HYDROGEN VEHICLES AND
THE NEW MEXICO SUPERCOMPUTING CHALLENGE
THEIR ATMOSPHERIC EFFECT

Final Report
April 5, 2006

Oñate High School, Team #73

TEAM MEMBERS:
Brittany Atteberry
Mihyun Hong
Jane Kim
Erica Swenson
Natalie Wells

SPONSORS:
Josefina Domínguez
Donald Downs

CHALLENGE MENTOR:
Eleanor Walther

Table of Contents

Executive Summary

Realizing that alternate forms of energy will soon need to be utilized, our group decided to investigate the possible future of hydrogen technology in the automotive industry, which we now believe could play an important role in the future of the planet. Our problem is that, if hydrogen vehicles were to replace gasoline vehicles in Doña Ana County, would this emission of water vapor affect the local air in that county. We obtained information from the Doña Ana County Planning Division, as well as several maps of our county and Las Cruces and a number measuring the amount of water a hydrogen vehicle emits per kilometer. Utilizing information from our Las Cruces map (we began with simulating Las Cruces, and then expanded to Doña Ana County), we obtained information measuring the amount of vehicles that would pass through a section of the city every minute, and thus how much water vapor they would produce in doing so. We then implemented the diffusion equation (derived from the law of the conservation of mass) into our JAVA matrix program (composed of a JAMA matrix package and our own programming) to simulate the diffusion of this water vapor across the city, and eventually the county.

Problem Definition

In an effort to reduce the amounts of pollution being distributed into the local air of Las Cruces and Doña Ana County, New Mexico, hydrogen vehicles may become the future of the automotive world. However, we seek to simulate the possible effect that these vehicles, which emit only water vapor, may have on the condition of the air in our county, assuming that all existing vehicles were replaced by hydrogen technology.

Method

1. Research

To gain a fundamental understanding of the concept of hydrogen technology, we researched how hydrogen vehicles function. This included obtaining a number measuring the amount of water that a hydrogen vehicle produces.

After finding and emailing scientists from The United Nuclear Scientific Supplies in Sandia Park, NM, we learned that these vehicles produce a steady, constant output stream of water vapor, amounting to .15 kg of water/mile. This amount surprised us, for we had expected the output of water vapor from hydrogen vehicles to be greater than combustion engine emissions (it is in fact the same, minus harmful pollutants), which led us to take a more positive attitude towards the beneficial potential of these vehicles.

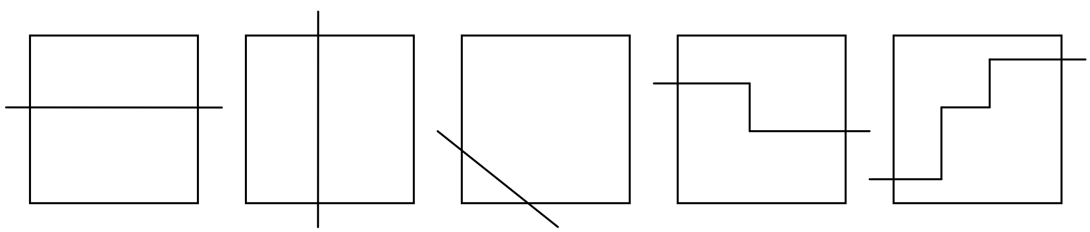
Furthermore, we made several calls to county offices in search of a map of Doña Ana County on which we could draw a grid and view major arteries. Fortunately, we obtained not only these maps, but a detailed map of Las Cruces listing AAWDT numbers (Annual Average Weekday Trips) for major roadways.

We divided this map into a grid with squares 1.27 km long on each side. After adding the AAWDT numbers for each roadway passing through each cell of our grid, we multiplied that number by .09321 (L/km; the amount of water vapor produced by 1 vehicle each kilometer it travels, converted from .15 kg/mile), multiplied this by 1.27 km (the distance the vehicle travels through), and finally divided by 24 (hours; AAWDT information covers 24 hours). Thus, for each cell, we obtained a number measuring the amount of water vapor produced in each cell per hour, which we further reduced to liters per minute.

In order to make our statements true, we must specify several assumptions that we have made:

1. Every vehicle included in the AAWDT information for 2002 - 2004 is replaced by a hydrogen vehicle.
2. Every vehicle that passes through a square on our grid of Las Cruces passes through the entire length (1.27 km) of the square.

   - There are obviously countless directions a vehicle could drive through a 1.27 km area, such as:



   - In order to greatly simplify our project, we decided to assume that every vehicle that passes through a cell travels 1.27 km in that square.

3. Every theoretical hydrogen vehicle in our study emits a constant stream of water vapor at a rate of .118377 L/km.
4. The AAWDT numbers we use for L/minute/section of grid are 24 hour averages, and do not adhere to daily traffic rushes and fluctuations.
5. We are disregarding evaporation from the Rio Grande and irrigation.

6. We are placing Dona Ana County into a virtual bubble, meaning that external areas will not affect or interact with our simulation.

2. Method

1. We computed a number (measuring water vapor produced per square per minute average) for every cell in our Las Cruces map.

2. We used the diffusion equation to discover how water vapor emitted from hydrogen cars will spread during a certain time period. The diffusion equation is derived from the continuity equation, which originates from the law of conservation of mass. In our model, water vapor mass is conserved.

$$\frac{du}{dt} = D\left(\frac{d^2 y}{dx^2} + \frac{d^2 y}{dy^2}\right)$$

du = diffusion constant ***dt*** = time

3. We set up a grid of Las Cruces, with divided sections which we will call cells:

	Δx	Δx
Δy	$u_{0,0}$	$u_{0,1}$
Δy	$u_{1,0}$	$u_{1,1}$

Δx = width
Δy = length
$u_{i,j}$ = water vapor concentration of cell i,j

4. To begin programming, we first learned to implement the diffusion equation into our Java Program:

2-Dimension Diffusion Equation:

$$\frac{du}{dt} = D\left(\frac{d^2y}{dx^2} + \frac{d^2y}{dy^2}\right)$$

D = some diffusion constant

5. In one dimension, we had to approximate the second derivative of u with respect to x in order to get an explicit equation:

$$\frac{u_i^{t+1} - u_i^{t}}{\Delta t} = D\left(\frac{u_{i+1}^{t} - 2u_i^{t} + u_{i-1}^{t}}{\Delta x^2}\right)$$

u = concentration of water vapor at any cell i
t = time

We then solve for the unknown u_i^t.

6. However, unless Δt is very small, the answer is unreliable, so we had to implement the 1-Dimensional Implicit Equation:

$$\frac{u_i^{t+1} - u_i^{t}}{\Delta t} = D\left(\frac{u_{i+1}^{t+1} - 2u_i^{t+1} + u_{i-1}^{t+1}}{\Delta x^2}\right)$$

Here, the only known concentration is $u_i^{\,t}$. We solve this for $u_i^{\,t}$.

$$u_i^{\,t+1}\left(1+\frac{2D\Delta t}{\Delta x^2}\right)-\frac{D\Delta t}{\Delta x^2}\left(u_{i+1}^{\quad t+1}\right)-\frac{D\Delta t}{\Delta x^2}\left(u_{i-1}^{\quad t+1}\right)=u_i^{\,t}$$

i = 0 to number of rows - 1

This is known as the fully implicit finite difference method.

7. To apply all of this information into a JAVA program, we placed the amount of water (in liters) into the matrix Las Cruces, and then added a computed amount of water vapor into it at each time step. After completing this, we ran this information through the diffusion equations for each cell in our Las Cruces grid.

Results

After running our program, we were able to see the actual results of our project. Water vapor was visibly diffused around traffic areas, with the highest concentration around the Las Cruces downtown area. Also visible was I-25 as well as I-10, the East and West Mesas, and Picacho Avenue. We doubled the number of vehicles which pass through our cells, and the concentration of water increased, however was not visibly apparent. We will continue to experiment with different variables and expand our project to Doña Ana County.

Conclusion

We have concluded that as the number of vehicles in Las Cruces and the entire world continuously becomes greater, if they ran on gasoline or hydrogen, there could be a significant alteration in the atmospheric conditions in our city as well as the world. Hydrogen offers the option of equal emissions minus harmful pollutants. However, if the water vapor emitted from each hydrogen vehicle was to be collected before it was released as exhaust, it could condense into liquid water and be utilized in various ways, including human consumption, for this water is clean enough to drink. Hydrogen technology, if given attention and focus on production and distribution, can offer a clean and earth-saving alternative to fossil fuels and oil dependency.

Program

```
import java.io.FileWriter;
import java.io.PrintWriter;
import java.io.IOException;
import java.io.FileReader;
import java.io.BufferedReader;
import java.util.StringTokenizer;
import java.lang.Double;

public class DriveMatrix
{
    public static void main ( String [] args ) throws IOException
    {
        final int NUMROWS = 15;
        final int NUMCOLS = 13;
           final int SIZE = NUMROWS * NUMCOLS;


        /* The matrices used in this program are constructed    *
         * and implemented using various methods from JAMA      *
         * shareware.  The matrix DonaAna consists of the      *
         * water vapor in liters in our grid squares.  U is the *
         * water vapor in the air, and waterVapor is a matrix   *
         * of water vapor being constantly emitted into any     *
         * given grid square.*/

           Matrix DonaAna = new Matrix( SIZE, SIZE );
        Matrix U = new Matrix( SIZE, 1 );
        Matrix waterVapor = new Matrix( SIZE, 1 );

        Double x;

        int i, j, l;
        int k = 0;


        /* deltaT represents the time step.  deltaY *
         * and deltaX are the lengths of the grid   *
         * squares on their respective axis.  D is  *
         * our diffusion constant. */
```

```
   final double deltaT = 60.0;
final double D = 0.000003;
final double deltaX = 1.27;
final double deltaY = 1.27;

double c1 = -D * deltaT / Math.pow( deltaX, 2 );
double c2 = ( 1.0 + 2 * ( 2D * ( deltaT )) / ( Math.pow( deltaX, 2 )));
   double c3 = (( deltaT * -D ) / ( Math.pow( deltaX, 2 )));

double d1 = (( -D * deltaT ) / ( Math.pow( deltaY, 2 )));
double d2 = c2;
double d3 = (( -D * deltaT) / ( Math.pow( deltaY, 2 )));


/* FileReader, BufferedReader, FileWriter, and PrintWriter*
 * are classes that allow us to easily access the numbers *
 * of liters of water vapor in the air easily from a .txt *
 * file instead of having to go through and declare each  *
 * position independently. */

FileReader reader = new FileReader ( "litersPerHour.txt" );
BufferedReader in = new BufferedReader( reader );
FileWriter writer = new FileWriter( "outputTest.txt" );
PrintWriter out = new PrintWriter( writer );

String inputLine;
StringTokenizer tokens;


   for( i = 0; i < SIZE; i++ )
{
    DonaAna.set( i, i, c2+DonaAna.get( i, i ));
       if( i > 0 )
    {
        DonaAna.set(i, i-1, c1+DonaAna.get( i, i-1 ));
    }
    if( i < SIZE-1 )
    {
        DonaAna.set( i, i+1, c3+DonaAna.get( i, i+1 ));
    }
}
```

```
for( j = 0; j < SIZE; j++ )
{
    if( j >= NUMCOLS )
    {
        DonaAna.set( j, j-NUMCOLS, d1+DonaAna.get(j, j-NUMCOLS ));
    }
    if( j < SIZE-NUMCOLS)
    {
        DonaAna.set( j, j+NUMCOLS, d3+DonaAna.get( j,j+NUMCOLS ));
    }
}


/* This for loop is the implementation of *
  the methods used to read .txt files. */

for( i = 0; i < NUMROWS; i++ )
{
    inputLine = in.readLine();
    tokens = new StringTokenizer( inputLine );
    while( tokens.hasMoreTokens() )
    {
        x = new Double( tokens.nextToken() );
        waterVapor.set( k, 0, x.doubleValue() / 60.0 );
        k++;
    }
}

/* Here the constant water vapor emitted at each *
 * timestep is put into the matrix U.*/

U = waterVapor;
Matrix DAinv = (new LUDecomposition( DonaAna )).solve
            ( Matrix.identity ( SIZE, SIZE ));
Matrix Unew = DAinv.times( U );


   for( i = 0; i < SIZE; ++i )
   {
           if( Unew.get( i, 0 ) < 0.0 )
           {
               Unew.set( i, 0, 0.0 );
```

```
            }
        }


        for( l = 0; l <= 1000; l++ )
        {
            U = Unew.plus( waterVapor );
            Unew = DAinv.times( U );
        }

        System.out.println();

        k = 0;

        for( i = 0; i < NUMROWS; ++i )
        {
            for( j = 0; j < NUMCOLS; ++j )
            {
                out.print( U.get( k, 0 ) + "  " );
                k++;
            }
            out.println();
        }
        writer.close();
    }
}
```

Charts and Graphs

This chart displays the number of vehicles that pass through each created cell of Las Cruces in 24 hours. Some of the AAWDT information is from 2002-2004 for lack of contemporary information in some areas.

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0	2367	2484	2190	4357	5669	0	0	0	0	0	2868	1798
1	0	3435	6924	9129	19522	11188	2922	0	0	0	0	27445	13525
2	0	1068	8003	2484	7894	3129	2355	0	0	0	25655	0	0
3	0	1455	1018	9311	4516	2363	11692	0	25655	25655	0	0	0
4	0	1455	0	9394	4984	7627	9477	47721	27968	0	0	0	0
5	0	1455	559	2887	7907	16058	12794	77511	22570	0	0	0	0
6	0	0	0	2260	20112	20681	36336	11091	31093	8557	10949	0	0
7	0	1836	0	3594	0	23008	27739	75216	61307	59292	14352	1203	0
8	1836	11451	17074	18081	26095	47494	219706	103956	80277	91829	9822	0	0
9	15527	8964	0	5605	42762	74453	67328	89674	82583	69527	38518	0	0
10	382	5605	5605	6365	5629	17533	38208	41370	72042	62514	29068	0	0
11	0	0	0	0	0	29166	6082	47146	43654	16389	11188	0	0
12	0	0	0	0	0	10180	1783	2779	28714	4173	15737	2158	0
13	0	0	0	0	0	707	461	1119	6141	0	8461	0	0
14	0	0	0	0	0	0	881	4524	595	0	0	8026	0

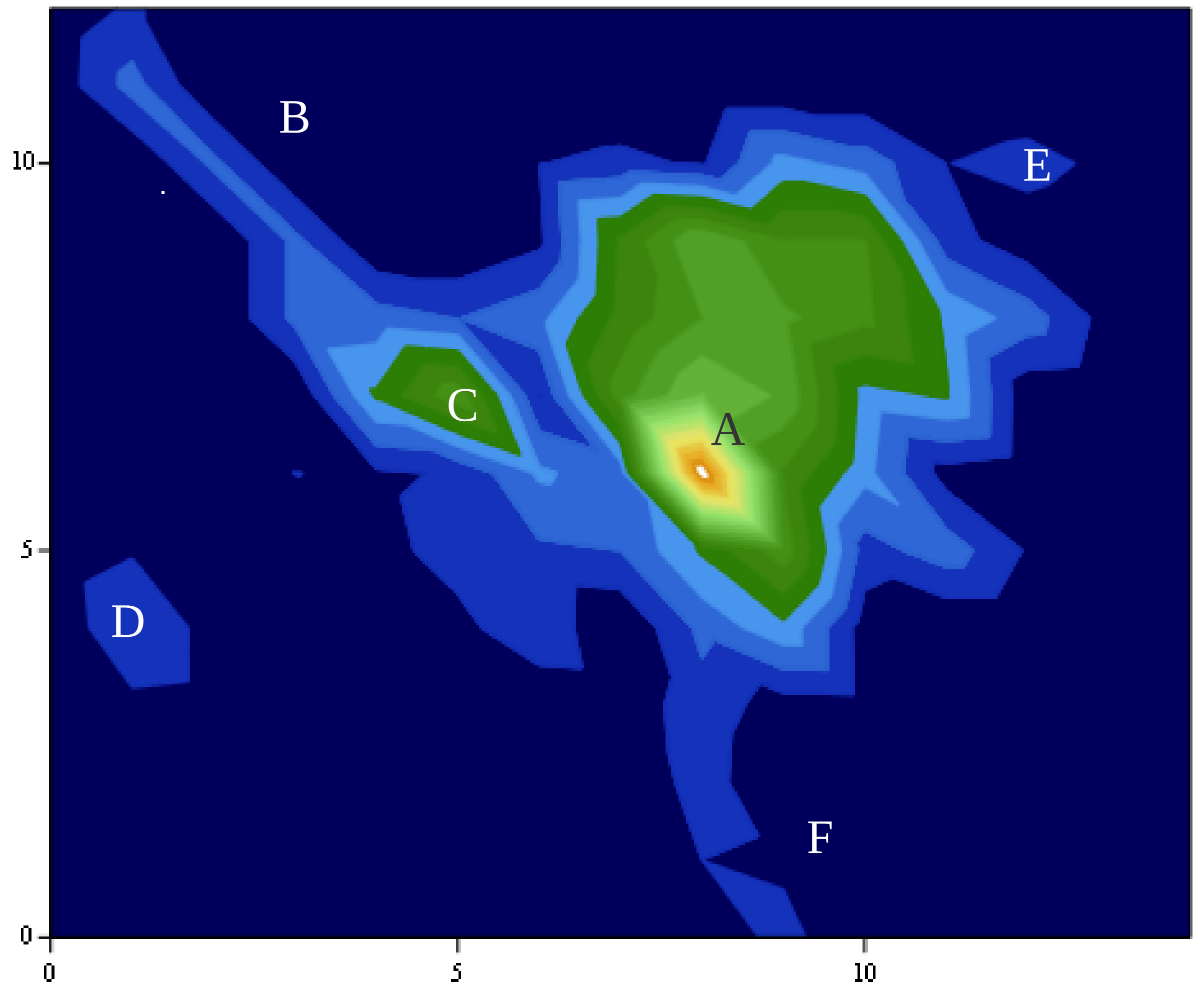
The numbered rows and columns correspond to the numbered grid on our map of Las Cruces.

This chart displays the emission of water vapor (in liters) over a 1-hour time period in Las Cruces:

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0	11.7	12.3	10.8	21.5	28.0	0	0	0	0	0	14.1	8.9
1	0	16.9	34.2	45.0	96.3	55.2	14.4	0	0	0	0	135.4	66.9
2	0	5.3	39.5	38.9	38.9	15.4	11.6	0	0	0	126.5	0	0
3	0	7.2	5.0	45.9	22.3	11.7	57.7	0	126	126	0	0	0
4	0	7.2	0	46.3	24.5	37.6	46.7	235	138	0	0	0	0
5	0	7.2	2.8	14.2	39.0	79.2	63.1	382	111	0	0	0	0
6	0	0	0	11.1	99.2	102.0	179.2	54.7	153	42.2	54.6	0	0
7	0	9.1	0	17.7	0	113.5	1361.8	371	302	293	70.8	5.9	0
8	9.05	56.5	84.2	89.2	128.7	234.3	1083.6	512	396	453	48.4	0	0
9	77	44.2	0	27.6	210.9	367.2	332.1	442	407	343	190.0	0	0
10	1.9	27.6	27.6	31.4	27.8	86.5	188.5	204	355	343	143.4	0	0
11	0	0	0	0	0	143.9	30.0	233	215	80.8	55.2	0	0
12	0	0	0	0	0	50.2	8.8	13.7	142	20.6	77.6	10.6	0
13	0	0	0	0	0	3.5	2.3	5.5	30.3	0	41.7	0	0
14	0	0	0	0	0	0	4.3	22.3	2.9	0	0	39.6	0

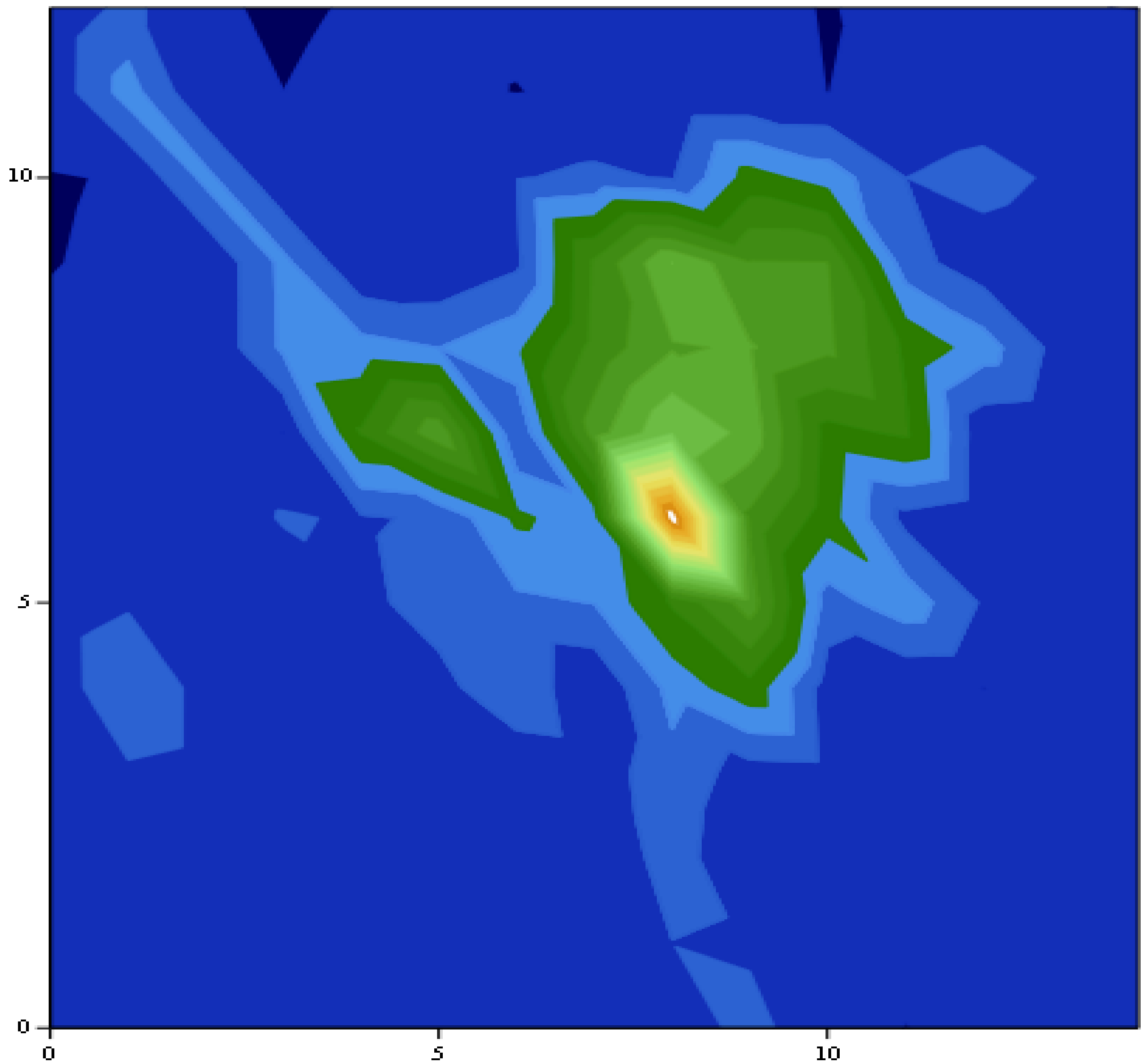
After entering this information into the matrix, we divided by 60 in the program, which gave us liters of water emitted per cell per minute.

This simulation models the above information, after being entered into the matrix and diffused through time. These results represent the diffusion of water vapor after 1000 minutes (16.667 hours) with a diffusion constant of .000003:



A
A= Las Cruces Downtown Area
B= Interstate 25
C= West Picacho
D= West Mesa
E= East Mesa
F= Interstate 10

This model represents the diffusion of water vapor after 10,000 minutes (166.667 hours) with a diffusion constant of 3:



A

From this model, we can see a larger spread of water vapor over Las Cruces, which could, attributed to wind, affect other locations.

Significant Achievement

We feel that having the ability to simulate the emission of water from vehicles, which may possibly be used in the future to conserve the welfare of the very planet, is indeed significant. Also, we find our ability to portray the growth of our own city and the consequential rise in vehicle emissions as a result equally noteworthy. The information that we learned from this project serves as a reminder of the large amount of emissions that our everyday vehicles send into our atmosphere (and thus the air that we breathe everyday), as well as the imminent need of a solution to reduce this harmful output. Furthermore, we have strategized that, if the important conversion to hydrogen technology is made, the problem of vehicle emissions could be altogether eliminated, for the output of water vapor could be collected in the vehicle itself, and this resulting liquid water could be disposed into the ground, or even used for clean drinking water. Initially skeptical of hydrogen technology, our project has led us to realize how real and beneficial their future could be.

Acknowledgments

We would like to thank:

- Frank Dodd at the Doña Ana Planning Division, who generously provided maps of Doña Ana County and Las Cruces.
- Donald Downs at Oñate High School, who guided and taught us throughout our entire project.

Also,

- Leslie Eudy at the National Renewable Laboratory in Colorado, who forwarded our questions to colleagues.
- James E. Francfort at the Idaho National Engineering and Environmental Laboratory, who led us to valuable and helpful websites.
- The United Nuclear Scientific Supplies in Sandia Park, NM, who shared information with us about their hydrogen vehicles.

Bibliography

- Sierra, Kathy; Bates, Bert. (2003,2005*). Head First Java 2nd Edition*. California: O'Reilly Media, Inc.
- The MathWorks and the National Institute of Standards and Technology. *JAMA: A Java Matrix Package.*
- "Fuel Cells," "The Hydrogen Future." Energy Efficiency and Renewable Energy. U.S. Department of Energy. 8 Mar 2006. <http://www.eere.energy.gov/>.
- "Why Fuel Cells?" Fuel Cell Shop. Collins Technologies, Inc. <http://www.dcht.com/why/why-fuel-cells.html>.
- "Hydrogen Use and Safety," "Hydrogen Fuel Cells." California Hydrogen Highway. <http://www.hydrogenhighway.ca.gov/>.
- Frank Dodd, a mapper at the Doña Ana Planning Division. (505) 647-7200.