in the loss-of-ventilation scenario.

4.2.2 Velocities

The gas velocity vectors are shown in Figure 15. The circulating pattern of the gases in the glovebox is similar to those when the exhaust fan is operating (Figure 9). This circulating flow pattern continues to disperse the flammable gases being released the precipitate in the boats, even when the exhaust fan is not functioning. As a result the half-flammable clouds above the hot boats are similar to preceding scenario, but the circulating flow does not help the overall mass build up in the entire glovebox.

4.2.3 CO Release with No Butene

Another sensitivity case was run with CO and CO₂ released from 4 boats, but no butene is released. The conservative scenario has the CO/CO₂ released at their bounding release rate for 2 minutes with a normal exhaust rate of 150 ft³/min. At 2 minutes, the glovebox ventilation is lost and the release rates are reduced by a factor of 3 as discussed previously because of the no-stir effect. The reduced release rates are simulated for another 54 minutes (56 minutes in total), which releases all of the 1270 grams of CO from the boats (i.e., 100% of the initial inventory).

The results of this case show that the incoming air continues to come in through the inlet after the ventilation is lost, although at a lower rate, and gas continues to exit through the exhaust port. After several minutes, some gas exits the inlet, but at a low rate. The incoming fresh air along with the gas released from the boats, causes a flow rate out of the exhaust port the entire time that ventilation is lost. As a result, the average CO mole fraction is between 7% to 10% in the entire glovebox. Also, the CO concentration is rather uniform due to the mixing caused by the natural circulation of hotplate and hot gases (200 °C). Velocity vectors are shown in Figure 16 after 56 minutes, which indicate good mixing. The normal exhaust rate of 150 ft³/min is more beneficial to reducing CO concentrations before and even after the ventilation is lost. The absence of butene also appears to be beneficial in that the heavy gas with large viscosity does not get in the way of the CO mixing and dispersing. Lastly, without butene, Le Chatelier's principle is not used since there is only one flammable gas, CO, and only its LFL is important, not its half-flammable cloud.

5.0 SUMMARY AND CONCLUSIONS

The FLUENT simulation of the two flammable gases, butene and carbon monoxide, released from decomposing oxalate precipitate in four boats placed on two hotplates, are summarized in Table 2 for each of the two scenarios. The first scenario is the low-exhaust-rate scenario, and the second scenario is the loss-of-ventilation scenario.

Table 2. CO and Butene Concentrations and Masses after Release into Glovebox

Gas	Release Rate per Hotplate	Maximum Mole Fraction	Maximum Mass in %-Flammable Cloud	Maximum Mass in Glovebox
Scenario #1 Low Exhaust Rate of 75 ft³/min: 20 minutes of bounding release rates				
CO	1.14 gmole/min, 31.8 grams/min	28% CO in boat, 14% just above boat rim	< 0.8 gram total, 0.37 gram above boats, 0.42 gram in boats	265 grams < 2.6%vol in entire glovebox
C ₄ H ₈	0.125 gmole/min, 7 grams/min	3.1% C ₄ H ₈ in boat, 1.5% just above boat rim	0.16 gram total, 0.07 gram above boats, 0.09 gram in boats	58 grams < 0.29%vol in entire glovebox
Mixture	NA	NA	NA	< 40% LFL _{mix}
Scenario # 2 Loss of Ventilation in Glovebox: 15 minutes at bounding rates above, and 15 minutes at rates below for a total of 30 minutes				
CO	0.46 gmole/min, 10.6 grams/min	14% CO in boat, < 9.0% just above boat rim	< 0.8 gram total, 0.49 gram above boats, 0.31 gram in boats	508 grams, < 4.9 %vol in entire glovebox
C ₄ H ₈	0.042 gmole/min, 2.3 grams/min	< 1.6 % C ₄ H ₈ in boat, < 1.0% just above boat rim	< 0.14 gram total, 0.07 gram above boats, 0.07 gram in boats	111 grams, < 0.54 %vol in entire glovebox
Mixture	NA	NA	NA	< 75% LFL _{mix}

In summary, for the first scenario (low-exhaust-rate scenario), all of the flammability results for glovebox HC-230C-3 are benign as they are bounded by previous calculations, which showed benign results (HNF-5389, HNF-9339). The CO concentration has a peak value in the boat interior of 28%, and a peak concentration of 14%, which is slightly above its LFL of 12.5%, just above the boat rim (< 1/2 inch) as shown in Figure 4. The butene concentration has a peak value in the boat interior of 3.1%, and a peak concentration of only 1.5%, which is below its LFL of 1.6%, just above the boat rim (< 1/2 inch) as shown in Figure 6. Using Le Chatelier's principle for adding partial LFLs of gases, the amount of CO and butene mass in the half-flammable clouds above the boat is very small at 0.37 gram for CO and 0.07 gram for butene. The amount of heat released from CO and butene upon combusting is less than the heat calculated in HNF-5389, and would increase the average gas temperature in glovebox by less than 2 °C. However, the local effects of such a burn would cause higher temperature increases in the local flammable region, but the resulting pressure pulse is insignificant and bounded by the benign pressure impulse calculated in HNF-5389 and HNF-9339, which was based on the combustion of 1 gram and 2 grams, respectively, of CO. The calculated impulse of 2 grams of CO (< 22 Pa-sec, HNF-9339) is not high enough to breach the windows or gloves in the glovebox (HNF-9339). The amount of CO and butene gas in the boat interiors of 0.42 gram for CO and 0.09 gram for butene is also small and benign. After 100% of the gas inventory is released from the precipitate in 20 minutes, the mixture in glovebox is less than 40% of its lower flammability limit.

These flammable masses are conservative because of the following:

- 1) the exhaust vent rate used in the simulations was 75 ft³/min, which is about half of the normal vent rate,
- 2) the peak release rates were used for the entire time of release,
- 3) the gases were released simultaneously from both hotplates, and Le Chatelier's principle was followed, and
- 4) low diffusion coefficients were used.

The normal vent rate of 150 ft³/min would lower the amount of flammable gas in the glovebox, or, in other words, would reduce the size of the half-flammable clouds shown in Figures 5 and 7 for CO and butene, respectively. Using time-varying gas release rates would decrease the peak concentrations. Having the hotplates heat up at different times would decrease the combined release rates and sum of gas concentrations. Higher diffusion coefficients would spread the gas concentrations out over a larger region, decreasing their concentrations and flammable clouds.

In summary, for the second scenario ("loss-of-ventilation" scenario), the results are also benign, provided the hotplate power is turned off or ventilation is restored within 15 minutes after glovebox ventilation is lost. There are two cases for "loss-of-ventilation" scenario defined by the state of hotplate power; one case has the hotplate power off, which is the more probable case, and the other case has the hotplate power on, which is the one analyzed here. For the "loss-of-ventilation" scenario, the flammable mixture cloud is about the same size as the one in the first scenario, even though the exhaust rate is lost. This is because the source rate decreases when the hotplate is not stirred. The release rates used in the simulations for the loss-of-ventilation scenario were 1/3 of the bounding release rates (bounding rates include stirring effects). The one-third release rates bound the release rates for the case with the hotplate power on, because no stirring will take place if the ventilation is lost. The lack of stirring of the precipitate, based on experiments (HNF-5389), lowers the release rates by a factor of 4 or more (Section 3.2). In conclusion, the flammability conditions are benign for at least 15 minutes after the glovebox ventilation is lost, which has some margin, primarily because of the conservative initial conditions based on low exhaust rate (Section 3.5).

However, the total CO and butene masses in glovebox increase, because the inactive (*oft*) exhaust fan is not removing the gases like an active exhaust fan. There are still some convective and diffusive losses through the exhaust vent, but these loss rates do not prevent some build up of gases in glovebox. After 100% of the gas inventory is released from the precipitate in 30 minutes, the mixture in glovebox is less than 75% of its lower flammability limit. These results indicate that the hotplate power can be on for at least 15 minutes after the glovebox ventilation is lost. This means that the hotplate power should be turned off or ventilation should be restored within 15 minutes after glovebox ventilation (exhaust) is lost. Workers should stay out of the room with glovebox HC-230C-3 until ventilation has been restored for some time period.

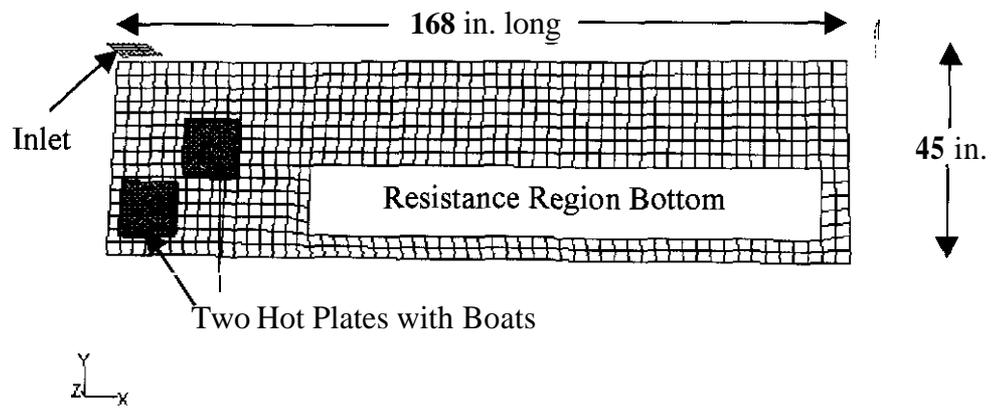
Another case related to the loss-of-ventilation scenario is the loss of inlet air, which is caused by the fire damper, located before the inlet vent, closing. The closing of fire damper is only possible if the fusible link, which holds the fire damper open, fails to keep the damper lifted. The consequences of a closed inlet are expected to be benign, primarily because of the alternate inlet with HEPA filter on top of glovebox. With this alternate inlet of air, an operating exhaust fan, and the natural circulation near hotplates, which is enhanced by the hot CO and butene releases from the boats, the flammable conditions of this case are expected to be bounded by the two scenarios shown in Table 2. The loss-of-ventilation scenario clearly bounds the total CO and butene masses in entire glovebox, because the exhaust fan is off in the loss-of-ventilation scenario. For the case with only CO/CO₂ release and no butene release, the CO mole fraction is below its LFL.

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- RPP-5667, Hey, B.E., S. Finrock, R. Marusich, and G. Ryan, 2000, *Stochastic Consequence Analysis for Waste Leaks*, Rev. 0, Fluor Federal Services, Richland, Washington.

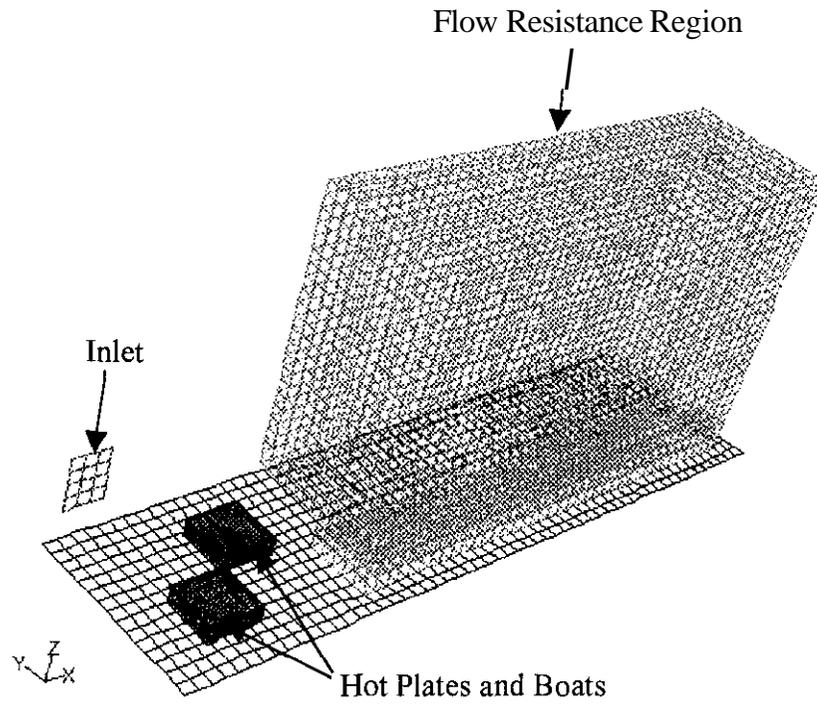
ZO-190-605, *Operating Procedure of the Magnesium Hydroxide Precipitation Process System*,
Section 4.12, PFP Operations Procedure ZO-190-605, Fluor Hanford Inc., Richland,
Washington.

Figure 1. Plan View of Grid Outline of FLUENT Model Domain



Grid Flame5f	Dec 12, 2001 FLUENT 5.5(3d, dp, segregated, spe4, rngke, unsteady)
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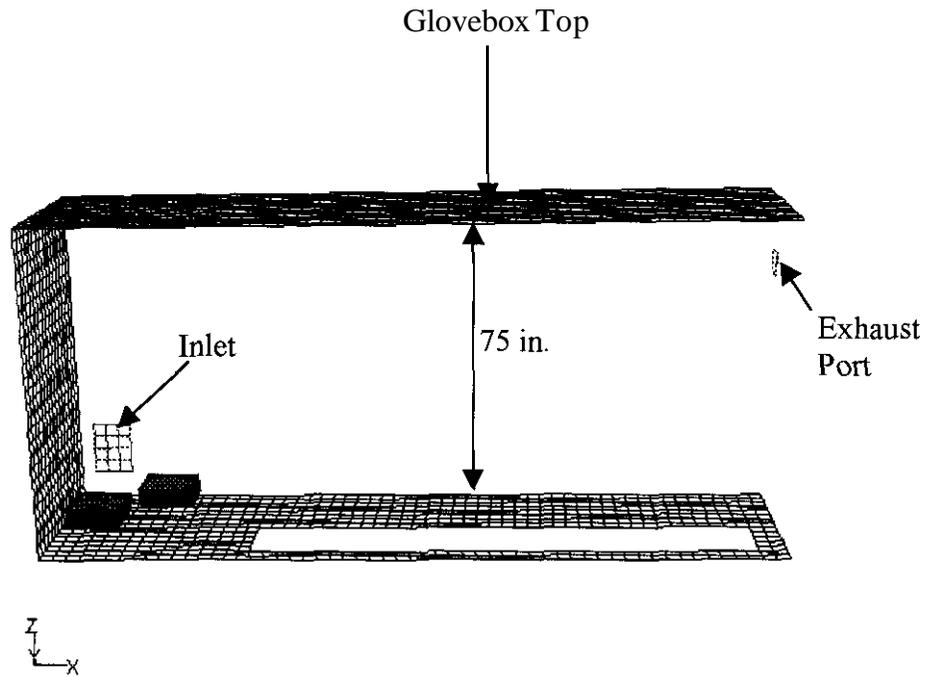
Figure 2. Isometric View of Model Domain Showing Flow Resistance Region



Grid
Flame8f

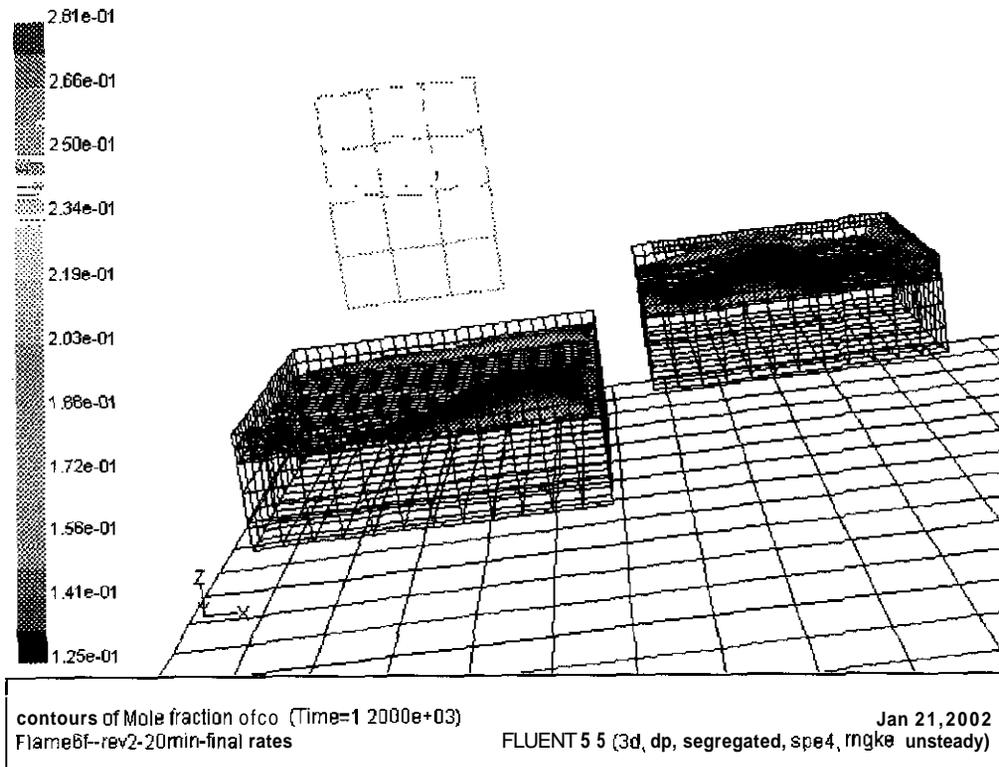
Dec 12, 2001
FLUENT5.5 (3d, dp, segregated, spe4, mgke, unsteady)

Figure 3. Isometric View of Model Domain with Inlet, Exhaust, Boat Locations

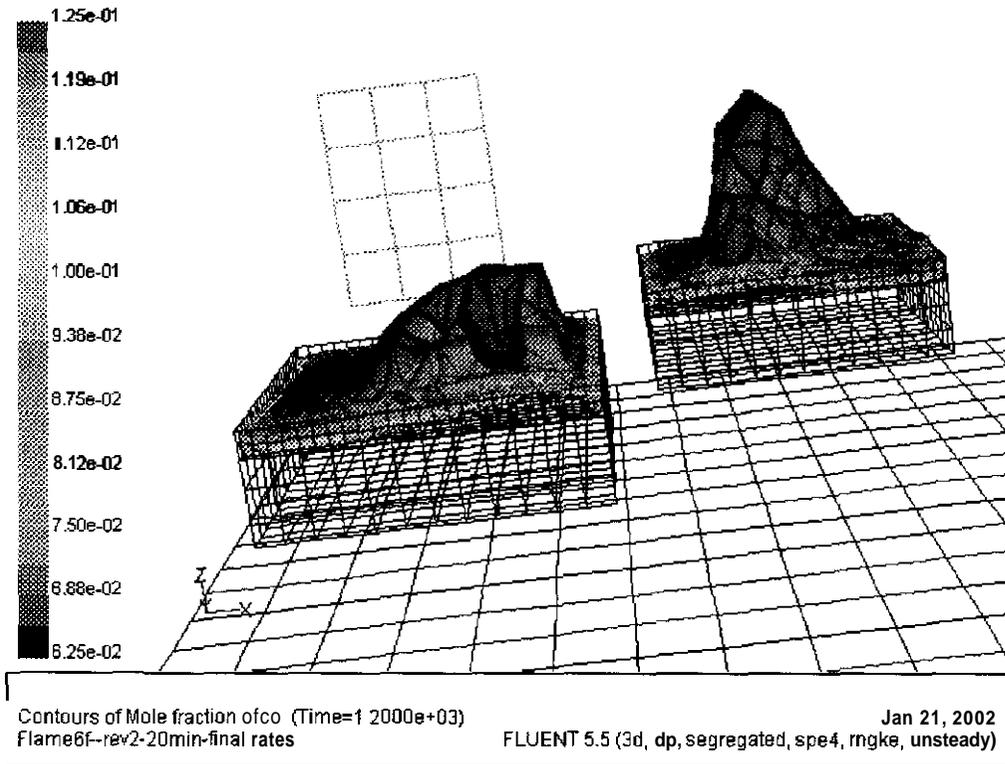


Grid Flame6f	FLUENT 5.5 (3d, dp, segregated, sped, mgke, unsteady)	Dec 12, 2001
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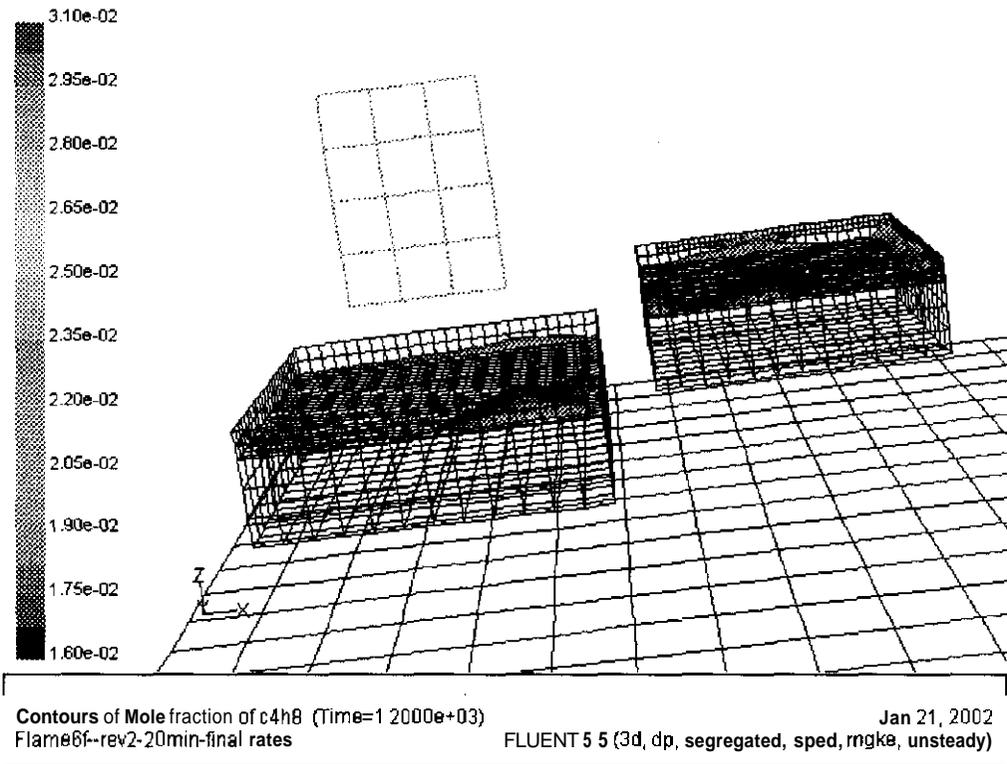
Figure 4. Side View of CO Flammable Cloud (Mole Fraction > 0.125) at 20 Minutes
(hotplate and boats sides are 4 inches high, CO is in top 1 in. of open boat and slightly above boat; Max. Percentage = 28% in boat, 14% above boat)



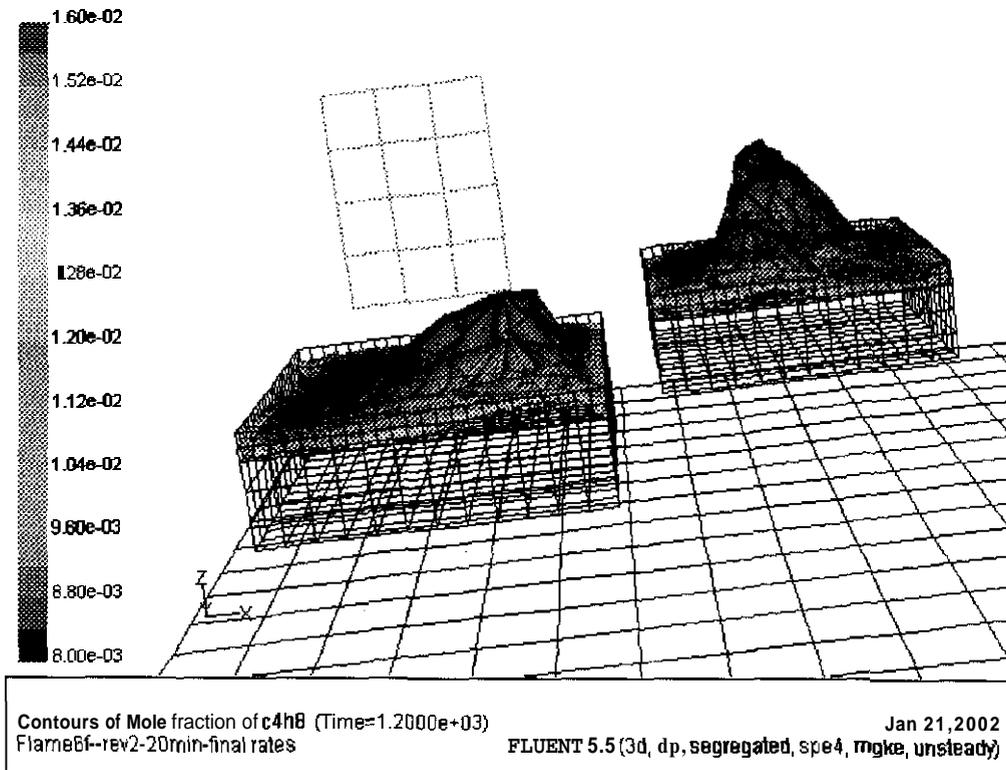
**Figure 5. Side View of CO Half Flammable Cloud at 20 minutes;
Mole Percentage Range is 6.25% (1/2 LFL) to 12.5% (1 LFL).**



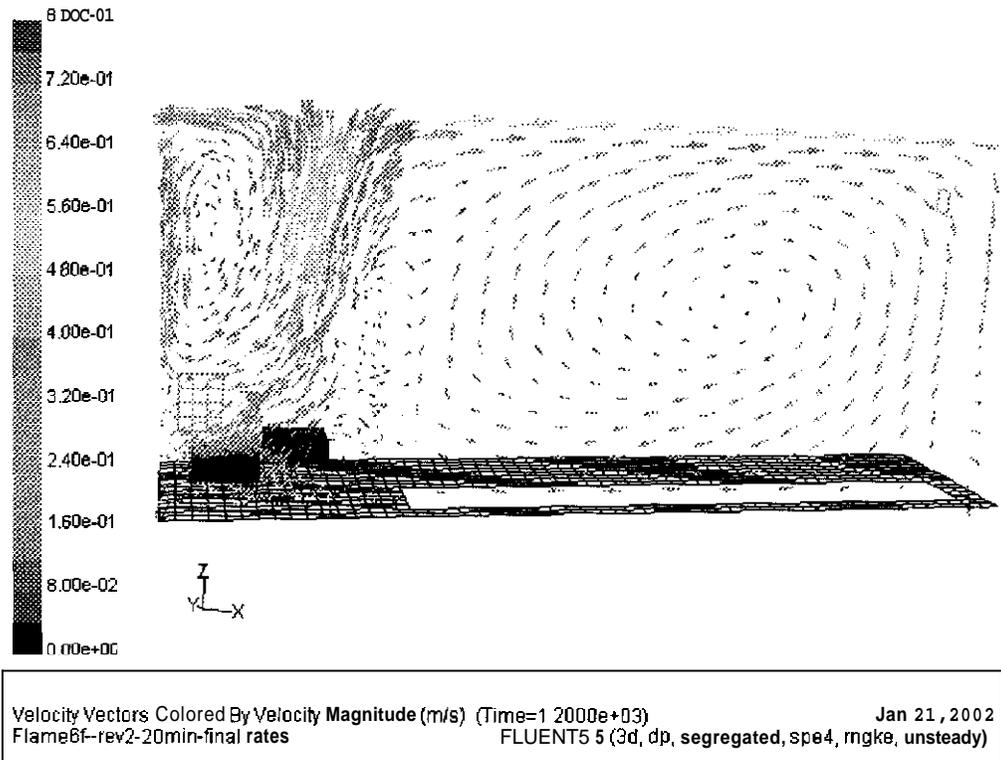
**Figure 6. Side View of Butene Flammable Cloud (Mole Fraction > 0.016) at 20 Minutes;
Boat Interior is Visible, Max. Fraction = 3.1% in Boat; No Flammable Cloud
Outside of Boat.**



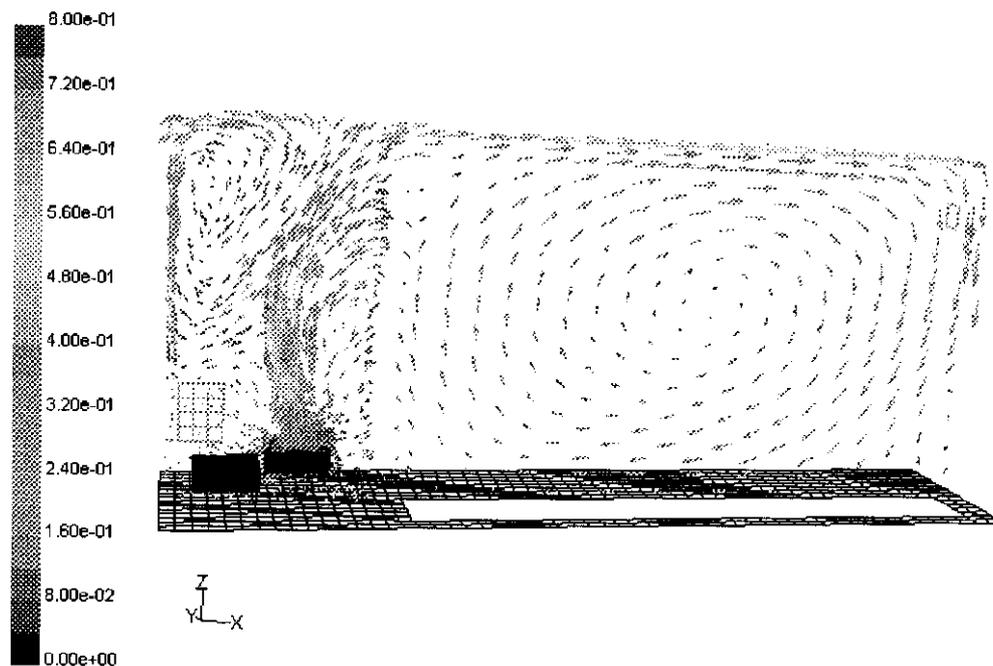
**Figure 7. Side View of Butene Half Flammable Cloud at 20 minutes.
Mole Percentage Range is 0.8% (1/2 LFL) to 1.6% (1 LFL), which Has Smaller Volume
than CO Half-Flammable Cloud (Figure 5).**



**Figure 8. Velocity Magnitude Vectors in Plane 25 cm from Front of Glovebox;
Plane Slices through First Hotplate and Boats**

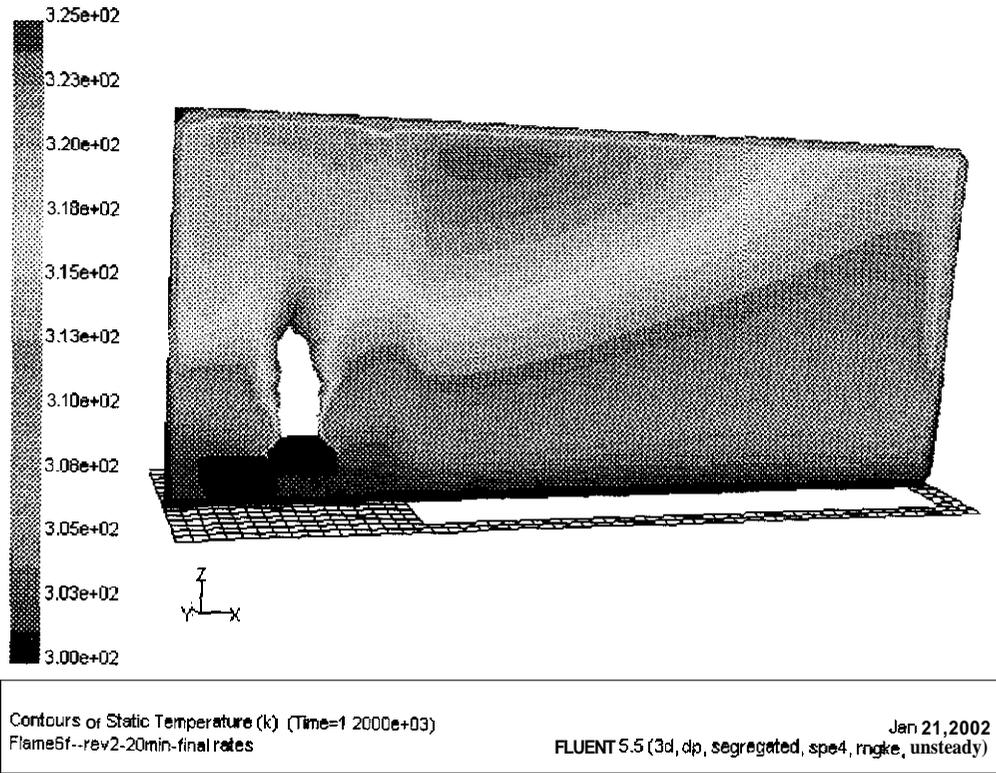


**Figure 9. Velocity Magnitude Vectors in Plane 50 cm from Front of Glovebox;
Plane Slices through Second Hotplate and Boats**

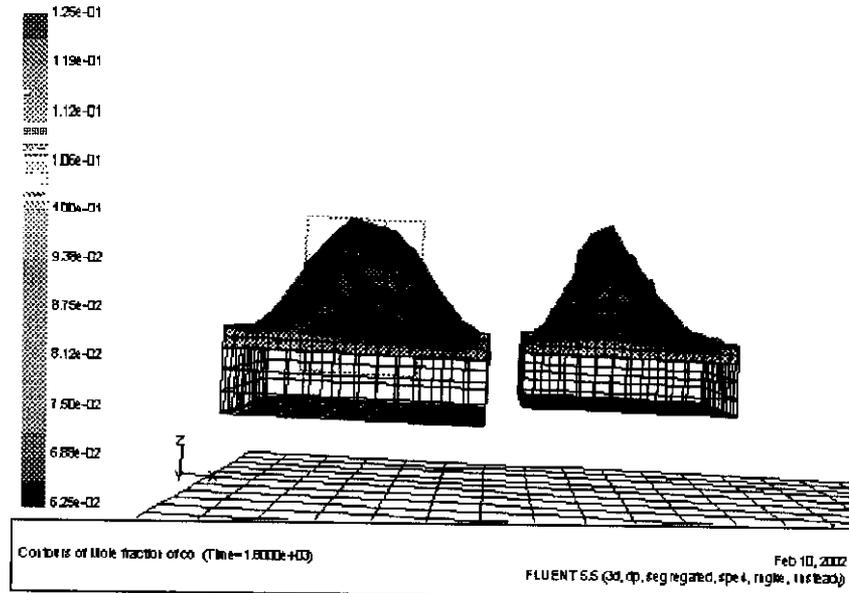


Velocity Vectors Colored By Velocity Magnitude (m/s) (Time=1.2000e+03) Jan 21, 2002
Flame6f--rev2-20min-final rates FLUENT 5.5 (3d, dp, segregated, spe4, rngke, unsteady)

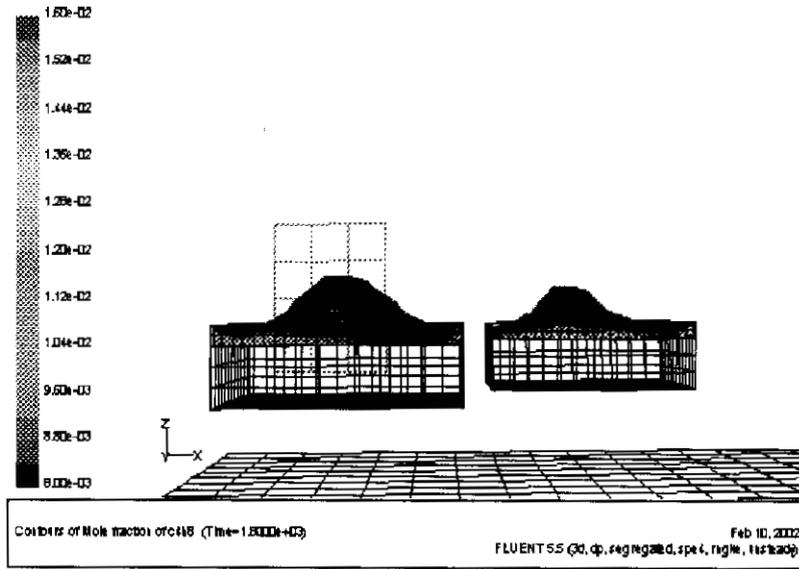
Figure 10. Temperature Contours (27 °C to 52 °C) on a Plane 50 cm from front of Glovebox at 20 Minutes (Open space above hotplate is far above 52 °C).



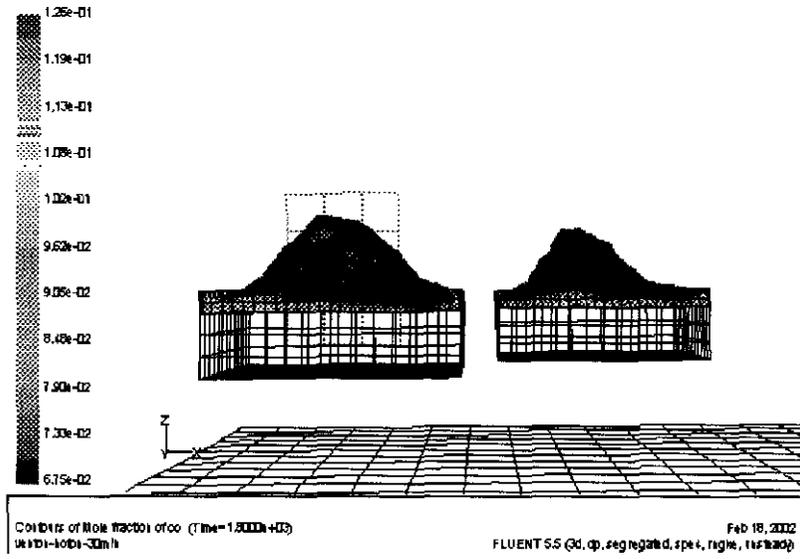
**Figure 11. Side View of CO Half Flammable Cloud at 30 minutes,
15 minutes with no ventilation; Mole Percentage Range is 6.25% (1/2 LFL) to
12.5% (1 LFL).**



**Figure 12. Side View of Butene Half-Flammable Cloud at 30 minutes,
15 minutes with no ventilation; Mole Percentage Range is 0.8% (1/2 LFL) to
1.6% (1 LFL).**



**Figure 13. Side View of CO 54%-Flammable Cloud at 30 minutes,
15 minutes with no ventilation;
Mole Percentage Range is 6.75% (0.54 LFL) to 12.5% (1.0 LFL).**



**Figure 14. Side View of Butene 46%-Flammable Cloud at 30 minutes,
15 min with no ventilation;
Mole Percentage Range is 0.736% (0.46 LFL) to 1.6% (1.0 LFL).**

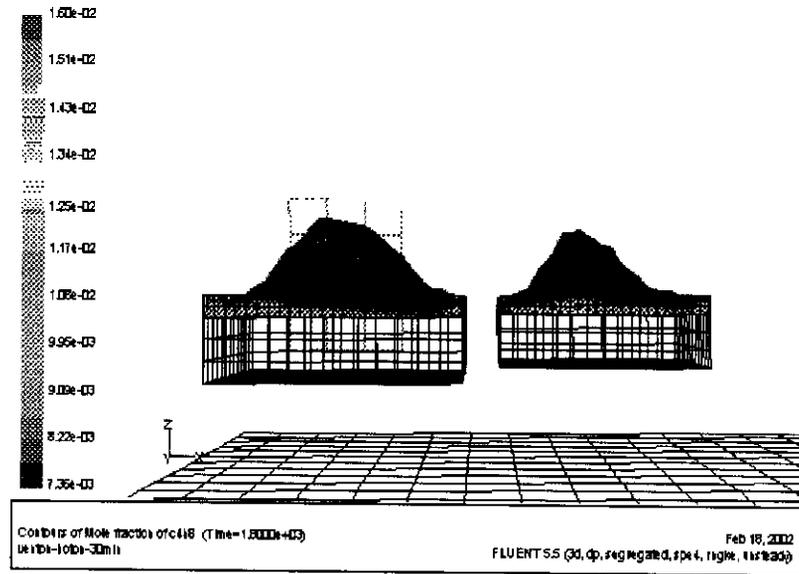


Figure 15. Velocity Magnitude Vectors (Loss-of-Ventilation Scenario) in Plane 50 cm from Front of Glovebox; Plane Slices through Second Hotplate and Boats

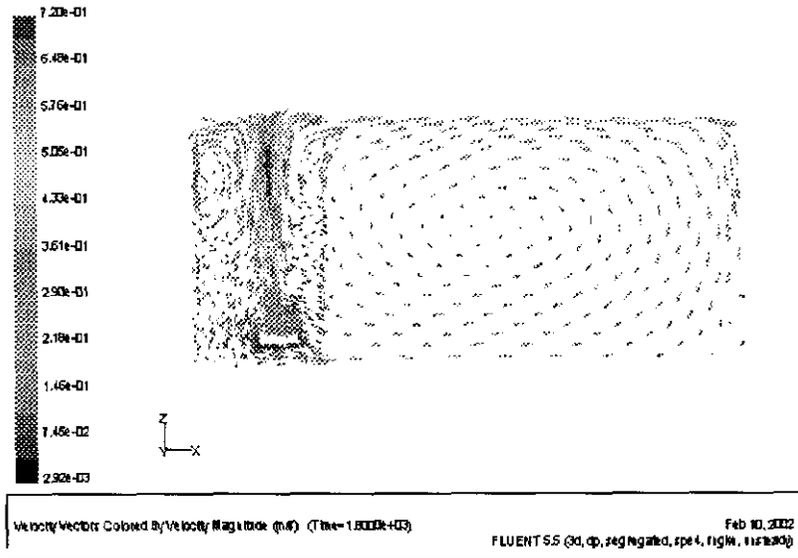
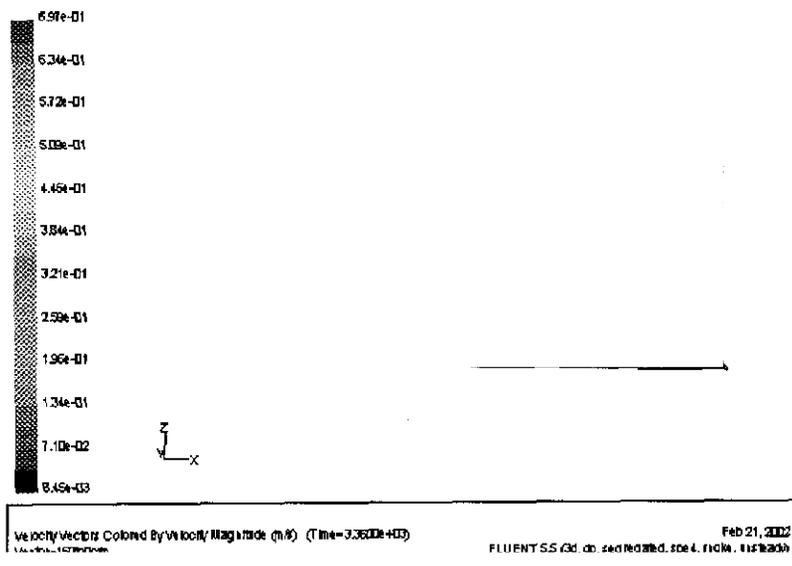


Figure 16. Velocity Magnitude Vectors (Loss-of-Ventilation Scenario with no butene in release) in Plane 50 cm from Front of Glovebox; Plane Slices through Second Hotplate and Boats



CHECKLIST FOR TECHNICAL PEER REVIEW

Document Reviewed - "HNO_x ne". 0

Title: Butene and Carbon Monoxide Flammable Clouds In A Glovebox With Two Hotplates

Author: M. G. Piepho

Date: February 2002

Yes	No*	NA	
<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Referenced analyses appropriate.
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Problem completely defined and all potential configurations considered.
<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Accident Scenarios developed in a clear and logical manner.
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Necessary assumptions explicitly stated and supported.
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Computer codes and data files documented.
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Data used in calculations <i>explicitly stated</i> in document.
<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Data checked for consistency with original source information BE applicable.
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Mathematical derivations checked including dimensional consistency of results
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Models appropriate and used within range of validity, or use outside range of established validity justified .
<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Hand calculations checked for errors . Spreadsheet results should be treated exactly the same as hand calculations.
<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Software input correct and consistent with document reviewed.
<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Software output consistent with input and with results reported in document reviewed.
<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Limits/criteria/guidelines applied to analysis results are appropriate and referenced. Limits/criteria/guidelines checked against references.
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Safely margins consistent with good engineering practices.
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Conclusions consistent with analytical results and applicable limits.
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Results and conclusions address all points required in the problem statement.
<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Format Consistent with applicable guides or other standards.
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	** Review calculations, comments, and/or notes are attached. <i>for Section 4.2, 3</i>
<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Document approved (for example, the reviewer affirms the technical accuracy of the document).

① See below

See ① below

R.M. Marusich *R.M. Marusich*
 Technical Peer Reviewer (printed name and signature)

2/22/02
 Date

- * All "no" responses must be explained below or on an additional sheet.
- ** Any calculations, comments, or notes generated as part of this review should be signed, dated and attached to this checklist. The material should be labeled and recorded in such a manner as to be understandable to a technically qualified third party.

SCOPE
 Fluent results in Figures 4-5, 11 and 12 checked using same method as in HNF-8091, App E. The results were found to be reasonable. The CO, CO₂ and butene release rates were checked against HNF-8091, HNF-5359. The model was checked and found to be quite similar to that used in HNF-8091. Did not check Figures 13 and 14. Checked logic.

① Suggest using < 10% for CO concentration in Section 4.2.3 rather than < 7% due to the uncertainties involved in the generation rates and flow rates. 7 to 10% is also acceptable.

FLUOR DANIEL



DATE

CONT. NO.

BY

CHK'D

SHEET NO. 1 of 2

check of Gas Concentration given
Loss of ventilation.

CALCULATIONS and SKETCHES

R Marusich
Feb. 21, 2002

Total Gas available for release

$$\text{CO} = (1.14 \text{ mole/min} - \text{hotplate})(20 \text{ min})(2 \text{ hotplates})$$

$$= 45.6 \text{ moles}$$

$$\text{CO}_2 = (0.62 \text{ mole/min} - \text{hotplate})(20 \text{ min})(2 \text{ hotplates})$$

$$= 24.8 \text{ moles}$$

$$\text{butane} = (2.4 \text{ moles/hotplate})(2 \text{ hotplates})$$

$$= 4.8 \text{ moles}$$

$$\text{Total} = 75.2 \text{ moles}$$

Air in glove box initially. Glove box volume 9300 L.
Subtract 200 L for equipment. Assume 30°C, 1 atm.

$$\# \text{ moles} = 9100 / (0.082 \text{ L-atm/mole-K})(303) = 366 \text{ moles}$$

Glove box volume is 9100 L or 322 ft³

Ventilation is 150 ft³/min. Glove box purged in 2 min.

Section 4.2.3 states that ventilation runs for 2 min.

$$\text{CO lost} = (1.14 \text{ mole/min} - \text{hotplate})(2 \text{ min})(2 \text{ hotplates})$$

$$= 4.6 \text{ moles}$$

$$\text{CO left} = 45.6 - 4.6 = 41 \text{ moles}$$

$$\text{CO}_2 \text{ lost} = 2.5 \text{ moles}$$

$$\text{CO}_2 \text{ left} = 22.3 \text{ moles}$$

$$\text{butane lost} = 4.8 \text{ moles} (2/20) = 0.5 \text{ moles}$$

$$\text{butane left} = 4.8 - 0.5 = 4.3 \text{ moles}$$

$$\text{total left} = 67.6 \text{ moles}$$

FLUOR DANIEL



CALCULATIONS and SKETCHES

DATE

CONT. NO.

BY

CHK'D

SHEET NO.

2 of 2

Check of Gas Concentration given
less of Ventilation

R Marwisch

Feb 21, 2002

To maintain 1 atm, gas and air must
leave the glove box through the exhaust
and intake. The factor for expansion is

$$\frac{366}{366 + 67.6} = 0.844$$

Gas left in glove box at end

$$\text{CO}_2 \quad 22.3 \text{ mole} (0.844) = 18.7$$

$$\text{CO} \quad 41 (0.844) = 34.6$$

$$\text{butane} \quad 4.3 (0.844) = 3.6$$

$$\text{Air} \quad 366 (0.844) = 308.9$$

Ignore butane

$$\% \text{ CO} = \frac{34.6}{308.9 + 34.6 + 18.7} = 9.6\%$$

The code value was < 7%.

A reasonably good agreement. A value
of < 10% should be used in the
analysis to cover uncertainties.