An integrated simulation system for traffic induced air pollution

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Abstract

In recent years the growing traffic demand combined with an increase in exhaust gas emissions is the main reason for a permanent decrease in air quality in urban areas. Especially during hot summer days, mainly traffic emissions are responsible for providing precursor substances for the ozone reaction. They account for approximately 70% of all emissions. In order to facilitate investigations analysing this situation, local authorities in environmental protection and urban planning agencies are interested in performing emission and air pollution simulation as well as scenario analysis by means of model based simulation systems. Therefore a realistic modelling of the physical behaviour of the atmosphere as well as the exact description of the emissions is necessary. Up to now mainly traffic countings combined with different statistical methods have been used to calculate these emissions. The obtained results are often incorrect and do not reflect the dynamic behaviour of the traffic flow. Traffic flow models provide a more promising approach. Currently, in the European Community funded SIMTRAP project, an integrated system for traffic flow information, air pollution modelling and decision support will be developed in a distributed High Perfomance Computing Network (HPCN), and subsequently tested in a number of European sites. SIMTRAP centres around two well-established core components: the air pollution model DYMOS and the mesoscopic dynamic traffic simulation tool DYNEMO. The project aims to integrate both modules in a remote HPCN environment in order to enable the detailed simulation of an area of sufficient geographical extent. Interpretation and visualization of results will take place in a local 3D GIS system. Communication will take place using existing computer networks and protocols. © 1998 Elsevier Science Ltd. All rights reserved.

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1. Introduction

In nearly all regions of the world, where industrialization is causing large urban areas supplemented with high traffic density, higher concentrations of photochemical oxidants can be observed periodically during the summer months. Especially critical examples are Mexico City, Sao Paulo, Los Angeles, Athens, Berlin and most of the other major European cities. Experts and public authorities are seriously involved in investigations searching for appropriate measures to improve air quality in these areas. One of the main sources of atmospheric pollution in urban areas are motor vehicle emissions. It is estimated that road transport contributes in most European cities more than 40% of emissions of volatile organic compounds (VOC), more than 70% of nitrogen oxides (NO_x) and over 90% of the emissions of

carbon monoxide (CO). Many of these pollutants have injurious effects on human health, vegetation and material, besides contributing to altering the atmospheric characteristics. Urban traffic is actually the main cause for the health-critical concentration of near-surface ozone typically for hot mid-summer periods in urban areas. Due to the nonlinearity of the chemical reactions contributing to the ozone production it is impossible to derive simple source–receptor relationships between the emitted primary species and the ozone concentration.

The growing traffic demand together with an increase of exhaust gas emissions and travel times on the one hand, and the likewise growing need for mobility on the other, requires the realization of measures for a better traffic control and planning. Aiming at shorter travel times and a reduction of air pollution, these measures include for example traffic control strategies (rerouting) and the shifting from car traffic to public transportation. Currently, the decision which measure serves the purpose best can not be simulated in advance. Therefore a

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simulation system for traffic flow, traffic emissions and air pollution dispersion is under development at GMD FIRST (Sydow et al., 1995) consisting of the following modules (see Fig. 1):

- a traffic flow model considering single vehicles,
- a traffic emission model processing a variety of parameters and vehicle characteristics,
- air pollutants dispersion models calculating transport and chemical transformation,
- a database storing and managing all input and output data,
- a decision support system visualizing data in spatial relations and deriving decision proposals.

2. The air pollution transport model DYMOS

At GMD FIRST the DYMOS system (Sydow, 1994) has been developed, a parallelly implemented simulation system to analyse the generation, dispersion, and chemical transformation of gaseous air pollutants and different aerosols. The model is well suited to reproduce most frequent occurring kinds of smog situations:

- winter smog: high concentration of inert (regarding the model domain) pollutants (e.g. SO_2, NO_x, dust, etc.) caused by high pressure weather situations in the winter months.
- summer smog: high concentration of ozone and other photochemical oxidants caused by strong insolation during high pressure weather situations in the summer months.

DYMOS consists of the air pollutants transport model REWIMET (Heimann, 1985) and the air–chemistry model CBM-IV (Gery et al., 1988).

REWIMET is a mesoscale atmospheric model which is officially distributed by the German Engineer Association VDI. Mesoscale models describe processes (e.g. thunderstorms, cloud clusters, low-level jets) occurring over a horizontal extension of about 20–200 km and therefore provide the foundation for simulations covering urban areas. REWIMET is based on a hydrostatic,

divergenceless and dry atmosphere. In contrast to true three-dimensional models calculating the variables at the nodes of a locally fixed spatial grid, REWIMET uses the fixed grid structure only horizontally. Vertically, the model is subdivided into 3 layers lying on top of each other. A part of the model variables, namely the horizontal wind components, the potential temperature, and the air pollutant concentrations, is calculated for each horizontal grid point as box average in all 3 layers. The vertical wind component, the pressure, and the turbulent flux of impulse, heat and air pollutants are determined at the boundaries between the layers.

The model REWIMET is driven by the suprascale stratification, the suprascale horizontal pressure gradient (geostrophic wind), and the surface temperature. The input of the geostrophic wind and surface temperature can be time-dependent. REWIMET considers the orography and the land utilization in the model domain. The transport of several air pollutants can be calculated simultaneously.

CBM-IV is a popular and sufficiently tested reaction scheme describing the most important chemical processes in the gas phase chemistry for the production of ozone and other photooxidants. It is officially distributed by the U.S. Environmental Protection Agency. CBM-IV is a condensed version of the original CBM. Carbon atoms with similar bonding are treated similarly. There is no need for the definition of an average molar weight so that this mechanism is mass balanced. Some species are handled explicitly, because of their special character in the chemical system (e.g. isoprene which is the most emitted biogenic species). The mechanism involves 34 species and 82 reactions, and contains 9 primary organic compounds. To profit from the features of the CBM-VI detailed information of the hydrocarbon mixture is necessary.

Simulation runs with these complex models REWIMET and CBM-IV have an extensive need for computation time. In order to supply users with results of case studies in acceptable time or to actually allow smog prediction (computation time less than simulation period) the DYMOS system is already parallelized and implemented as message-passing version on parallel computers with Intel i860 and PowerPC processors using tools like PVM. As the model domain of REWIMET and CBM-IV is represented by a 3D grid the model parallelization is performed by grid partitioning.

The parallized version of the DYMOS model described above is incorporated in the SIMTRAP system as the air pollution dispersion and chemistry model part. The major input and output data necessary for a simulation run are given in Table 1.
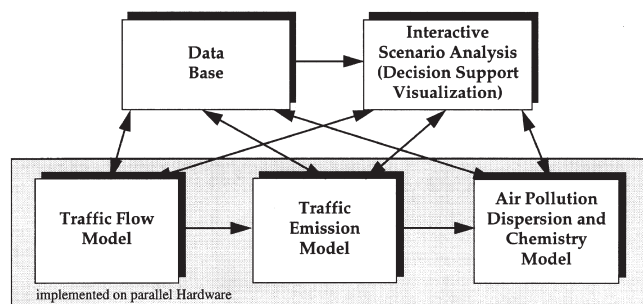

Fig. 1. System architecture and communication links of SIMTRAP.

Table 1
Input–output relations of the submodels

Traffic flow model DYNEMO		Traffic emission model		Air pollutions simulation system DYMOS	
Input	Output	Input	Output	Input	Output
Origin-destination matrix	Traffic volume	Traffic volume		Geostrophic wind (velocity, direction)	Local mean wind per grid and vertical layer
Road network data	Road section coordinates	Road section coordinates		Vertical air temperature and pressure profile	Local mean temperature per grid
Traffic light signals	Driven way from start per vehicle	Driven way from start per vehicle		Mean water temperature	
Fundamental diagrams	Velocity of single vehicle	Velocity of single vehicle		Land use classes per grid	
Desired speed distribution		Exhaust emission factors	Grid emissions per update interval (NO_x, HC, CO)	Grid emissions per update interval (NO_x, HC, CO)	Mean concentrations of air pollutants including photooxidants per grid
		Cold start exhaust emission factors		Mean altitude per grid	
		Emission update interval of the air pollution model		Emission update interval	
		Grid size (1–5 km) of the air pollution model		Grid size	
		Domain size (50–200 km)		Domain size	

3. Traffic emission modelling

3.1. Vehicle type analysis

In view of their different emission characteristics vehicles are classified by engine type. Vehicles with similar parameters, e.g. age, mileage and engine type are grouped in one vehicle layer. It is advisable to classify vehicles according to the following features:

- vehicle type (car, van, truck, bus etc.)
- engine type (gasoline 4-stroke, 2-stroke, diesel)
- engine size
- the concept of emission reduction
- the engine mileage and catalyst mileage.

The percentage of each vehicle layer compared to all vehicles could be extracted from statistical collections of governmental institutions. As yearly mileage reduces with increasing vehicle age, it is recommendable to weight the percentage of every vehicle layer according to its yearly mileage.

3.2. Driving behaviour and exhaust gas emissions factors of the vehicles

Recent studies (TÜV Rheinland, 1987, 1994, 1995) have shown that fuel consumption and emission depend to a large extent on the vehicle speed and its acceleration. Better approaches to estimate traffic emissions can

be assisted by measuring exhaust gases from vehicles under different driving conditions. Comprehensive measurements were carried out by the TÜV Rheinland to obtain the exhaust gas emission factors of different vehicle types depending on their driving parameters. The measured emission factors provide the basis for the calculation of more realistic emission models.

Existing traffic emission models are based on statistical approaches to estimate the driving parameters of the vehicles. Two of the most common approaches use driving cycles or driving pattern for the determination of the emission of a single vehicle. The basis of driving cycles are standardized driving modes with fixed periods of acceleration, continuous speed and stops. Such driving cycles reflect the mean heuristic driving behaviour of vehicles on different kinds of roads.

By driving under the fixed conditions of each cycle the exhaust gas emissions and fuel consumption of different vehicles could be measured in a uniform way. The most common cycles are the 'New European Driving Cycle' (NEFZ), the 'US Test', the 'Motorway Cycle', and the 'Highway Cycle'. Table 2 shows the most important parameters of these cycles. Approximate classifications of road types, local road conditions, and traffic density limit the quality of the calculated emissions, especially in urban areas.

A more advanced statistical approach, that is the approach of driving patterns, is based on statistical investigations of the driving behaviour of vehicles on

Table 2
Parameter of the driving cycles

Driving cycle	Mean speed (km/h)	Speed $v_{min} - v_{max}$ (km/h)	Percentage of stops
New European Driving Cycle (NEFZ) inside of cities	19	0–50	31
NEFZ outside of cities	63	0–120	10
NEFZ	34	0–120	24
US-Test-75, Phase 1/3	41	0–91	20
US-Test-75, Phase 2	26	0–55	19
US-Test-75	34	0–91	19
Highway	78	0–96	< 1
Motorway, $v_{max} > 150$ km/h	118	86–162	0
Motorway, 130 km/h $< v_{max} \leq 150$ km/h	110	86–139	0
Motorway, $v_{max} \leq 130$ km/h	107	90–124	0

Table 3
Classes of driving pattern on urban roads

| Driving pattern	Characteristcs	Percentage of constant speed	Percentage of stops	Mean speed (km/h)
1	Area sources (side streets)	31.8	5.3	18.6
2	Line sources with non controlled traffic lights, high density of buildings	23.3	32.5	19.9
3	Line sources with non controlled traffic lights, low density of buildings	36.6	13.5	32.0
4	Highway (lower category), driving in towns	26.2	15.3	37.5
5	Line sources (main streets), low density of buildings, controlled traffic lights	52.2	0.6	46.2
6	Highway (unsteady)	27.9	1.1	60.6
7	Highway (lower category) Line sources (controlled traffic lights, speed > 50 km/h)	46.2	0.7	58.4
8	Highway with acceleration shares (e.g. leaving towns)	35.3	0.2	78.3
9	Highway (steady) with braking shares (e.g. driving into towns) Highway (lower category)	39.5	0.7	72.0
10	Highway (steady)	59.6	0.7	76.7
11	Stop and Go inside cities	48.0	52.0	5.3
12	Stop and Go on motorways	16.3	23.0	9.4
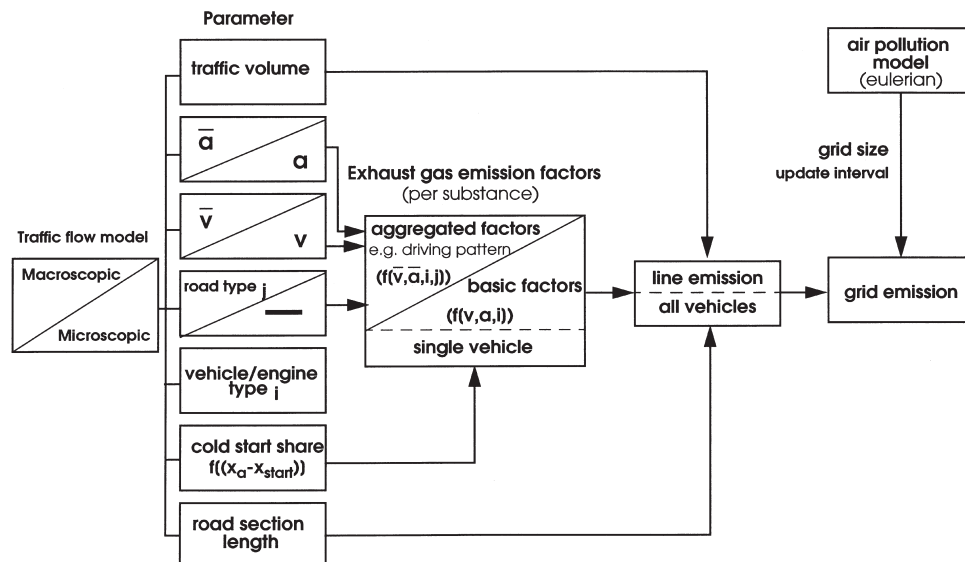
Fig. 2. Emission modelling flow chart.

different kinds of city roads and highways. In several cities in Germany measurements of speed, acceleration and exhaust gas of vehicles as well as the registration of the geometry and the traffic conditions on the road were carried out to find significant classes of driving pattern with its specific emission factors for each vehicle layer. In Table 3 the observed pattern with similar features is described (TÜV Rheinland, 1994). The application of this approach involves a considerable effort to classify the road network.

A disadvantage of all statistical emission models is the limited accuracy of the dynamic behaviour of a single vehicle and the determination of the traffic density. An exact analysis of speed and acceleration in certain situations (e.g. stop-and-go at traffic lights, stop-and-go scenarios in overcrowded roads) can only be performed by means of traffic flow models. Currently, simulation systems for traffic emission coupled with a traffic flow model do not exist. However, they would greatly improve the dynamic description of the emissions.

In Fig. 2 an emission calculation flow chart is shown. Traffic flow models are classified by its type into microscopic or macroscopic models, which differ in the number of parameter and their level of detail, e.g. in expressing the dynamics of the vehicles, the number of included submodels to describe the interaction between the vehicles as well as the features of the road network (for further details see next section).

After coupling the emission model with a microscopic traffic model, the emission calculation requires exhaust emission factors for each vehicle layer (class of vehicles with similar engine features) as a function of velocity and acceleration.

If such a level of detail cannot be provided, aggregated emission factors for each vehicle type layer have to be used. In this case the exhaust emission factors reflect the average emission with respect to the road type (including mean velocity and acceleration behaviour) on which the vehicle is actually driving. The traffic flow model has only to provide the traffic volume per road section as well as the actual road type.

However, there is one important fact considerably affecting the amount of emission that has to be pointed out here. As long as the engine and the catalyst (when available) have not reached their operating temperatures, the cold start emissions are considerably higher. Especially during the first five kilometres the exhaust emissions per substance increase by a percental add in depending on the outside temperature and the vehicle type. In Fig. 3 the cold start behaviour of a catalyst car is shown for different exhaust gases (CO, NO$_x$ and HC).

In the SIMTRAP project the traffic emission model is included in the traffic flow model. The input data required for a simulation run and the received output data are given in Table 1.
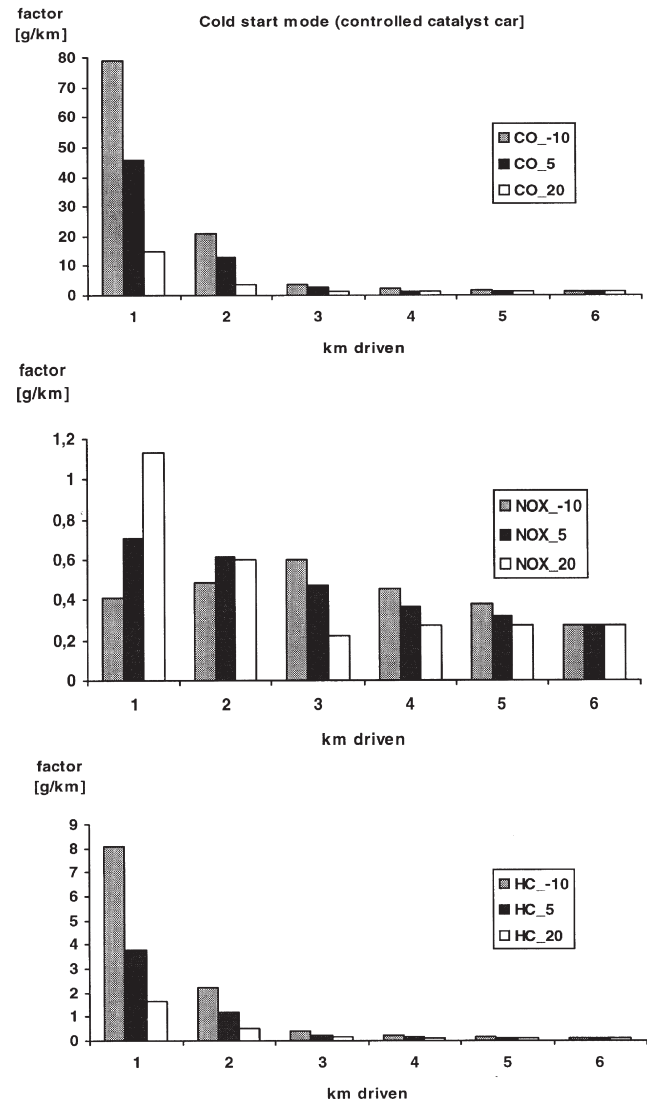

Fig. 3. Cold start mode for catalyst cars (1.4–2 litres), temperatures − 10, 5, 20°C). Source: TÜV Rheinland (1994).

4. Traffic flow models

4.1. Overview

Traffic flow models are an approximated description of specific phenomena within the traffic flow operations, normally based on a set of mathematical equations or on an analogy to other physical systems.

There are two basic concepts in traffic flow simulation: the microscopic concept based on the driver behaviour and the interaction of individual vehicles, and the macroscopic concept based on the hydrodynamic theory. Apart from this classification, some modifications and derivations exist such as the follow-the-leader concept, gas kinetic (Boltzmann-like) models, fluid dynamic models and cellular automaton models (Prigogine and Herman, 1971; Kerner and Konhäuser, 1993; Helbing, 1995). However, the scientific world is

still searching for the most suitable approach for an effective and environmentally tolerable traffic control.

Microscopic traffic flow models describe the interaction of individual vehicles which in turn depend on the vehicle drivers. Depending on the sophistication of the model, each vehicle in a road network may be described by its position $x(t)$, its actual velocity $v(t)$, its desired velocity $v_{wu}(t)$, its route from an origin to a destination, its tendency to pass other vehicles, characteristics of the drivers behaviour, and the vehicle type. Clearly, the computational effort for these models is increasing rapidly with the number of vehicles within the system. The advantage of microscopic simulation of the traffic flow is that the user has complete information about the state of the vehicles in the system over time and space.

The second model class, the macroscopic models, use aggregate variables such as traffic density ρ, mean speed $\bar{v}$, and volume q to describe the traffic flow. This model class is based on the hydrodynamic theory. Under the assumption that the traffic flow can be considered as a compressible medium, the following equation of continuity for a one-dimensional flow reads as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho \bar{v}) = 0.$$

Due to the representation of the state by aggregate variables, the computational requirements here is much smaller than with microscopic variables. On the other hand, macroscopic models are not able to provide information about travel time, fuel consumption or route choice.

4.2. The traffic flow model DYNEMO

The mesoscopic traffic flow model DYNEMO (Schwerdtfeger, 1994), as shown below, combines the advantages of microscopic and macroscopic models. For each stretch in the network the model needs as input the relationship between traffic density and mean speed. Fig. 4 shows this fundamental relationship, which represents the macroscopic behaviour of the model.

The relationship reflects the fact that the behaviour of a driver strongly depends on how many vehicles he/she notices on the road and particularly on the distance to the vehicle immediately in front. Actually, this relation is only valid in the stationary and spatially homogeneous case. The maximum value of traffic density ρ_{max} depends upon the vehicle length, and on the distance bumper to bumper (spacing when they come to a stop). The value v_{free} characterizes the free flow state where the mean speed is nearly independent of the traffic volume.

A basic assumption of the microscopic part of DYNEMO is that each individual vehicle-speed at a given traffic condition characterized by its density varies within the interval $[\tilde{v}(\rho), \tilde{v}(\rho)]$. The actual speed v of a vehicle depends on its desired speed v_{wu} and is restricted by the given interval. Therefore, for vehicles with the maximum desired speed (i.e. $v_{wu} = \tilde{v}_{wu}$) we have $v = \tilde{v}$, whereas for vehicles with the minimum desired speed (i.e. $v_{wu} = \tilde{v}_{wu}$) we have $v = \tilde{v}$. Furthermore the transition from partly constrained to constrained traffic is assumed to occur in the neighbourhood of the maximum of the curve shown in Fig. 4. Here, the mean speed of this point is denoted as v_{opt}, although it is an open ques-
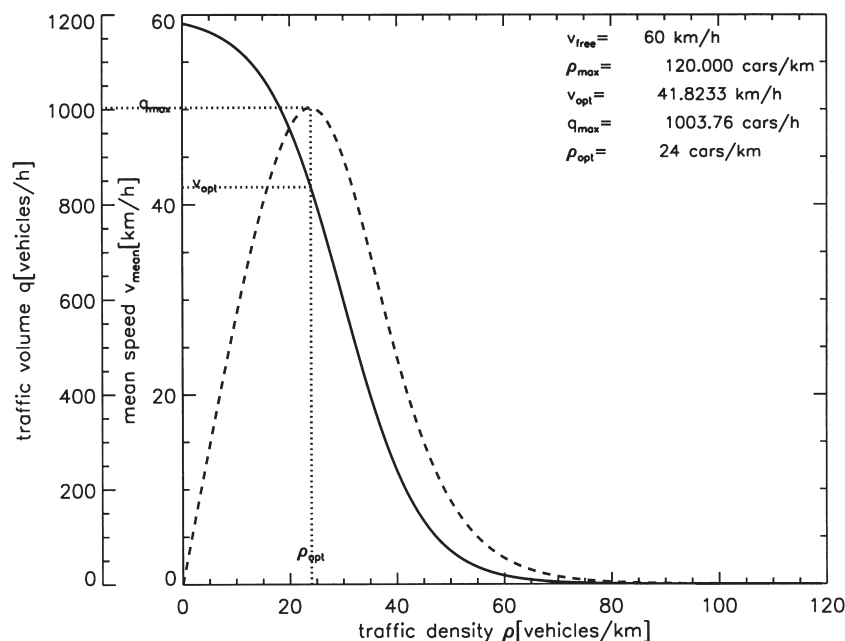

Fig. 4. Fundamental diagram of the street: relation between the mean speed respectively traffic volume and traffic density.
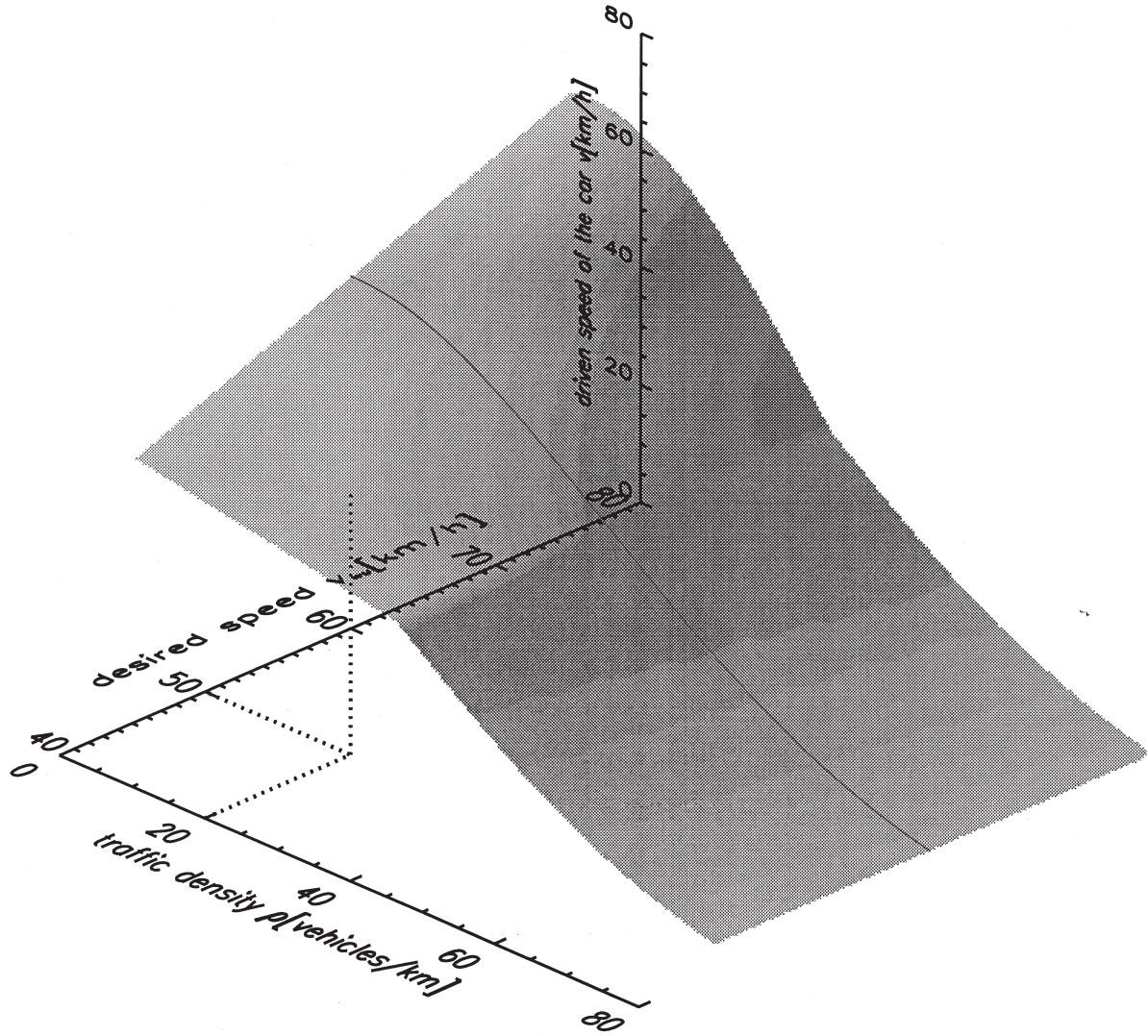
Fig. 5.   Behaviour of the speed of an individual vehicle depending on the traffic density and the desired speed of the driver.

tion whether the traffic flow at the maximum volume is in every respect optimal. Under these assumptions the speed of an individual car is

$$v(\rho) = \begin{cases} \tilde{v}(\rho) + \dfrac{v_{wu} - \underset{\sim}{v}_{wu}}{\tilde{v}_{wu} - \underset{\sim}{v}_{wu}}\,(\tilde{v}(\rho) - \tilde{v}(\rho)), & \rho > \rho_{opt} \\ \bar{v}, & \rho \le \rho_{opt} \end{cases}.$$

The limiting values $\tilde{v}(\rho)$ and $\tilde{v}(\rho)$ have to be chosen so that the expected value of the individual speeds is equal to the mean speed of the fundamental diagram, that is

$$E(v(v_{wu})) = \int_{\underset{\sim}{v}_{wu}}^{\tilde{v}_{wu}} v(v_{wu}) f(v_{wu})\, dv_{wu} = \bar{v},$$

where $f(v_{wu})$ denotes the probability function of the desired speed. When v_{wu} belongs to a symmetric distribution and

$$\tilde{v}(\rho) = 2\underset{\sim}{v} - \underset{\sim}{v}(\rho),$$

the equation above is always satisfied. Finally, the actual speed of the vehicle is obtained from

$$v = \left(1 - \frac{x}{l}\right)v_i + \frac{x}{l}\,v_{i+1},$$

where x denotes the actual position, i the number of the stretch, and l the length of the stretch. This reflects the anticipation of changing traffic conditions. The resulting speed of an individual vehicle depending on the traffic density and the desired speed of the driver is shown in Fig. 5.

The model described above is implemented on a paral-

lel computer to speed up the calculations. The inherent structure of this traffic model favours a domain decomposition as a general approach to parallelization. Nevertheless, traffic modelling partly generates irregular problems.

4.3. Parallelization of the traffic flow model

The simulation of large traffic networks with huge numbers of cars requires considerable run times. The traffic flow model DYNEMO has been parallized in order to speed up this simulation process. One of the major problems is to develop a suitable communication structure of the parallel processes. First results shown that an ordinary master slave topology seems to be well suited.

The master process is responsible for supervising the slaves, the initialisation and decomposition of the traffic network as well as for such tasks which require information of the state of the whole network, e.g. the dynamic route choice. During one time step, each slave calculates the spatial motion of the vehicles situated on their subnetworks. The slaves are arranged on a nonregular grid. The shape of this 2D-grid depends on the decomposition of the network.

In fact the decomposition has to satisfy partly contradictory aims. On the one hand the decomposition should provide possibly large coherent regions of the subnetworks with minimal interconnections (stretches) between the subnetworks. The number of stretches influence the number of cars moving to a neighbouring subnetwork. Since car exchange between subnetworks

requires time for interprocessor communication this approach guarantees a minimal communication effort. On the other hand the decomposition has to ensure a nearly equal-distributed workload on all physical processors. This workload depends not only on the number of stretches or lanes but also on the number of vehicles driving on the subnetwork. Unfortunately the traffic on the roads is a priori unknown and may change rapidly. Consequently, a dynamic loadbalancing may be required. In case of a dynamic load balancing a rearrangement of the topology of the communication structure has to be performed from time to time. Since this procedure is very time consuming we only have set up this option at the moment. At a later time we will decide whether to implement the dynamic load balancing depending on the run-time results or not.

The traffic flow model has been implemented by means of the PVM (Geist et al., 1994) message passing model. This version is incorporated in the SIMTRAP system. Major input and output data are given in Table 1.

5. First results of an application example

The example will briefly represent some results which were received in simulation scenarios running on the system components as described before. The considered region comprises the German cities Berlin, Potsdam and Brandenburg, covering an area of 150×150 km with about 5 million inhabitants. For the calculation of the traffic induced emission rates a road network has been used taking both major city and rural roads into account.

Fig. 6.   Calculated CO traffic emissions (g/km·h) of the inner city of Berlin.
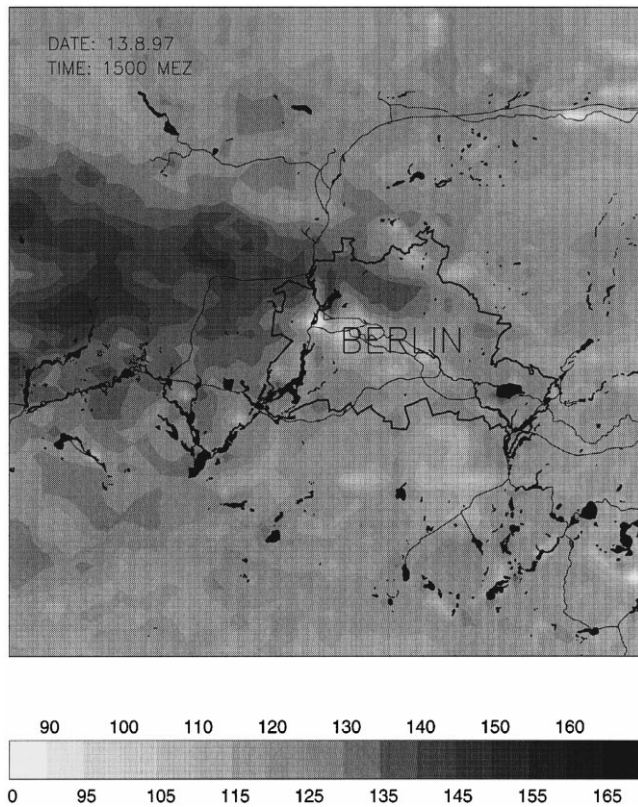
Fig. 7. Calculated ozone concentration in $\mu g/m^3$ for the Berlin/Brandenburg region.

simulation results are similar to the measurements taken at the Berlin Air Quality Monitoring Network (BLUME) with more than 70 measuring points, and to former measurement flights of a special equipped aircraft.

In addition to the traffic, most of the essential industrial pollutants are represented in the emission inventory. The contribution of the households has been estimated on the base of the number of inhabitants.

For a better illustration of the results the following figure only concentrates on a smaller part of the network-the inner city region of Berlin. This subnetwork consists of 152 traffic zones, 443 nodes, and 1076 links and it has been built by the Senate of Berlin. The traffic simulation includes priority rules and traffic light phasing schemes for the intersections. Fig. 6 illustrates the cumulated CO ejections of the cars on different roads. The gray shades denote different emission levels.

The dynamic traffic emissions together with pollution from industry and households are transferred to the DYMOS air pollution dispersion model. In Fig. 7, the result of a simulation with DYMOS showing the ozone concentration for a hot summer day in 1997 with temperatures up to 32°C and low winds from the east. The values of the ozone concentration are given on a 2×2 km grid for the extended region of Berlin/Brandenburg. The figure indicates that the highest ozone level usually occurs in the wind plume outside of the inner city. The

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