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TITLE: # Development of the Transims Environmental Module

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DEVELOPMENT OF THE TRANSIMS ENVIRONMENTAL MODULE

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1.0 Overview

The TRansportation ANalysis and SIMulation System (TRANSIMS) is one part of the multi-track Travel Model Improvement Program sponsored by the U. S. Department of Transportation, the Environmental Protection Agency, and Department of Energy. Los Alamos National Laboratory is leading this major effort to develop a new, integrated transportation and air quality forecasting procedures necessary to satisfy the Intermodal Surface Transportation Efficiency Act and the Clean Air Act and its amendments.

TRANSIMS is a set of integrated analytical and simulation models and supporting data bases. The TRANSIMS methods deal with individual behavioral units and proceed through several steps to estimate travel. TRANSIMS predicts trips for individual households, residents and vehicles rather than for zonal aggregations of households. TRANSIMS also predicts the movement of individual freight loads. A regional microsimulation executes the generated trips on the transportation network, modeling the individual vehicle interactions and predicting the transportation system performance.

The purpose of the environmental module is to translate traveler behavior into consequent air quality, energy consumption, and carbon dioxide emissions. Transportation systems play a significant role in urban air quality, energy consumption, and carbon-dioxide emissions. Recently, it has been found that current systems for estimating emissions of pollutants from transportation devices lead to significant inaccuracies (Oliver et al, 1993). When these inaccuracies are coupled to air quality models and limited meteorological data, it is difficult to tell whether the most appropriate path is being taken to achieve air quality goals. Most of the existing emission modules use very aggregate representations of traveler behavior and attempt to estimate emissions on typical driving cycles. However, recent data suggests that typical driving cycles produce relatively low emissions, while most emissions come from off-cycle driving, cold-starts, and evaporative emissions. Furthermore, some portions of the off-cycle driving such as climbing steep grades are apt to be correlated with major meteorological features such as downslope winds. These linkages are important, but they are not systematically treated in the current modeling systems.

Among the important problems to which transportation activities contribute are: (1) excessive ozone concentrations in urban areas, (2) excessive concentrations of carbon-monoxide in urban areas, (3) excessive levels of respirable particulate matter in urban areas, (4) global build-up of greenhouse gases, (5) regional visibility degradation and (6) deposition of nitrates onto metals and into bodies of water. Three of these areas are major subjects of regulatory action: (1) excessive ozone concentrations, (2) excessive respirable particulate matter concentrations and (3) excessive carbon-monoxide concentrations. At present there are well-defined rules specifying how emissions and air quality are to be modeled for these

pollutants and the materials that create these pollutants through chemical reactions in the atmosphere. It's likely that the respirable particulate matter rules and regulations will be changed in the near future and possibly be replaced by new standards dealing with fine particulate matter.

There are four major tasks required to translate traveler behavior into environmental consequences: (1) estimate the emissions, (2) describe the atmospheric conditions into which the contaminants are emitted, (3) describe the local transport and dispersion, and (4) describe the chemical reactions that occur during transport and dispersion of the contaminants. For some environmental problems, fewer tasks are relevant. For carbon dioxide we only need to consider the first step; the estimation of emissions. The environmental relevance of carbon-dioxide lies in its role as a green house gas and the global behavior is the area of concern not its urban-scale behavior. Carbon-monoxide, on the other hand, is primarily of concern for its local consequences. The highest concentrations of carbon-monoxide are usually found very near to local sources and the most important local sources are mobile sources. In the case of carbon-monoxide, chemical reactions are of secondary concern while the transport and dispersion within street canyons is important.

The air quality community has developed a number of tools to address these problems. Emissions have typically been estimated by assuming that people use driving patterns similar to those over which the emissions of vehicles have been tested. The basic premise is that the emissions are dominated by average behavior. With these formulations, estimates of vehicle miles traveled and average speeds can be used to estimate emissions. This basic formulation has been supplemented by corrections for cold starts, evaporation from fuel tanks, and non-conforming vehicles. However, recently it has become clear that deviations from the standard driving cycles can produce dramatically increased emissions so that total emissions may be dominated by atypical behavior.

There are two basic ways of describing atmospheric conditions: (1) simple models can be used to distribute measurements over the area of interest, or (2) models that attempt to solve the basic equations of motion for the atmosphere can be use. The former, called diagnostic models, use the measurements to provide the basic physics of the atmosphere and thus are limited by the representativeness of the measurements. The second approach involves the use of models, called prognostic models, with a relatively complete description of the physics and less extensive measurements. Prognostic models use measurements to describe important features produced by atmospheric conditions originating beyond the boundaries of the model domain. In many cases prognostic models are used with measurements to help keep them on track.

There are several ways to describe the dispersion and transport of pollutants: (1) simple Gaussian plume models, (2) Gaussian puff models, (3) random particle models, and (4) Eulerian grid models. The Gaussian plume models normally use a single wind direction and assume that plume spreads in a Gaussian manner and extends indefinitely in the downwind direction. This type of model ignores the change of wind speed with height and changes in wind direction or speed along the path. The Gaussian puff model is slightly more sophisticated in that puffs of the contaminants follow the local average wind so that the model does consider changes in the average wind which occur

along the path traveled by the pollutants. Gaussian puff models do not consider the effects of wind changes with height. In random particle models, the models simulate the motion of contaminants transported with an instantaneous wind that is composed of the mean wind plus a randomly selected turbulent wind. Concentrations can be obtained by either defining small volumes and counting the simulated particles (particle in cell method) or by considering that each particle represents the center of a distribution (Monte Carlo kernel method) whose characteristics are defined by the turbulence history of the particle. Monte Carlo kernel methods are computationally efficient and representative of the key physics of atmospheric transport. Eulerian methods involve defining a three dimensional grid and calculating the exchange of materials between cells through turbulent mixing or through drifting with the mean wind. In the Eulerian system the concentrations are considered constant over a cell and a narrow plume may be artificially spread as its material is averaged over a cell volume. Eulerian systems are very good for dealing with situations where the chemistry is important and where pollutants are well mixed over volumes larger than the grid cells.

There are principally three ways in which air chemistry is being done: (1) box models, (2) trajectory models, and (3) airshed models. In box models the atmosphere is looked upon as though it were a simple box in which the pollutants react, relatively clean air is added (to approximate the effect of clean air mixing down from aloft) and pollutants are added (to represent the effects of sources within the box). Obviously box models don't tell us how pollutants vary in space and cannot treat situations where winds carry aged materials back into the urban setting. In trajectory models the winds are used to define a path and a box model is used which incorporates the emissions that would be found along the path. The trajectory model provides a little more spatial information than does a box model, but it doesn't describe what happens as material mixes in from adjacent trajectories. Airshed models use an Eulerian grid and describe the interactions between cells and the reactions that occur in each cell.

2.0 Methodology

The TRANSIMS architecture includes four major elements: (1) a household and commercial activity disaggregation module, (2) an intermodal route planner, (3) a travel microsimulation module, and (4) an environmental module. The disaggregation module uses census and survey data to construct a regional synthetic population. In the future, it will also estimate travel related activities for each member of the synthetic population. Currently, travel activities are inferred from origin and destination matrices developed by regional planning authorities. The intermodal planner produces planned travel link by link and mode by mode on the travel network. The TRANSIMS environmental module is composed of a system of environmental modules that can describe both the average conditions and the fluctuations about the averages. It uses a prognostic meteorological model, HOTMAC, to describe the atmospheric conditions. The environmental module will use modal emissions models to define the emissions. Transport and dispersion of conservative pollutants will be described with a Monte-Carlo Kernel model (RAPTAD). Air chemistry will be described by an airshed model with the current choice being the CIT model developed at the California Institute of Technology and the Carnegie Mellon Institute of Technology

Input for the system will consist of surface characteristics, large-scale meteorology, terrain, traveler behavior, and vehicle characteristics. Terrain and surface characteristics for current conditions are available for US cities. For future applications, estimates will have to be made of the changes expected in the future. The required large-scale meteorology is available through airport radio balloon soundings or through meteorological analyses done by the National Meteorological Center.

2.1 Household and Commercial Activity Disaggregation Module

The disaggregation module includes two components: (1) a synthetic population submodule and (2) an activity demand submodule. The synthetic population is developed from the Census Standard Tape File 3 (STF-3) and the Public Use Microdata Sample (PUMS). The PUMS has all the desired attributes of the population but it represents a sample from a much larger population than desired while the STF-3 represents a much smaller population, but it doesn't provide all the information of interest. A statistical technique called iterative proportional fitting is used to estimate the desired data at the census tract or block group level based on the PUMS correlations. The actual synthetic population is randomly drawn from the multi-way tables produce by iterative proportional fitting.

The activity demand module is not yet developed. In the interim, a module that uses the metropolitan planning organization's estimated origin and destination tables to produce synthetic activities is being used.

2.2 The Intermodal Route Planner

The planner generates routes for each load from the activity-based travel demand. A load is a traveler or a commodity. A trip plan is a sequence of modes, routes and planned departure and arrival times at the origin, destination(s), and mode changing facilities to move the load to its activity locations. We assume that travel demand derives from a load's desire or need to perform activities. The household and commercial activity disaggregration module provides the planner with disaggregated activity demand and travel behavior. The planner assigns activities, modes, and routes to individual loads in the form of trip plans. The individual trip plans are input to the travel microsimulation for its analysis.

Trip plan selection is related directly to a load's desire to satisfy individual (or in the case of freight, corporate) goals. Goals measure a trip plan's acceptability and depend on the load's socioeconomic attributes and trip purpose. Typical goals include cost, time, and distance minimization, and safety and security maximization. The load's objective is to minimize the deviations from these goals.

The travel demand problem is formulated as a mathematical program based on a multi-goal objective function. The Planner's solution method has four phases: (1) trip generation, (2) goal measurement, (3) preference adjustment, and (4) trip plan superposition. In the first three phases, the individual's travel behavior preferences such as departure time or origin-destination directness, are adjusted iteratively to satisfy the travel goals. After

very load has a feasible trip plan, the fourth phase superimposes all trip plans on one another in space and time. The network characteristics are then updated based upon the projected interaction of all trips and steps (1) through (4) are repeated.

2.3 Travel Microsimulation

The Travel Microsimulation module mimics the movement and interactions of travelers throughout a metropolitan region's transportation system. The approach is to use a cellular automata (CA) microsimulation. CA traffic models divide the transportation network into a finite number of cells. In the current form each cell's length is the average distance between vehicles when traffic is at a complete standstill. A cell may be empty or contain a single vehicle. If it contains a vehicle, the vehicle has an integer velocity between zero and maximum velocity, Vmax=5. The integer velocity represents the number of cells that vehicle moves the next step. The step size is exactly one second, in which case Vmax corresponds to 135 km/hour, or about 84 mph. This step size abets fast computation because the updated vehicle position is computed by integer arithmetic and without multiplication of velocity and time step.

Updating the vehicle's next velocity and position is quite simple. First, we define the number of unoccupied cells ahead of the vehicle as its "gap". Then, we update the velocity by accelerating to the maximum velocity without running into the vehicle ahead:

$$V(t+1)=\min[V(t)+1,Vmax,gap].$$

But, with probability P, we reduce this tentative velocity by one (without going backwards):

$$V(t+1)=\max[V(t+1)-1,0].$$

Finally, we update the vehicle's position:

$$X(t+1)=X(t)+V(t+1).$$

This rule set is called the Nagel-Schreckenberg model. The random velocity reduction process captures driver behavior such as free-speed driving fluctuations, non-deterministic accelerations, and overreactions when braking. The simple one-lane model has been extended to cover lane changing, passing, merging, and left-turn behavior.

The simple model produces dynamics observable in everyday freeway traffic. First, we can display an individual vehicle's movement in space and time as shown in Figure 1. Vehicles moving at constant velocity leave straight-line tracks slanting downward to the right. A stopped vehicle moves in time, but not in space, creating a vertical line. The figure shows the spontaneous formation of well-known traffic shock waves that propagate backward in space.

This model also produces the fundamental flow-density relationship shown in Figure 2 where density has been normalized to 1.0 for a completely jammed system. At low densities, flow increases linearly with more vehicles in the system. Near a density of 0.1 the system achieves maximum throughput or

'capacity,' but the flow is quite chaotic and its variability increases dramatically.

2.4 Emissions modules

An essential component for TRANSIMS is an emissions model that can give emissions that are specific to the type of driving being done. There is one such model in existence now that uses a so-called engine map to define the emissions. The model called VEHSIME was developed from a fuel economy model called VEHSIM. One disadvantage of this model is that it needs measurements of the emissions of each vehicle type as a function of engine load. In fact, there are relatively few cars for which such measurements are available. Consequently, VEHSIME is viewed as an intermediate solution, which will permit us to gain experience with TRANSIMS. In the longer term, an approach based on the physics and chemistry of the automobile engine will be used. Investigators at the University of Michigan are working on such a model.

We also expect to use the results of work being done at Georgia Tech, the California Air Resources Board, National Cooperative HIghway Research Program, and EPA.

Our work with VEHSIME discovered a number of deficiencies. First, the fuel consumption tended to be significantly lower than that reported for similar vehicles driving either the highway or city driving cycle (Carlson et al, 1994). This was not true for the two 1977 vehicles where the engine maps were developed from measured engine torques as opposed to the late model engine maps that used estimated torques. The first effort to correct this problem involved scaling the measured torques by a factor so that the engine's maximum rated horsepower was the same as the maximum horsepower from the engine map. This adjustment was not used for vehicles, such as pickup trucks with powerful engines where the measurements did not include full throttle loads at higher rpm. Another step was to turn the fuel consumption off for negative torque rather than use the idle fuel consumption at the same rpm. Finally, Professor Marc Ross and his students have described a vehicle's fuel consumption in terms in a two parameter form as:

$$\text{fuel consumption} = a*rpm + b*rpm*torque,$$

and the parameters a and b are functions of engine displacement and highest gear ratio (An and Ross, 1993). We adjusted the factors a and b from their theoretical values to produce new values that gave a better agreement with the EPA reported city and highway fuel economies. The adjustments do not give exactly the EPA reported fuel economies because we did not permit large changes from the theoretical values. The emissions of NOX, CO, and hydrocarbons were assumed to be proportional to the fuel consumption. We further adjusted the emissions to be consistent with the reported EPA highway emissions for similar vehicles. The results of these adjustments was to produce modified engine maps that approximately matched the EPA fuel economy measurements for similar vehicles and matched the EPA tailpipe emissions for NOX, CO, and hydrocarbons for the highway driving cycle. The goal was to make the engine maps more representative of those found in the EPA database.

An illustration of the use of the modal emissions model is shown in Figure

3. Figure 3 describes the average CO emissions while driving half the time up the specified grade and half the time down the grade with a distribution of speeds and accelerations derived from EPA's three cities study (USEPA,1993). The camaro is a 350 cubic inch displacement model and it is not affected by any but the highest grades, while the effects are much greater for lower powered cars.

There are three other elements to the motor vehicle emissions module: (1) evaporative emissions, (2) cold start emissions, and (3) non-conforming vehicle emissions. Evaporative emissions are captured in a canister that is purged during vehicle operation. If the vehicle is not operated for a long period of time the canister becomes full and the fuel is evaporated and released to the atmosphere. We have the evaporative emissions model that is used in Mobile 5A and we are incorporating it into our emissions module. The TRANSIMS planner will provide information on the vehicles that are in use or idle so that we will be able to tell when the canister is full and the emissions are released to the atmosphere.

A vehicle starting with a cold engine has considerably higher emissions than one with an engine at normal operating temperature. There are two reasons for this. When the engine is cold, the commanded air-fuel mixture is rich in fuel compared to the ideal stoichiometric conditions normally commanded for an engine and thus there is not enough oxygen in the air-fuel mixture to completely combust the fuel. This increased amount of fuel is commanded to reduce the tendency of the engine to stall when it is cold. The incomplete combustion of the fuel results in emissions of CO and hydrocarbons that cannot be completely handled by the catalytic converter. Also the catalytic converter will not start working until it reaches the "light-off" temperature. Thus if there is a situation where many of the vehicles in the fleet are taking frequent short trips, the cold-start emissions can account for a significant fraction of the vehicle's emissions. We are using a formulation wherein the CO engine-out emissions are doubled during startup and the catalyst transitions from zero effectiveness to the level obtained from a hot catalyst.

The last large source of emissions that has not been modeled precisely is emissions from non-conforming vehicles, or vehicles with malfunctioning emissions control systems. Measurements have indicated that emissions from as little as 10% of the vehicles can account for most of the emissions. Some of the uncertainty in the measurements of high emitting vehicles is because that vehicles with properly functioning emissions control systems can have very high emissions if they are under high engine load at the time of the measurement. Thus there is some doubt whether the vehicles identified in measurements as high emitters have continuous high emissions or were measured during the short period of time they had high emissions due to engine load. Initially, we are going to divide the vehicles into two sets: (1) those with damaged catalysts (probably about 10% of the fleet, based on remote sensing data) and (2) those with malfunctioning fuel metering systems (probably about 0.1% of the fleet). Remote sensing data will be used to estimate the fraction of the fleet in each category and the average catalyst efficiency for those with impaired catalysts. We will estimate the emissions from damaged fuel metering systems by using VEHSIME with high accelerations and high grades to force enrichment behavior.

In the longer term, University of Michigan investigators plan to develop

models describing vehicles with engine problems and with malfunctioning emissions control systems. Once these models have been developed we plan to incorporate them into TRANSIMS.

The primary output of the transportation micro-simulation module will be summarized cellular-automata (CA) data. The CA describes the vehicle position in units of cells, velocity in units of cells per second and the acceleration in units of cells per second per second. A typical cell size is 7.5 meters so that the resulting motion is too lumpy to be used directly as input to the emissions module. We are developing an approach using the Kalman filter to produce realistic, smooth vehicle trajectories that can be used in the emissions module. The Kalman filter is designed to treat a physical process that has random elements and is observed with a noisy measuring device. In this application, the equations describing vehicle motion become:

$$X(n+1)=X(n)+V(n),$$

$$V(n+1)=V(n)+a,$$

and

$$Xc(n+1)=X(n+1)+err,$$

where X(n) is the position at update n, V(n) is the velocity at update n, a is the random velocity fluctuation (acceleration) at update n, Xc(n) is the cell location at update n, and err is an error term produced by the uncertainty of the position within the cell.

The Kalman filter applies to a zero-mean process so that the positions and velocities must be described in a frame of reference moving with the desired speed at each time. We have done some testing of the use of the filter. We began with actual vehicle trajectories from a database developed by the California Air Resource Board (Effa and Larson, 1993). We overlaid a grid on the vehicle's trajectory and deduced equivalent CA positions and velocities. The trajectories were grouped into 10 sets; three sets of arterials, slow, medium, and fast, and 7 freeway sets ordered by increasing congestion. The most uncongested freeway set had average speeds of about 60 mph while the most congested set had average speeds of about 10 mph. In each case we used only the first 30 seconds of the driving.

From the synthetic CA data we collected the fraction of the vehicles in each CA speed bin in each CA cell plus the fraction that increased CA speeds in a cell and the fraction that decreased speeds in a cell. We used the information to construct a new set of CA trajectories that were ordered by aggressiveness and were begun within sub-interval speeds that covered each CA speed bin at approximately 2 mph intervals. We also used Baltimore driving data to estimate the distribution of accelerations associated with a positive acceleration from a given speed. We also estimated the distribution of decelerations from a given speed. The new set of CA trajectories was constructed by using the original CA acceleration and deceleration probabilities to estimate the probability of an acceleration in a cell. If the acceleration occurred as determined a random draw, we increased the velocity by the acceleration appropriate to the level of aggressiveness of the trajectory. Once the new trajectories, ordered by

aggressiveness were formed, we constructed new aggressiveness ordered trajectories in the same fashion as the original CA trajectories were constructed. We chose not to use the original CA trajectories directly because we expect that actual CA data will not preserve aggressiveness from one second to the next. There is one step in the process that needs refinement; the deduction of the probability of an acceleration from the CA speed change distributions. This task is complicated by the fact that vehicles traveling with constant speeds will appear to undergo accelerations or decelerations unless they have exactly the central speed in a CA cell.

Once the new aggressiveness-distributed CA trajectories were defined, the Kalman was used to produce new, continuous trajectories. The averages of speeds, CO emissions, NOX emissions, hydrocarbon emissions, and fuel consumption were compared to those from the original trajectories. Figure 4 reports such a comparison for CO emissions for a medium speed freeway link. Figure 5 reports such a comparison for NOx emissions for a medium speed freeway segment, while Figure 6 gives the comparison for hydrocarbon emissions on a medium speed freeway link. The average speeds on the medium speed freeway link are shown in Figure 7. Figures 8 through 11 show the comparisons for a very congested freeway link for CO, NOx, hydrocarbon emissions and average speeds respectively. Overall the comparisons show the need for further development, but they also show that the system can produce respectable results over a wide range of driving conditions.

2.5 Meteorological Module

The meteorological module is HOTMAC (Higher Order Turbulence Model for Atmospheric Circulation). HOTMAC is a three-dimensional time-dependent model (Yamada and Bunker, 1988). It uses the hydrostatic approximation and a terrain-following coordinate system. HOTMAC solves conservation relations for the horizontal wind components, potential temperature, moisture, turbulent kinetic energy, and the turbulence length scale. HOTMAC describes advection (properties moving with the wind), Coriolis effects (motion induced by the earth's rotation), and turbulent transfer of heat, momentum, and moisture. It also describes solar and terrestrial radiation effects of forest and urban canopies. The lower boundary conditions are defined by a surface energy balance and similarity theory. The soil heat flux is obtained by solving a heat conduction equation that ignores lateral heat flux. In an urban context, the surface energy balance requires an additional term that represents the heat released by human activities. The additional heat, along with differences in thermal and albedo properties between urban and non-urban surfaces, produces the urban heat island.

HOTMAC uses two major sets of inputs: (1) topography and (2) a single vertical profile of winds, temperatures, and relative humidity. The topography consists of terrain heights at half grid intervals over the domain and indices that show the land use or land coverage of each computational cell. For existing situations, the land use/land coverage is available in commercial databases or can be deduced from satellite images. The meteorological profile is used to describe the synoptic (large-scale) conditions of winds, temperatures, and moisture. The model is initialized with the potential temperature assumed to be the same in every location for any given height above mean sea level. Potential temperature is the temperature of a parcel of air adiabatically compressed to sea-level pressure. In a well-mixed atmosphere, the potential

temperature tends to be constant with height except for very near the surface. On the lateral boundaries the winds, moisture, and temperatures are the result of solving a one-dimensional form of the model in which parameters vary only in the vertical direction. The placement of the boundaries is normally chosen so that all the major terrain influences on the region of interest are included within the computational grid.

Mesoscale models, such as HOTMAC, are designed for circumstances in which the local terrain influences are significant and make the meteorology more predictable than might otherwise be the case. The top boundary of the model is fixed at a constant height above sea-level and is a no flow boundary. The model uses a vertical grid that is linear for a specified number of cells, but then increases parabolically to the top. In a typical application the first 4 cells would be 4 meters in size, after which the cell size would expand from 37 meters for the fifth cell to over 600 meters for the last cell. The horizontal grid is staggered so that the east-west and north-south wind components are calculated at points that are off-set one-half grid in the corresponding directions. The model uses the alternating-direction implicit differencing technique which provides high accuracy and stability. The model uses a nested grid system so that areas of importance can be treated in much greater detail. In the current version, the innermost grid is one third the scale of the next larger grid. The computational time is dominated by the requirements of the innermost grid so that the outer grids require little computational time. The model forms clouds, but it does not permit precipitation.

Proper initialization and incorporation of changing large-scale conditions is a challenge for mesoscale models. The current version of HOTMAC (Williams et al, 1995) addresses this by first calculating winds at a measurement site, such as an airport, with very light low-level large-scale winds. The solutions from the light wind case are used to describe the local-wind effects and the measured winds are adjusted according and used to update the model throughout the model domain.

HOTMAC has been used successfully in many contexts. It has been used in the Geysers region of California that is in the Pacific Coast Range near the Pacific Ocean. It has been used to describe flow in narrow, deep canyons of western Colorado. It has described the formation and dissipation of clouds during evening hours over the south coast of England. It has successfully described the linked sea-breeze between the Pacific Ocean and the Japanese Alps. It has also been used on sub-continental transport problems in the eastern US and the southwestern US. It was used in the Mexico City Air Quality Research Initiative and it is currently being used by officials in Mexico City to plan their air quality improvement program.

HOTMAC provides grid-averaged winds, temperatures, moisture, clouds, and turbulent wind energies for the model domains that cover hundreds of kilometers with a maximum resolution of about one kilometer. HOTMAC does not describe the complex motion found in urban street canyons. As a result of vehicle emissions in urban areas, air pollution can become trapped between buildings in what is called an "urban canyon". Studies have shown that air pollution concentrations can be 2 to 10 times higher in an urban canyon than in the case without buildings. Typically, a large recirculation zone forms between the buildings that transports the traffic emissions from street-

level to building top. However, only a small portion of the air pollution is vented out of the urban street canyon top, as the buildings cause the air flow within the canyon to become separated from the larger-scale air flow above.

Our approach for accounting for the urban canyon effect on air pollution concentrations will consist of two levels of sophistication: first, a derivation of a simple parameterization that can be easily implemented into our existing modeling system to roughly approximate the urban canyon effect and second, development of a microscale air flow model for explicitly simulating the air flow in the urban canyon.

In the first approach, an urban-canyon-induced eddy circulation will be added to the dispersion model RAPTAD in order to approximate the entrapment of air pollution between buildings. In the second approach, we will jointly develop a finite difference Navier-Stokes numerical flow model with researchers from the Theoretical Division of Los Alamos National Laboratory. The computer model will allow for explicit simulation of many different building configurations and flow scenarios. In addition, the computer model can be used to improve the parameterization used in the RAPTAD model.

2.6 Local Transport and Dispersion Module

The dispersion module will be based on the RAPTAD (Random Particle Transport and Dispersion) model (Yamada and Bunker, 1988). Pseudo-particles are transported with instantaneous velocities that include the mean wind field and the turbulence velocities. The turbulence velocity is generated randomly so that it is consistent with the standard deviation of the wind at the particle location. The location of each pseudo-particle represents the center of mass of a concentration distribution for the volume of air that encloses the material associated with the pseudo-particle (puff). The total concentration at any point is obtained by adding the concentration contributions of each puff at that point (a kernel method). The Monte Carlo kernel method requires that a functional form for the distribution kernel be chosen and that parameters that describe the width, breadth, and depth of the distribution be calculated. The approach used here is to assume a Gaussian distribution where particle position variances are determined from the time integration of the velocity variances encountered over the history of the puff. The position variances are estimated based on the random force theory of turbulent diffusion (Lee and Stone, 1982). The random force theory is also known as the Brownian-motion analogy, or the Langevin model. An equation is written which describes the motion of particles under the influence of random accelerations and a resistive force term. Lee and Stone extend the theory to the treatment of clusters of particles from finite-size, finite-duration sources.

The system has many advantages for applications involving complex terrain. The use of a higher-order turbulence model means that there are three-dimensional time-dependent wind fields and turbulence fields available for the representation of dispersion and transport. Transport can be treated in more detail because important terrain influences are represented in both the mean fields and the turbulence fields. Consider a situation in which the pollution is being released in the upper end of a canyon. The flow in the canyon

bottom is down canyon because of the cold air draining down hill. The flow aloft is may be up-canyon. A normal Gaussian puff model would follow the mean wind down the canyon and ignore the material that dispersed upward and was taken up canyon by the winds aloft. The situation can be treated either by a Monte Carlo kernel model such as RAPTAD, or it could be treated by a random particle model that did not use a kernel. Other random particle codes calculate concentrations by counting random particles in cells. The cell approach, however, has the disadvantage that the cell sizes must be carefully chosen and they must vary in size. If the cell size is too small, the concentrations will be very noisy with some cells having no particles and thus no concentrations, while an adjacent cell may have very large concentrations if it has one or two particles in its small volume. If the cells are too large, the concentrations will be smeared out in an unrealistic fashion. The kernel system, as used by RAPTAD, avoids this problem because the pollution associated with a particle is not concentrated at a point but extends over a volume surrounding a point. The volume around the point is calculated based on the turbulence history of the particle. In an afternoon turbulent circumstance, the volume expands very rapidly, while at night it expands very slowly.

A second example of the importance of a more sophisticated treatment of dispersion is afforded by the following real-world example. A tracer material was released for one hour in a valley in Utah and some 65 monitors were used to record the concentrations. During the night few monitors actually recorded significant amounts of tracer because the plume was so narrow during nighttime conditions. The measurements showed that the concentrations measured at ten km downwind extended for several hours. Gaussian puff calculations gave low concentrations for all hours except one. RAPTAD gave concentrations that remained high for a few hours. The Gaussian puff model moved all the material with the same wind speed. In actuality, some of the material near the ground moved very slowly, while some aloft moved much more rapidly. RAPTAD was able to treat the wind speed differences and provide a much better description of the actual pollution behavior.

An interim urban-street canyons model will be constructed by using simple parameterizations that describe the formation of eddies between rows of buildings. The local wind and turbulence will be based on the eddy geometry and the winds at the tops of the buildings.

2.7 Air Chemistry Module

The air chemistry module will be the CIT airshed model. The area to be modeled is divided into an Eulerian three-dimensional grid. The equations that describe the pollutant concentration are solved within each cell of the grid, which imposes a large computational effort. The concentration of species may vary by the incorporation of new emissions, transport of chemical species in and out of each cell, dilution, and chemical reactions, all as a function of time. One advantage of this type of model is geographical resolution for control strategies and impacts.

The CIT airshed model (Russell, et al, 1988) is an Eulerian photochemical air quality model that calculates the transport and chemical reactions of pollutants in the atmosphere. The current version of the CIT model contains a condensed version of the Lurmann, Carter, and Coyner (LCC) mechanism.

(Lurmann, Carter, and Coyner 1987) The extended LCC mechanism includes 106 chemical reactions involving 35 different inorganic and organic species. In the mechanism the organic species are lumped by molecular classes. Compounds that have similar structure and reactivity are grouped together. The chemistry of all molecules within a single lumped class is then represented using one or more surrogate species (e.g., toluene is used to represent the chemistry of all monoalkylbenzenes). The chemical mechanism includes separate reactions with the hydroxyl radical for each of the lumped organic species. In addition, the mechanism includes the reactions of ethene and lumped C3+ alkenes with O3, the nitrate radical, and atomic oxygen. In the chemical mechanism, the photolysis reactions involving the aldehydes and ketones are also considered. The removal of pollutants at the ground surface by dry deposition is included in the model. Dry deposition velocities are computed using local meteorology, surface roughness, and land use data in each square cell of the simulation grid (Russell et al. 1992). The CIT model is continually being improved, and a major focus of the current work to extend the formulation to address organic aerosols. The extension to organic aerosols and the improvements to the treatment of inorganic aerosol formation is very important because of the increased concern over fine particles in the urban setting.

3.0 Summary of Major Features

The TRANSIMS environmental module will include: (1) a modal emissions module, (2) a prognostic meteorological module, (3) a Monte-Carlo kernel dispersion module, and (4) an airshed air chemistry module. It will require inputs from the TRANSIMS planner and traffic microsimulation. It will estimate emissions of relevant species and it will use large-scale meteorology and land coverage to estimate concentrations of ozone, secondary aerosols, carbon-monoxide, nitrogen-dioxide, sulfur dioxide, and respirable particulate matter.

It will be capable of estimating both mean concentrations and fluctuations about the mean concentrations. It will also be able to estimate nitrate deposition. It will be a flexible tool for "what if" questions and it can be applied to any city given appropriate topography and surface characteristics. It will be a good platform for future improvements.

4.0 References

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Figure Captions

Figure 1. Waterfall plot of traffic dynamics produced by a cellular automata model.

Figure 2. Fundamental flow-density relationships produced by a cellular automata model.

Figure 3. Average CO emissions from VEHSIME for vehicles driving with speed and acceleration distributions derived from the EPA three cities study with half the driving up the specified grade and half down the grade.

Figure 4. Comparison between average CO emissions estimated from VEHSIME with real driving on a moderately congested freeway link and those produced from synthetic CA data on the same link.

Figure 5. Comparison between average NOx emissions estimated from VEHSIME with real driving on a moderately congested freeway link and those produced from synthetic CA data on the same link.

Figure 6. Comparison between average hydrocarbon emissions estimated from VEHSIME with real driving on a moderately congested freeway link and those produced from synthetic CA data on the same link.

Figure 7. Comparison between average speeds with real driving on a moderately congested freeway link and those produced from synthetic CA data on the same link.

Figure 8. Comparison between average CO emissions estimated from VEHSIME with real driving on a very congested freeway link and those produced from synthetic CA data on the same link.

Figure 9. Comparison between average NOx emissions estimated from VEHSIME with real driving on a very congested freeway link and those produced from synthetic CA data on the same link.

Figure 10. Comparison between average hydrocarbon emissions estimated from VEHSIME with real driving on a very congested freeway link and those produced from synthetic CA data on the same link.

Figure 11. Comparison between average speeds with real driving on a very congested freeway link and those produced from synthetic CA data on the same link.

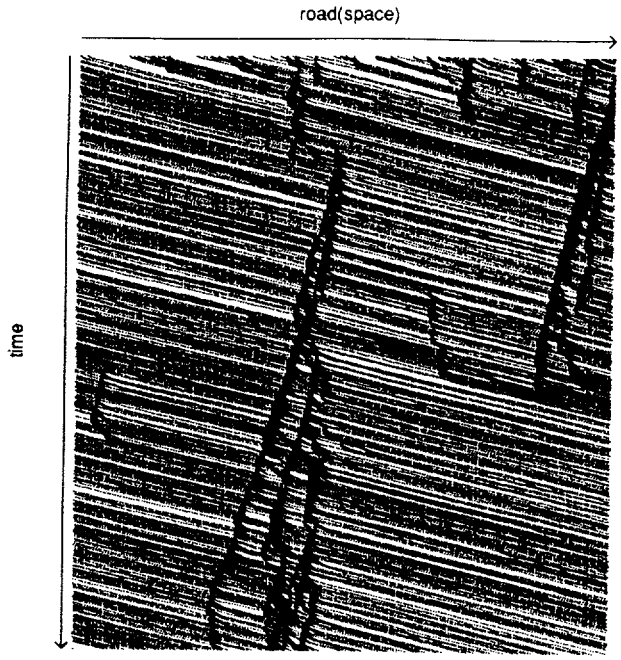


Figure 1. Waterfall plot of traffic dynamics produced by a cellular automata model.

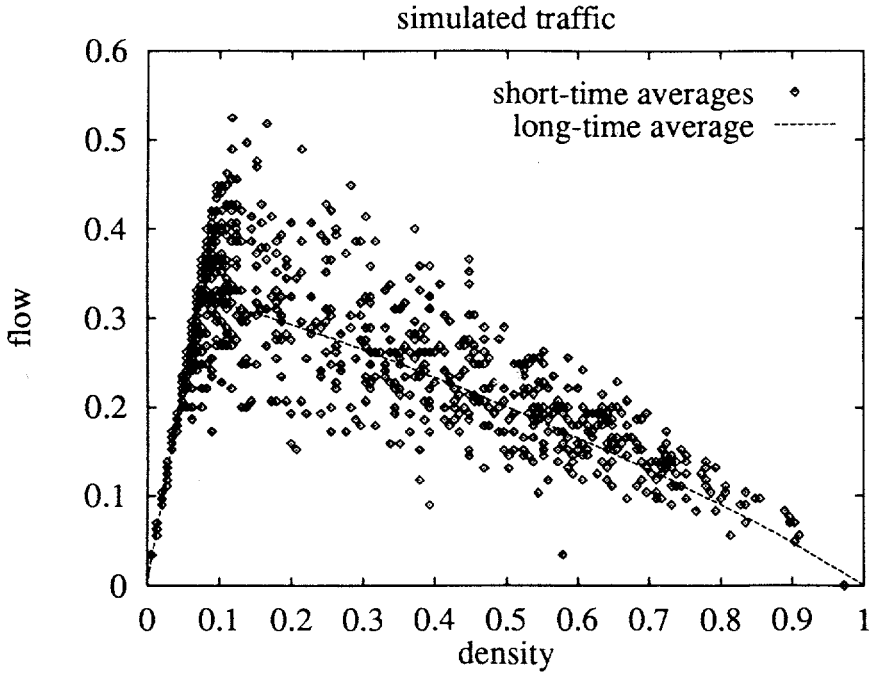
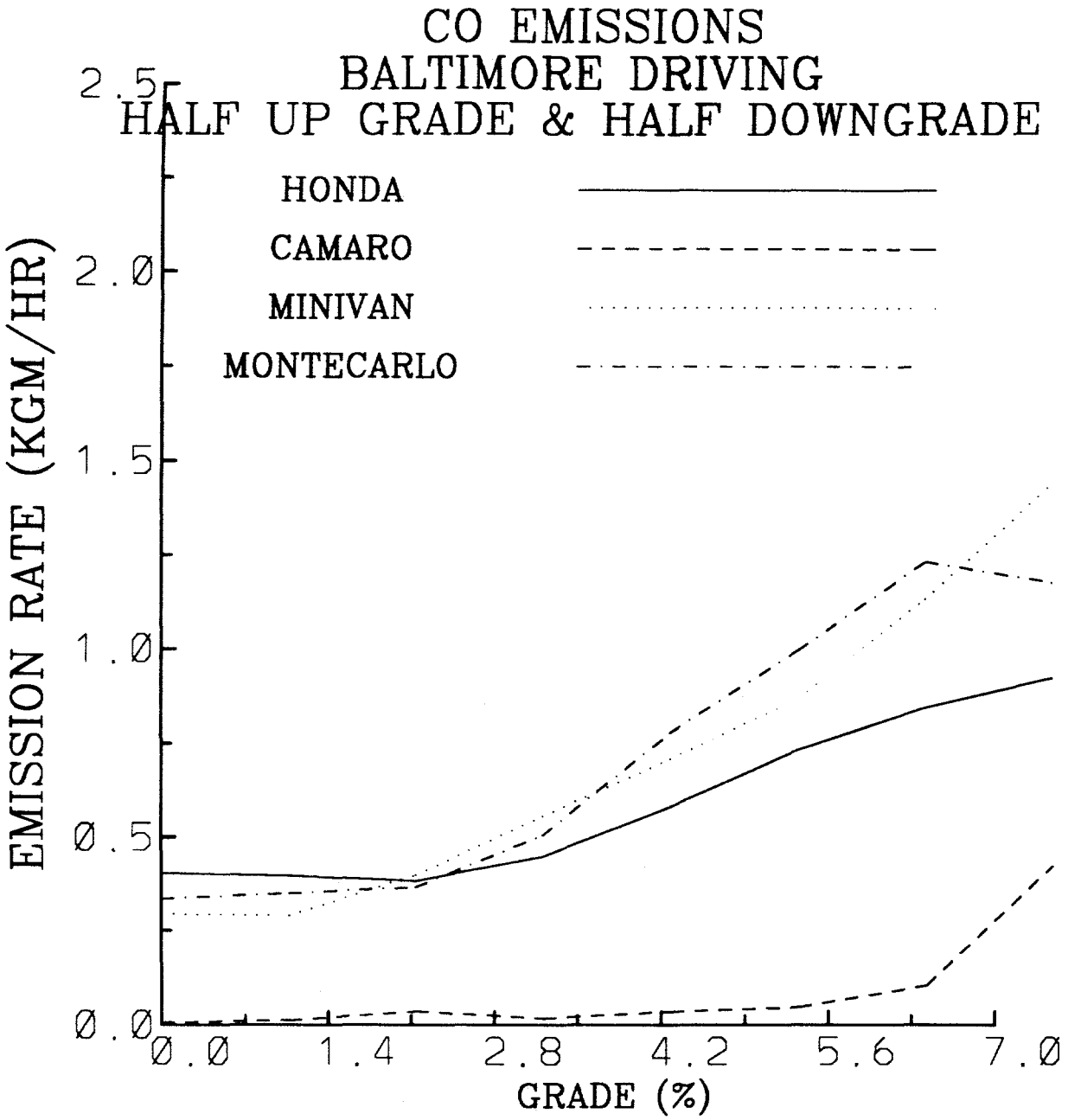


Figure 2. Fundamental flow-density relationships produced by a cellular automata model.



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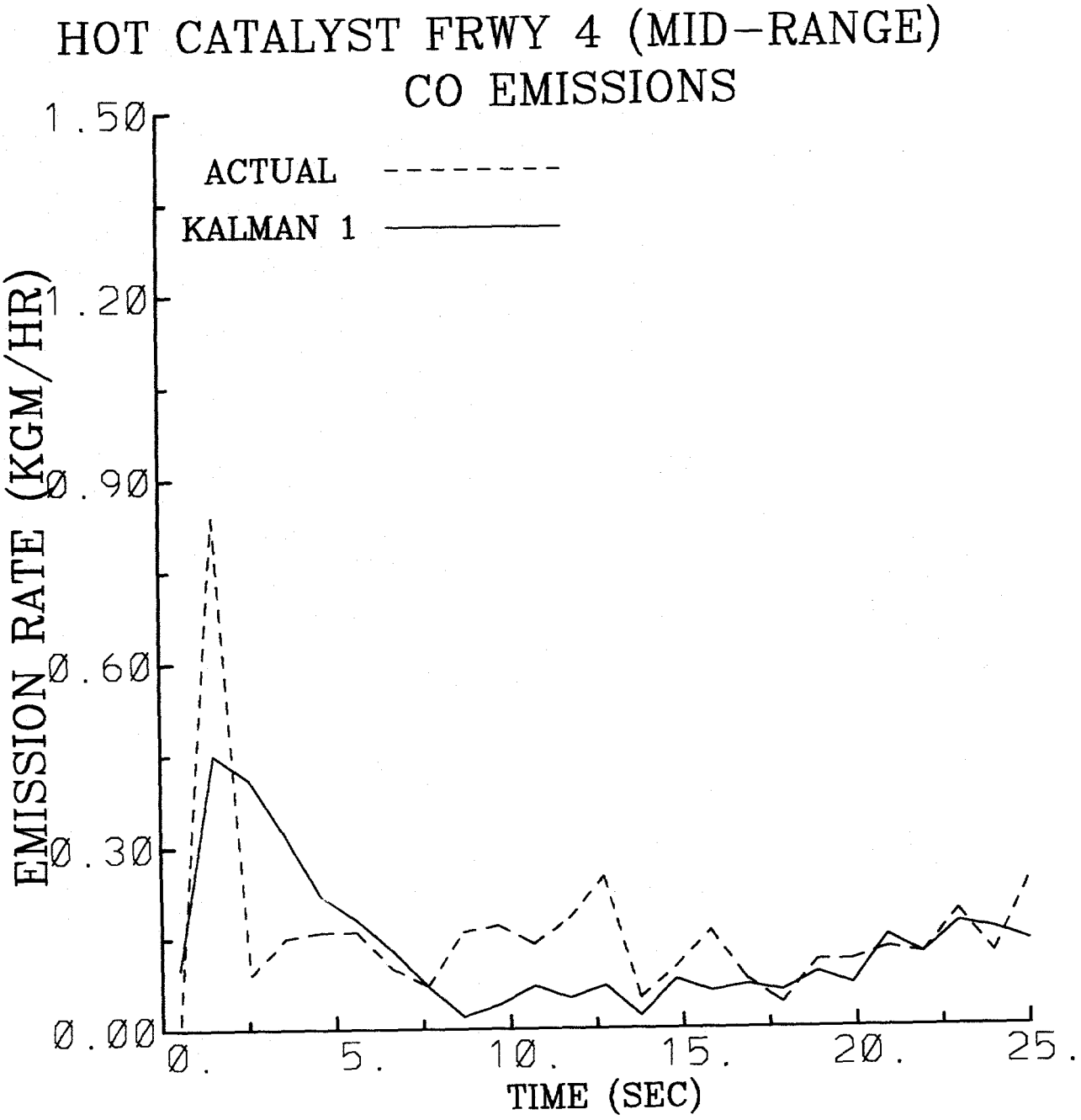

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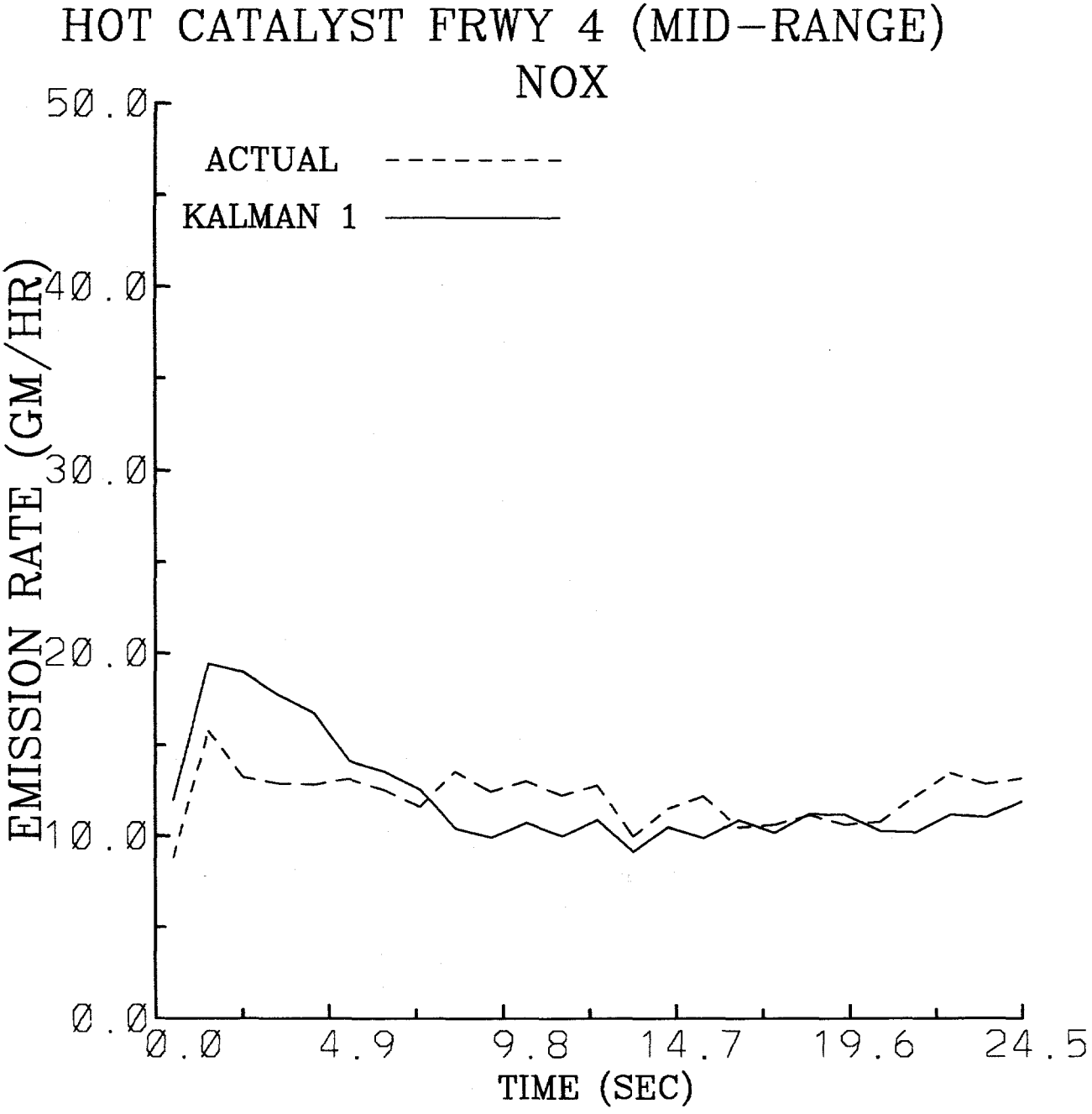

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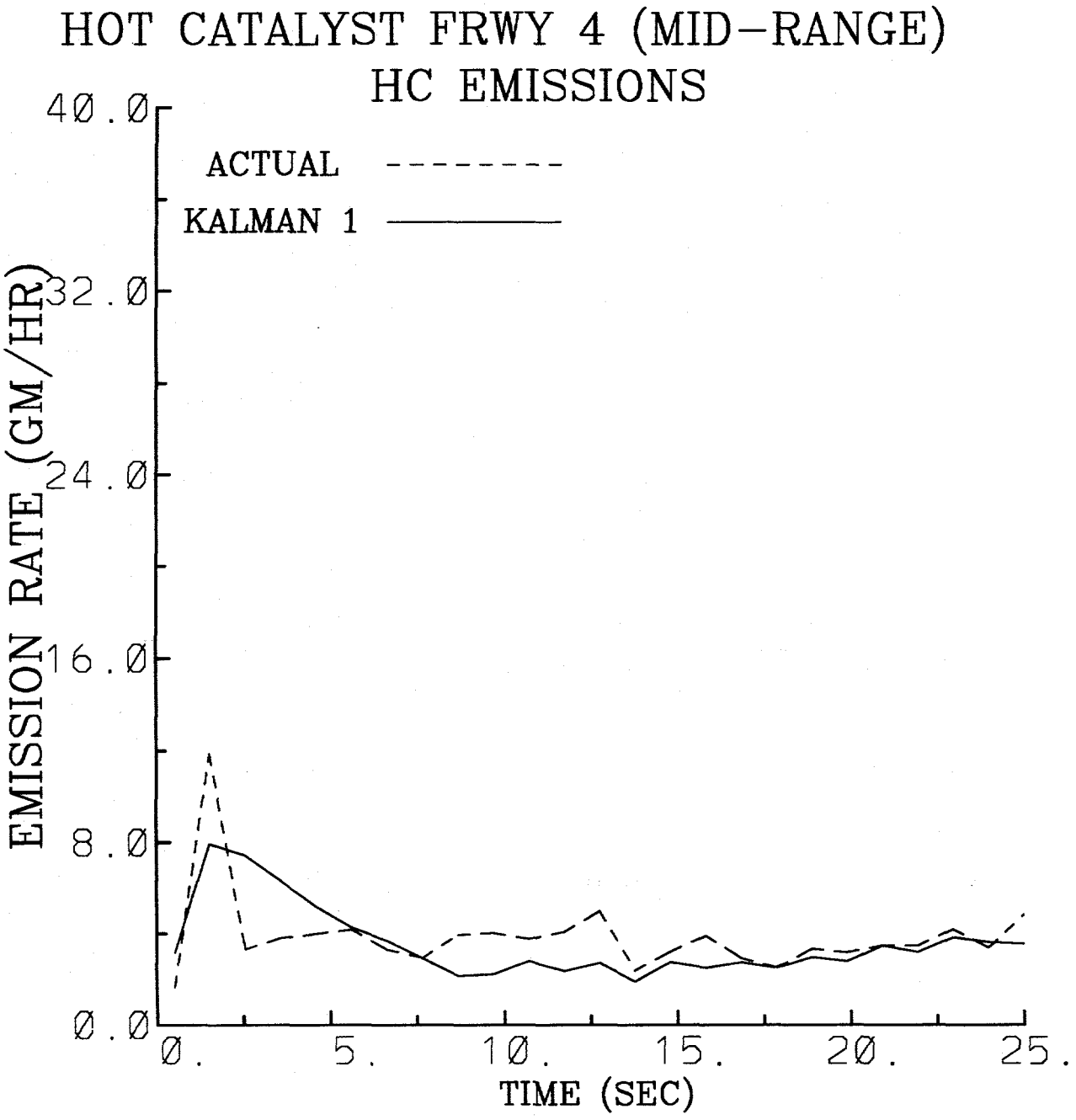

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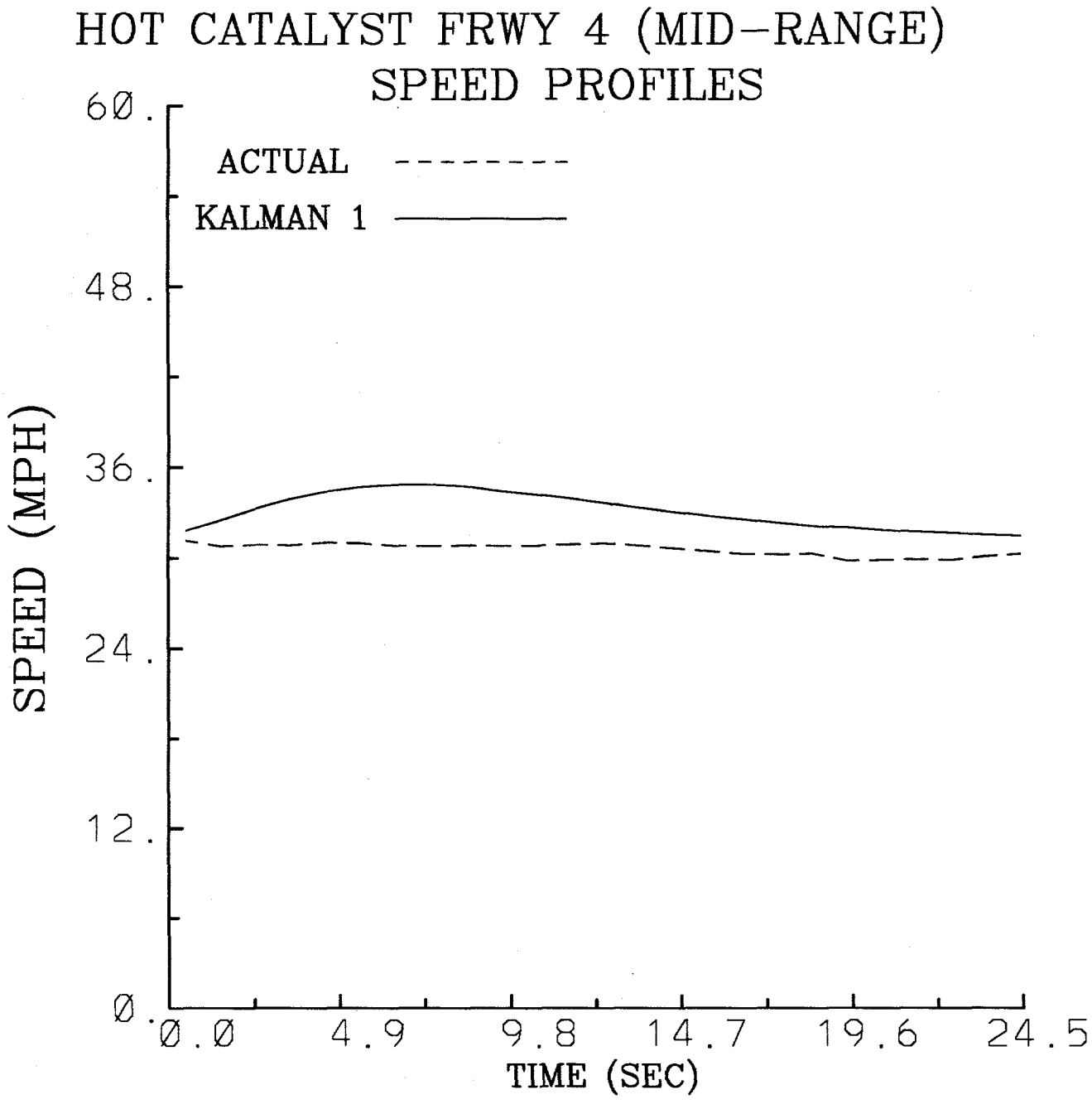

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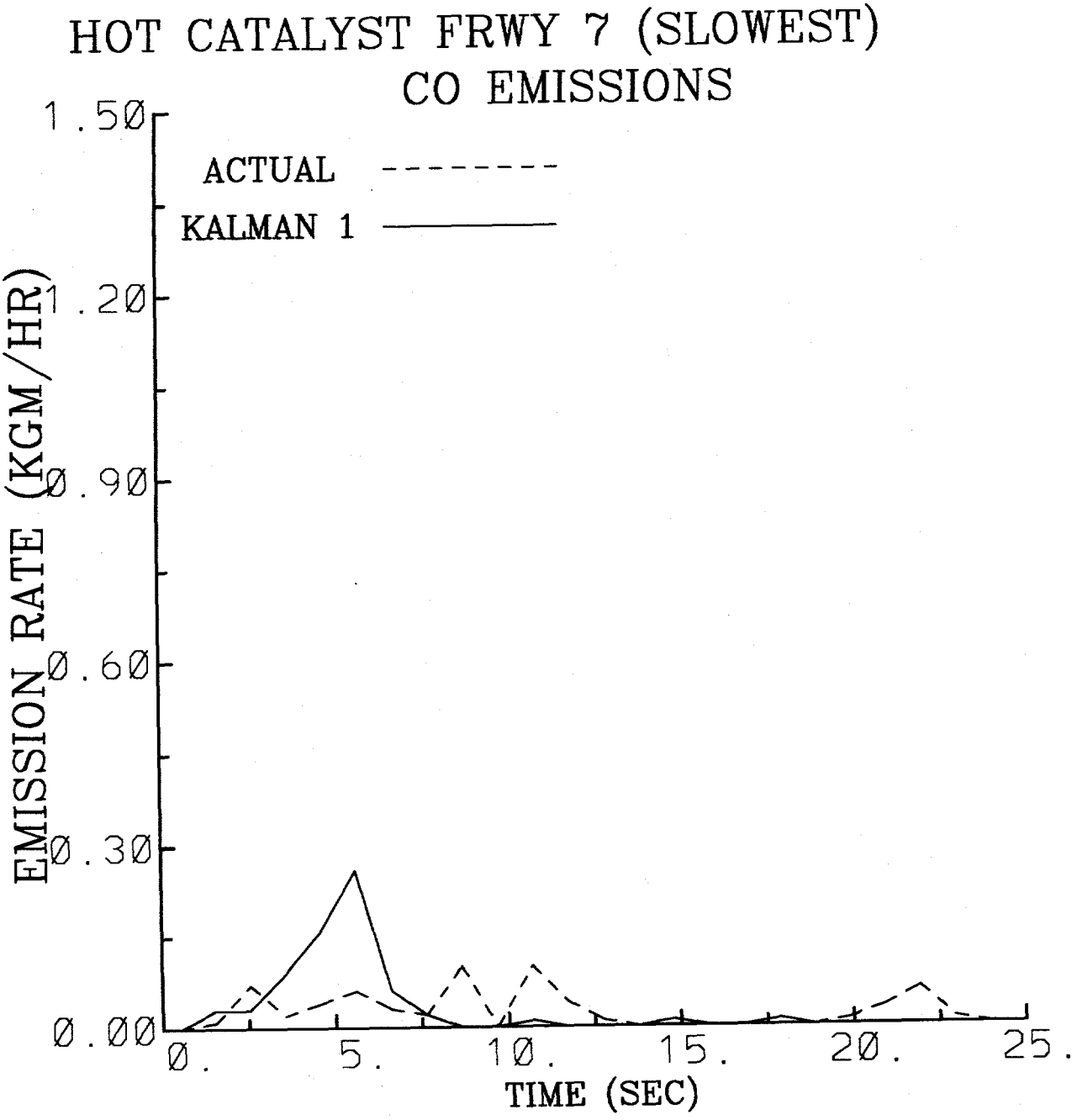

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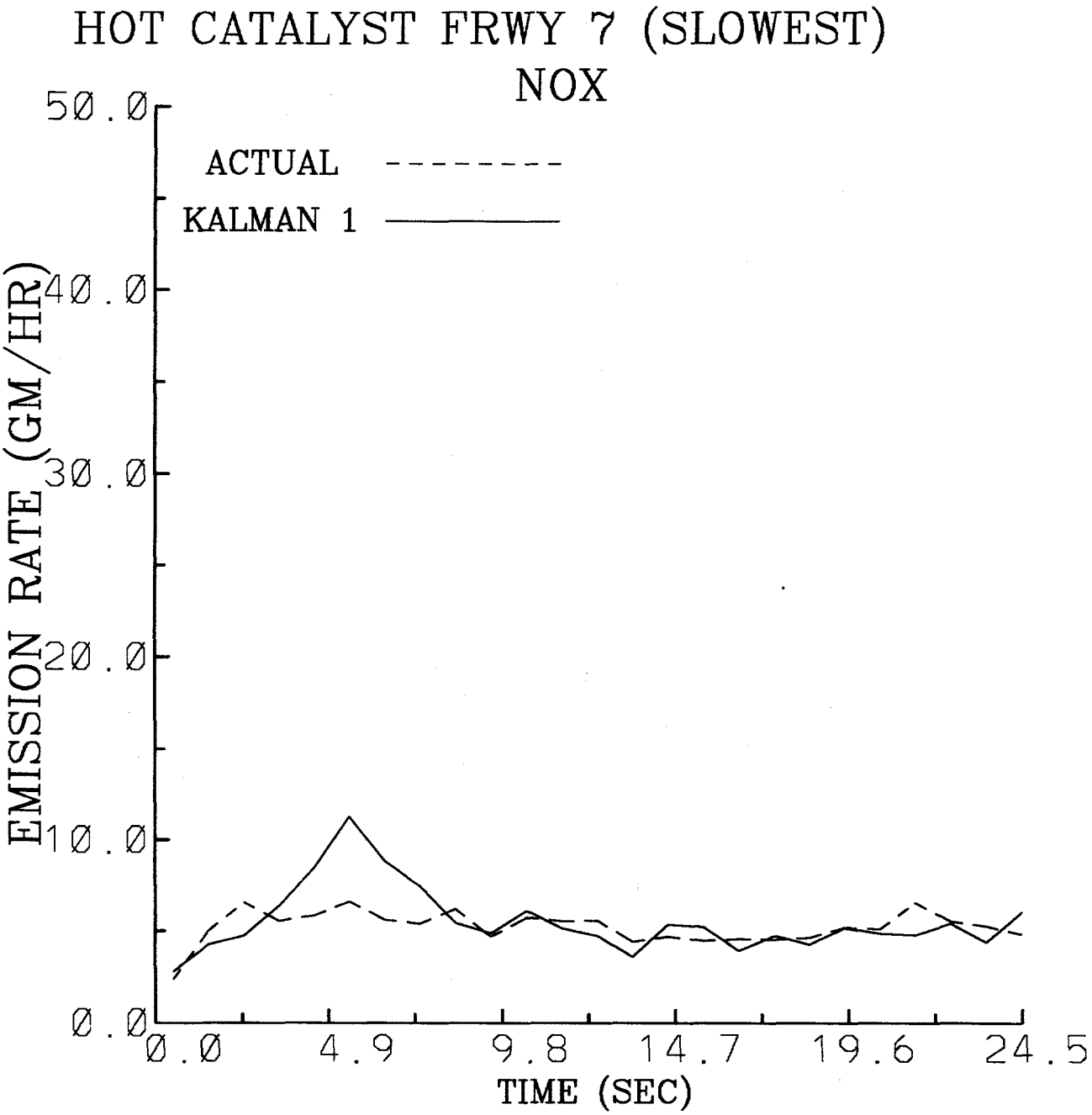

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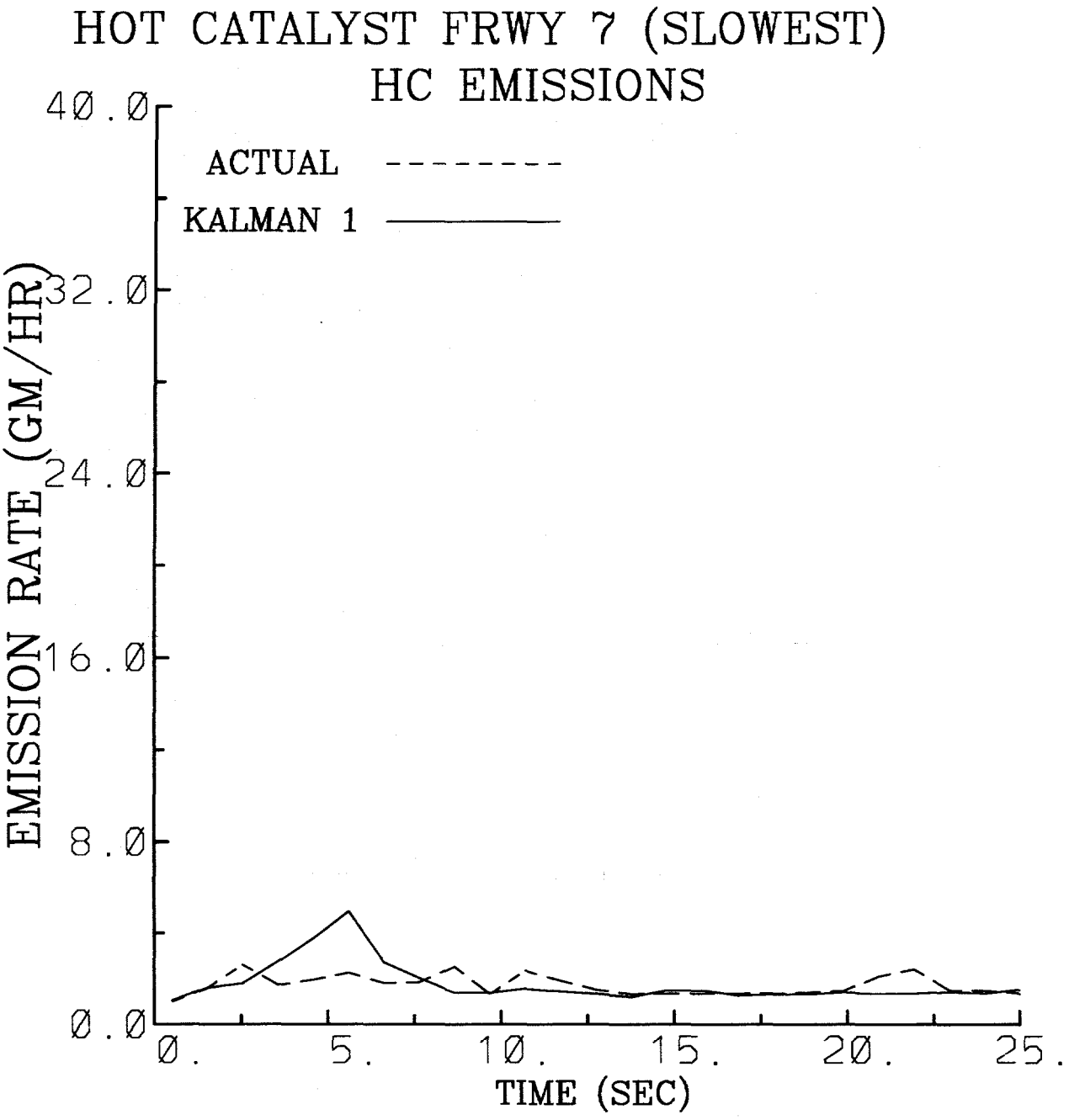

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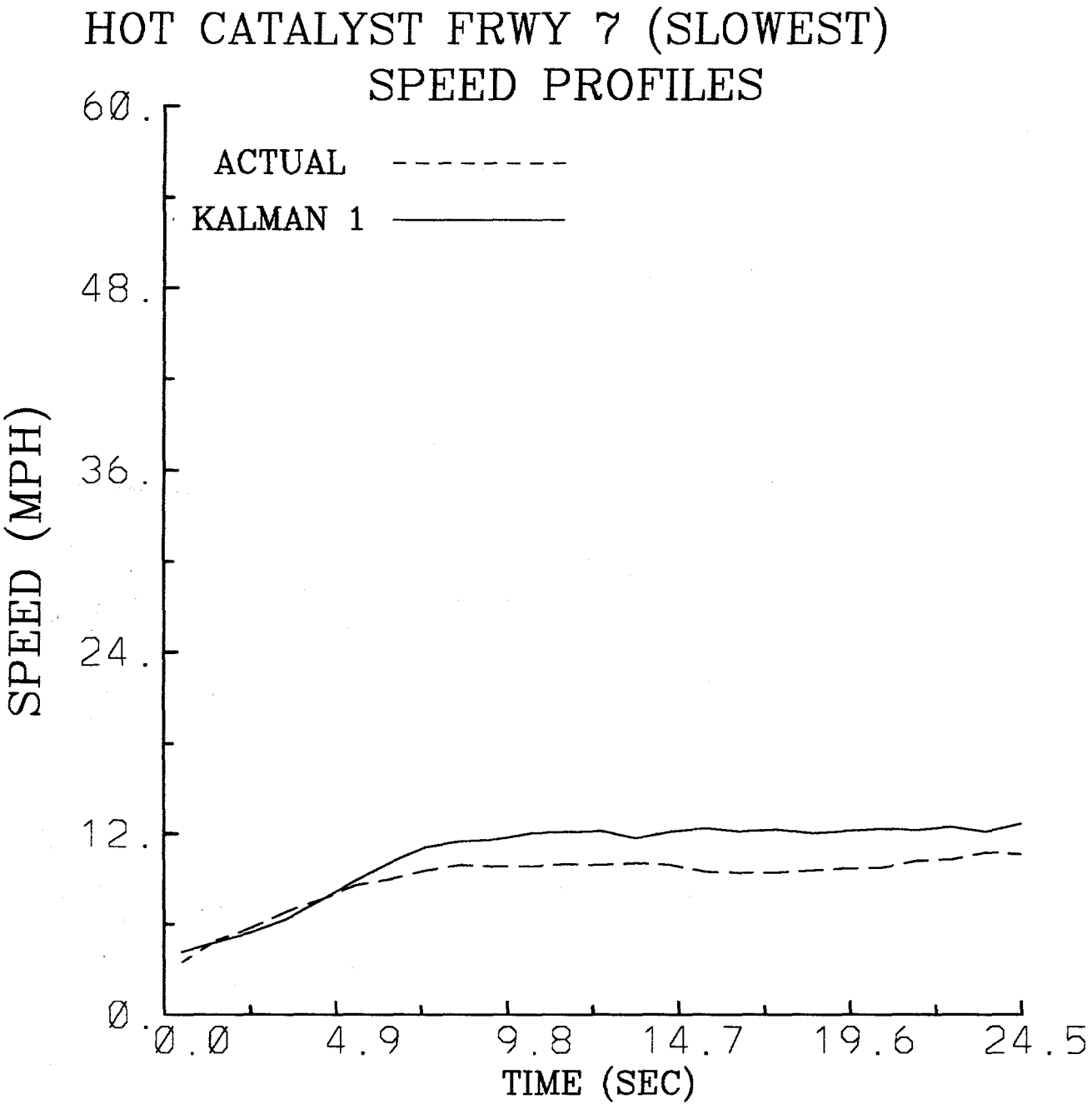

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