A Model Based Tool for Environmental Risk Management after Accidental Atmospheric Release of Toxic Substances

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Abstract The paper describes the system design of an air pollution emergency system and presents application results. The simulation system is able to compute the dispersion of toxic substances from stationary or mobile sources with better-than real time performance. The air pollution emergency system consists of a set of source strength estimation modules, a three-dimensional wind field model which serves as a meteorological preprocessor and a 3D dispersion model. It considers different potential release types to estimate the release rate of the toxity. Monte Carlo methods are used to take into account input data uncertainties. A time dependent source term probability function gives the emission rates serving as an input for a Lagrangian dispersion model. The code of the individual software packages was parallelized using different parallelizing strategies according to its inherent programming structure. This offers the possibility of using advanced models in conjunction with uncertainty analysis methods for emergency management calculations but also enhances the acceptance of model use for training and analyzing tasks.

1. INTRODUCTION

LAGSIM (**LAG**rangian **SIM**ulation System) is a model-based software system to compute release and dispersion of chemically inert substances in complex terrain. Using distributed parallel computing, LAGSIM aims at reaching better-than real time performance for the simulation of accidental release of hazardous substances into the atmosphere, using state-of-the-art 3D simulation models. This information can be used in the framework of decision support and advisory systems for the support of emergency management tasks and related staff training, for transportation and stationary accidents involving hazardous substances, and for hazardous installations. In addition to connecting the HPC (High Performance Computing) simulations to various data sources, primarily environmental and meteorological monitoring, LAGSIM explores an additional important aspect of HPCN (High Performance Computing and Networking) based decision support applications, namely, the on-line integration of uncertainty and error analysis, based on Monte-Carlo methods again realized by parallel simulation. With distributed parallel high-performance computing resources, dispersion calculation results can be provided in better than real-time mode.

2. LAGSIM-THE MODELS

LAGSIM uses a number of models for describing technological risk and emergency situations. These primarily include models for:

- the computation of the release of (toxic) chemicals (release models)
- dispersion calculation (a Lagrangian transport model)
- wind field estimation (a 3D diagnostic wind field model).

One of the most important features of an atmospheric emergency simulation system is the computation of a realistic wind field in a complex terrain. The methodology used to design the core part of the LAGSIM wind field model is similar to the well-know Diagnostic Wind Model [Douglas 1990]. The wind field model generates gridded wind fields at a specified time. Initialized with a stability dependent 1D profile of wind and temperature, it adjusts the domain-scale mean wind for terrain effects [Allwine 1985, Liu 1980, O'Brien 1970] , e.g. kinematic effects, such as lifting and acceleration of the air flow over terrain obstacles, as well as thermodynamically generated slope flows. It performs a divergence minimization to ensure mass conservation. The diagnostic wind model is based on a digital elevation map of the model domain. A grid based mean elevation for

every grid for the desired resolution must be provided by the customer.

A typical application range of the model extends from medium scale to regional scale and covers vertical levels up to the mixing height. The model is not able to resolve very local wind structures, e.g. lee waves at a building, however it provides a mean wind field and diffusion parameters for the area of interest.

The model system for the computation of the source strength consists of different individual submodules with regard to the release type. The LAGSIM system includes:

- jet release of gas,
- stack release,
- evaporating pool release,
- time-dependent line sources emissions.

If the source strength is known, the release models are no longer necessary or perform very simply. However in case of an accident, very often only some geometric quantities (e.g. of a spill) are known. Most of the parameters needed for the source strength estimation are very uncertain. To take these uncertainties into account, a Monte Carlo simulation is used to determine a source strength distribution over time instead of a single number for the source strength. Key parameters of these time dependent distributions are used as an input for the dispersion model. Such key parameters can be, for example, the emission rate at the mean and at the 95th percentile of the probability functions.

Although explosion or burning may also be important release types, their explicit handling in the system is impossible for practical reasons (no data, expensive computational burden). With a high level of probability, an immediate total release of the substance can be assumed for explosions. For release types due to burning, the determination of the source strength and the properties of the released substances may be very uncertain. However, this is a basic problem, and not merely a problem of the modelling tools. For fire type release, the applied methodology is similar to buoyant jet release, taking into account the especially broad range of uncertainty for the model input parameters. The input for the release models is formed by a set of substance specific parameters and a set of release specific parameters such as release type, release and meteorological conditions.

Release and atmospheric quantities form the input of the Lagrangian type atmospheric transport model [Gerharz 1997]. The basic concept of Lagrangian models is the observation of air volumes or airborne particles, which is why these models are also referred to as Lagrangian particle simulation models. The term "particle" denotes any air pollutant or any buoyant substance in the air. In case of gaseous dispersion, every particle represents a certain mass although it is assumed to be mass free regarding to its transport behavior. Additionally, it has no spatial extension. In contrast to Gaussian models, which are based on an analytical solution of the advection diffusion equation applicable only under very restricted conditions such as homogeneous, stationary meteorology and flat terrain, Lagrangian trajectory models are appropriate for the description of dispersion in complex meteorological situations or heavily structured topography.

The Lagrangian model uses winds and fluctuation caused by turbulence to predict the pathways of individual particles or air volumes and register modifications in their characteristics for each time step. Particles or air volumes, respectively, may be released from any number of locations. The type of source, e.g. point or line source, is of no influence. The underlying basic methodology of the model can be described as follows: The position of a particle is given by its previous position plus a term describing the motion by advection processes and turbulence. The advective wind is completely determined by the velocity and direction of the wind, while the fluctuation or turbulent component describes the actual fluctuation. The simulation of turbulence is based on the statistical theory of Taylor [1921] for diffusion effects, and an extension made by Obukhov [1959] and Smith [1968]. The fluctuation is simulated by a Markov process of first order, a random component describes the coincidental effects in diffusion. If required and the deposition velocity of the substance is known, deposition effects can also be considered each time the new position of a particle is determined. The main advantages of the Lagrangian model to the analytical solution of the advection diffusion equation or even to the numerical solution in a Eulerian approach of the equation can be summarized as follows. It

- is able to describe transport in complex terrain,
- is easy to parallelize and is therefore suitable for HPCN,
- shows good accuracy/performance ratio
- is scalable over a wide range (from a few centimeters to some kilometers).

On the other hand, the particle methodology is not well suited to treat chemical reactive species. As long as the reactions can be described by a linear rate, chemistry can easily be included. But for complex nonlinear chemical reactions, a Eulerian approach should be used. For emergency management purposes, the computation of chemical changes is irrelevant due to the lack of

detailed information of the chemical reaction paths and reaction rates.

3. PARALLELIZATION

For emergency planning and especially for emergency management purposes, the system has to provide a result in a period of time at least an order of magnitude shorter than real time. This requires rapid data management as well as a fast execution of the underlying models.

To date, simple screening models have been used for these purposes. These models are very fast, but very limited in their application because they normally assume a flat terrain and do not allow complex wind fields as an input, although a realistic determination of the wind field and its use in the transport model provides the basis for a reliable concentration calculation. Another drawback of these models is that, although the quality of the input parameters is often very questionable, they are considered as known.

The LAGSIM approach uses advanced models in conjunction with uncertainty analysis methods. In general, the execution of this system in an appropriate resolution is too slow for emergency management purposes. To accelerate the execution, the numerical algorithm must be optimized with respect to the run-time requirements. Also, the use of fast hardware platforms is necessary which implies, of course, an expensive supercomputer. However, only a small number of customers possess or have permanent access to such a machine. To guarantee fast execution and flexible installation options, the time-consuming parts of the model code have been parallelized. An advantage of this approach lies in the flexibility of the installation. Wherever a cluster of workstations is available, irrespective of type, the program can be employed with the appropriate underlying software. The code remains scalable, depending on the actual number of workstations or CPU's the program is able to run on different configurations. The parallelizations use the paradigm of Parallel Virtual Machine (PVM) [Geist 1994]. PVM is a software package that allows the use of a heterogeneous computer cluster interconnected by a network as a single parallel computer. This guarantees a maximum of flexibility and portability to a variety of hardware platforms.

One of the main features of the wind field model is the solution of the continuity equation. In its simplified formulation, a divergence minimization procedure ensures the construction of a mass-consistent wind field. The divergence minimization is an iterative process using a predefined tolerance (a reasonably small margin of around 0.0001). This

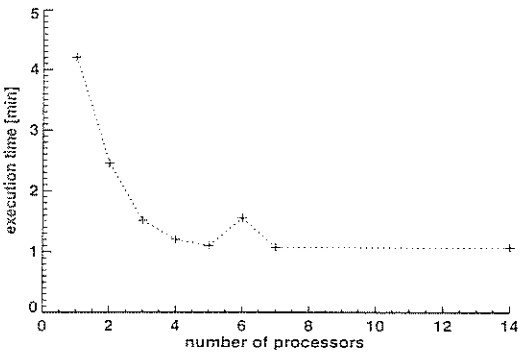

Fig. 1: Execution time vs. number of processors for the wind field model

process can easily count for more than 90 % of the total CPU time of the sequential execution of the wind field model. The parallelization exploits the independence of the divergence computation in every vertical level. The different vertical levels are distributed step-wise among the processors, beginning from the bottom. Usually, the layers close to the surface show the largest divergences, therefore requiring many more iteration steps before obtaining the accepted tolerance criteria for the levels at the top of the domain. This results in a strong load balance problem if the number of nodes is not appropriate in relation to the number of vertical levels used. An alternating distribution scheme of the vertical levels and a proper selection of the number of levels improves the load balancing significantly. The optimum configuration of a SUN cluster for the wind field model consists of 5 machines for the given test grid. The speed-up is rather high, reaching a value of approximately 4.2 with a total execution time in the range of 1 minute which meets the user requirements (Fig. 1).

The parallelization of the Monte Carlo process for the evaporation model is based on the complete independence of each parameter run. Thus the same segment of code runs for the total time sequence on the selected number of nodes (or workstations). The user must specify the number of input parameters which are not precisely known. In addition, an uncertainty range must be given for every parameter. This range can vary in positive or negative direction. In the initialization phase of the program, the master starts with a large but reasonable number for defining the first-guess source strength distribution. A predefined rule system for the program truncation helps to check whether a nearly smooth distribution has been reached. If not, more runs are executed until the truncation rules are valid. The truncation rules take into account the derivation of statistical characteristics of the distribution, e.g. the mean of the distribution, between two steps. If it exceeds a

given epsilon (reasonably small number), another set of simulation starts.

In the Lagrangian approach to the dispersion calculation, concentrations are represented by particle densities. The model uses winds and fluctuation computed by the wind field model to predict the trajectories of individual particles or air volumes. As long as an output time step has not been reached, the individual particles can be considered as fully independent. This makes the model well suited for numerical parallelization. The amount of emitted particles per time step representing a certain released mass is usually chosen to an acceptable but relatively small number. Unfortunately, no method has been established for determining the appropriate number of particles for a desired application. Thus the selection of this number is often left to choice, or the number is limited by the hardware resources. Insufficient particle numbers lead to unrealistic results, bad resolution and rippled concentration patterns. Nevertheless, the question of determining the appropriate particle number still remains. Test runs cannot be generalized and can only serve as a first approach. In order to ensure that calculations are, in most cases, on the "right side", the use of somewhat large particle ensembles derived from test runs with different particle numbers is recommended. However, neglecting the time required for an output (and computing the related concentration patterns), the execution time is nearly linearly proportional to the number of transported particles. A parallel implementation offers the possibility of using a large set of particles and guarantees a reasonable execution time. Fig. 2 shows a result of a run-time study with the Lagrangian particle model. The results indicate an

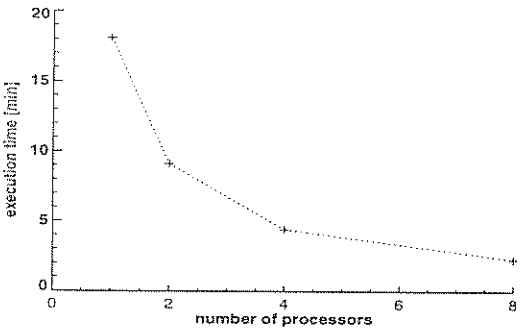

Fig. 2: Execution time vs. number of processors for the Lagrangian model

ideal speed-up of 8 for 8 processors and a reduction of the total execution time from approximately 1085 seconds for the single processor run to 136 seconds for the cluster of 8 processors. Additionally, the problem remains scalable which offers the possibility to enlarge the number of processors considerably, with an expected further reduction of the execution time.

The bottleneck of efficiency can be found in the final output computation. As soon as a concentration calculation is required (because an output is desired), the particles are no longer independent and communication becomes necessary. Therefore, the number of output intervals should be reasonably small in order to avoid excessive decrease of the speed-up of the parallel implementation.

Run-time studies indicate that with the help of a code parallelization of the core parts of the model system a considerable decrease of the run-time can be achieved. By conducting some further optimizations, the total execution time of a full run of the model system in the air domain including Monte Carlo uncertainty analysis, three-dimensional wind field generation and Lagrangian transport calculation can be reduced to approximately 10% of real time.

4. APPLICATION EXAMPLE: TOXIC SPILL OF CHLORINE IN THE SWISS REUSS VALLEY

Transsecting the Swiss Reuss valley, a major transeuropean transportation route links the north of Europe to the south, from Switzerland to Italy, via the Alpine Gotthard pass. It is frequently used by trucks as well as railways transporting toxic substances and other chemicals.

The Reuss valley is relatively flat at the bottom, approximately 450 m above sea level with steep mountain slopes rising to a height of 3000 m. The alpine wind systems driven by kinetic and thermal effects are very complex. Therefore, predictions of areas affected by toxins in case of an accident are nontrivial. An example of a predicted surface wind field with North-West synoptic scale wind and slightly stable meteorological conditions is shown in Fig. 3. Within the Reuss valley, the wind comes from different directions. On the slopes, a tendency of weak down-slope winds is visible. Accidental release of toxic materials in the atmosphere, especially in this environment, can severely damage human health. To investigate the results of an accidental release of toxic materials in the valley, three typical meteorological conditions were analyzed:

- scenario 1: strong winter inversion layer, weak synoptic wind from north-west
- scenario 2: moderate winter inversion, moderate synoptic wind from north-east (see Fig. 3)

- scenario 3: Föhn, strong synoptic-scale wind from south, deep convection

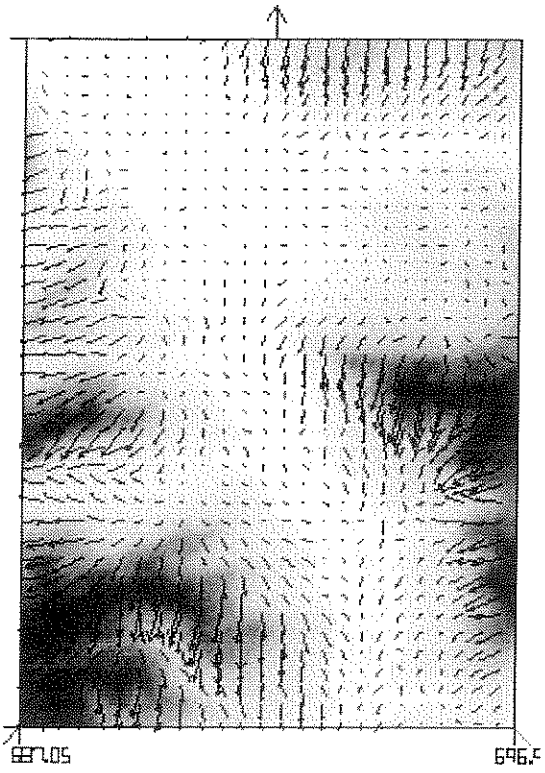

Fig. 3: Wind field above orography in the Swiss Reuss valley for scenario 2

The release location was close to the entry of a side valley, near the village Bürglen. Toxic spill of 5 tons of liquid chlorine was assumed. The liquid chlorine vaporizes relatively fast depending on the leakage geometry and the meteorological conditions. A Monte Carlo method was used to vary these input parameters for the evaporation pool release model. Rather than using a single value, a time dependent source strength probability function serves as the input for the dispersion calculation. The emission maxima for the three different scenarios for the mean and the 95th percentile are given in Tab. 1. For the same meteorological scenario, the rates are considerably different caused for the most part by the [illegible] because of the [illegible] the mean and the emission rate at the 95th percentile of the time dependent source term probability function are used as an input for the Lagrangian dispersion model. The mean represents a rate close to the most probable emission rate, whereas the 95th percentile represents a worst case scenario for the emission rate excluding a small probability of 5 percent of higher emission rates. The difference between the rates of the three scenarios reflects the dependence of the evaporation from meteorological quantities at the source location. The simulated average

scenario	maximum mean emission rate [g/s]	maximum emission rate of the 95th percentile [g/s]
scenario 1	280	750
scenario 2	450	1100
scenario 3	1100	3000

Tab. 1: Maximum emission rates for three different meteorological scenarios

maximum concentration in an area of about $100x100m^2$ is given in Tab. 2. Although the maximum emission rate increases from scenario 1 to scenario 3, the maximum concentration decreases because of the given meteorological conditions. Under stagnant meteorological conditions, represented by scenario 1, a low inversion layer develops. This prevents deeper thermal convection and can lead, in conjunction with calm synoptic winds, to high surface concentrations of toxic materials close to the release location. In contrast to scenario 1, higher wind speeds at the ground, upslope winds and higher vertical mixing lead to a faster dilution with the ambient air for scenario 3.

scenario	maximum concentration for the mean emission rate [$g*m^{-3}$]	maximum concentration for the emission rate of the 95th percentile[$g*m^{-3}$]
scenario 1	138	360
scenario 2	100	253
scenario 3	85	205

Tab. 2: Maximum simulated concentrations for three different meteorological scenarios

The surface concentration distribution in the model domain 20 minutes after the accident for scenario 2 is shown in Fig. 4. The toxic plume remains within the valley, the influence of the valley's geometry determines its shape. Although the main wind blows from the north-east, the flow is north-

westerly directed in the source-near areas due to local wind systems. Later on, it follows the shape of the valley and side-valleys.

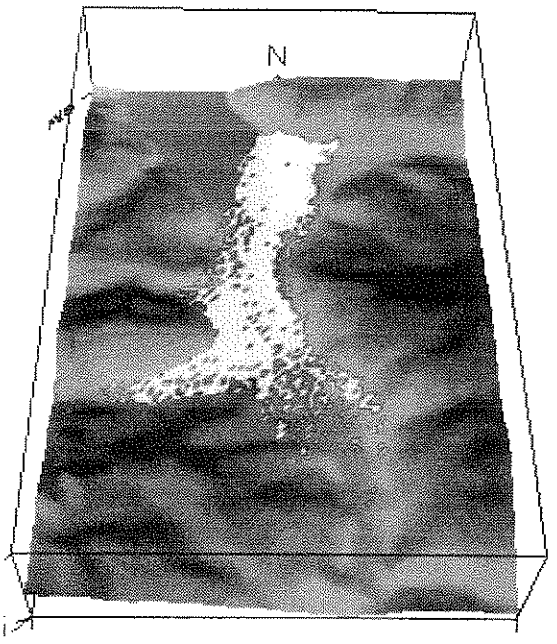

Fig. 4: Simulated chlorine concentration in the Reuss valley after 20 minutes for scenario 2

The dispersion calculation for the alpine terrain in the Swiss Reuss valley exhibits completely different and very complex concentration patterns of chlorine for different meteorological conditions. These results provide qualitatively new insights for intervention forces and management authorities.

5. CONCLUSIONS

LAGSIM has been successfully applied in a number of investigations of toxic release in complex terrain, for example in the Swiss Reuss valley and in Gavirate near Milan (Italy). It has also been chosen as the core model part for the development of an emergency management system (HITERM - High-Performance Computing for Technological Risk Management). The HITERM system integrates various simulation models (e.g. it includes most of the LAGSIM components) for describing technological risk and emergency situations. In particular HITERM is based on:

- models for chemical spills or runaway/ undesirable reactions, leading to atmospheric dispersion of a toxic gas or evaporating liquid, fires and explosions of a gas, liquid or evaporating liquid, transport and dispersion in soil, groundwater and surface water systems,
- pre-processor codes such as 3D diagnostic wind field models and source models such as spill/ pool or tank evaporation models,
- routing algorithms for transportation risk analysis,
- impact models.

The applications of the HITERM system cover also dynamic adaptive traffic routing taking into account dynamically updated environmental risk criteria and transportation accident simulation to address transportation risks of hazardous goods by road and rail.

6. ACKNOWLEDGMENTS

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7. REFERENCES

Allwine K.J., Whiteman C.D., MELSAR: A Mesoscale Air Quality Model for Complex Terrain: Volume1-Overview, Technical Description and Users Guide. Pacific Northwest Laboratory, Richland (PNL-5460), 1985.

Douglas G.S., Kessler R.C., Carr L., User's Manual for the Diagnostic Wind Model. EPA-450/4-90-007C, 1990.

Geist A., Beguelin A., Dongarra J., Jiang W., Manchek R., Sunderam V., PVM: Parallel Virtual Machine, A User's Guide and Tutorial for Networked Parallel Computing. The MIT Press, Cambridge, Massachusetts, 1994.

Gerharz I., Lux Th., Sydow A., Inclusion of Lagrangian Models in the DYMOS System. In Proceedings of the IMACS World Congress 1997. (Berlin, Germany, August 25-29). W&T, Berlin, 6: 53-58, 1997.

Liu M.K., Yocke M.A., Siting of wind turbine generators in complex terrain. J. Energy, 4: 10-16, 1980.

O'Brien J.J., Alternative solutions to the classical vertical velocity profile. *J. Applied Meteorol.*, 9: 197-203, 1970.

Obukhov, A. M., Description of Turbulence in Terms of Lagrangian Variables. *Advances in Geophysics*, 6, 113-116, 1959.

Smith, F. B., Conditioned Particle Motion in a Homogeneous Turbulent Field. *Atmospheric Environment*, 2 , 491-508, 1968.

Taylor G.I., Diffusion by Continuous Movements. London Mathematical Society, 20: 196-211, 1921.