

Risk Assessment for Propane Gas Leakage in Valleys

IMA Summer Program for Graduate Students
Mathematical Modeling

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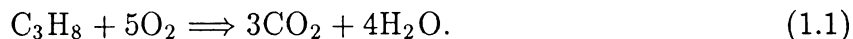
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Section I: Introduction and Assumptions

Introduction

We want to analyze the risk of explosion resulting from the leakage of propane gas into a valley. Liquefied propane gas has escaped from a pipeline. Since propane is more dense than air the propane has collected in a valley. In the valley the propane has mixed with air to form a combustible mixture. A wind with constant velocity blows across the top of the valley and carries away some of the air/propane mixture.

The combustion proceeds according to this greatly simplified chemical reaction equation:



Hence, since air is approximately one-fifth oxygen, we see that to totally burn all our reactants, we need 25 moles of air for every mole of propane.

The risk of explosion is controlled by two factors: (1) the amount of heat that could be produced by the combustion, and (2) the probability of ignition. We have defined the risk of explosion as

$$\tilde{R} = \int_0^{\infty} \tilde{Q}(\tilde{t})p(\tilde{t}) d\tilde{t}, \quad (1.2)$$

where $\tilde{Q}(\tilde{t})$ is the amount of heat released by combustion at time \tilde{t} and $p(\tilde{t})$ is the probability of ignition at time \tilde{t} . Also of interest to us is the sensitivity of the risk of explosions to changes in the wind speed and changes in the initial concentration of propane in the air/propane mixture.

Assumptions

1. The valley has rectangular cross section and is infinitely long (so end effects can be ignored). The valley has uniform depth Z and uniform width X .
2. Temperature and pressure are constant throughout the valley and surrounding area.
3. The air/propane mixture obeys the ideal gas law. Since the volume of the valley is constant then we know the number of moles of air/propane mixture is constant.
4. At initial time $\tilde{t} = 0$ the valley is filled with the air/propane mixture, which has mixed thoroughly. The initial average concentration of propane is \tilde{C}_0 .
5. Wind of constant speed U blows across the top of the valley.

Section II: Nomenclature

In the notation used below, the subscript i is either 1 (for propane) or 2 (for air).

A_n : (used in spatially dependent model) Fourier cosine series coefficient.

$\tilde{A}(\tilde{t})$: (used in rising plume model), area of gas cloud between the limits of the walls of the valley extended into space (units m^2), defined by

$$\tilde{A}(\tilde{t}) = X \left[Z + \tilde{h}(\tilde{t}) \right] \quad (2.1)$$

C_l : minimum volume fraction at which combustion can occur, value 0.022.

C_m : stoichiometric limit for combustion, value 1/26.

C_u : maximum volume fraction at which combustion can occur, value 0.095.

\tilde{C} : concentration of both species, units mol/m.

\tilde{C}_0 : initial average concentration (units mol/m)

$\tilde{C}_i(\tilde{z}, \tilde{t})$: concentration of species i , units mol/m. To be calculated from equations.

D : mixing diffusivity of propane and air, units m^2/sec .

$\tilde{h}(\tilde{t})$: height of eddy currents in air, units m.

p : proportionality constant for probability density, units sec^{-1} .

$\tilde{p}(\tilde{t})$: probability of ignition at time \tilde{t} , units sec^{-1} .

q : heat released per mole of substance, units J.

$\tilde{Q}(\tilde{t})$: heat released by an ignition at time \tilde{t} , units J.

\tilde{R} : heat risk of explosion (units J), defined by

$$\tilde{R} = \int_0^\infty \tilde{Q}(\tilde{t}) \tilde{p}(\tilde{t}) d\tilde{t}. \quad (2.2)$$

R_i : (used in rising plume model) Richardson number.

\tilde{S}_c : sensitivity of heat risk to input concentration \tilde{C}_0 (units m/mol), defined by

$$\tilde{S}_c = \frac{1}{\tilde{R}} \frac{\partial \tilde{R}}{\partial \tilde{C}_0}. \quad (2.3)$$

\tilde{S}_u : sensitivity of heat risk to wind speed U (units sec/m), defined by

$$\tilde{S}_u = \frac{1}{\tilde{R}} \frac{\partial \tilde{R}}{\partial U}.$$

s : Laplace transform variable.

\tilde{t} : time, units sec.

\tilde{t}_1 : (used in spatially independent model) time at which $C_1 = C_u$, units sec.

- \tilde{t}_2 : (used in spatially independent model) time at which $C_1 = C_m$ (stoichiometric limit), units sec.
 \tilde{t}_3 : (used in spatially independent model) time at which $C_1 = C_l$, units sec.
 \tilde{t}_4 : (used in spatially dependent model) time at which $\tilde{z}_1 = Z$, units sec.
 \tilde{t}_5 : (used in spatially dependent model) time at which $\tilde{z}_1 = 0$, units sec.
 \tilde{t}_6 : (used in spatially dependent model) time at which $\tilde{z}_2 = Z$, units sec.
 \tilde{t}_7 : (used in spatially dependent model) time at which $\tilde{z}_2 = 0$, units sec.
 \tilde{t}_8 : (used in spatially dependent model) time at which $\tilde{z}_3 = Z$, units sec.
 \tilde{t}_9 : (used in spatially dependent model) time at which $\tilde{z}_3 = 0$, units sec.
 \tilde{u}_1 : entrainment velocity, units m/sec.
 U : wind velocity, units m/sec.
 V_e : amount of air involved in the entrainment process, units m^2 .
 \tilde{x} : horizontal distance along channel, units m.
 X : width of channel, units m.
 \tilde{z} : vertical distance along channel, units m.
 \tilde{z}_1 : (used in spatially dependent model) height at which $C_1(z) = C_u$, units m.
 \tilde{z}_2 : (used in spatially dependent model) height at which $C_1(z) = C_m$, units m.
 \tilde{z}_3 : (used in spatially dependent model) height at which $C_1(z) = C_l$, units m.
 Z : height of channel, units m.
 $\tilde{Z}_{e1}(\tilde{t})$: explosion zone (zone where gas will explode if ignited in the flammability zone at time \tilde{t}) where $C_1(z) < C_m$, units m.
 $\tilde{Z}_{e2}(\tilde{t})$: explosion zone (zone where gas will explode if ignited in the flammability zone at time \tilde{t}) where $C_1(z) > C_m$, units m.
 $\tilde{Z}_f(\tilde{t})$: flammability zone (zone where gas can be ignited at time \tilde{t}), units m.
 ϕ : the empty set.

Nondimensionalized variables will have no tildes. Laplace transformed quantities have hats.

Section III: Spatially Independent Model

It is assumed the wind blowing across the valley forms a turbulent layer of thickness on the order the height of the ground-based obstructions in its path. This wind layer will carry off propane gas from the valley. Since molecular diffusion of the propane takes place at a much slower rate, the wind is assumed to be the dominant mechanism by which propane is depleted from the valley. We also assume that mixing within the valley occurs at such a rapid rate that concentration differences are instantaneously distributed evenly throughout the valley. Mathematically, we say that \tilde{C} is independent of \tilde{z} and is a function of \tilde{t} only.

If the turbulent layer has dimension \tilde{h} (measured in meters, which in this model we assume to be a constant), then propane leaves the valley at the rate given by the product of the wind speed, the thickness of the turbulent layer, and the current concentration of propane in the valley. In our nomenclature

$$\frac{d(\tilde{C}_1 Z X)}{d\tilde{t}} = -U\tilde{h}\tilde{C}_1. \quad (3.1)$$

To nondimensionalize (3.1) we will normalize \tilde{C}_1 by C , all distances by Z , and time by the transit time of the wind across the valley, X/U . Summarizing, we have the following:

$$C_1 = \frac{\tilde{C}_1}{C}, \quad t = \frac{\tilde{t}U}{X}, \quad h = \frac{\tilde{h}}{Z}. \quad (3.2)$$

Substituting (3.2) into (3.1) we arrive at the following dimensionless differential equation:

$$\frac{dC_1}{dt} = -hC_1. \quad (3.3)$$

Using the initial condition $C_1(0) = C_0$, this differential equation has solution

$$C_1(t) = C_0 e^{-ht}. \quad (3.4)$$

Whether the propane will ignite and how much will burn (and thus the amount of heat produced) depend on the concentration of propane in the air. If $C_1(t) < C_l = 0.022$ or $C_1(t) > C_u = 0.095$ the air/propane mixture will not ignite. Since five moles of oxygen are required to support the combustion of one mole of propane and since air is approximately one fifth oxygen, if $C_u \geq C_1(t) > C_m = 1/26$ then only $(1 - C_1)ZX/25$ moles of propane will burn before all the oxygen is consumed. If $C_l \leq C_1(t) \leq C_m$ then C_1ZX moles of propane will burn and there will be oxygen left over. Thus the times at which C_1 reaches

these crucial values are of interest. The time at which the propane concentration reaches the upper limit of flammability is

$$t_1 = \max \left\{ 0, -\frac{1}{h} \ln \frac{C_u}{C_0} \right\}. \quad (3.5)$$

The time at which the concentration reaches the point at which all the propane will burn is

$$t_2 = \max \left\{ 0, -\frac{1}{h} \ln \frac{C_m}{C_0} \right\}. \quad (3.6)$$

The air/propane mixture reaches the lower limit of flammability at time

$$t_3 = \max \left\{ 0, -\frac{1}{h} \ln \frac{C_l}{C_0} \right\}. \quad (3.7)$$

If we now consider the equation describing the risk of explosion, we have

$$\tilde{R} = \int_{\tilde{t}_1}^{\tilde{t}_2} \tilde{Q}_1(\tilde{t}) \tilde{p}(\tilde{t}) d\tilde{t} + \int_{\tilde{t}_2}^{\tilde{t}_3} \tilde{Q}_2(\tilde{t}) \tilde{p}(\tilde{t}) d\tilde{t}. \quad (3.8)$$

The integral involving \tilde{Q}_1 represents the dimensional form of the heat produced from the burning propane from the time at which the concentration is low enough for ignition to occur until the time at which the concentration of propane is equal to the stoichiometric limit. The second integral is the heat produced from the time at which the concentration of propane is equal to the stoichiometric limit until the time at which the concentration of propane has been lowered to the point at which the air/propane mixture will not burn.

We assume in this case that the probability density is uniform in any time period during which ignition can occur. Hence, we let $\tilde{p}(\tilde{t}) = p$, where p is chosen so that the integral of the probability density is 1. Thus equation (3.8) becomes

$$\tilde{R} = pqXZC \left[\int_{\tilde{t}_1}^{\tilde{t}_2} \frac{1 - C_1(\tilde{t})}{25} d\tilde{t} + \int_{\tilde{t}_2}^{\tilde{t}_3} C_1(\tilde{t}) d\tilde{t} \right].$$

Then if we make the substitution $t = \tilde{t}U/X$ we get

$$\tilde{R} = \frac{pqX^2ZC}{U} \left[\int_{t_1}^{t_2} \frac{1 - C_1(t)}{25} dt + \int_{t_2}^{t_3} C_1(t) dt \right]. \quad (3.9)$$

which we can evaluate using equations (3.4)-(3.7) as

$$\tilde{R} = \begin{cases} \frac{pqX^2ZC}{hU} \left(\frac{1}{25} \ln \frac{C_u}{C_m} + \frac{C_m - C_u}{25} + C_m - C_l \right) & \text{if } C_u \leq C_0 \\ \frac{pqX^2ZC}{hU} \left(\frac{1}{25} \ln \frac{C_0}{C_m} + \frac{C_m - C_0}{25} + C_m - C_l \right) & \text{if } C_m \leq C_0 < C_u \\ \frac{pqX^2ZC}{hU} (C_0 - C_l) & \text{if } C_l < C_0 < C_m \\ 0 & \text{if } C_0 \leq C_l. \end{cases} \quad (3.10)$$

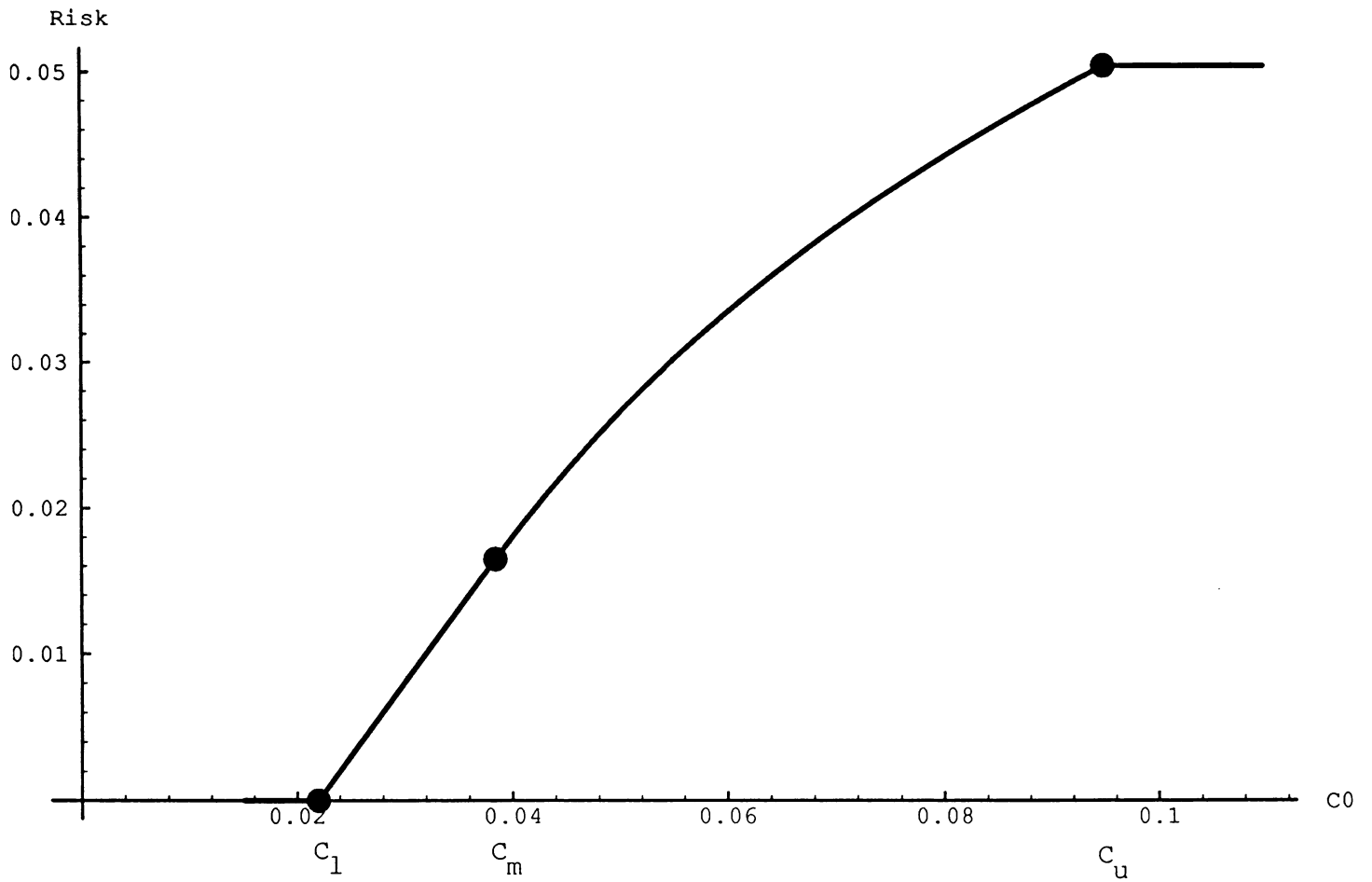
Thus the sensitivity to changes in wind speed becomes

$$\tilde{S}_u = \frac{1}{\tilde{R}} \frac{d\tilde{R}}{dU} = \begin{cases} -\frac{1}{U} & \text{if } C_l < C_0 \\ 0 & \text{if } C_0 \leq C_l. \end{cases} \quad (3.11)$$

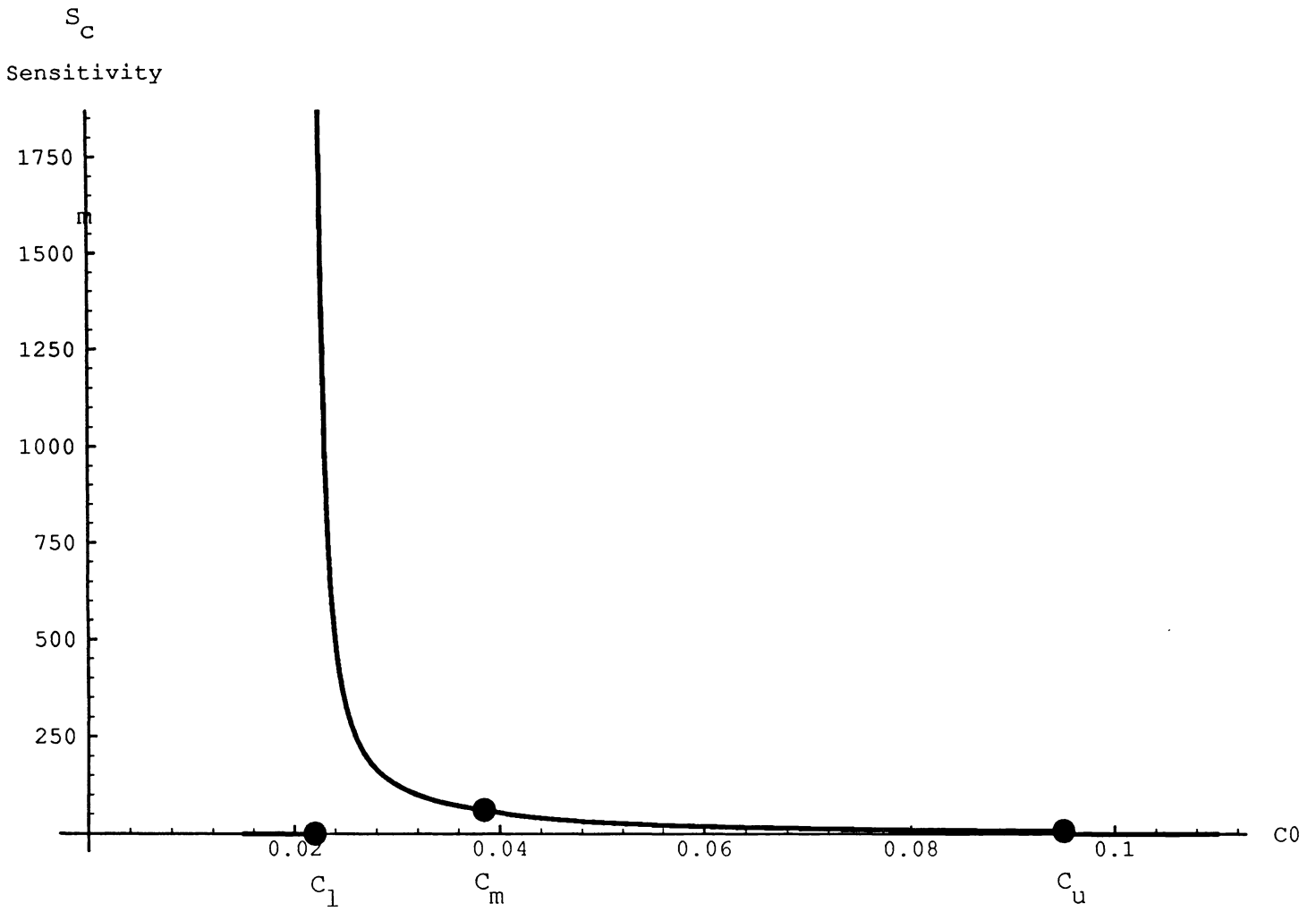
The sensitivity to changes in the initial concentration of propane is

$$\tilde{S}_c = \frac{1}{\tilde{R}} \frac{d\tilde{R}}{dC_0} = \begin{cases} 0 & \text{if } C_u \leq C_0 \\ \frac{\frac{1}{25} \left(\frac{1}{C_0} - 1 \right)}{\frac{1}{25} \ln \frac{C_0}{C_m} + \frac{C_m - C_0}{25} + C_m - C_l} & \text{if } C_m \leq C_0 < C_u \\ \frac{1}{C_0 - C_l} & \text{if } C_l < C_0 < C_m \\ 0 & \text{if } C_0 \leq C_l. \end{cases} \quad (3.12)$$

Risk versus Concentration
Spatially Independent Model



Sensitivity versus Initial
Concentration for Spatially
Independent Model



Section IV: Spatially Dependent Model

Now we wish to complicate our model somewhat. We assume that the mixing inside the valley is only great enough to guarantee a striated concentrated distribution, rather than a uniform one; *i.e.*, we assume that the concentration profile varies as a function of \tilde{z} according to a standard Fickian diffusion law:

$$\frac{\partial \tilde{C}_1}{\partial \tilde{t}} = D \frac{\partial^2 \tilde{C}_1}{\partial \tilde{z}^2}. \quad (4.1)$$

For boundary conditions, we assume that no flux is coming in from the bottom:

$$\frac{\partial \tilde{C}_1}{\partial \tilde{z}}(0, \tilde{t}) = 0. \quad (4.2)$$

For our boundary condition at $\tilde{z} = Z$, we look at the following *global* mass balance principle:

$$X \frac{\partial}{\partial \tilde{t}} \left[\int_0^{Z+\tilde{h}} \tilde{C}_1(\tilde{z}, \tilde{t}) d\tilde{z} \right] = -U\tilde{h}\tilde{C}_1(Z + \tilde{h}, \tilde{t}). \quad (4.3)$$

Equation (4.3) simply states that the change in the amount of propane in the entire system is given by the mixing rate. However, we may simplify equation (4.3) using equation (4.1) to obtain the following:

$$\left[D \frac{\partial \tilde{C}_1}{\partial \tilde{z}}(\tilde{z}, \tilde{t}) \right]_0^{Z+\tilde{h}} + \frac{U\tilde{h}}{X} \tilde{C}_1(Z + \tilde{h}, \tilde{t}) = 0.$$

However, since $\tilde{h} \ll Z$, we may approximate our function values by those at Z . Using equation (4.2), we have

$$\frac{\partial \tilde{C}_1}{\partial \tilde{z}}(Z, \tilde{t}) + \frac{U\tilde{h}}{DX} \tilde{C}_1(Z, \tilde{t}) = 0. \quad (4.4)$$

Now we proceed to nondimensionalize our equations. We normalize \tilde{z} by Z , our height. Since we are modeling a diffusion process, we normalize \tilde{t} by the diffusion time scale, Z^2/D . We normalize our \tilde{C}_1 by C to get mole fractions. Summarizing, we have the following:

$$z = \frac{\tilde{z}}{Z}, \quad t = \frac{D\tilde{t}}{Z^2}, \quad C_1 = \frac{\tilde{C}_1}{C}. \quad (4.5)$$

Substituting into equations (4.1), (4.2), and (4.4), we have the following system:

$$\frac{\partial C_1}{\partial t} = \frac{\partial^2 C_1}{\partial z^2} \quad (4.6)$$

$$\frac{\partial C_1}{\partial z}(0, t) = 0 \quad (4.7)$$

$$\frac{\partial C_1}{\partial z}(1, t) + \frac{ZU\tilde{h}}{DX}C_1(1, t) = 0 \quad (4.8)$$

$$C_1(z, 0) = C_0. \quad (4.9)$$

Now equation (4.8) tells us that a natural diffusion coefficient for this problem is given by $ZU\tilde{h}/X$. This is the coefficient we choose. Doing so, equation (4.8) becomes

$$\frac{\partial C_1}{\partial z}(1, t) + C_1(1, t) = 0. \quad (4.10)$$

Now we wish to solve our system of equations [(4.6), (4.7), (4.9), and (4.10)] to give us C_1 . Unfortunately, exact solutions are always messy and seldom useful. However, we may glean asymptotic information from them to yield results to within the order of accuracy of our assumptions. We begin by postulating a Fourier cosine series expansion:

$$C_1(z, t) = \sum_{n=1}^{\infty} A_n \exp(-\lambda_n^2 t) \cos(\lambda_n z). \quad (4.11)$$

The eigenfunctions are guaranteed to be orthogonal in this problem.

This series automatically satisfies equations (4.6) and (4.7). To satisfy equation (4.10), we take one eigenfunction and plug in:

$$\begin{aligned} -\lambda_n \sin(\lambda_n) + \cos(\lambda_n) &= 0 \\ \lambda_n \tan(\lambda_n) &= 1. \end{aligned} \quad (4.12)$$

To solve our initial condition, we see that since the eigenfunctions are orthogonal, we have

$$\begin{aligned} A_n &= 2 \int_0^1 C_1(z, 0) \cos(\lambda_n z) dz \\ &= 2C_0 \int_0^1 \cos(\lambda_n z) dz \\ &= \frac{2C_0 \sin(\lambda_n)}{\lambda_n}. \end{aligned} \quad (4.13)$$

Now, since all of our eigenvalues are decaying, we see from equation (4.11) that the eigenvalue corresponding to $n = 1$ will determine the leading order behavior of our solution for long time. Hence we have

$$C_1(z, t) \sim \frac{2C_0 e^{-\lambda_1^2 t} \sin(\lambda_1)}{\lambda_1} \cos(\lambda_1 z). \quad (4.14)$$

This is now our long-time approximation. For reference, $\lambda_1 = 0.86$.

However, we must be careful when we use the words “long-time”. We stated in section I that when $\tilde{t} = 0$, the gas had mixed thoroughly. If this is true, we may assume that at our $\tilde{t} = 0$ (dawn), the gas has *already diffused* into the leading order solution. Hence, we may adapt our initial condition to be of the following form:

$$C_1(z, 0) = A_1 \cos(\lambda_1 z). \quad (4.15)$$

Since C_0 is our average initial condition, we have

$$\int_0^1 C_1(z, 0) dz = C_0.$$

Substituting equation (4.15) into the above and solving for A_1 gives us the following expression:

$$A_1 = \frac{C_0 \lambda_1}{\sin \lambda_1}. \quad (4.16)$$

Now since our initial condition consists of only one eigenfunction, our *exact* solution becomes

$$C_1(z, t) = \frac{C_0 \lambda_1 e^{-\lambda_1^2 t}}{\sin \lambda_1} \cos(\lambda_1 z). \quad (4.17)$$

Now that we have an expression for C_1 , we may construct an expression for our risk. We know that the dimensional risk is the following:

$$\tilde{R} = \int_0^\infty \tilde{Q}(\tilde{t}) \tilde{p}(\tilde{t}) d\tilde{t}. \quad (4.18)$$

Hence we need to know \tilde{Q} and \tilde{p} . We first postulate that the probability of explosion at any time \tilde{t} is proportional to the volume of gas in the flammability zone, hence we assume $\tilde{p} = p|\tilde{Z}_f(\tilde{t})|$.

For $\tilde{Q}(\tilde{t})$, we make the following argument: if gas in the flammability zone explodes *above* gas that is not in the flammability zone, then the pressure from the explosion will force the gas below the explosion into a new flammability zone caused by the fact that increased pressure changes our flammability limits. Hence, any explosion automatically uses up all gas from $\tilde{Z} = 0$ to the top of the flammability zone. We call this extended region the *explosion zone*. However, the converse is not true. If gas explodes *below* gas not in the flammability zone, the pressure wave will disperse the gas and not explode it.

The heat \tilde{Q} is going to depend only on the concentration of the rate-controlling reactant at any point and time. The discussion of how to determine this was given in section II. Hence we may represent the risk symbolically by the following:

$$\tilde{R} = \int_{\tilde{t}_4}^{\tilde{t}_9} p|\tilde{Z}_f(\tilde{t})| \left\{ \int_{\tilde{Z}_{e1}(\tilde{t})} qX \tilde{C}_1(z, t) dz + \int_{\tilde{Z}_{e2}(\tilde{t})} qX \left[\frac{1 - \tilde{C}_1(z, t)}{25} \right] dz \right\} d\tilde{t}.$$

Nondimensionalizing the right-hand side, we have the following:

$$\tilde{R} = \frac{pqX^2Z^2C}{\tilde{h}U} \int_{t_4}^{t_9} p|Z_f(t)| \left\{ \int_{Z_{e1}(t)} qXC_1(z,t) dz + \int_{Z_{e2}(t)} qX \left[\frac{1 - C_1(z,t)}{25} \right] dz \right\} dt. \quad (4.19)$$

From equation (4.19), it is clear that \tilde{R} is proportional to $1/U$. Hence, we have the following:

$$\tilde{S}_u = \frac{1}{\tilde{R}} \frac{\partial \tilde{R}}{\partial U} = -\frac{1}{U}. \quad (4.20)$$

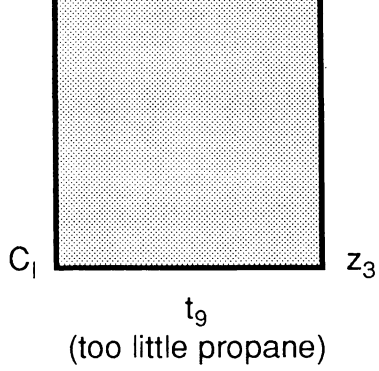
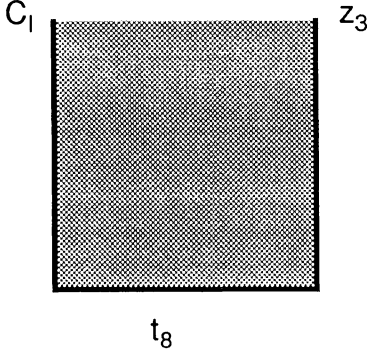
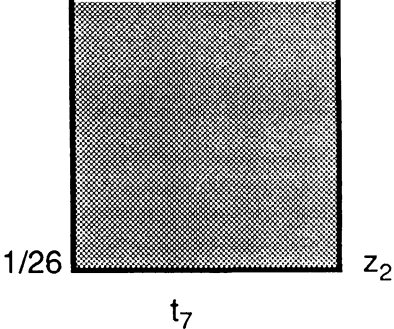
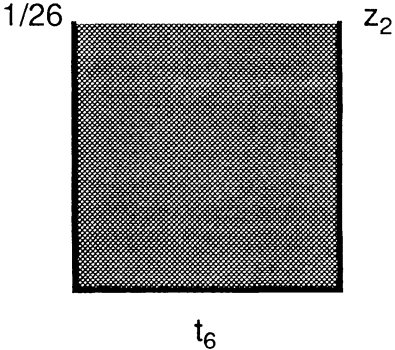
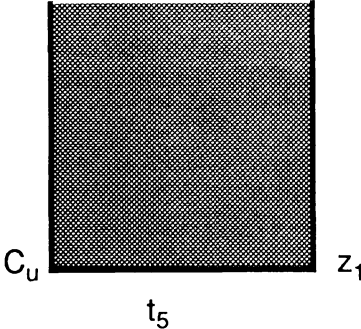
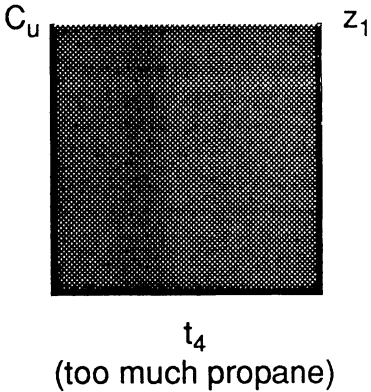
Note that equation (4.24) agrees with the results from model 1.

To calculate \tilde{S}_c , we must be more careful. We have calculated that $t_j < t_{j+1}$, $j = 4, 5, \dots$. However, $|Z_f(t)|$ and $Z_e(t)$ are different. Here is a brief summary of our regions for different time periods:

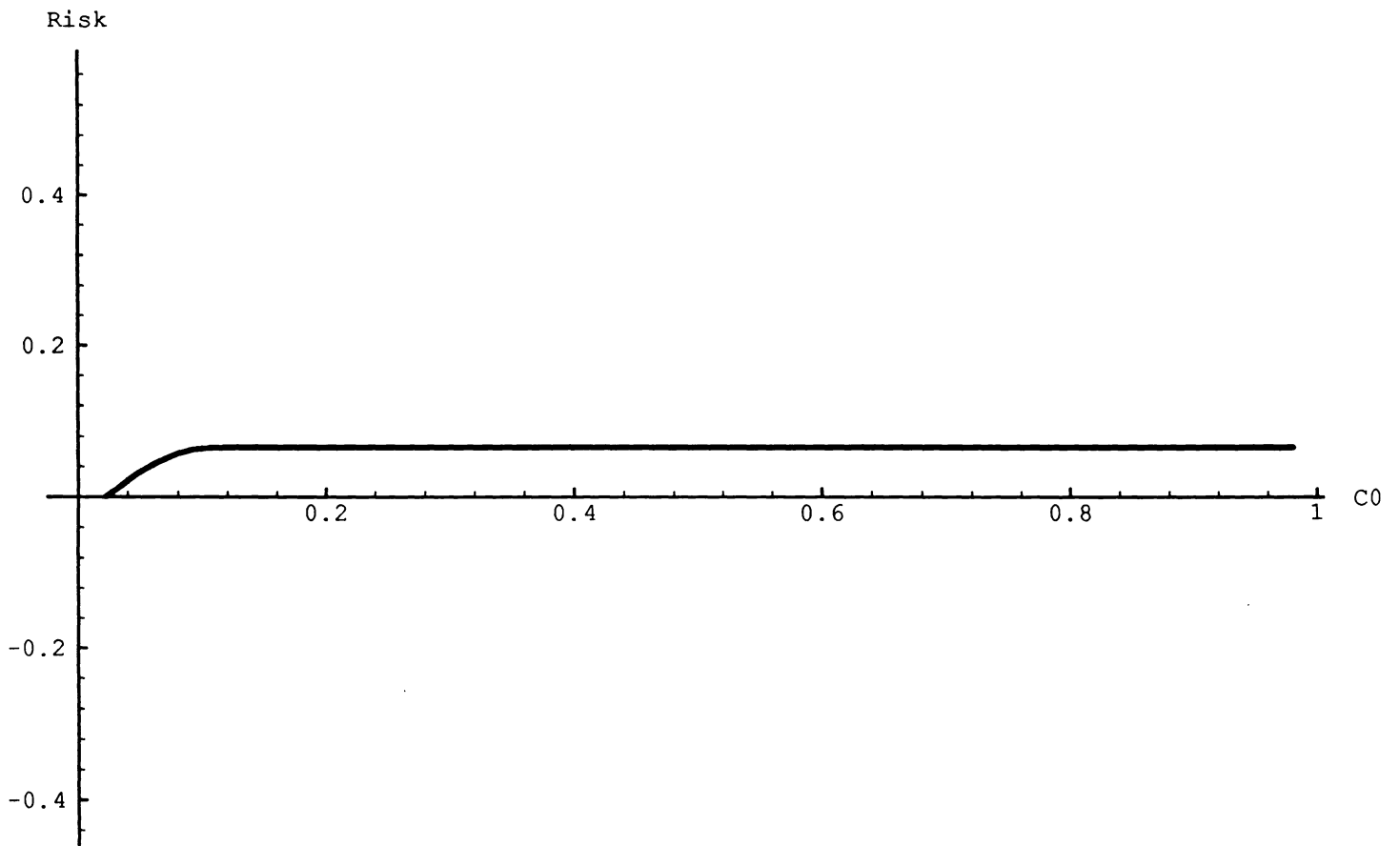
$$\begin{aligned} t_4 < t < t_5 : & \quad Z_f(t) = (z_1(t), 1); & \quad Z_{e1}(t) = \phi; & \quad Z_{e2}(t) = (0, 1) \\ t_5 < t < t_6 : & \quad Z_f(t) = (0, 1); & \quad Z_{e1}(t) = \phi; & \quad Z_{e2}(t) = (0, 1) \\ t_6 < t < t_7 : & \quad Z_f(t) = (0, 1); & \quad Z_{e1}(t) = (z_2(t), 1); & \quad Z_{e2}(t) = (0, z_2(t)) \\ t_7 < t < t_8 : & \quad Z_f(t) = (0, 1); & \quad Z_{e1}(t) = (0, 1); & \quad Z_{e2}(t) = \phi \\ t_8 < t < t_9 : & \quad Z_f(t) = (0, z_3(t)); & \quad Z_{e1}(t) = (0, z_3(t)); & \quad Z_{e2}(t) = \phi. \end{aligned} \quad (4.21)$$

The integral is quite complicated and was done numerically using a rectangular rule. Graphs of the risk versus the initial concentration C_0 and graphs of the sensitivity \tilde{S}_c versus the initial concentration C_0 follow.

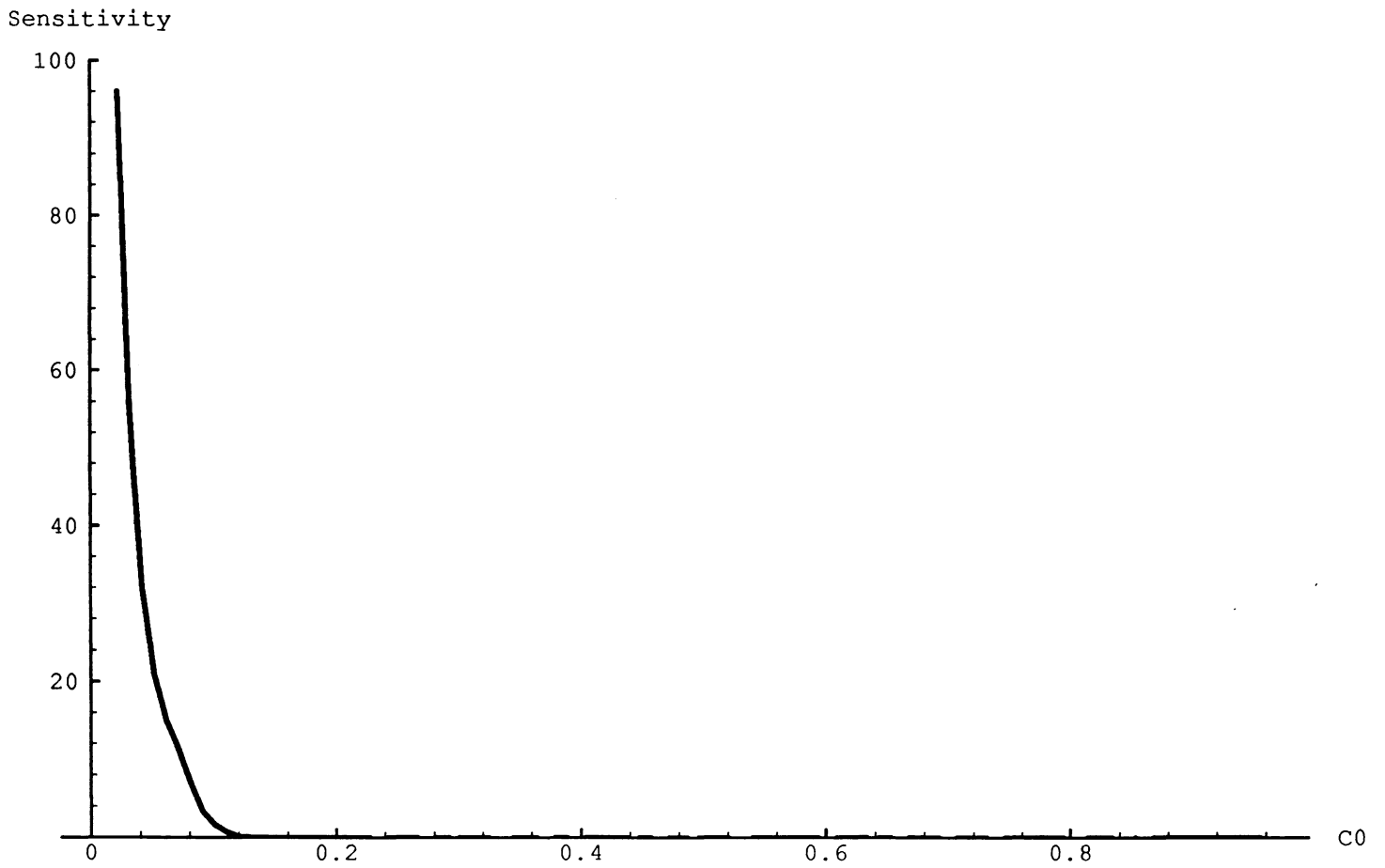
Combustion Sequence



Risk versus Initial
Concentration for Spatially
Dependent Model



Sensitivity S_c versus Initial
Concentration for Spatially
Dependent Model



Section V: Consideration of Entrainment

Introduction

In model I and II, we ignored the physical process of entrainment. It is the process by which air is mixed into the gas cloud (propane-air mixture) due to turbulence from shear flow of pure air passing the cloud. This process will effectively increase the height H of the cloud above the valley, thus resulting in a faster dissipation.

Because the gas is at constant temperature and pressure and we have assumed an ideal gas, the volume balance gives us:

$$\frac{\partial(LA)}{\partial \tilde{t}} = \frac{\partial V_e}{\partial \tilde{t}} - ULH$$

where L is a standard length of the valley, and A is the cross-sectional area of the cloud. Thus, the volume of gas changes as a result of the entrained air minus the volume of gas blown beyond the valley. Assuming V_e as a volume per length, the equation becomes

$$\frac{\partial A}{\partial \tilde{t}} = \frac{\partial V_e}{\partial \tilde{t}} - UH \quad (5.1)$$

The other governing equation comes from model I, with the well-mixed cloud assumption, namely, the propane balance equation:

$$\frac{\partial(C_1 A)}{\partial \tilde{t}} = -UC_1 H \quad (5.2)$$

Using the “box model” for entrainment, we assume that the shape of the cloud, after slumping, maintains a rectangular cross-section, and thus $A = X(Z + H)$. Also for this model

$$\frac{\partial V_e}{\partial \tilde{t}} = \frac{\alpha^3 \rho_a X U^3}{(\rho - \rho_a) g H} \quad (5.3)$$

where α is the ratio of entrainment velocity to wind velocity. We assume from other similar experiments, that $\alpha = 0.0532$. Since the molecular weight of C_3H_8 is 44 and the average molecular weight of air is 29, and the air and the gas have the same concentration because of the constant temperature and pressure, we have

$$\rho = 44C_1 + 29C_2 = 44C_1 + 29(C - C_1) = 15C_1 + 29C = 15C_1 + \rho_a$$

thus

$$\rho - \rho_a = 15C_1.$$

Therefore (3) can be written as

$$\frac{\partial V_e}{\partial \tilde{t}} = \frac{\alpha^3 \rho_a X U^3}{15 C_1 g H}. \quad (5.4)$$

Substituting this result in (1) and introducing the following dimensionless variables

$$t = \frac{U}{X} \tilde{t}, \quad x_1 = \frac{C_1(Z+H)}{CZ}, \quad x_2 = \frac{H}{Z}$$

we can transform governing equations (1) and (2) to the following dimensionless form

$$\begin{aligned} \frac{dx_1}{dt} &= -\frac{x_1 x_2}{1+x_2} \\ \frac{dx_2}{dt} &= a \frac{1+x_2}{x_1 x_2} - x_2 \end{aligned}$$

where

$$a = \frac{\alpha^3 \rho_a U^2 X}{15 g Z^2 C}.$$

Phase Plane Analysis

The equations for x_1, x_2 are nonlinear autonomous ODEs. We can perform a phase plane analysis to reveal some features of a solution of the system of ODEs. From the above equations we have

$$\frac{dx_2}{dx_1} = \frac{(1+x_2)[x_1 x_2^2 - a(1+x_2)]}{x_1^2 x_2^2}$$

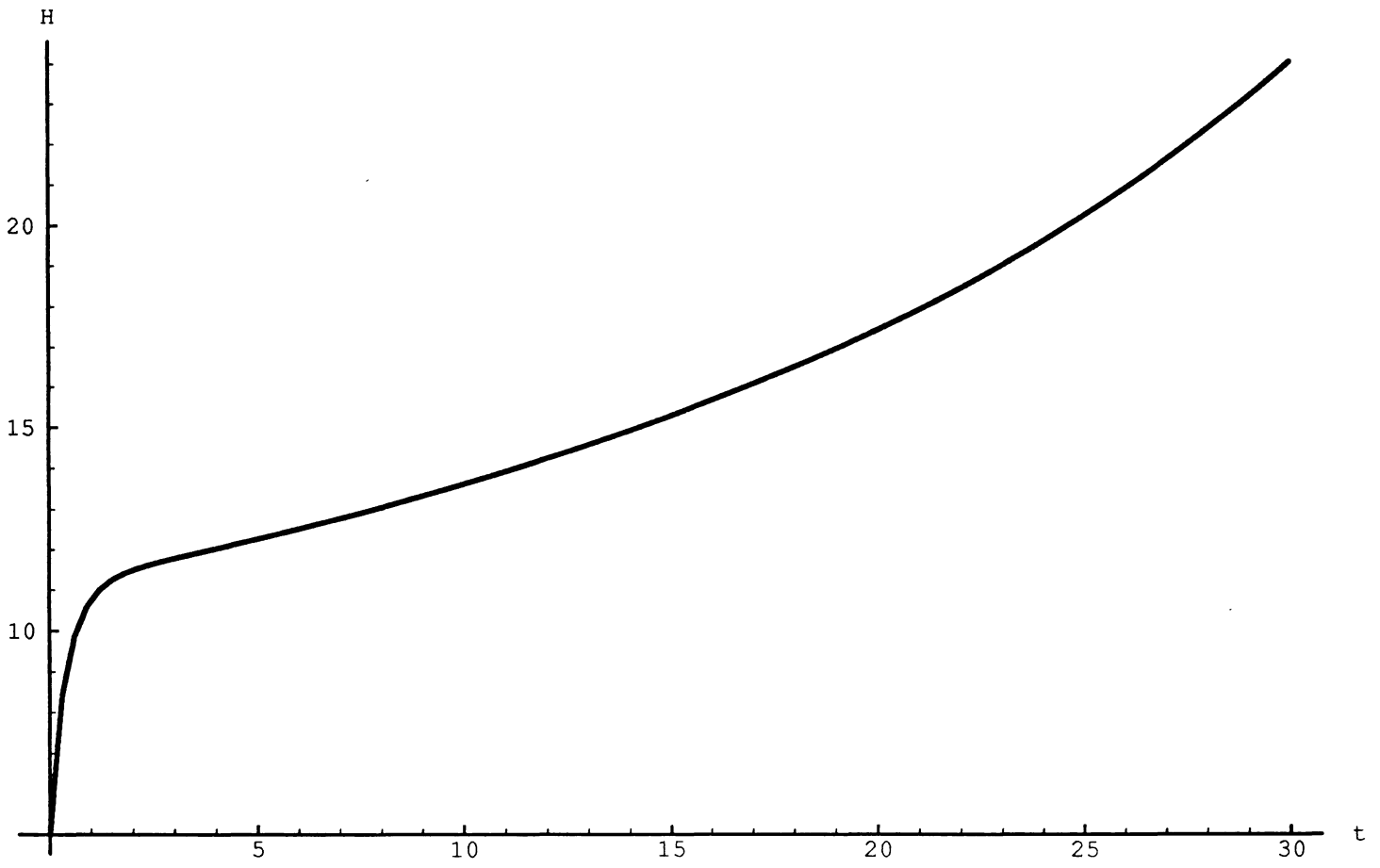
The trajectories of (x_1, x_2) are shown on the following phase plane diagram. On the phase plane, we see that for various starting concentrations, there is an initial large increase in x_2 (the cloud height) followed by a drop in concentration with a slower height increase.

Numerical Analysis

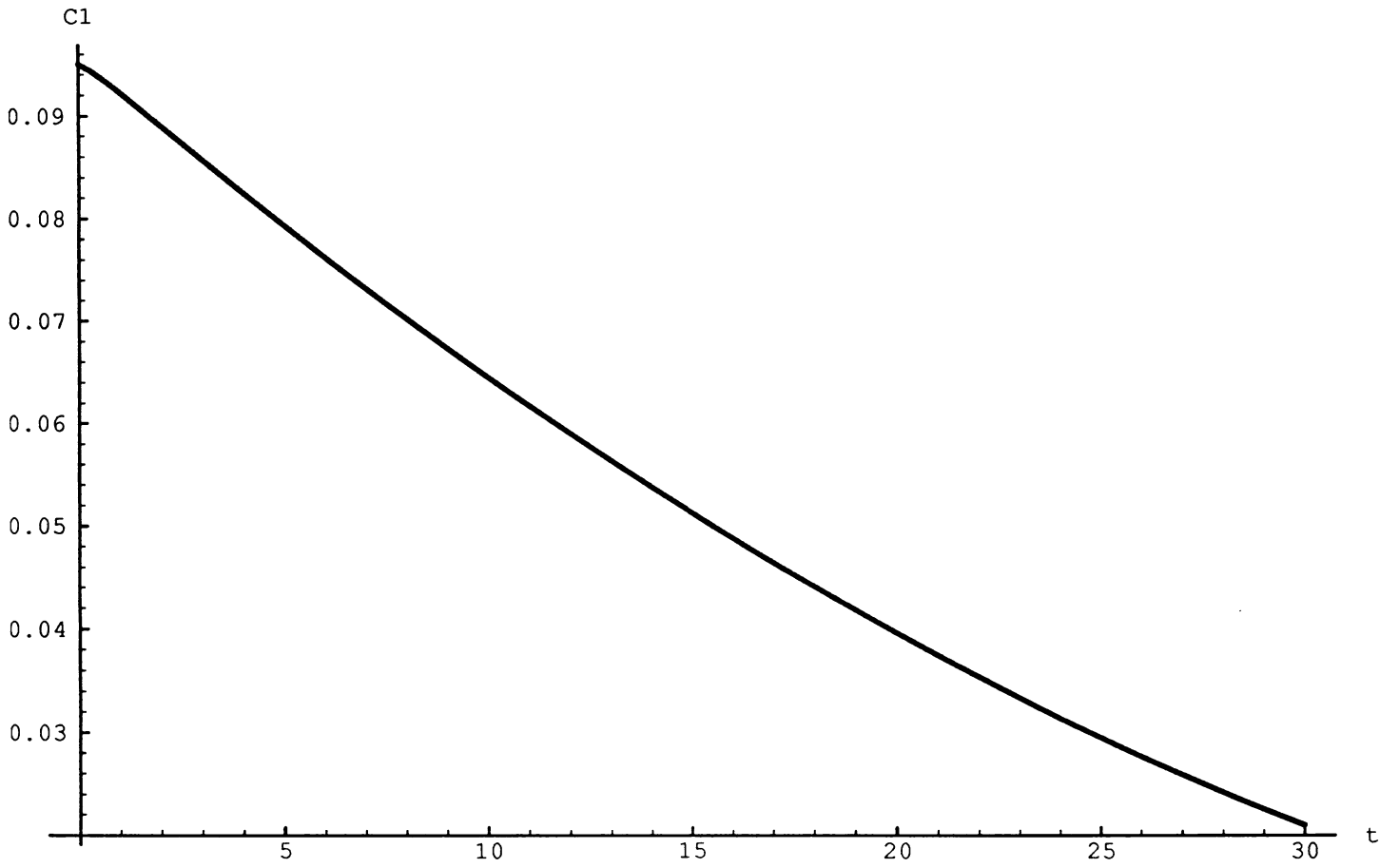
Since we could not get a closed-form solution of the nonlinear system, we performed numerical calculations.

The Runge-Kutta method of order 4 has been used to solve the system with time step size 0.001 for the given values of C_0 and U . We then used the numerical solution to determine the risk, R , using a trapezoid rule integrating scheme, based on the two-integral formula from model I. The forward difference formula was used to approximate the sensitivities $S_U = \frac{1}{R} \frac{\partial R}{\partial U}$ and $S_{C_0} = \frac{1}{R} \frac{\partial R}{\partial C_0}$ for this model.

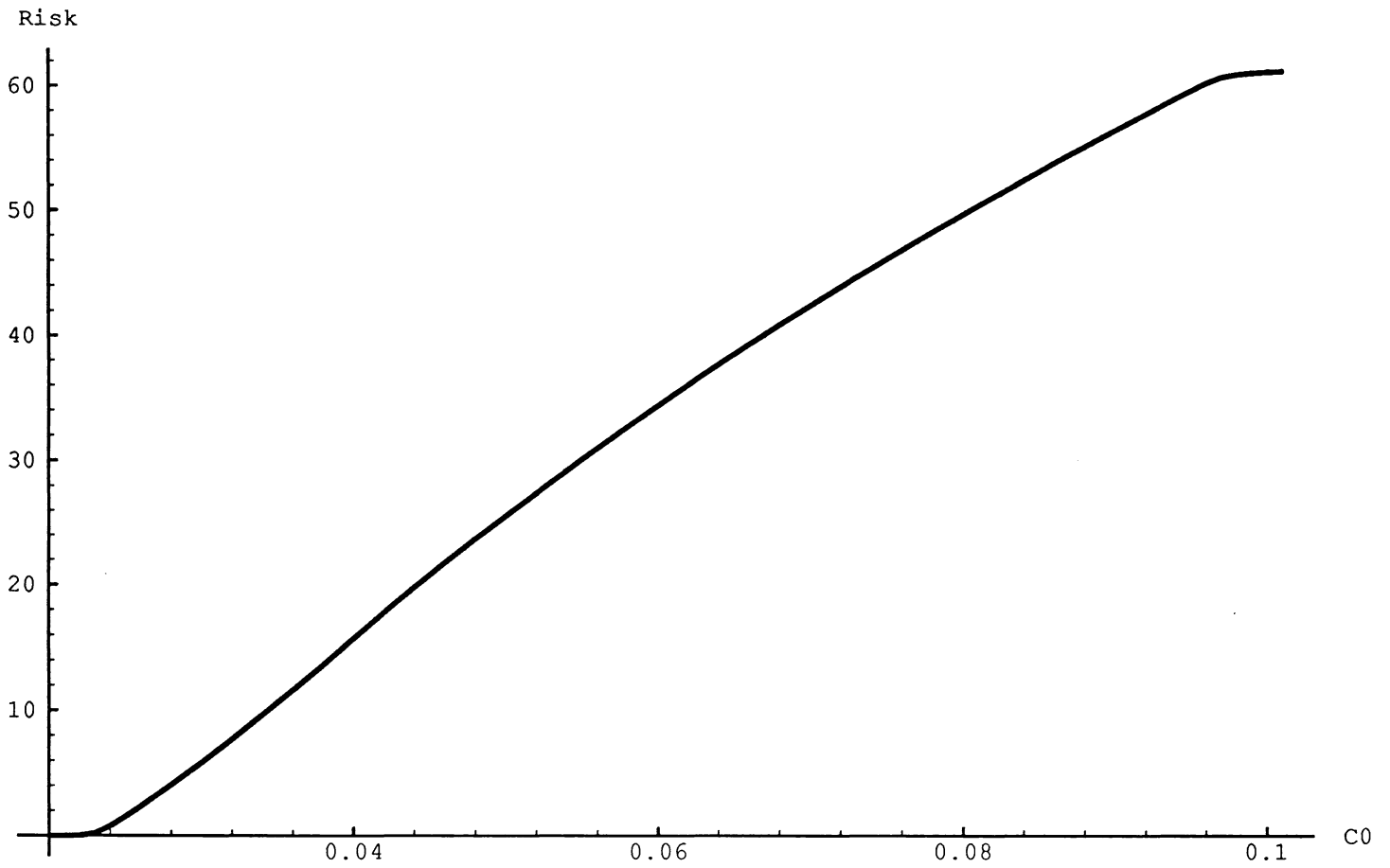
Height of Propane Plume
versus Time, Entrainment
Model



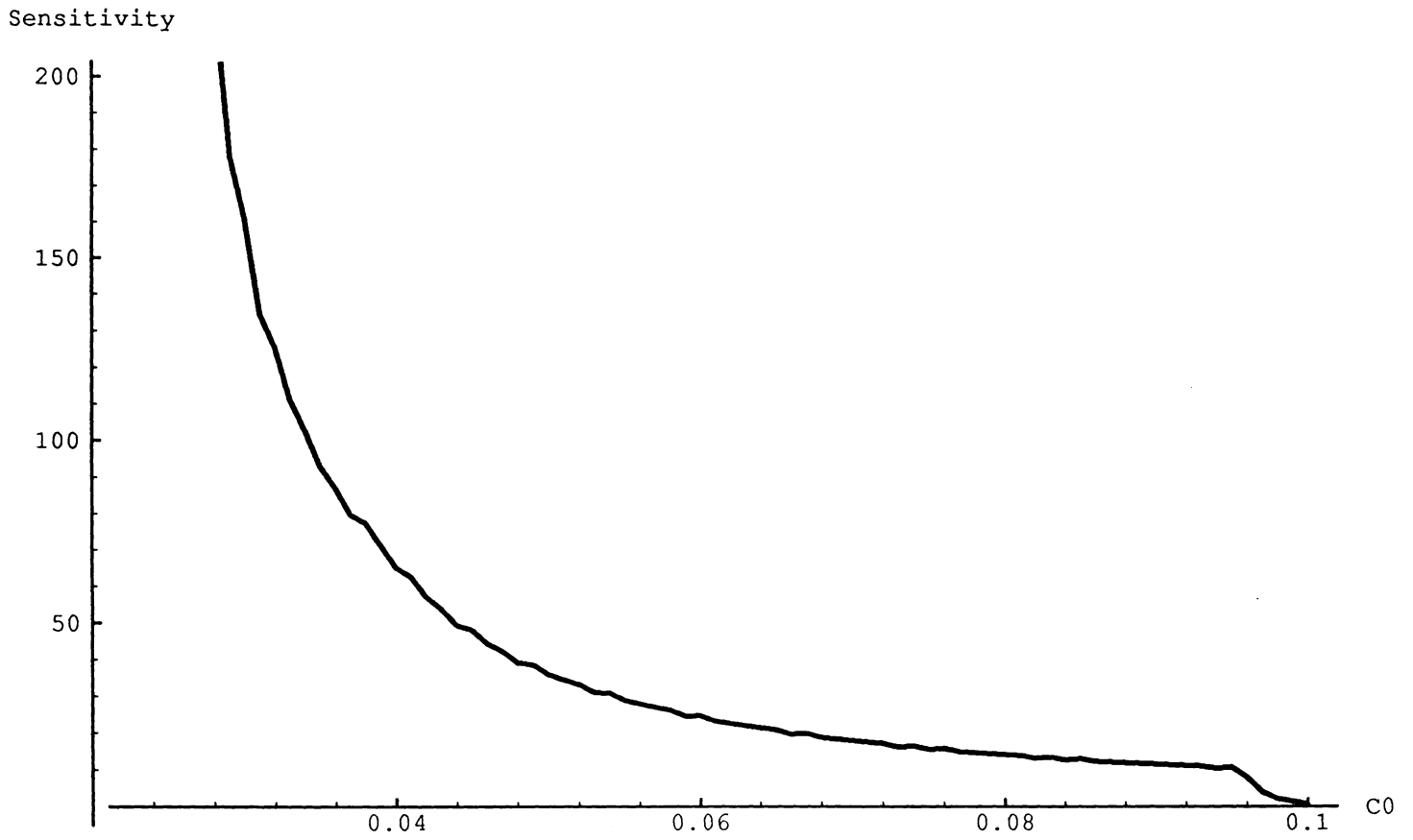
Value of Concentration
versus Time for Entrainment
Model



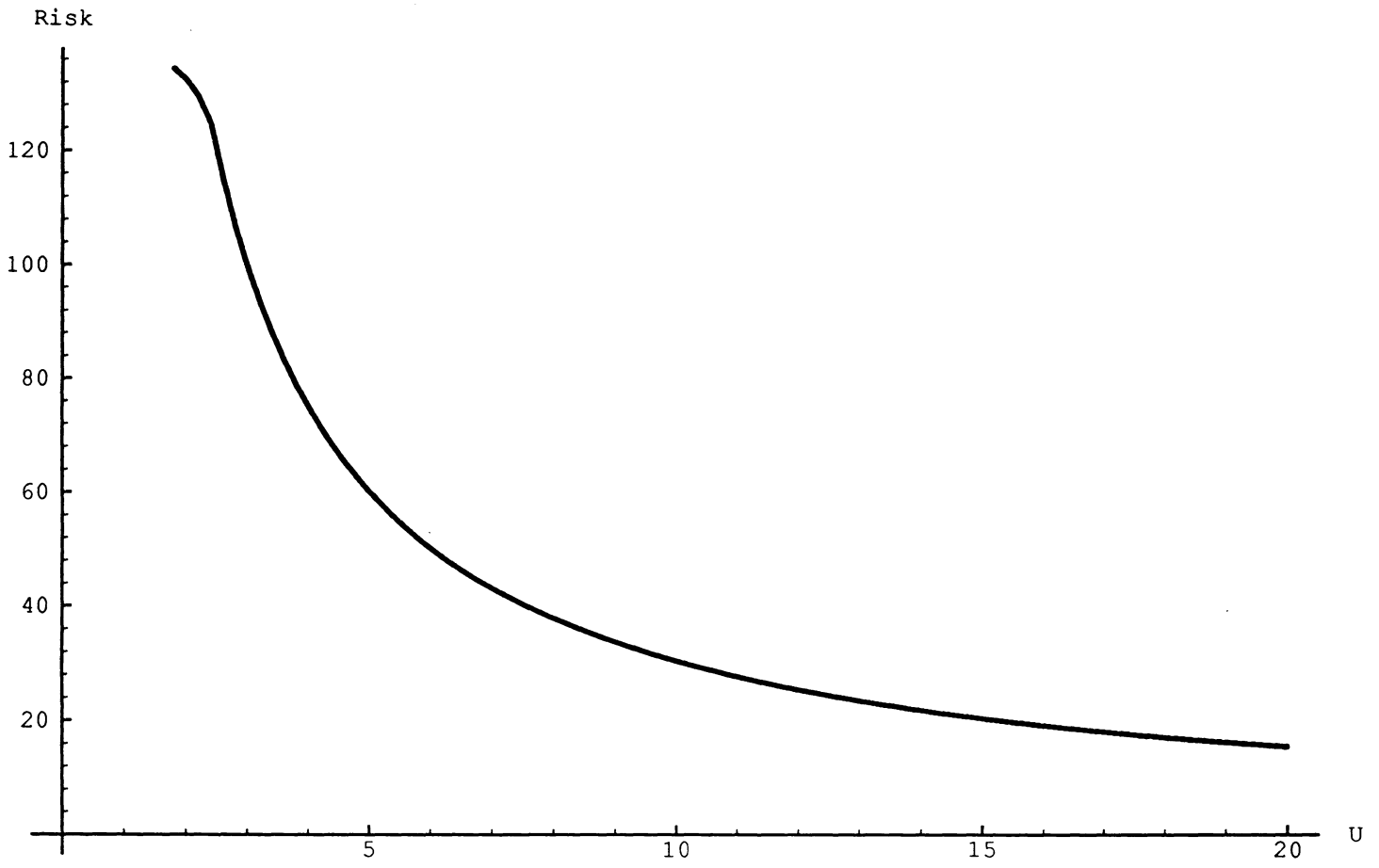
Risk versus Initial
Concentration C_0 for Entrainment
Model



Sensitivity S_c versus
Initial Concentration C_0
for Entrainment Model

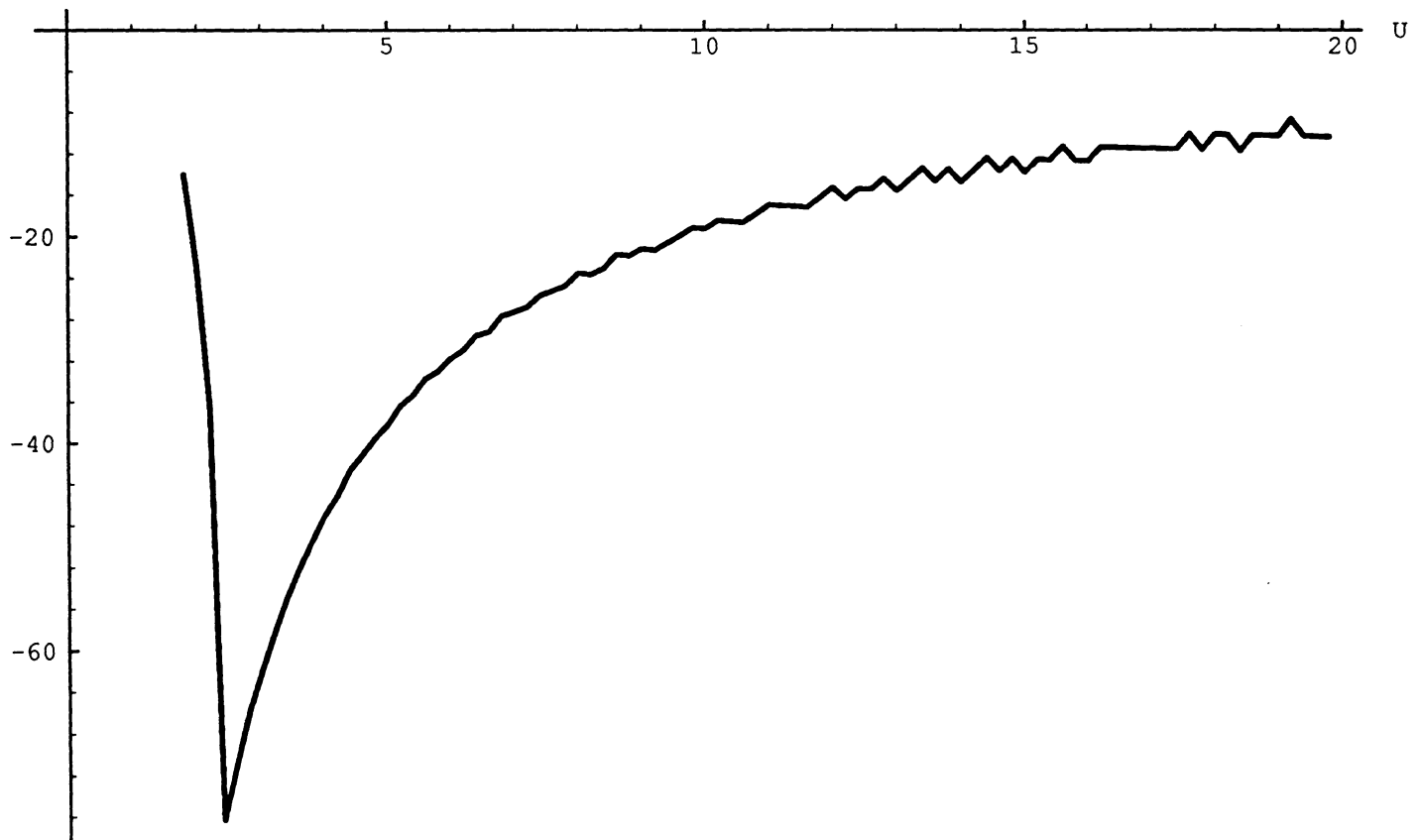


Risk versus Wind Speed U
for Entrainment Model

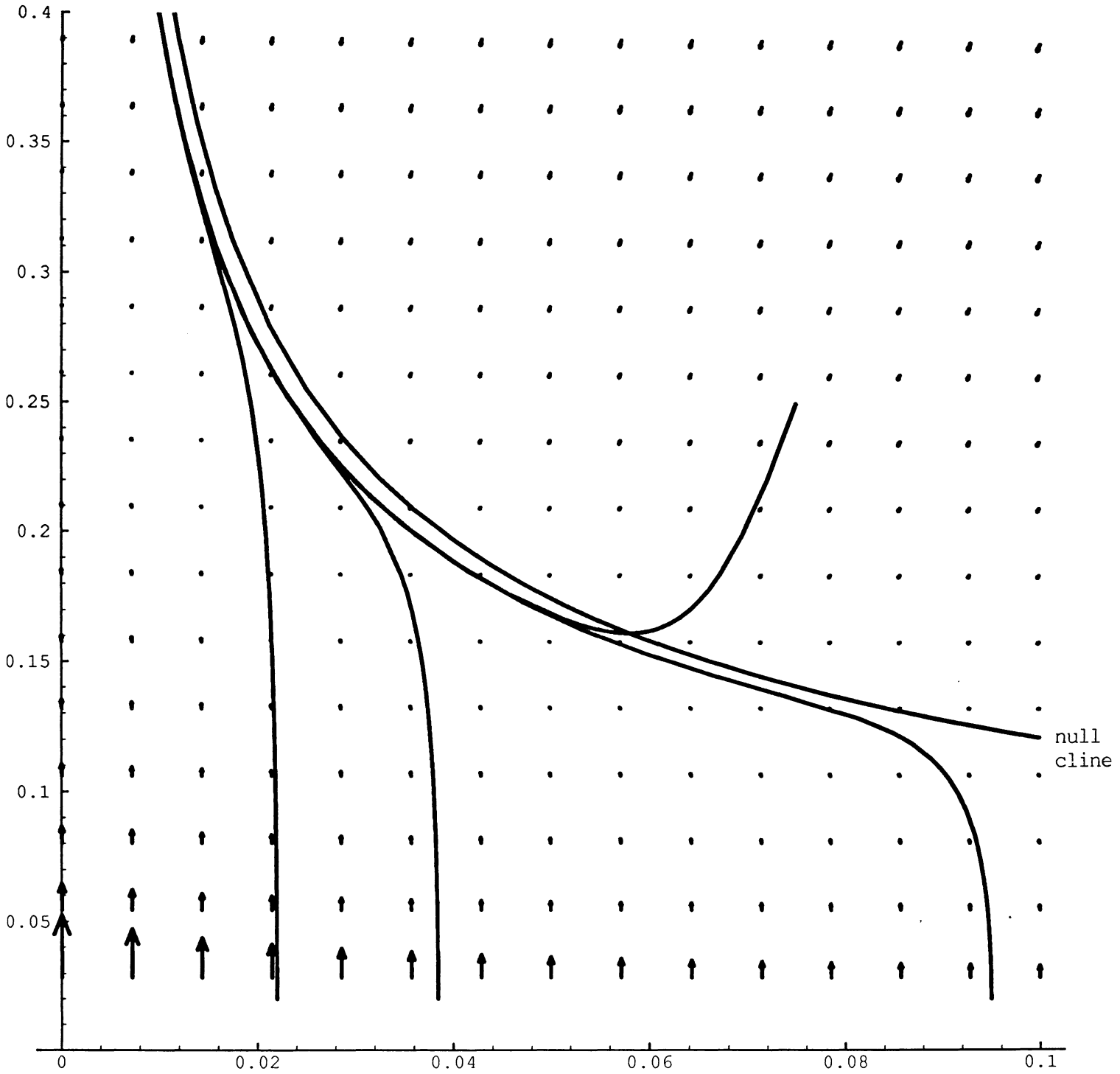


Sensitivity S_u versus
Wind Speed U for Entrainment
Model

Sensitivity



Velocity Field Superimposed
on Graph of Height of Plume
versus Concentration



Section VI: Conclusions and Future Research

Conclusions

Throughout each of our three models, we found a clear dependence of risk on the important physical parameters of wind velocity U and initial average concentration of propane in the valley C_0 . In the first model, the dependence was found in closed form as the sensitivity $\tilde{S}_u = -1/U$ and as \tilde{S}_c , which is graphed in Figure 1. The second model, which incorporated diffusion, also resulted in the closed form solution $\tilde{S}_u = -1/U$. The sensitivity \tilde{S}_c , calculated numerically, appeared to qualitatively agree with the first model. The entrainment model also gave numerical solutions for \tilde{S}_u and \tilde{S}_c with \tilde{S}_c again qualitatively unchanged. However, the risk now appears to be proportional to U^α for some $\alpha \in (-4, -3)$ rather than $\alpha = -1$ as in the other models. Note that the sensitivity and the risk are related as: $\tilde{S}_u = \alpha/U$ is equivalent to $R(C_0, U) = K(C_0)U^\alpha$.

Since each model with its own key assumptions produces physically reasonable results, further work needs to be performed to study, modify, and develop these models to determine the most accurate process representative.

Future Research

Future work on this project could be directed towards the following:

1. combining the diffusion and entrainment models.
2. working with more complicated geometric valley shapes, such as triangular and semi-circular valleys. We could also vary the aspect ratio of our valleys.
3. modeling the explosion process in the valley and the effects of ignition location.
4. modeling continuous propane leaks.
5. checking our results against any data available.

These efforts would hopefully then lead to a clearer understanding of the relationship between risk and U and C_0 as measured by the calculated sensitivities.