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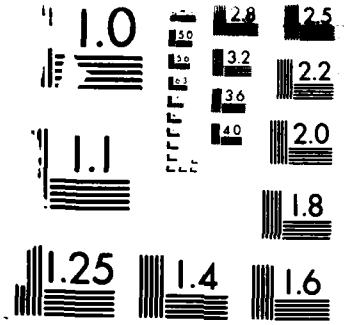
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DEVELOPMENT OF A MONTE CARLO SHUTTLE CONTAMINATION MODEL.

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Spectral Sciences, Inc.
111 South Bedford Street
Burlington, MA 01803

30 September 1986

Scientific Report No. 1

AIR FORCE GEOPHYSICS LABORATORY
AIR FORCE SYSTEMS COMMAND
UNITED STATES AIR FORCE
HANSCOM AFB, MASSACHUSETTS 01731

UNCLASSIFIED
SECURITY CLASSIFICATION OF THIS PAGE

AD-A175 409

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED	1b. RESTRICTIVE MARKINGS NONE
2a. SECURITY CLASSIFICATION AUTHORITY UNCLASSIFIED	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S) SSI-TR-113	5. MONITORING ORGANIZATION REPORT NUMBER(S) AFGL-TR-86-0204
6a. NAME OF PERFORMING ORGANIZATION Spectral Sciences, Inc.	6b. OFFICE SYMBOL (If applicable) 7U272
7a. NAME OF MONITORING ORGANIZATION Air Force Geophysics Laboratory	
6c. ADDRESS (City, State, and ZIP Code) 111 South Bedford Street Burlington, MA 01803	7b. ADDRESS (City, State, and ZIP Code) Hanscom Air Force Base Bedford, MA 01731
8a. NAME OF FUNDING/SPONSORING ORGANIZATION Air Force Geophysics Laboratory	8b. OFFICE SYMBOL (If applicable) AFGL/PHK
9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER F19628-85-C-0195	
8c. ADDRESS (City, State, and ZIP Code) Air Force Geophysics Laboratory Hanscom Air Force Base Bedford, MA 01731 Contract Monitor: Shu T. Lai/PHK	10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO.
62101F	7661	11	AH

11. TITLE (Include Security Classification)
Development of a Monte Carlo Shuttle Contamination Model

12. PERSONAL AUTHOR(S)
James B. Elgin and Robert L. Sundberg

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Scientific No. 1	FROM 9/85 TO 9/86	86 September 30	20

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	space shuttle, Monte Carlo, contamination

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Progress is described in the development of the SOCRATES model of space shuttle orbiter contamination. Monte Carlo techniques are reviewed, and adaptations required from previous plume descriptions are discussed. Representation of the shuttle in terms of simple surfaces and molecular intersections with these surfaces are presented.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION	
☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS	UNCLASSIFIED	
22a. NAME OF RESPONSIBLE INDIVIDUAL Shu T. Lai	22b. TELEPHONE (Include Area Code) (617) 377-2933	22c. OFFICE SYMBOL AFGL/PHK

DD FORM 1473, 84 MAR 83 APR edition may be used until exhausted. All other editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE
UNCLASSIFIED

CONTENTS

ILLUSTRATIONS

1. INTRODUCTION

This is the first yearly scientific report on a three year effort to develop a Monte Carlo model of contamination for the space shuttle orbiter. Contamination of instruments on the space shuttle orbiter is an issue of major concern. The shuttle gives off matter through surface outgassing, via various thrusters and from flash evaporators. At altitudes where the atmospheric mean free path is comparable to or less than shuttle dimensions, the deposition back onto shuttle-borne instruments will be largely determined by the multiple collision environment surrounding the shuttle. Even at higher altitudes, this may be the dominant source of contaminants for some portions of the shuttle. In addition to physical contamination of shuttle surfaces, "radiation contamination" is also a potential problem as gases surrounding the shuttle collide at high speed with atmospheric molecules. These energetic collisions can lead to vibrational excitation and subsequent radiative decay. A similar issue of some concern is the presence of ions in the vicinity of the shuttle which can (possibly) be produced via the critical ionization velocity effect. Ions in the shuttle environment may remain there for some time due to electric field forces, and radiative recombination is another potential source of radiation contamination. The situation is depicted schematically in Figure 1.

Spectral Sciences, Inc., (SSI) is developing a three dimensional Monte Carlo model of the flow field about the shuttle so that the contamination can be accurately characterized and understood. A comprehensive model of the contaminant field surrounding the space shuttle orbiter is crucial to the design of experiments which are to fly on the shuttle and to the development of procedures for minimizing the contamination.

SSI is adapting an existing three dimensional plume code (CHIMERA) to the space shuttle problem. The code is designed in a highly modularized fashion, so that additional physical and geometric complexity can be added as deemed necessary without requiring major rewriting of the model. The existing code already treats complex chemical and photochemical reactions for a neutral gas composed of molecules with energy dependent collision cross sections. The model allows for internal degrees of freedom for the molecules which can exchange energy with the translational mode. It has been named the SOCRATES code, which is an acronym for Shuttle Orbiter Contamination Representation Accounting for Transiently Emitted Species.

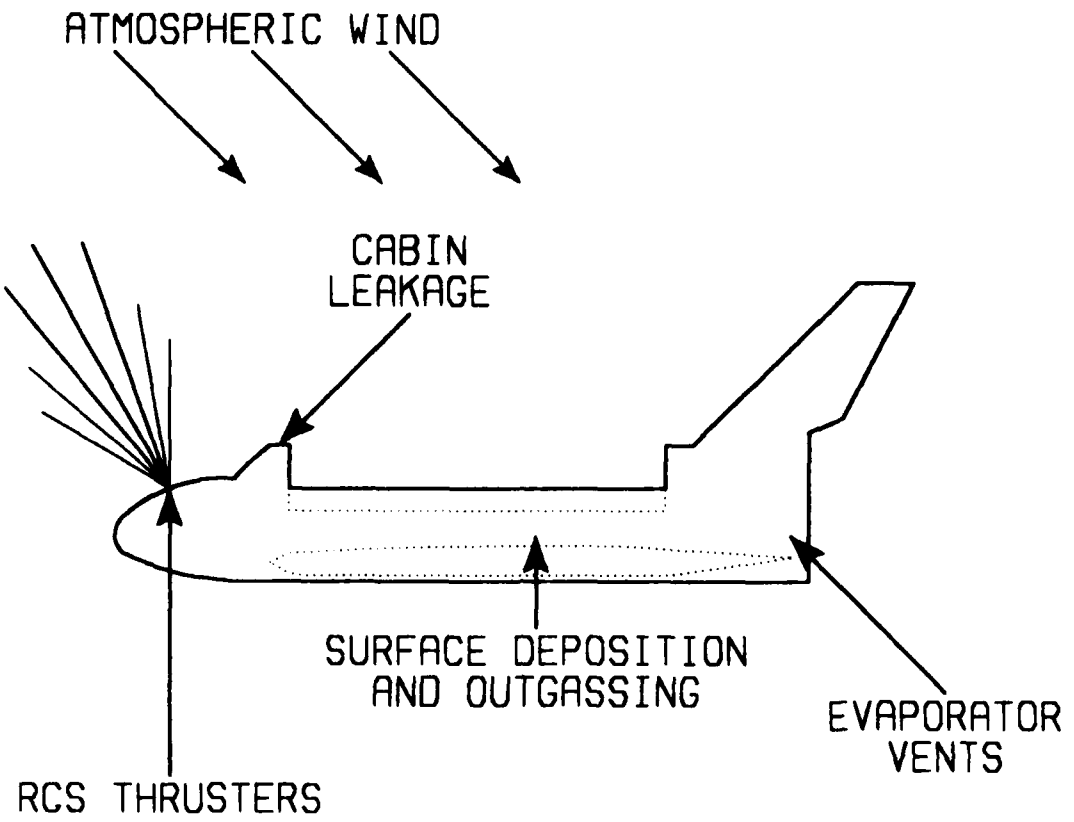

Figure 1. A Schematic Representation of the Major Elements of the Shuttle Contamination Problem.

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2. MONTE CARLO REVIEW

A complete description of the Monte Carlo procedure is beyond the scope of the present report, and can be found in References 1-3. However, it is instructive to briefly review how a typical Monte Carlo simulation proceeds. The method involves storing a discrete number of molecules (via

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1. Bird, G. A., Molecular Gas Dynamics, Clarendon Press, Oxford, 1976.

their velocities, positions and other pertinent information) in a computer. The solution region is broken up into a number of separate cells, and the solution is stepped forward in time in a two stage process. First, the molecules are advanced along their trajectories by an amount appropriate to their velocity and a time increment Δt_m. In this first stage some molecules will leave the solution region and some will be introduced as determined by the boundary conditions for a particular problem. The second stage is to simulate collisions in each cell appropriate to Δt_m so that collision frequencies are properly simulated. A basic hypothesis of the method is that if the time step is made small enough the processes of translations and collisions can be uncoupled in this manner.

Periodically, the solution is sampled to accumulate statistical sums of number densities, velocities and other basic properties. The solution is run repeatedly until statistical deviations are reduced to a desired limit, and then physically meaningful output quantities are computed from the statistical sums. The number of molecules represented is typically a few thousand at a time, which is vastly fewer than the number occurring in virtually all real flows. Hence, the construction of a dynamically similar flow to be simulated in the computer is an essential feature of the method. This is accomplished by artificially increasing the cross section of the molecules by the same factor that the number density is decreased, so that the mean free path between collisions is the same for the simulated flow as in the real flow. The logical flow of the solution procedure is shown in Figure 2, which includes the steps described above.

2.1 Collision Sampling Procedure

A basic hypothesis of the technique is that the solution cells should be small enough so that properties can be assumed constant within the cell. This assumption is necessary since the only spatial requirement placed on molecules which are selected for collisions is that they be within the same cell - they need not be within a molecular diameter of each other. The justification for this assumption is that molecules in a cell are considered representative of molecules which might equally well appear anywhere within the cell, due to the constancy of properties within the

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2. Elgin, J. B., "Getting the Good Bounce: Techniques for efficient Monte Carlo Analysis of Complex Reacting Flows", Report SSI-TR-28, Spectral Sciences, Inc., Burlington MA, 1983.

3. Elgin, J. B., "The CHARM Monte Carlo Transition Flow Modules", Report SSI-TR-103, Spectral Sciences, Inc., Burlington MA, 1986.

cell. The benefit of this assumption is substantial, since it means that all pairs of molecules do not have to be separately investigated; rather potential collision partners can be selected at random. The collision sampling procedure (which is described in detail in Reference 3) can be outlined via the following steps:

1) Two molecules are selected at random from the cell.

2) The product of their collision cross section times their relative velocity is computed.

3) The pair is accepted as a collision pair with a probability which is proportional to this product. If the pair is not accepted, the process is continued until some pair is accepted.

4) When a pair is accepted for a collision, then their velocities are altered appropriately to reflect the collision, and a "collision time counter" is incremented. Collisions are simulated in the cell until the collision time counter advances to the overall flow time.

2.2 Collision Sampling Concerns

It would be quite difficult to construct a cell structure which conformed to the shuttle surface. For the most part, the shuttle surfaces can protrude into the solution cells without adversely affecting the solution procedure. There are some difficulties, however, which arise during the collision sampling if a solution cell has part of the shuttle inside of it. These are enumerated below.

1) The assumption that position within the cell doesn't matter is no longer valid. This can be seen by considering the extreme case where a wing has portions of the cell above and below it. The flow field can be quite different on the two sides of the wing, and molecules from the two sides should not be allowed to collide with each other.

2) The time counter increment, which produces the proper collision frequency, is based on the mean density of molecules in the cell which, in turn, is based on the cell volume. If part of the cell is taken up by the shuttle, that portion should not count as available cell volume.

Ways around these concerns do exist. One approach under consideration is to simply not simulate collisions in these cells; and another approach is to consider only first collisions. The first collisions could be accurately treated during the molecular advancement portion of the

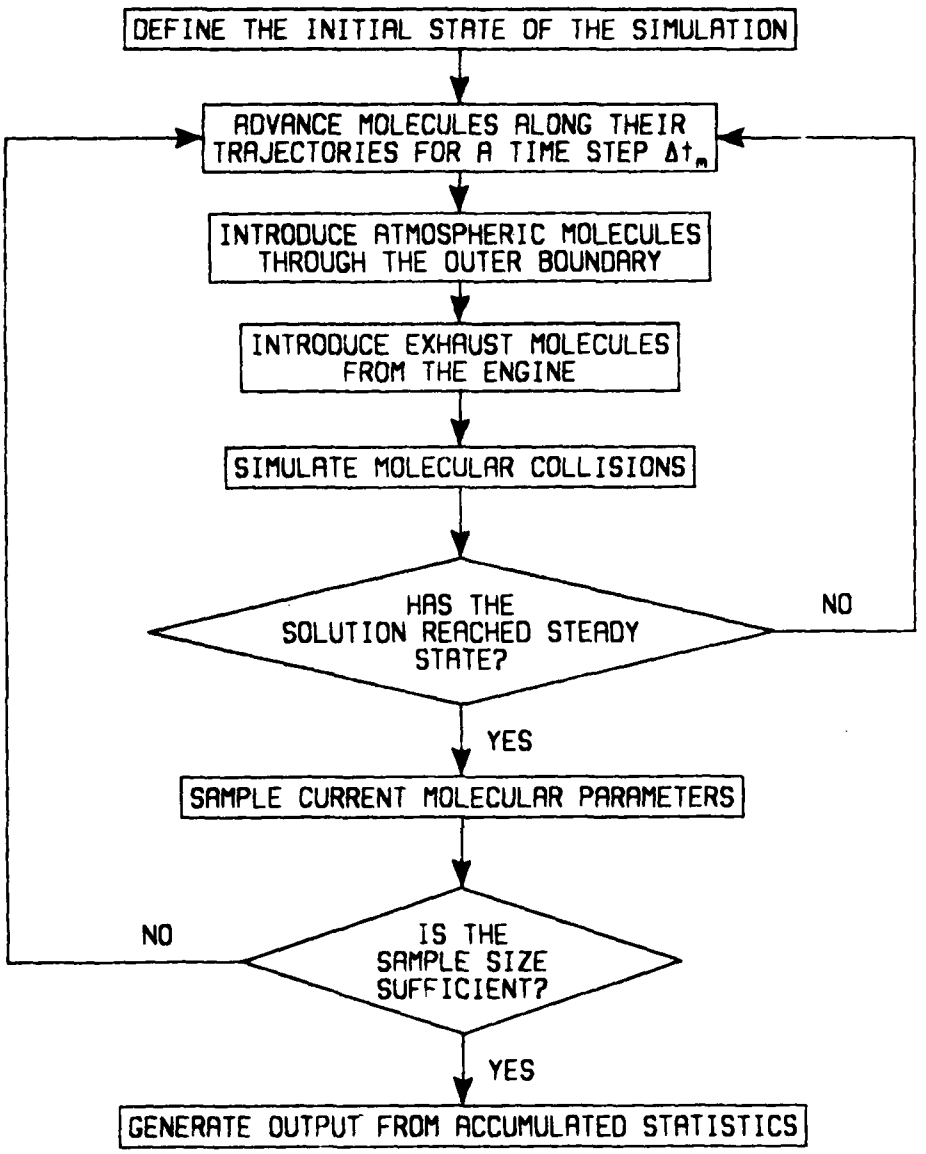

Figure 2. A Diagram of the Basic Solution Procedure Utilized in the Direct Simulation Monte Carlo Method.

simulation by calculating the probability that a molecule will suffer a collision during its advancement, and simulating the change in direction if it occurs. Since the mean free path will be much larger than the cell size, there is physical justification for such approaches.

3. REQUIRED CODE MODIFICATIONS

The model to be developed is envisioned as a research tool, which will undoubtedly have many features added to it over time. A minimal set of working features must exist, however, before the tool can be used at all. In order to develop a usable model for shuttle contamination from the CHIMERA plume code, a number of technical milestones must be achieved. Most of the required new features have to do with gas-surface interactions, since there are no solid surfaces in the plume code and surfaces are an essential feature of a contamination model. Only after the working model is constructed can work proceed on the investigation of important physical issues such as critical ionization velocity. A minimum set of steps to achieve a usable contamination model is described below:

1) The shuttle must be represented in terms of mathematically tractable surface elements. These surface elements should be pieces of common shapes (rectangles, triangles, cones, cylinders, etc.).

2) The routines which advance molecules along their trajectories in the Monte Carlo simulation must be modified to recognize when and where intersection with a surface element takes place.

3) A gas-surface interaction model must be developed to define what occurs when the intersection takes place. This model will probably be a combination of sticking and diffuse reflection. (Specular reflection could be treated easily, but it is an infrequently realized ideal.)

4) Collision sampling in cells which include shuttle components must be modified. This point is discussed at more length in Section 2.2.

5) The plume code cell geometry, which utilizes a symmetry plane which exists for the plume problem but not for the shuttle problem, must be modified.

6) Various sources of contaminants must be modeled.

7) A procedure for representing, and accumulating statistics on, position dependent surface quantities must be developed.

8) The diverse length scales of a shuttle and its plumes operating at typical altitudes must be addressed.

4. CODE MODIFICATIONS COMPLETED

Many of the required code modifications listed in the previous section have been addressed in the first year of the contract. The modifications which have been implemented are enumerated in the following subsections.

4.1 Shuttle Representation

A preliminary version of the shuttle has been constructed. This model was intentionally simplified since it makes no sense to deal in precise geometric detail before the code is checked out. The initial model for the shuttle geometry was designed to form a completely closed (i.e., no "holes"), non-overlapping surface which approximates the shuttle geometry with a minimum number of surface elements. The surface elements are simple geometric shapes such as rectangles, triangles, disks, cylinders and cones. This first model employs four surface types with a total of eleven surface elements. In particular, the wings are represented by triangular planes which currently have no thickness, but necessarily have a top and bottom. The tail is modeled using a combination of four triangular planes, the shuttle body as the outer surface of a cylinder, the shuttle nose as a cone, and the aft end of the shuttle as a disk. The model is specified in cartesian coordinates with the origin placed along the axis of the cylinder at the end of the tail section. This preliminary model is shown in front, top and side views in Figures 3-5, respectively.

4.2 Determination of Surface Intersections

The interaction of species with the shuttle is a crucial portion of the contamination model, and it has two distinct facets:

1) Calculating the point in space and time at which a contaminant molecule makes contact with a shuttle surface.

2) Characterizing what happens to the molecule after contact (e.g., adsorption, specular reflection, diffuse reflection, etc.).

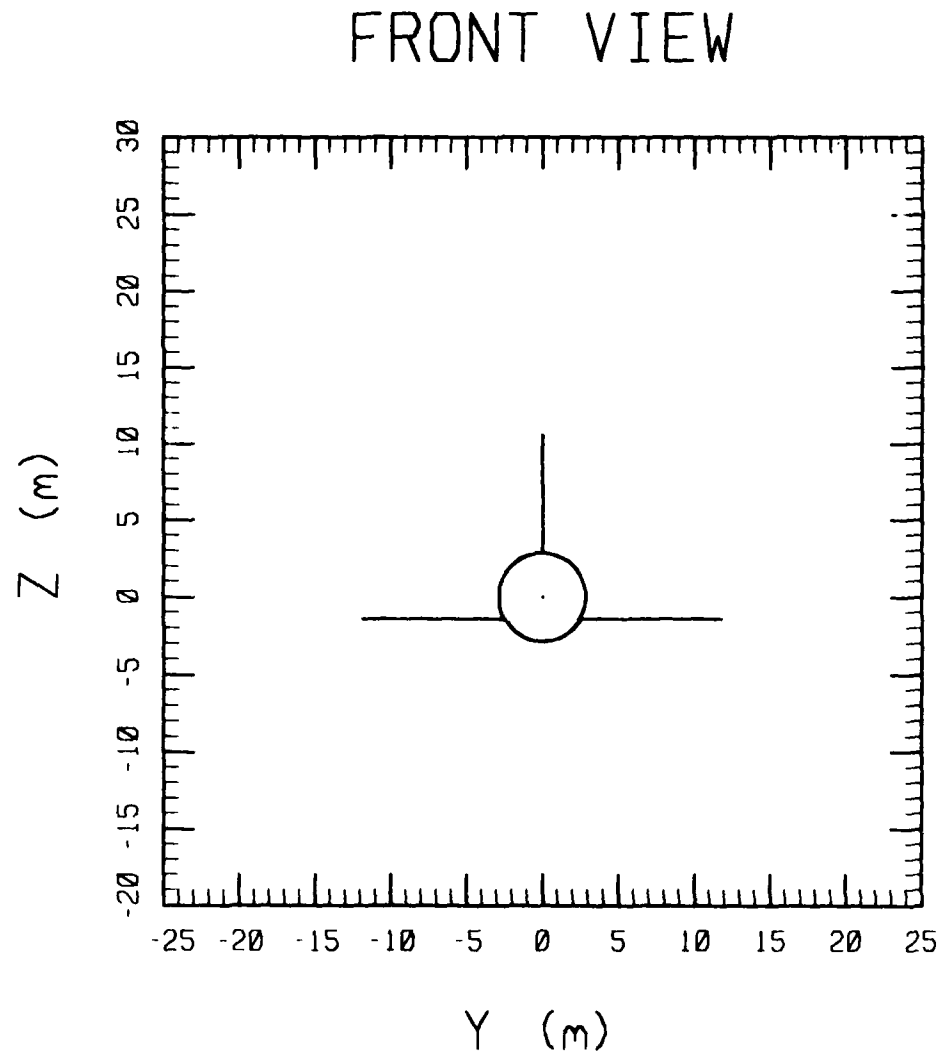

Figure 3. A Frontal View of the Crude Shuttle Model.

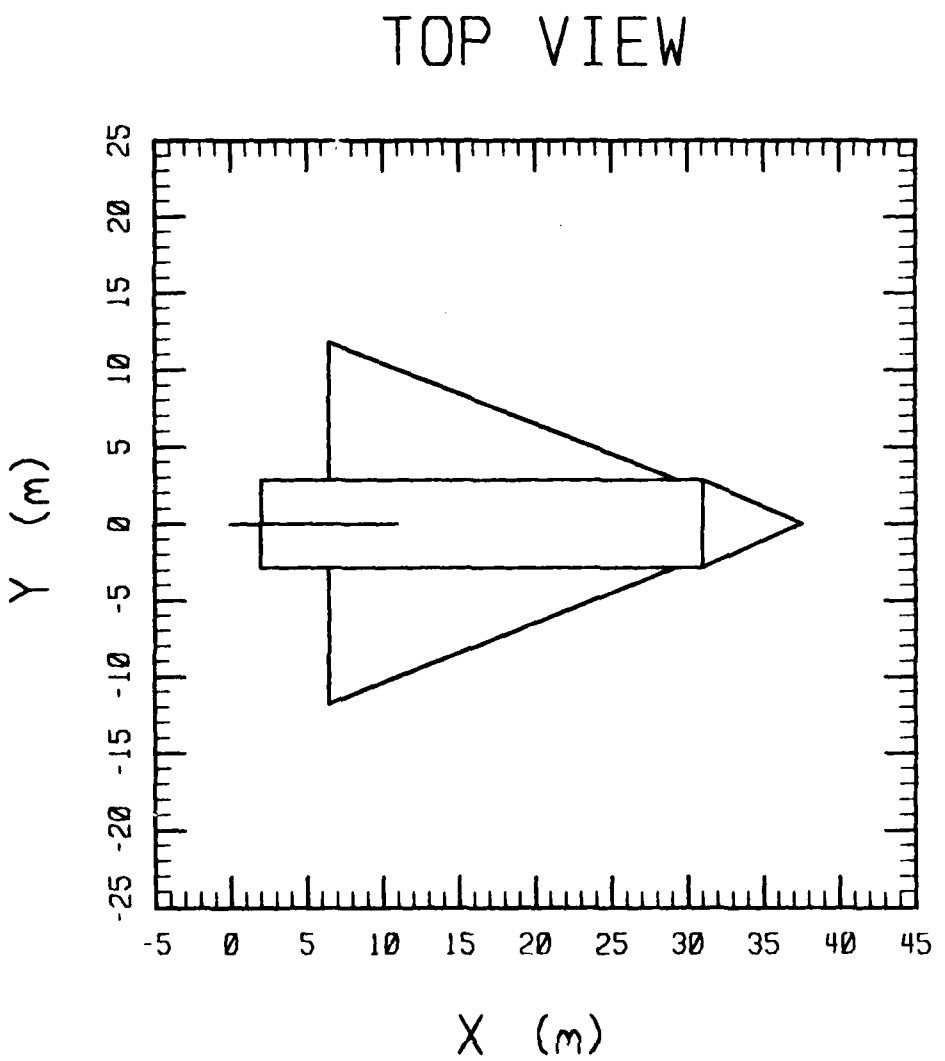

Figure 4. A Top View of the Crude Shuttle Model.

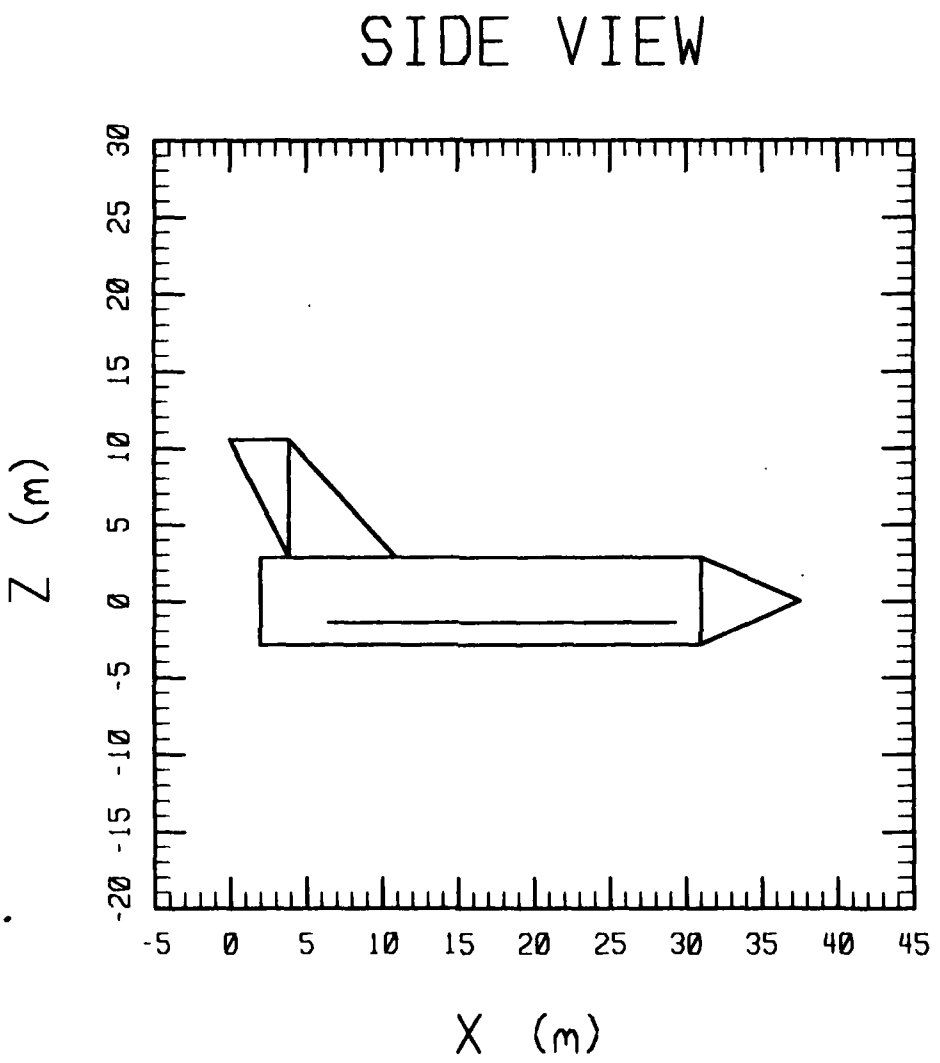

Figure 5. A Side View of the Crude Shuttle Model.

This subsection deals with the development of an algorithm for the first point above. The calculation of an intersection point, while conceptually straightforward, is a potential source of considerable computational effort. Routines have been written to calculate the intersection point in space and time for a molecule starting from an arbitrary position and velocity for each of the simple geometric shapes to be used in the shuttle description. These routines also return the local triple of unit vectors at the intersection point which is useful for the calculation of surface reflections. The procedure will be illustrated for the case of a rectangular surface element. The surface, as shown schematically in Figure 6, is defined by the following quantities:

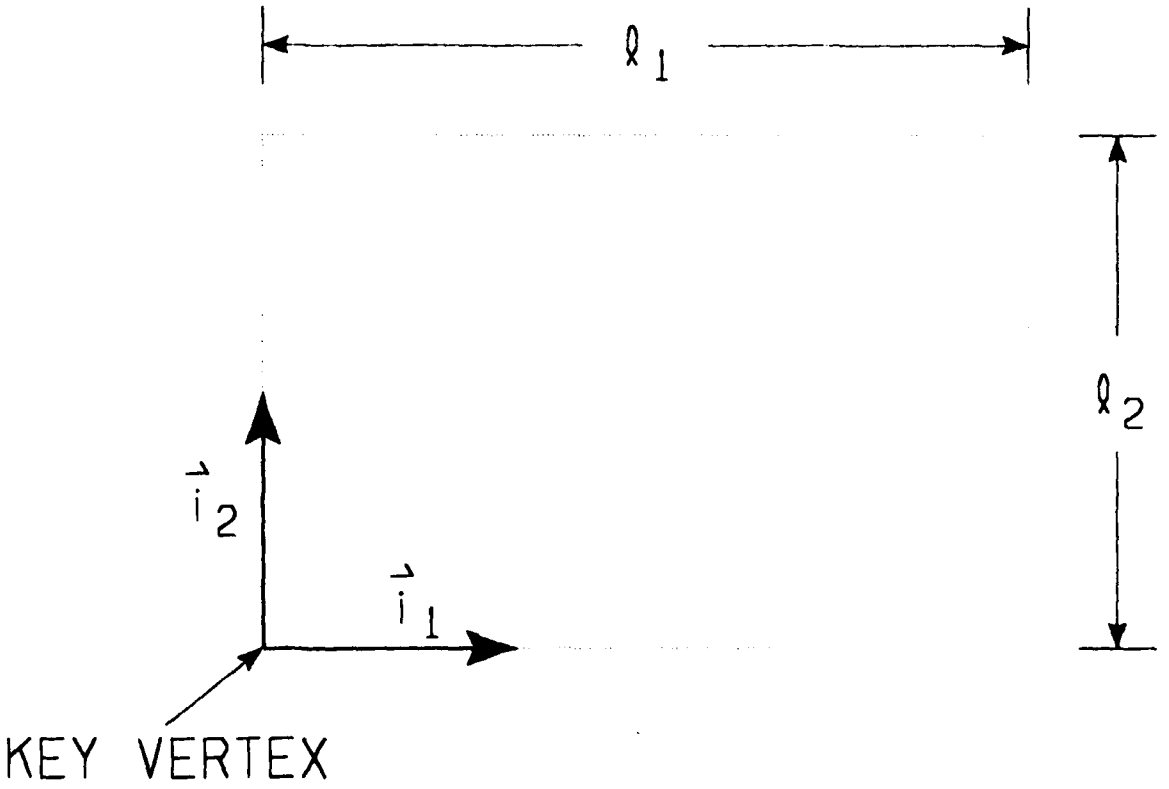

Figure 6. An Illustration of the Quantities Used to Calculate Intersection with a Rectangle.

a) A vector, $\vec{r}_s$, giving the absolute location of the "key vertex" of the rectangle in code coordinates.

b) An orthonormal triple of unit vectors which define the orientation of the surface. $\vec{i}_1$ and $\vec{i}_2$ define the directions from the key vertex to the two adjacent vertices of the rectangle and $\vec{i}_3$ is the outward surface normal. A right handed coordinate system is used, so

$$\vec{i}_3 = \vec{i}_1 \times \vec{i}_2 \quad . \tag{1}$$

c) The lengths, ℓ_1 and ℓ_2, of the two sides. (See Fig. 6.)

If a molecule has a position $\vec{r}_m$ and a velocity $\vec{v}_m$, then the analysis for intersection proceeds as follows:

1) The component in the $\vec{i}_3$ direction of the molecule's position and velocity relative to the key vertex, x_3 and v_3, are computed via

$$x_3 = \vec{i}_3 \cdot (\vec{r}_m - \vec{r}_s) \tag{2}$$

and

$$v_3 = \vec{i}_3 \cdot \vec{v}_m \quad . \tag{3}$$

2) In order for an intersection to take place on the proper side of the rectangle, x_3 must be positive and v_3 must be negative. If these criteria are not met, no further analysis is performed.

3) If the above criteria are met, the intersection with the plane of the rectangle takes place at a time, t, given by

$$t = - \frac{x_3}{v_3} \quad . \tag{4}$$

4) The position of the intersection point, x_{1i} and x_{2i}, relative to the key vertex is then given by

$$x_{1i} = \vec{i}_1 \cdot (\vec{r}_m + t\vec{v}_m - \vec{r}_s) \tag{5}$$

and

$$x_{2i} = \vec{i}_2 \cdot (\vec{r}_m + t\vec{v}_m - \vec{r}_s) \quad . \tag{6}$$

5) An intersection with the rectangle occurs if and only if ($0 \leq x_{1i} \leq \ell_1$) and ($0 \leq x_{2i} \leq \ell_2$).

The procedure for the other surface types is not given here, but it is quite similar. Each surface is defined by a location vector, a triple of orientation vectors, and a few pieces of auxiliary information. The use of simple geometric shapes allows the checks for intersection for all of the surfaces to be made expeditiously.

There will be thousands of molecules in a simulation, and each one of these molecules is advanced along its trajectory at every solution time step. Some check for intersection must be made for each molecule, at every time step. The shuttle is modeled as a combination of several simple surfaces. Although the initial model does not involve a large number of surfaces, it is an obvious growth path for the contamination model to use a more and more sophisticated model of the shuttle itself. (Previous models[4] have used hundreds of distinct surfaces to describe the shuttle.) It is not necessarily valid to stop checking for intersections when one is found, since it is the first intersection point that is the real one. Hence, it is desirable to have an algorithm which does not suffer greatly from a large number of surfaces.

A concept to speed up the calculation of surface intersections has been implemented. An element was added to the "state vector" to indicate the time at which a given molecule will experience a surface collision if its trajectory is not altered. (The state vector is simply the entire list of information which the code has about each simulated molecule.) The element is used as follows:

1) Whenever a molecule is introduced into the simulation, this element is set to zero. This serves as a flag indicating that a possible surface intersection has not yet been calculated for this molecule.

2) During collision sampling, whenever a molecule has its trajectory changed, the state vector element for surface intersection is reset to zero. This flags the molecule to have its possible surface intersection recomputed when it is advanced along its trajectory.

3) The routines which advance a molecule along its trajectory examine this element. If it is zero, then all surfaces are checked for possible intersection. If an intersection is found, then the time at which the intersection will take place is put in the state vector element. If it is determined that the current trajectory will not intersect any surfaces, then the value of 10^{20} (a computer approximation for infinity) is put in the element.

4) If it is known that a molecule will not intersect a surface within the time interval corresponding to the molecular advancement, then the molecule is simply moved along its trajectory without further checking of surfaces. This will be the case for the large majority of molecules which are inspected.

5) If a molecule does intersect a surface within the current time interval, then it is advanced to the point of intersection. The state vector corresponding to the post-reflection conditions are calculated and the element corresponding to surface collision time is reset to zero. The molecule is then advanced along its new trajectory for the remainder of the time interval, allowing for any new reflections which may occur.

Another concept that has been developed for speeding up the calculation of surface intersections is to surround many surface elements with an artificial surface such as a sphere. If a molecule starts on the outside of the sphere and doesn't penetrate it, then it cannot hit any of the surface elements within the sphere. In this manner, the calculation of intersection for many surface elements can frequently be replaced by the calculation of one intersection. (If the sphere is penetrated, of course, then the detailed calculations must then be carried out. The expectation is, however, that a large fraction of molecules will not need the detailed analysis.) This concept will be implemented if computationally required.

4.3 Surface Reflections

Routines were written to describe a diffuse reflection of a molecule from a surface after complete accommodation. This is felt to be the most reasonable physical model, so it is the natural initial choice. Other options will be added as the model is expanded.

4.4 Grid Structure Changes

The cell geometry for the CHIMERA plume code was based on cylindrical polar coordinates so it could naturally yield the axisymmetric limit for a plume aligned with the free stream. Additionally, it utilized the symmetry plane that exists when an initially axisymmetric plume interacts with a uniform atmosphere. This enabled half of the overall solution to be inferred from the other half.

The symmetry plane does not exist for the shuttle problem and cannot be used. Similarly, there is no reason to utilize the cylindrical polar

coordinate system for the cell geometry since the axisymmetric limit does not exist. Hence, the grid structure was changed to a more convenient three dimensional Cartesian coordinate system. There are parameters for varying the number and spacings of the cells independently in all six directions from the origin, so cells will not be placed where they are not needed.

The alteration of the cell grid structure required the following changes to the code:

1) The initialization routines calculating cell volumes and boundary locations had to be modified.

2) The procedure to determine the cell in which a molecule resides from its position had to be altered.

3) The routines to introduce new atmospheric molecules across the outer solution boundary had to be changed to reflect the different geometry of the flux. (I.e., molecules were no longer coming across a curved outer boundary.)

4) The calculation of output quantities had to be modified to reflect the different positions at which the output was occurring.

These changed have all been made and verified.

5. FUTURE WORK

As is evident from Section 4, many of the required steps in the model development have been completed. Contaminant sources remain to be modeled and procedures have to be developed for simulating collisions in cells containing surface elements, and keeping surface statistics. At that point, preliminary calculations of surface contamination will be performed. More rigorous calculations will require a better representation of the shuttle geometry and the inclusion of ions into the simulation.

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1. Bird, G. A., Molecular Gas Dynamics, Clarendon Press, Oxford, 1976.

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