ATLANTIC AREA
Transnational Programme
INVESTING IN OUR COMMON FUTURE

European Union
European Regional Development Fund

ARCOPOL

Airborne Pollution Propagation from water incidents:

State of the art of air pollution models

Activity 4

Task 4.2.1

ARCOPOL

The Atlantic Regions' Coastal Pollution Response

Version:	**Version 2**
Last updated on:	**05/11/2010**
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1. Executive Summary

Pollution caused by spillage of hazardous and noxious substances (HNS) is an extremely challenging issue that represents a severe threat to coastal regions. Some of the HNS or hydrocarbon substances have the potential to rapidly evaporate in contact with the water surface. Hence releasing of some chemical substances evaporating under the weather conditions can generate vapour clouds that might be toxic or form an explosive mixture with air. As a result, there may be potential health and safety implications for vessel crew, responders and population nearby. In order to plan a response, it is relevant to understand the behaviour of gas or vapour and the likely trajectory of hazardous clouds. Modelling of the spreading of airborne contaminants will help to forecast the movement and fate of the plume as it disperses, allowing the advisory of the public of potential dangerous zones or finding safety places.

To achieve this goal it is necessary to review the currently available models that can be applied in the geographic area ARCOPOL project. This collection shows the advantages and disadvantages of explained models, and a discussion about their degree of suitability to the objectives of ARCOPOL project.

2. Context and aims of the task

This document deals with the application of air quality models. These models are mathematical tools used to quantify concentrations of air pollutants as a result of emissions to ambient air. These mathematical tools are chiefly based on physical and chemical processes but may also be derived based on statistical relationships.

The structure and form of this document is intended to facilitate model users in determining the requirements, possibilities and limitations when using models for applications in regard to safety rules and air quality laws. The document covers the following topics:

- ✓ a summary of the European Air Quality Directive

- ✓ an interpretation of the European Air Quality Directive in regard to the use of modelling
- ✓ a summary on reporting requirements to the European Commission when modelling is used
- ✓ an overview of model types and model requirements for application to air quality rules
- ✓ information on the availability of input data for models

2.1. Summary of the 2008 Air Quality Directive

The "Directive 2008/50/EC" of the European Parliament and of the Council on ambient air quality and cleaner air for Europe was officially adopted by the European Parliament on the 21 May 2008 (EC, 2008). In addition, reference is also made to the Directive on heavy metals and PAH (EC, 2005), as this is will remain valid. In this document we refer to these two collectively as the "European Air Quality Directive" or simply the "AIR QUALITY Directive".

This chapter summarises the AIR QUALITY Directive in regard to the thresholds, limit values, critical levels, reduction targets, target values, etc. Most of this information is contained in *Annex II, VII, XI, XII, XIII and XIV of AIR QUALITY Directive.*

2.1.1. Concepts and definitions

In this section a number of terms and concepts necessary to understand the air quality directives are given. For an official interpretation of all terms the reader is referred to the Air quality laws themselves.

Table 1. List of the terms and their definition contained in the Air Quality Directive

Concept	Meaning
Emissions	Fumes discharged from vehicle exhaust pipes, chimneys and other sources, which then mix with the ambient air, are diluted and dispersed by the wind. In the course of this transportation process, foreign substances are able to interact, forming new pollutants .
Immission or ambient air quality	Concentration of pollutants at ground level. Immission levels or air quality determines the effect of a pollutant on health or the environment. Therefore, to minimize air pollution, it is necessary, first, control of atmospheric emissions (emission) and, on the other, control and monitoring of the presence of pollutants in the air at various receptor sites (immission levels).
Buoyant emission plume	Plumes which are lighter than air because they are at a higher temperature and lower density than the ambient air which surrounds them, or because they are at about the same temperature as the ambient air but have a lower molecular weight and hence lower density than the ambient air. For example, the emissions from the flue gas stacks of industrial furnaces.
Dense gas emission plume	Plumes which are heavier than air because they have a higher density than the surrounding ambient air. A plume may have a higher density than air because it has a higher molecular weight than air (for example, a plume of carbon dioxide). A plume may also have a higher density than air if the plume is at a much lower temperature than the air. For example, a plume of evaporated gaseous methane from an accidental release of liquefied natural gas (LNG) may be as cold as -161 °C.
Passive or neutral plumes	Plumes which are neither lighter or heavier than air
Pollutants levels and values	
Limit value	A pollutant level not to be exceeded, in regard to human health, for every year. These are legally binding.
Critical level	A pollutant level not to be exceeded, in regard to human health, for every year. These are legally binding.
Margin of tolerance	Relates to the limit value and its given as a percentage. This provides, under specifies conditions, a flexibility for compliance with the limit value.
Target value	A pollutant level that one tries to avoid. Generally applicable over longer periods, 3-5 years. These are not legally binding.
Alert threshold	A short term pollutant level for which immediate steps must be taken.
Information threshold	A pollutant level for which immediate information to the public must be given.

Upper assessment threshold	A pollutant level, beneath the limit value, where a combination of modeling and monitoring (and/or indicative measurements) may be used for assessment.
Lower assessment threshold	A pollutant level, beneath the upper assessment threshold, where a modeling (or objective-estimation techniques) may be used for assessment.
Long term objective	A pollutant level to be obtained in the long term.
Exposure levels and values (related to PM2.5)	
Average exposure indicator (AEI)	This is the urban background pollutant level and has been introduced in relation to PM 2.5
Exposure concentration obligation	A level applied to the AEI that should be obtained over a given (3 year) period.
National exposure reduction target	A percentage reduction in the AEI to be achieved over a given period.
Measurement types	
Fixed measurements	These are measurements with the most strict data quality objectives, which are to be used when pollutant is above the upper assessment threshold
Indicative measurements	These are measurements with less strict data quality objectives than normal fixed measurements. For some pollutants, e.g. particulates, this has the same data quality objective as modeling.
Objective-estimation techniques	These are methods (not specified) with even less strict data quality objectives than the indicative measurements. The relative uncertainty in these method should be < 100%.

2.2. Where does the Air Quality Directive apply?

The Air Quality Directive applies everywhere outdoors excluding workplaces. It is applied within individual zones and these zones are defined by the Member States to cover their complete territory. The air quality requirements for health, such as limit and target values, apply everywhere within the zone but are not to be assessed:

a) at any locations situated within areas where members of the public do not have access and there is no fixed habitation
b) on factory premises or at industrial installations to which all relevant provisions concerning health and safety at work apply
c) on the carriageway of roads and on the central reservations of roads except where there is normally pedestrian access to the central reservation.

Note that these exceptions exclude exposure during road transport activities. E.g. the Air Quality Directive does not cover the environment within a bus but will cover the ambient environment when the public steps out of the bus.
In regard to the protection of vegetation and natural eco-systems the Air Quality Directive aims to protect areas distant from urban and industrial sources, leaving protection in these near source regions to the Member States.

2.2.1. Limits and target values for the protection of human health

The various health related limits and levels for the legislated pollutants are provided in Table 2. This includes the limit values, target values, the assessment threshold values, the long term objectives and the information and alert thresholds, as stated in Table 1. Some of these values come with specific conditions so for a definitive confirmation of these values the reader is referred to the Air Quality Directive itself.

Table 2. Summary of the air quality directive limit, target, assessment threshold, long term objective, information threshold and alert threshold values for the protection of human health

HUMAN HEALTH	Limit or target (1) value					Assessment threshold values		Long term objective		Information (i) and alert thresholds	
Pollutant	Averaging period	Value	Maximum number of allowed occurrences	Margin of tolerance	Date applicable	Upper	Lower	Value	Date	Period	Threshold value
SO_2	Hour Day	350 μgm^{-3} 125 μgm^{-3}	24 3	43% (150 μgm^{-3}) none	2005 2005	none 75 μgm^{-3}	none 50 μgm^{-3}			3 hours	500 μgm^{-3}
NO_2	Hour Year	200 μgm^{-3} 40 μgm^{-3}	18 0	50% in 2000 to 0% in 2010 50% in 2000 to 0% in 2010	2010 2010	140 μgm^{-3} 32 μgm^{-3}	100 μgm^{-3} 26 μgm^{-3}			3 hours	400 μgm^{-3}
Benzene	Year	5 μgm^{-3}	0	100% in 2005 to 0% in 2010	2010	3.5 μgm^{-3}	2 μgm^{-3}				
CO	Maximum daily 8 hour mean	10 mgm^{-3}	0	60%	2005	7 mgm^{-3}	5 mgm^{-3}				
PM_{10}	Day Year	50 μgm^{-3} 40 μgm^{-3}	35 0	50% 20%	2010 2010	35 μgm^{-3} 28 μgm^{-3}	25 μgm^{-3} 20 μgm^{-3}				
$PM_{2.5}$	Year	25 μgm^{-3} 25 μgm^{-3} (t)	0 0	20% in 2008 to 0% in 2015	2015 2010	17 μgm^{-3}	12 μgm^{-3}	25 μgm^{-3}	2020		
Pb	Year	0.5 μgm^{-3}	0		2005	0.35 μgm^{-3}	0.25 μgm^{-3}				
As	Year	6 ngm^{-3} (t)	0		2013	3.6 ngm^{-3}	2.4 ngm^{-3}				
Cd	Year	5 ngm^{-3} (t)	0		2013	3 ngm^{-3}	2 ngm^{-3}				
Ni	Year	20 ngm^{-3} (t)	0		2013	14 ngm^{-3}	10 ngm^{-3}				
B(a)P	Year	1 ngm^{-3} (t)	0		2013	0.6 ngm^{-3}	0.4 ngm^{-3}				
O_3	Maximum daily 8 hour mean averaged over 3 years	120 μgm^{-3} (t)	25		2010			120 μgm^{-3}	Not defined	1 hour 3 hours	180 μgm^{-3} (i) 240 μgm^{-3}

2.2.2. Limits and target values for the protection of vegetation

In this section the various ecosystem related limits and levels for the legislated pollutants are provided, as stated in Table 1. These have been grouped and are listed together in Table 3. Some of these values come with specific conditions so for a definitive confirmation of these values the reader is referred to the Air Quality Directive itself.

Table 3. Summary of the air quality Directive critical, target, assessment threshold and long term objective values for the protection of vegetation.

VEGETATION	Critical Level or target value				Assessment threshold values		Long term objective	
Pollutant	Averaging period	Value	Margin of tolerance	Date applicable	Upper	Lower	Value	Date
SO_2	Calendar year and winter (1 October to 31 March)	20 μgm^{-3}	none		12 μgm^{-3}	8 μgm^{-3}		
NO_x	Calendar year	30 μgm^{-3}	none		24 μgm^{-3}	19.5 μgm^{-3}		
O_3	May to July	AOT40* 18 000 $\mu gm^{-3} \cdot h$ averaged over five years		2010			AOT40* 6000 $\mu gm^{-3} \cdot h$	Not defined

* AOT40 (expressed in $\mu gm^{-3} \cdot$ hours) is the sum of the difference between hourly concentrations greater than 80 μgm^{-3} (= 40 parts per billion) and 80 μgm^{-3} over a given period using only the one-hour values measured between 8:00 and 20:00 Central European Time (CET) each day from 1 May to 31 July each year, for vegetation protection and from 1 April to 30 September each year for forest protection).

2.2.3. Air quality web portals in Europe

Most Member States now have their own web portals for communicating their air quality to the public. In Table 4 a list of these is provided. Most of these web portals provide updated information on monitoring activities within the country and some provide forecasts using models. All provide background information and links to reports

Table 4. Links to public information web sites for the EEC (European Economic Community)

Country (EEC)	Air quality public information site link	Monitoring information	Modelling information
Austria	http://www.umweltbundesamt.at/umweltsituation/luft/luftguete_aktuell/	Daily average	
Belgium	http://www.irceline.be/	Hourly graphs Hourly maps	Three day forecasts for Belgium
Bulgaria	http://www.icsr.bas.bg/icsrwebsite/departments/rdts/htdocs/index_EN.html	Daily average	
Cyprus	http://www.airquality.dli.mlsi.gov.cy/	Hourly graphs	
Czech Republic	http://www.chmi.cz/uoco/act/indexe.html	Hourly average Hourly graphs	
Denmark	http://www2.dmu.dk/atmosphericenvironment/byer/forside.htm	Hourly graphs	3 day forecasts for Denmark
Estonia	http://mail.klab.ee/seire/airviro/		
Finland	http://www.ilmanlaatu.fi/index.php http://silam.fmi.fi/AQ_forecasts/Finland_nested_v4_5_1/index.html	Hourly graphs Hourly maps	6 hours forecast for Finland
France	http://www.prevair.org/fr/index.php	Hourly Twice daily maps	1 day French and European forecasts Near real time analysis maps
Germany	http://www.env-it.de/umweltbundesamt/luftdaten/index.html	Hourly graphs	3 day ozone forecasts for Germany
Greece	http://www.minenv.gr/1/12/122/12204/e1220400.html http://lap.phys.auth.gr/gems.asp http://lap.physics.auth.gr/forecasting/airquality.htm	Daily average	General forecasting for Athens 3 day forecasting for Athens Daily forecasting
Hungary	http://members.chello.hu/dasy.kft/forecast/Budapest.htm	Daily map	2 day forecasting for Budapest
Ireland	http://www.epa.ie/whatwedo/monitoring/air/	Hourly graphs	
Italy	http://ita.arpalombardia.it/ITA/qaria/Home.asp http://www.aria-net.eu/QualeAria/	Daily maps Daily graphs	Air quality forecasting for Lombardy region 48 hour forecasts of air quality for Italy
Latvia			
Lithuania	http://stoteles.gamta.lt/	Hourly average Hourly graphs	
Luxembourg	http://www.environnement.public.lu/air_bruit/index.html	Hourly average Hourly graphs	
Malta	http://www.mepa.org.mt/airquality	Hourly average	
Netherlands	http://www.lml.rivm.nl/data/smog/index.html	Hourly maps Hourly graphs	2 day forecasting for Netherlands
Poland	http://armaag.gda.pl/en/results.htm	Hourly maps Hourly graphs	
Portugal	http://www.qualar.org/	Daily graphs Daily average	3 day forecasting for Portugal
Romania	http://www.calitateaer.ro/	Hourly average Hourly graphs	
Slovakia			
Slovenia	http://nfp-		

	si.eionet.europa.eu/Dokumenti/GIS/zrak		
Spain	http://www.mma.es/portal/secciones/enlaces/enl_auton.htm http://www.bsc.es/caliope http://www.gencat.cat/mediamb/qaire/pronostic/pronostic_aire.htm http://gestiona.madrid.org/aireinternet/html/web/ModeloPredictivoAccion.icm?rangoModelo=24&ESTADO_MENU=4_1 http://www.ingurumena.ejgv.euskadi.net/r49-n82/es/vima_ai_vigilancia/prevision48.apl	General provincial portal for AQ data	2 day forecasts for Europe and Spain Regional forecast for Cataluña Regional forecast for Madrid Regional forecast for Pais Vasco
Sweden	http://www.slb.mf.stockholm.se/e/ http://macc-raq.gmes-atmosphere.eu/som_forecast.php?datemodel=20100811&mod=SMH&niv=SFC	Hourly graphs	2 day forecasting
United Kingdom	http://www.airquality.co.uk/ http://www.airqualityni.co.uk/ http://gems.ecmwf.int/d/products/raq/forecasts/plot_UKN!Nitrogen%20Monoxide!Surface!00!gems!od!enfo!plot_MFM!2010090600!/	Hourly graphs	1 day forecasts for the UK 1 day forecasts for Northern Ireland
Albania			
Bosnia and Herzegovina			
Croatia			
Iceland	http://www.reykjavik.is/desktopdefault.aspx/tabid-1007	Hourly average Hourly graphs	
Macedonia FYR			
Norway	http://www.luftkvalitet.info/	Hourly graphs	Winter forecasts for several cities in Norway
San Marino			
Serbia and Montenegro			
Switzerland	http://www.bafu.admin.ch/luft/luftbelastung/aktuell/index.html?lang=en	Hourly average Daily graphs Daily maps	

3. Methodology

The focus of this study is to collect and review the existing information from most important airborne pollution models all over the world.

3.1. When can models be used for the assessment of existing air quality?

The Air Quality Directive defines a range of situations where models can be applied for assessment instead of, or in combination with, fixed measurements. In principle modelling can be used anywhere but unlike monitoring there are no minimum requirements regarding the use of models, i.e. there is no demand that modelling be used at all for the assessment of existing air quality. Concretely, the Air Quality Directive defines the following situations where models can be applied:

1. Models can always be used to supplement fixed measurement data no matter the pollutant levels. The advantage of this is that the number of monitoring stations may be reduced.

2. Air Quality Directive stipulates when, and in what way, modelling may be used for air quality assessment, not including ozone, based on the level of pollutants. These are:

- Modelling can be used to supplement monitoring when a zone is in exceedance of the upper assessment threshold
- Modelling can be used in combination with monitoring when a zone is in exceedance of the lower assessment threshold
- Modelling can be used to replace monitoring when a zone is below the lower assessment threshold

3.2. Combined use of measurements and models for assessment

In the Air Quality Directive the combined use of measurements and modelling is encouraged and allowed for in reporting when exceedances are below the upper assessment threshold. There are no specifics provided as to the level of combination or

how the combination can be made. There is clearly a multitude of methods available for combining monitoring and modelling, ranging from advanced data assimilation methods to simple validation of models.

3.3. What types of models can be used?

There are a wide variety of model types available for use in air quality modelling. There is generally no single model suitable for all scales, all compounds or all applications so the rule in selection of models is that they should be 'fit for purpose'. Models can be generally divided into four categories, based on the methods used for the calculations. Some models may make use of more than one methodology and may fall into more than one category.

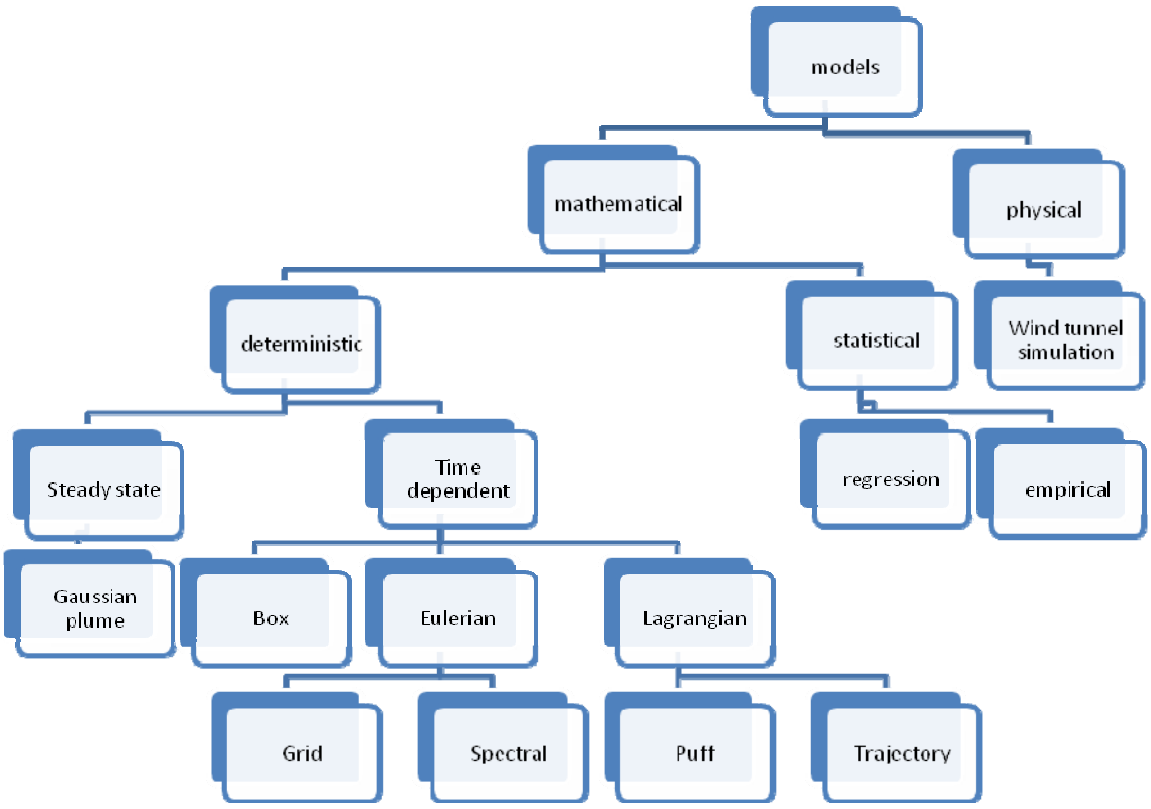

Figure 1: Different types of air quality models according to their foundation

In Table 5 a list of the application scales, the pollutants and the typical types of models, or required processes, is provided. A comprehensive listing of air quality models used in Europe can also be found at the EIONET Model Documentation System web site (http://air-climate.eionet.europa.eu/databases/MDS/index_html).
The list below should be considered to be indicative. For every modelling application a more thorough assessment of the required model types should be made.

Table 5. List of typical model characteristics, formulations and processes, for the various scales and pollutants needed for air quality assessment.

	Area of assessment		
Description	Local /hotspot (1-1000 m)	Urban /agglomerate (1-300 km)	Regional (25-10000 km)
Model type	Gaussian and non-Gaussian paraeterised models Statistical models Obstacle resolving fluid dynamical models Lagrangian particle models	Gaussian and non-Gaussian paraeterised models Eulerian chemical transport models Lagrangian particle models	Eulerian chemical transport models Lagrangian chemical models
Meteorology	Local meteorological measurements Obstacle resolving fluid dynamical models Diagnostic wind field models	Mesoscale meteorological models Localised meteorological measurements Diagnostic wind field models	Synoptic/mesoscale meteorological models
Chemistry	Limited or none	Ranging from none to comprehensive, depending on application	Comprehensive
Emission modelling	Bottom up traffic emissions Source specific emissions	Bottom up and/or top down traffic emissions Emission process models	Top down emission modeling Emission process models

The Air Quality Directive does not provide any suggestions for the actual models to be used. As long as the model complies with the quality objectives then it may be applied. However, U.S. EPA have defined several models as preferred for particular case studies.

3.4. What are the Components of an Air Modeling Analysis?

The dispersion models require the input of data which includes:

- Meteorological conditions such as wind speed and direction, the amount of atmospheric turbulence (as characterized by the "stability class"), pressure, relative humidity, the ambient air temperature and the height to the bottom of any inversion aloft that may be present.
- Emissions parameters, such as source location and height, source vent stack diameter and exit velocity, exit temperature and mass flow rate.
- Terrain elevations at the source location and at the receptor location, urban/rural classification.
- The location, height and width of any obstructions (such as buildings or other structures) in the path of the emitted gaseous plume.

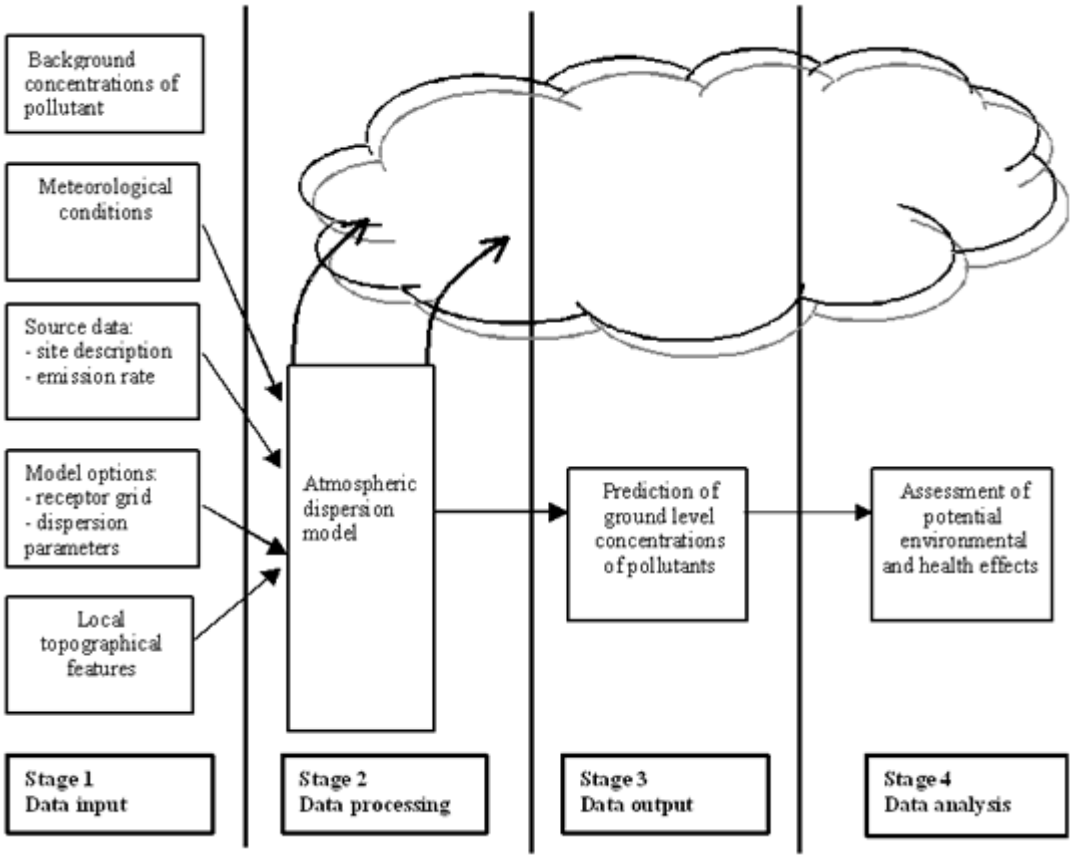

Figure 2: Block diagram of air quality modeling, showing main input data

3.5. Air quality forecasting for alert thresholds, information to the public and short term action plans in Europe

The Member States have an obligation to provide information to the public concerning to levels of information and alert thresholds for SO_2, NO_2 and ozone. Though purely statistical methods may be applied for determining any future modification of these threshold levels, air quality models are well suited for forecasting air pollution levels at both the regional and urban scales. In addition Air Quality Directive states that short term action plans are required if there is a risk that alert thresholds, limit values or target values are to be exceeded. Models are suitable tools for assessing the effects of any short term measures employed to reduce the air pollution or protect the public as well as for predicting, through forecasts, potential risks of exceedance.

There are a number of established air quality forecasting systems for both regional and urban air quality (see Table 4). A number of these, but not all, can be accessed through the PROMOTE web site (http://www.gse-promote.org). On the European scale both PROMOTE and GEMS (http://gems.ecmwf.int/d/products/rair_quality)projects provide a feasibility study related to the use of ensemble forecasts for all of Europe. These forecasts are based on an integrated ensemble of up to eight European air quality models running fully operationally in a number of countries (most are listed in table 4). As continuation of the PROMOTE and GEMS projects, operational ensemble forecasts are being provided within the MACC project (Monitoring Atmospheric Composition and Climate – FP7, http://www.gmes-atmosphere.eu) which will be the cornerstone of the future GMES Atmospheric Service (Global Monitoring for Environment and Security). Such regional scale forecasts are useful information for providing regional scale concentrations, particularly in regard to compounds such as ozone, but also provide background contributions for urban scale forecasts.

Model studies have shown that short term action plans can be effective if they are decided and implemented at least two or three days before the pollution episode occurs. Therefore, the forecasting capacity that provides, in many cases, an assessment on the origin of the episode (e.g. long range transport, transport of natural species, local emissions, local meteorological conditions) can help in deciding the most

appropriate information and emergency measures to be taken. Generally these measures concern road traffic (speed limits, alternating circulation) and industrial emission controls. Though it is recommended in the Air Quality Directive, use of forecasting results for designing emergency measures is still a new approach and not fully adopted by the Member States. Its relevance depends on the forecasting models' quality and accuracy, meaning their ability to avoid false alarms and missing events.
The forecasting capacity of an air quality model is strongly determined by the quality of the meteorological forecasts driving the system, as well as by the accuracy of the emissions inventory used. In regard to meteorology many weather forecasts models are not designed to provide accurate results for typical episodic pollution events, such as low wind speeds, inversions and local recirculation.

3.6. A joint EU - North-American initiative

The EU - North-American Air Quality Model Evaluation International Initiative (AQMEII), was recently established (2008), having recognized the necessity for exploring advanced methodologies for model evaluation as well as the necessity to categorize the existing methods, including the identification of their limits. The main aims of this initiative are to bring together NA and EU regional scale modelling communities, for an effective and efficient exchange of views and experiences through common activities, and to promote exploratory research in the field. The latter is achieved through thematic workshops that try to focus research activities and to identify research priorities. AQMEII (http://aqmeii.jrc.ec.europa.eu) is organized around the model evaluation frameworks of Operational, Diagnostic, Dynamic and Probabilistic evaluation that include:

- Operational evaluation: evaluation based on routine observation for both meteorology and air quality. The comparison is mainly focusing on a one-to-one pairing of model output with monitoring data.
- Diagnostic evaluation: investigates the way in which specific physio-chemical model processes can influence model results.

- Dynamic evaluation: deals with the model's ability to predict changes in air quality concentrations in response to changes in either source emissions or meteorological conditions. This also includes an assessment of the uncertainties in these inputs and their influence on the air quality predictions.
- Probabilistic evaluation: characterizing the uncertainty of air quality model predictions and used to provide a credible range of predicted values rather than a single "best-estimate".

Activities are being organized around and across these four themes that will involve the EU and North American modelling communities in a common modelling effort that will feature both North American and EU in air quality modelling case studies.

3.7. U.S. Experience

The U.S. Environmental Protection Agency (EPA) uses a wide range of models with different complexity for regulatory decision making. The EPA Quality system, defined in 2000, covers also environmental data produced from models (EPA, 2000). Guidance on how to document quality assurance planning for modelling (e.g., model development, model application, as well as large projects with a modelling component) was published in 2002, (EPA, 2002). In March 2009 the ―Guidance on the Development, Evaluation, and Application of Environmental models was also published. It presents recommendations and provides an overview of best practices for ensuring and evaluating the quality of environmental models

4. Results: Compilation of Models

4.1. U.S. Environmental Protection Agency Models

This compilation of atmospheric dispersion models describes the models currently in use by the U.S. EPA briefly.

Many of the dispersion models developed by or accepted for use by the U.S. EPA are accepted for use in many other countries as well.

4.1.1. Dispersion modeling

Dispersion modeling uses mathematical formulations to characterize the atmospheric processes that disperse a pollutant emitted by a source. Based on emissions and meteorological inputs, a dispersion model can be used to predict concentrations at selected downwind receptor locations. These air quality models are used to determine compliance with National Ambient Air Quality Standards (NAAQS), and other U.S regulatory requirements such as New Source Review (NSR) and Prevention of Significant Deterioration (PSD) regulations. These models are addressed in Appendix A of EPA's *Guideline on Air Quality Models* (also published as Appendix W), which was originally published in April 1978 to provide consistency and equity in the use of modeling within the U.S. air quality management system. These guidelines are perodically revised to ensure that new model developments or expanded regulatory requirements are incorporated.

4.1.1.1. Preferred/Recommended Models

Refined air quality models that are currently listed in Appendix W and are required to be used for State Implementation Plan (SIP) revisions for existing sources and NSR and PSD programs.

Table 6. AERMOD model.

Name	AERMOD (AMS/EPA Regulatory Model)
Version	09292 (October 19, 2009)
Model developer	AERMIC (AMS (American Meteorological Society)/U.S. EPA (Environmental Protection Agency) Regulatory Model Improvement Comittee)
Web url	http://www.epa.gov/scram001/dispersion_prefrec.htm#aermod
Description	A steady-state plume model that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain. In the autumn of 2005, AERMOD became established as the preferred air dispersion model in the U.S. EPA's "Guideline on Air Quality Models". From December 9, 2005 onwards, AERMOD should be the appropriate application used as a replacement for the ISC3 model.
Knowledge level	Level of knowledge needed to operate model : Intermediate
User community	Consultants, industries, authorities, research and educational establishments.
Model code available?	Yes, EPA web url. User-friendly interfaces on later versions are available from Lakes Environmental company commercially. http://www.weblakes.com/index.html
Pre & Post processors	Two pre-processors: AERMET deals with meteorological data. AERMAP generates receptor grids and characterizes the terrain features. Other non-regulatory components are: AERSCREEN, AERSURFACE and BPIPPRIME.
Computer requirements	Easily installed on PC. AERMOD was developed specifically for MS Windows and runs under Windows 95, 98, Me, NT, 2000, Xp, Vista and 7. CPU time: very fast, seconds for one hour of meteorological data. Storage: typically 0.5 GB.
Model scale	Near field impacts (within 50 km). Short and long term.
Features and capabilities	Sources types: multiple point, area and volume source. Sources releases: surface, near surface and elevated sources. Terrain types: simple or complex terrain. Plume types: continuous, buoyant plumes. Meteorological data profiles: Vertical profiles of wind, turbulence and temperature are created
Input data	Source data, dispersion data, receptor and terrain data (AERMAP), meteorological data (AERMET), downwash related information (BPIPPRIME).
Output data	1h, 24h and yearly concentration and deposition values in tables or in territorial distribution are calculated.
Model limitations	Calms winds, rapidly changing weather conditions, restricted to non-reactive pollutants. Dispersion of heavier-than-air gases is not considered.

Table 7. CALPUFF model.

Name	CALPUFF
Version	Two versions free available: - Version 5.8- Level 070623 EPA-approved version - Version 6 – Level 080725
Model developer	Sigma Research Corporation (SRC) under contract with the California Air Resources Board (CARB)
Web url	http://www.epa.gov/scram001/dispersion_prefrec.htm#calpuff http://www.src.com/calpuff/calpuff1.htm http://www.meteosim.com/es/modelizacion_meteorologica/CALPUFF_mapas.php?region=tarragona_op
Description	CALPUFF is a multi-layer, multi-species, non-steady-state puff dispersion integrated modeling system used for a wide variety of air quality modeling studies, including toxic pollutant deposition, near-field impacts from point, line, area, and volume sources, forest fire impacts, visibility assessments, and long range transport studies. The model has been adopted by the U.S. Environmental Protection Agency in its Guideline on Air Quality Models as the preferred model for assessing the long range transport of air pollutants.
Knowledge level	Level of knowledge needed to operate model : Intermediate - Advanced
User community	Consultants, industries, authorities, research and educational establishments.
Model code available?	Yes, source code of EPA-approved version is free at developer website. http://www.src.com/calpuff/calpuff1.htm New features on later versions are available from Lakes Environmental Inc under commercial agreement. http://www.weblakes.com/index.html
Pre & Post processors	The main components of the modeling system are CALMET (a diagnostic 3-dimensional meteorological model), CALPUFF (an air quality dispersion model), and CALPOST (a postprocessing package). Each of these programs has a graphical user interface (GUI). In addition to these components, there are numerous other processors that may be used to prepare geophysical (land use and terrain) data in many standard formats, meteorological data (surface, upper air, precipitation, and buoy data), and interfaces to other models such as the Penn State/NCAR Mesoscale Model (MM5), the National Centers for Environmental Prediction (NCEP) Eta/NAM and RUC models, the Weather Research and Forecasting (WRF) model and the RAMS model.
Computer requirem	PC Windows. CPU time: vary considerably depending on the model application. Storage: 3 MB for unzipped files, 18 MB for installed system

ents	
Model scale	The model has been enhanced to make it more suitable for meso-scale applications. Long term.
Features and capabilities	Some examples of applications for which CALPUFF may be suitable include: -Near-field impacts in complex flow or dispersion situations • complex terrain • stagnation, inversion, recirculation, and fumigation conditions • overwater transport and coastal conditions • light wind speed and calm wind conditions -Long range transport -Visibility assessments and Class I area impact studies -Criteria pollutant modeling, including application to State Implementation Plan (SIP) development -Secondary pollutant formation and particulate matter modeling -Buoyant area and line sources (e.g., forest fires and aluminum reduction facilities)
Input data	Control file inputs: -Geophysical and hourly meteorological data, created by the CALMET meteorological model -Emissions data for point, line, area or volume sources with time-varying emission parameters.
Output data	CALPUFF produces files of hourly concentrations of ambient concentration s for each modeled species, wet deposition fluxes, dry deposition fluxes, and for visibility applications, extinction coefficients. Postprocessing programs (PRTMET and CALPOST) provide options for analysis and display of the modeling results.
Chemical reactions	A pseudo-first-order chemical reaction mechanism for the convesion SO2 to SO4-- and NOx to NO3- based on scheme used in the MESOPUFF II model or The RIVAD/ARM3 scheme for clear non-urban areas. User-specified diurnal cycles of transformation rates. No chemical conversión can be specified.
Model limitations	Heavier-than-air releases are not considered and chemical transformations are available for five chemicals. Probably, the most significant limitation is the lack of a front end spills model that computes evaporation, jet effects, etc. The model does not compute the area of impact above ERPG (Emergency Response Planning Guideline) level.

Table 8. BLP model.

Name	BLP (Buoyant Line and Point Source Dispersion)
Version	Julian date 99176
Model developer	Environmental Research and Technology, Inc
Web url	http://www.epa.gov/ttn/scram/dispersion_prefrec.htm#blp
Description	Blp is a Gaussian plume dispersion model designed to handle unique modeling problems associated with aluminum reduction plants, and other industrial sources where plume rise and downwash effects from stationary line sources are important
Model code available?	Yes, EPA web url.
Pre & Post processors	The model consists of three programs: BLP, BLPSUM AND POSTBLP.
Input data	Source data: Stack location, elevation of stack base, physical stack height, stack inside diameter, stack gas exit velocity, temperature and pollutant emission rate; line sources require coordinates of the endpoints of the line, release height, average line-source width, average spacing between buildings, and average line-source buoyancy parameter. Meteorological data: hourly surface data including stability class, wind direction and speed, temperature and mixing height. BLP can reda ISCST meteorological data when in the ASCII format. Receptor data: Location and elevation of receptors, or location and size of receptor grid
Output data	It generates short term (1, 3, and 24 hours) concentration output on a maximum of 100 points at ground level, but can average these values on a monthly or yearly horizon. It also provides the contribution of each source to the total concentration at each receptor.
Chemical reactions	Chemical transformations are treated using linear decay. Decay rate is input by the user.
Model limitations	BLP may be used to model primary pollutants. BLP does not treat settling and deposition. It recommends be used in flat, rural areas within a range of 50 km of distance and can include up to 50 point sources and 10 parallel line ones. One hour to one year averaging times. Maximum: 100 receptors.

Table 9. CALINE3 model.

Name	CALINE3
Version	Julian date (89219)
Model developer	California Department of Transportation (CALTRANS)
Web url	http://www.epa.gov/scram001/dispersion_prefrec.htm#caline3
Description	A steady-state Gaussian dispersion model designed to determine air pollution concentrations at receptor locations downwind of highways located in relatively uncomplicated terrain. CALINE3 is incorporated into the more refined CAL3QHC and CAL3QHCR models.
Model code available?	Yes, EPA web url.
Input data	Source data: Up to 20 highway link endpoint coordinates, traffic volume, mixing zone width, source height, emission factor. Meteorological data: wind speed, wind angle, stability class, mixing height, ambient concentration, surface roughness (optional) Receptor data: coordinates and height above ground
Output data	Printed output includes concentration at each receptor for the specified meteorological condition.
Chemical reactions	Not treated.
Model limitations	Plume rise is not treated. CALINE-3 is appropriate for the following applications: Highway (line) sources; Urban or rural areas; Simple terrain; Transport distances less than 50 kilometers; and One-hour to 24-hour averaging times. Model primary pollutants.

Table 10. CAL3QHC/CAL3QHCR models.

Name	CAL3QHC/CAL3QHCR
Version	Dated 04244
Model developer	California Department of Transportation (CALTRANS)
Web url	http://www.epa.gov/ttn/scram/dispersion_prefrec.htm#cal3qhc
Description	CAL3QHC is a CALINE3 based model with queuing and hot spot calculations and with a traffic model to calculate delays and queues that occur at signalized intersections; CAL3QHCR is a more refined version based on CAL3QHC that requires local meteorological data.
Model code available?	Yes, EPA web url.

Table 11. CTDMPLUS model.

Name	CTDMPLUS (Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations)
Version	dated 93228
Model developer	Atmospheric Sciences Research Laboratory (U.S. EPA), Computer Sciences Corporation, Environmental Research and Technology, Inc. And Sigma Research Corporation (SRC)
Web url	http://www.epa.gov/ttn/scram/dispersion_prefrec.htm#ctdmplus
Description	CTDMPLUS is a refined point source gaussian air quality model for use in all stability conditions for complex terrain. The model contains, in its entirety, the technology of CTDM for stable and neutral conditions. CTSCREEN is the screening version of CTDMPLUS.
Model code available?	Yes, EPA web url.
Input data	There are five required input files and two optional input files for CTDMPLUS: -A general file of program specifications, which consist of program switches, source data, meterological tower coordinates and hill surface roughness lengths; -A terrain data file which is obtained directly from the terrain preprocessor; -A file containing receptor names, locations, and the associated hill numbers; -A surface meterological data file which is obtained directly from the meteorological preprocessor program; -A user-created meterological profile data file which contains conventional meterological data measured by multiple levels; -An optional file of hourly emissions parameters; -An optional file containing upper air data from rawinsonde data
Output data	-Stack data for each source; -Meteorological variables at plume height; -Geometrical relationships between the source and the hill; -Plume characteristics at each receptor for stable and unstable hours;
Chemical reactions	Chemical transformation is not treated
Model limitations	CTDMPLUS may be used to model non-reactive, primary pollutants. Physical removal is not treated by CTDMPLUS (complete reflection at the ground/hill surface is assumed). Lack of the ability to accommodate dense gas dispersion is a weakness. Up to 40 point sources, 400 receptors and 25 hills may be used. Receptors and sources are allowed at any location. Hill slopes are assumed not to exceed 15 degrees, so that the linearized equation of motion for Boussinesq flow are applicable. CTDMPLUS does not simulate calm meteorological conditions.

	CTDMPLUS is appropriate for the following applications: -Elevated point sources; -Terrain elevations above stack top; - Rural or urban areas; -Transport distances less than 50 kilometers; and -One hour to annual averaging times when used with a post-processor program such as CHAVG (http://www.epa.gov/ttn/scram/dispersion_related.htm#chavg)

Table 12. OCD model.

Name	OCD (Offshore and Coastal Dispersion Model)
Version	Version 5
Model developer	Environmental Research And Technology, inc.
Web url	http://www.epa.gov/ttn/scram/dispersion_prefrec.htm#ocd
Description	OCD is a straight line Gaussian model developed to determine the impact of offshore emissions from point, area or line sources on the air quality of coastal regions. It incorporates overwater plume transport and dispersion as well as changes that occur as the plume crosses the shoreline. It assumes short distances and short time intervals.
Model code available?	Yes, EPA web url.
Input data	Hourly meteorological data are needed from both offshore and onshore locations. Specifications of emission characteristics and receptor locations are similar to the standard EPA UNAMAP (User's Network for Applied Modelling of Air Pollution) models. Hourly emission rate, exit velocity, and stack gas temperature may also be specified.
Output data	Average concentration, five highest concentrations at each receptor
Chemical reactions	Treated using exponential decay (half-life input by user); allows different rates during day and at night
Model limitations	OCD may be used to model primary pollutants, no settling or deposition. Constant, uniform horizontal winds. Up to 250 point sources, 5 area sources, or one line source and 180 receptors may be used. Coastal grid- up to 3600 rectangles.

4.1.1.2. Alternative Models

Models, that can be used in regulatory applications with case-by-case justification to the Reviewing Authority as noted in Section 3.2, "*Use of Alternative Models*", in Appendix W.

Model code available at EPA web url, or at developer url for: ADMS-3, HGSYSTEM, HOTMAC, PANACHE.

Table 13. List of U.S. EPA Alternative Models.

Correlative number	Model name	Description
1	**ADAM**	Air Force Dispersion Assessment Model (ADAM) is a modified box and Gaussian dispersion model which incorporates thermodynamics, chemistry, heat transfer, aerosol loading, and dense gas effects.
2	**ADMS-3**	Atmospheric Dispersion Modeling System (ADMS-3) is an advanced dispersion model developed in England for calculating concentrations of pollutants emitted both continuously from point, line, volume and area sources, or discretely from point sources.
3	**AFTOX**	A Gaussian dispersion model that handles continuous or instantaneous, liquid or gas, elevated or surface releases from point or area sources.
4	**ASPEN**	The Assessment System for Population Exposure Nationwide (ASPEN) consists of a dispersion and a mapping module. The dispersion module is a Gaussian formulation based on ISCST3 for estimating ambient annual average concentrations at a set of fixed receptors within the vicinity of the emission source. The mapping module produces a concentration at each census tract. Input data needed are emissions data, meteorological data and census tract data. The Emissions Modeling System for Hazardous Pollutants (EMS-HAP) is needed to process the emission inputs into the ASPEN model or the ISC3 model. The ASPEN model was used in estimating annual ambient concentrations for air toxics pollutant in the National Air Toxics Assessment (NATA) Study.
5	**DEGADIS**	Dense Gas Dispersion (DEGADIS) is a model that simulates the dispersion at ground level of area source clouds of denser-than-air gases or aerosols released with

		zero momentum into the atmosphere over flat, level terrain.
6	**HGSYSTEM**	A collection of computer programs designed to predict the source-term and subsequent dispersion of accidental chemical releases with an emphasis on dense gas behaviour.
7	**HOTMAC and RAPTAD**	HOTMAC is a model for weather forecasting used in conjunction with RAPTAD which is a puff model for pollutant transport and dispersion. These models are used for complex terrain, coastal regions, urban areas, and around buildings where other models fail.
8	**HYROAD**	The HYbrid ROADway Model (HYROAD) integrates three individual modules simulating the pollutant emissions from vehicular traffic and the dispersion of those emissions. The dispersion module is a puff model that determines concentrations of carbon monoxide (CO) or other gaseous pollutants and particulate matter (PM) from vehicle emissions at receptors within 500 meters of the roadway intersections.
9	**ISC3**	A Gaussian model used to assess pollutant concentrations from a wide variety of sources associated with an industrial complex. This model accounts for: settling and dry deposition of particles; downwash; point, area, line, and volume sources; plume rise as a function of downwind distance; separation of point sources; and limited terrain adjustment. ISC3 operates in both long-term and short-term modes.
10	**ISC-PRIME**	(Plume RIse Model Enhancements) is a model with building downwash incorporated into the Industrial Source Complex Short Term Model (ISCST3).
11	**OBODM**	A model for evaluating the air quality impacts of the open burning and detonation (OB/OD) of obsolete munitions and solid propellants. It uses dispersion and deposition algorithms taken from existing models for instantaneous and quasi-continuous sources to predict the transport and dispersion of pollutants released by the open burning and detonation operations.
12	**OZIPR**	OZIPR is a one-dimensional photochemical box model that is an alternative version of the OZIP model that deals with air toxic pollutants.
13	**PANACHE**	PANACHE is an Eulerian (and Lagrangian for particulate matter), 3-dimensional finite volume fluid mechanics model designed to simulate continuous and short-term pollutant dispersion in the atmosphere, in simple or complex terrain. Available from Transoft US. Inc.

14	**PLUVUEII**	A model that estimates atmospheric visibility degradation and atmospheric discoloration caused by plumes resulting from the emissions of particles, nitrogen oxides, and sulfur oxides. The model predicts the transport, dispersion, chemical reactions, optical effects and surface deposition of such emissions from a single point or area source.
15	**SCIPUFF**	A puff dispersion model that uses a collection of Gaussian puffs to predict three-dimensional, time-dependent pollutant concentrations. In addition to the average concentration value, SCIPUFF predicts the statistical variance in the concentrations resulting from the random fluctuations of the wind.
16	**SDM**	Shoreline Dispersion Model (SDM) is a Gaussian dispersion model used to determine ground-level concentrations from tall stationary point source emissions near a shoreline.
17	**SLAB**	A model for denser-than-air pollutant releases that utilizes the one-dimensional equations of momentum, conservation of mass and energy, and the equation of state. SLAB handles ground-level and elevated jet releases, liquid pool evaporation releases, and releases from volume sources.

4.1.1.3. Screening Models

These are models that are often used before applying a refined air quality model to determine if refined modeling is needed.

Model code available at U.S. EPA web url.

Table 14. List of U.S. EPA Screening Models.

Correlative number	Model name	Description
1	AERSCREEN	The screening version of AERMOD. It produces estimates of concentrations without the need for meteorological data that are equal to or greater than the estimates produced by AERMOD with a full set of meteorological data.
2	COMPLEX1	A multiple point source screening model with terrain adjustment that uses the plume impaction algorithm of the VALLEY model.
3	CTSCREEN	The screening version of CTDMPLUS model.
4	RTDM3.2	Rough Terrain Diffusion Model (RTDM3.2) is a sequential Gaussian model for estimating ground-level concentrations of one or more co-located point sources in rough (or flat) terrain.
5	SCREEN3	The screening version of ISC3
6	TSCREEN	Toxics Screening Model (TSCREEN) is a Gaussian model for screening toxic air pollutant emissions and their subsequent dispersion from possible releases at superfund sites. It contains 3 modules: SCREEN3, PUFF, and RVD (Relief Valve Discharge).
7	VALLEY	VALLEY is a steady-state, complex terrain, univariate Gaussian plume dispersion algorithm designed for estimating either 24-hour or annual concentrations resulting from emissions from up to 50 (total) point and area sources.
8	VISCREEN	VISCREEN calculates the potential impact of a plume of specified emissions for specific transport and dispersion conditions.

4.1.2. Photochemical Models

Photochemical air quality models have become widely utilized tools for assessing the effectiveness of control strategies adopted by regulatory agencies. These models are large-scale air quality models that simulate the changes of pollutant concentrations in the atmosphere by characterizing the chemical and physical processes in the atmosphere. These models are applied at multiple geographical scales ranging from local and regional to national and global.

There are two types of photochemical air quality models commonly used in air quality assessments: the Lagrangian trajectory model that employs a moving frame of reference, and the Eulerian grid model that uses a fixed coordinate system with respect to the ground. Earlier generation modeling efforts often adopted the Lagrangian approach to simulate the pollutants formation because of its computational simplicity. The disadvantage of Lagrangian approach, however, is that the physical processes it can describe are somewhat incomplete. Most of the current operational photochemical air quality models have adopted the three-dimensional Eulerian grid modeling mainly because of its ability to better and more fully characterize physical processes in the atmosphere and predict the species concentrations throughout the entire model domain.

Table 15. CMAQ model.

Name	CMAQ (Community Multi-scale Air Quality Model)
Version	v 4.7.1 (06/2010)
Model developer	US. EPA
Web url	http://www.epa.gov/asmdnerl/CMAQ/index.html http://www.cmascenter.org/ http://verde.lma.fi.upm.es/cmaq_eu/
Description	The latest version of the Community Multi-scale Air Quality (CMAQ) model has state-of-the-science capabilities for conducting urban to regional scale simulations of multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation.
Knowledge level	Users should have familiarity with air quality modeling principles, UNIX/LINUX platforms, and scientific programming.
User community	Government, Industry, Academia, Research, Consultants, Stakeholder groups
Model code available?	Yes, source code are available at http://www.cmascenter.org
Pre & Post processors	The CMAQ modeling system consists of several processors and the chemical-transport model: -Meteorology-chemistry interface processor (MCIP) -Photolysis rate processor (JPROC) -Initial conditions processor (ICON) -Boundary conditions processor (BCON) -CMAQ chemical-transport model (CCTM)
Computer requirements	Unix/Linux platform (single processor, or multi-processor), 2 Ghz chip speed or better, 1Gb memory per processor; Unix/Linux clusters (8 CPUs is typical); or PC Pentium IV 2.4 GHz, 1GB RAM. Other Software Required to Run the Model **:** netCDF, IOAPI libraries. Time needed for run: Approximately 25 min. for 7 days run, 6 vertical layers, 35x35 cells, CB-IV chemical mechanism. Storage: 60 GB Hard drive
Model scale	Mesoscale
Features and capabilities	The CMAQ system was designed to have a flexible community modeling structure based on modular components. The CCTM includes the following major processes: Horizontal advection Vertical advection Mass conservation adjustments for advection processes Horizontal diffusion Vertical diffusion Emissions injection Deposition Gas-phase chemical reactions

	Air qualityueous-phase reactions and cloud mixing Aerosol dynamics, thermodynamics, and chemistry Plume chemistry effects Photolytic rate computation Process analysis
Input data	-Hourly (or finer temporal resolution) gridded meteorological data from either MM5 or WRF meteorological model; processed through CMAQ's Meteorology-Chemistry Interface Processor (MCIP) -Hourly (or finer temporal resolution) gridded Emissions data from SMOKE emissions modeling system (including biogenic and anthropogenic source emissions of CO, NO, NO2, VOCs, SO2, NH3, and particulate matter) -Initial gridded chemical concentrations and hourly or static lateral boundary concentrations
Output data	Hourly three-dimensional grid of estimated air trace gas concentrations (e.g., ozone, NO, NO2), and fine particulate matter (PM2.5 and its size-distributed chemical constituents). Hourly two-dimensional gridded wet and dry deposition amounts of chemical species, and gridded atmospheric visibility. Temporal resolution of output can be defined by user.
Model limitations	CMAQ is a deterministic model. Thus, some discrepancies in comparing grid-average values with point measurements should be expected. Majority of the current regional application involve 12 km horizontal resolution grids while urban scale applications typically use 1-4 km resolutions. Finer scale applications would require enhancements in the representation of turbulent transport in the model. The accuracy of CMAQ predictions is also intricately linked to the accuracy and resolution of the input meteorological and emission data sets.

Table 16. CAMx model.

Name	CAMx (Comprehensive Air quality model with extensions)
Version	v5.20.1
Model developer	ENVIRON International Corporation (USA)
Web url	http://www.camx.com/
Description	The Comprehensive Air quality Model with extensions (CAMx) is a publicly available Eulerian computer modeling system for the integrated assessment of photochemical and particulate air pollution over many scales ranging from urban to super-regional. It handles a variety of inert and chemically active pollutants, including ozone, particulate matter, inorganic and organic PM2.5/PM10, and mercury and other toxics.
Knowledge level	Advanced. Model should be applied by skilled users.
User community	Environmental agencies, private companies, researchers for regulatory applications. 3-day air quality are carried out by two greek universities using a modeling system which consists of the meteorological model MM5 coupled to CAMx. The forecast is performed in two spatial scales: Regional scale (Europe, Balkan), and Urban scale (Athens) http://lap.phys.auth.gr/gems/
Model code available?	CAMx is publicly available for free at: www.camx.com . The code is subject to the GNU general public license.
Computer requirements	CAMx is most commonly run on Unix/Linux workstations and PCs using shell scripts. Third-party graphics are needed to visualize output fields. CAMx is distributed with tools to prepare data in several widely used formats. The time required to run CAMx depends on grid resolution, grid size, duration of the period to simulate, complexity of chemistry, use of "Probing Tool" extensions. The following examples are for a simple single-grid CAMx run employing CB4 gas-phase chemistry only, on a 2.1 GHz Linux PC with 256 MB RAM: * 97x90x14 grid - 24 min/day * 97x90x14 grid - 16 min/day (2 CPU)
Model scale	1 km to 1000 km spatial scales, hourly to annual time scales
Features and capabilities	Most notable features: - two-way nested grid structure and flexi-nesting - three gas-phase chemical mechanism options (CB-IV, CB05, and SAPRC99) - three gas-phase solver options (IEH, EBI or LSODE) - Treatment of particulate matter, inorganic (ISORROPIA) and organic (SOAP) - Mercury and toxics chemistry - Plume-in-Grid module - Horizontal Advection Solver options (Bott or PPM)

	- Dry and wet deposition - advanced photolysis model - detailed cloud impact on photolysis rates and aqueous chemistry - parallel processing on shared-memory systems (OMP) or distributed memory systems (MPI) - Ozone and Particulate Source Apportionment Technology - Decoupled Direct Method - Process Analysis
Input data	CAMx requires inputs to describe photochemical conditions, surface characteristics, initial/boundary conditions, emission rates, and various meteorological fields over the entire modeling domain. Preparing this information requires several preprocessing/premodeling steps to translate "raw" emissions, meteorological, air quality and other data into final input files for CAMx.
Output data	Hourly (or user-defined interval) two- or three-dimensional concentration fields (ppm for gases, ug/m3 for aerosols). Hourly (or user-defined interval) two-dimensional surface deposition fields (m/s for deposition velocity, mol/ha for gases, g/ha for aerosols). Diagnostic and mass balance output files.
Model limitations	Model scope limited by the computing resources available to the user

Table 17. REMSAD model.

Name	REMSAD (Regional Modeling System for Aerosols and Deposition)
Version	V 8.00
Model developer	ICF Consulting Inc.
Web url	http://remsad.com/
Description	The Regional Modeling System for Aerosols and Deposition (REMSAD) calculates the concentrations of both inert and chemically reactive pollutants by simulating the atmospheric processes that affect pollutant concentrations over regional scales. It includes processes relevant to regional haze, particulate matter and other airborne pollutants, including soluble acidic components and mercury
Knowledge level	Some prior experience in modeling and atmospheric science is helpful. User should be comfortable running applications in a Unix/Linux environment. User must be capable of organizing and handling large data sets.
Model code available?	See www.remsad.com for registration and download instructions. Available for free.
Pre & Post processors	The REMSAD system consists of a series of preprocessor programs, the core model, and several postprocessing programs.
Computer requirements	PC or Workstation, min 500Mb RAM, 100 Gb disk storage
Model scale	The REMSAD system is built on the foundation of the variable-grid Urban Airshed Model (UAM-V) – a regional-scale photochemical modeling system. Thus many of features of the UAM-V are also available in REMSAD. The REMSAD model is capable of "nesting" one or more finer-scale subgrids within a coarser overall grid. This two-way fully interactive nesting feature allows the user to apply higher resolution over selected source and/or receptor regions. The modeling system may be applied at scales ranging from a single metropolitan area to a continent containing multiple urban areas. To date, most applications have focused on the continental-scale.
Features and capabilities	REMSAD includes: A detailed gas phase chemical mechanism (the Carbon Bond V mechanism) consisting of 30 gas phase species and over 100 reactions. An algorithm treating the formation of secondary organic aerosols. The MARS-A algorithm to calculate particulate partitioning of nitrates Particulate partitioning algorithms for toxics and organic aerosols.

	Algorithms for transport and diffusion of all pollutants. Convective transport effects. Detailed treatments of dry and wet deposition processes. Aqueous and gas phase chemistry of mercury. Chemical transformations of toxics such as POM and dioxins. Particle and Precursor Tagging Methodology (PPTM) for sulfur, nitrogen, and mercury to allow estimation of source contributions
Input data	REMSAD requires a number of input files containing spatially resolved (3-dimensionally gridded) and temporally resolved (time-varying) data on meteorological parameters, emissions and physical characteristics.
Output data	REMSAD provides gridded, averaged surface and multi-layer instantaneous concentrations, and surface deposition output for all species and grids simulated. The averaged surface concentrations and deposition are intended for comparison with measurements and ambient standards.
Model limitations	Highest resolution is about 1 – 2 km. Long simulation periods and high resolution require considerable computer resources. Preparation of input data for large applications can be time and computer resource intensive.

Table 18. UAM-V model.

Name	**UAM-V** (Urban Airshed Model-V)
Version	v1.50
Model developer	ICF Consulting Inc.
Web url	http://www.uamv.com
Description	The UAM-V Model is a three-dimensional, multi-scale photochemical grid model that calculates concentrations of pollutants by simulating the physical and chemical processes in the atmosphere. The model is the latest of the Urban Airshed Model (UAM) lineage, which was initiated in the early 1970s and has undergone nearly continuous cycles of application, performance evaluation, update, extension, and improvement.
Knowledge level	Some prior experience in modeling and atmospheric science is helpful. User should be comfortable running applications in a Unix/Linux environment. User must be capable of organizing and handling large data sets.
Model code available?	See http://www.uamv.com for registration and download instructions. Available for free.
Pre & Post processors	Vertical turbulent exchange coefficients are estimated using either output from a prognostic meteorological model, such as MM5, or a preprocessor that utilizes gridded UAM-V input wind and temperature information.
Computer requirements	PC or Workstation, 100 Mb memory, 20 Gb disk space
Model scale	The typical time step is 10–30 minutes for coarse (10–40 km) grids and a few minutes for fine (1–2 km) grids.
Features and capabilities	The model contains the following features: capability of simulating multiple nested grids of variable resolution, two-way communication between nested grids, multiple coordinate system capabilities, and plume-in-grid (PiG) treatment. The UAM-V also includes Process Analysis capabilities that allow the user to quantify the contributions from the physical and chemical processes to simulated concentrations in selected grid cells. The model employs the Carbon Bond V chemical kinetics mechanism, an updated version CB-IV mechanism (Gery, at al., 1989)
Input data	The model requires input data specifying the emissions and initial and boundary concentrations of gaseous precursors of ozone (VOC, NOx, and CO). The model also requires a full set of three-dimensional meteorological inputs, which can be provided by dynamic meteorological models (such as MM5) or diagnostic models (such as DWM). The UAM-V also has the capability of running without photochemistry (nonreactive), to simulate urban-

	or regional-scale CO concentrations.
Output data	The output provided by the UAM-V model includes a three-dimensional array of pollutant concentrations for all species simulated in two files: an average file provides hourly (or other averaging period specified by the user) concentrations that are an average of the concentrations at each advection time step; and an instantaneous file, that provides concentration fields at the beginning of the hour (or other user-specified time period). The model also provides a full list of input specifications, including emission summaries, mass fluxes across boundaries, history of the simulation, and a record of useful diagnostic parameters for each time step of the simulation.
Model limitations	Highest resolution is about 1 – 2 km. Long simulation periods and high resolution require considerable computer resources. Preparation of input data for large applications can be time and computer resource intensive.

4.2. Other U.S.A. models

U.S. EPA and the National Oceanic and Atmospheric Administration (NOAA) developed CAMEO (Computer-Aided Management of Emergency Operations). CAMEO is a set of software modules and programs designed to assist first responders and emergency planners.

- Access chemical property and response information, (CAMEO CHEMICALS)
- Model potential chemical releases, (ALOHA)
- Display results on a map, (MARPLOT, also ARCVIEW and ARCMAP)

The modules and programs work interactively to display critical information in an easy-to-understand manner. During a response to a chemical release, CAMEO can help decision makers quickly get the information they need for a safe, effective response.

Table 19. ALOHA model.

Name	ALOHA (Areal Locations of Hazardous Atmospheres)
Version	Version 5.4.1.2
Model developer	U.S. EPA /NOAA
Web url	http://www.epa.gov/oem/content/cameo/aloha.htm
Description	ALOHA is an atmospheric dispersion model used for evaluating releases of hazardous chemical vapors. ALOHA allows the user to estimate the downwind dispersion of a chemical cloud based on the toxicological/physical characteristics of the released chemical, atmospheric conditions, and specific circumstances of the release. ALOHA can estimate threat zones associated with several types of hazardous chemical releases, including toxic gas clouds, fires, and explosions. Threat zones can be plotted on maps with MARPLOT or ARCVIEW to display the location of other facilities storing hazardous materials and vulnerable locations, such as hospitals and schools.
Knowledge level	Basic, ALOHA is designed to be extremely user friendly. It contains pull down menus with prompts and warning and caution messages. ALOHA's output is designed for easy use and interpretation.
User community	Intended users: First responders (such as fire and police services); State, local, and industry planners; Environmental organizations and academics. ALOHA is used by thousands of people and organizations, and it has been introduced into about 50 countries. CAMEO has been adopted by the United Nations Environment Programme's APELL (Awareness and Prevention of Emergencies at the Local Level) program, which promotes planning and preparedness for chemical accidents, especially in newly-industrializing countries. http://www.unepie.org/scp/sp/links/disasterprev.htm
Model code available?	Yes, source code is available under commercial agreement with American Institute of Chemical Engineers (AICHE). Executables are available at U.S. EPA website.
Computer requirements	ALOHA runs on Apple Macintosh computers and Microsoft Windows (Version 3.0 or later). It requires at least 1 megabyte of RAM and a hard drive. It enjoys extremely good portability and can be used by a first responder at the scene of an emergency. **Run execution time** (for a typical problem)**:** 1-2 minutes
Model scale	Microscale and short term releases.
Input data	Required Inputs ▪ Enter basic scenario information (such as date, time, and location). ▪ Choose a chemical from ALOHA's chemical library. ▪ Enter atmospheric information (such as wind speed and direction, air temperature, and cloud cover) by hand or

	automatically using a portable station for atmospheric measurements (SAM). ▪ Choose a source: direct, puddle, gas pipeline, or tank. ▪ Enter source information (such as release amount, tank dimensions, and whether the chemical is burning). ▪ Specify the Levels of Concern (LOCs) you want ALOHA to use when estimating the threat zones or use the default LOCs ALOHA offers. ▪ Choose the type of hazard (such as a toxic vapor cloud or a vapor cloud explosion) you want ALOHA to use when estimating the threat zones.
Output data	Text summaries of user inputs and model results; graphs of predicted source strength and on- and off-centerline indoor and outdoor concentrations; dose over time at specified locations; and a "footprint" plot of the area downwind of a release where concentrations may exceed a user-set threshold level. Complete scenario sets can be saved as archive files.
Chemical reactions	Not modeled
Model limitations	ALOHA has many strengths on the chemical source term side and many weaknesses on the dispersion model side. ALOHA models releases and disperses pure, nonreactive chemicals only. It does not account for terrain steering or changes in wind speed and horizontal direction, nor does it model particulate dispersion or chemical mixtures. It does not account for initial positive buoyancy of a gas escaping from a heated source, nor byproducts of combustion (such as smoke) or chemical reactions. ALOHA assumes the ground is flat and does not model the trajectories of the hazardous fragments.

4.3. Models developed in Europe

4.3.1. European Air Quality Monitoring and Forecasting GEMS and MACC European community projects

Table 20. CHIMERE model.

Name	CHIMERE
Version	Chimere2008
Model developer	Institut Pierre Simon Laplace (IPSL) /Laboratoire Inter-universitaire des Systèmes Atmosphériques (LISA) / Institut National de l'EnviRonnement industriel et des rISques (INERIS) -France
Web url	http://www.lmd.polytechnique.fr/chimere/ http://macc-raq.gmes-atmosphere.eu/som_forecast.php
Description	The CHIMERE multi-scale model is primarily designed to produce daily forecasts of ozone, aerosols and other pollutants and make long-term simulations for emission control scenarios. CHIMERE runs over a range of spatial scale from the regional scale (several thousand kilometers) to the urban scale (100-200 km) with resolutions from 1-2 km to 100 km.
Knowledge level	Intermediate
User community	Chimere users mailing list: chimere-users@lmd.polytechnique.fr questions: chimere@lmd.polytechnique.fr Complete documentations available, ranging from the scientific description down to users manuals with details on the machine code. Scientific and technical documentation in english is avaliable in PDF file on the chimere web site.
Model code available?	Yes, online free access to the code under the General Public License
Computer requirements	LINUX systems. CPU time: Depending on resolution, application. The model is now parallelized and may run over an European domain with 10km resolution and for 5 days in less that 10min (with gas and aerosols) on a PC linux cluster. Storage: Depending on resolution, application. For example, a forecast of 5 days, over a large western europe domain needs 2G disk storage.
Model scale	Temporal resolution: From 5min to 1 hour, depending on the user choice. Horizontal resolution: 1km to 100km
Input data	All chimere input data are free and available on line on the chimere web site with references and documentation. **Emissions** The model provides an interface combining several emissions sources such as EMEP (Yearly totals), IER (Time variations), TNO (Aerosol emissions), UK Dept of Environment (VOC speciation). **Meteorological**: A CHIMERE interface for the MM5 and WRF models have been developed. **Concentrations** A set of boundary conditions from the MOZART II model is proposed as a default solution.
Output data	Four dimensional (x-y-z-t) concentrations fields of all active species, following the usr selection. Diagnosed turbulent parameters (boundary layer height, friction

	velocity etc.), dry and wet deposition fluxes.
Chemical reactions	CHIMERE offers the option to include different gas phase chemical mechanisms. The original, complete scheme, hereafter called MELCHIOR1, describes more than 300 reactions of 80 gaseous species. The hydrocarbon degradation is fairly similar to the EMEP gas phase mechanism. Adaptations are made in particular for low NOx conditions and NOx-nitrate chemistry. Heterogeneous formation of HONO from deposition of NO2 on wet surfaces is now considered, using the formulation of [Aumont, 2003]. In order to reduce the computing time a reduced mechanism with 44 species and about 120 reactions is derived from MELCHIOR, following the concept of *chemical operators*. This reduced mechanism is called MELCHIOR2 hereafter.
Model limitations	Lower tropospheric description. No global version. Long simulation periods (more than 24 hours)

Table 21. EURAD model.

Name	EURAD (European Air Pollution Dispersion Model)
Version	CTM 3.0
Model developer	Institut fuer Geophysik und Meteorologie, Universitaet zu Koeln (Germany)
Web url	http://www.uni-koeln.de/math-nat-fak/geomet/eurad/index.e.html http://macc-raq.gmes-atmosphere.eu/som_forecast.php
Description	EURAD is a threedimensional Eulerian model designed to predict air pollution episodes, trends and to study emission reduction scenarios. Therefore, EURAD simulates the transport, chemical transformations and depositions of atmospheric constituents in the troposphere over Europe. Its comprehensive description of atmospheric processes includes chemical processes in clouds and rain and also the development of aerosols.
Knowledge level	Advanced
Model code available?	Standard version is available to selected groups for scientific purposes. Please check with ctmuser@eurad.uni-koeln.de
Computer requirements	Linux PC cluster. Time needed for run15 minutes up to several hours for 24 hours model simulation storageUp to 1 GB for 24 hours model simulation
Model scale	Time scale: analysis of long and short term AQ indicators, on-line analysis of AQ indicators during episodes. Spatial scale: from local to continental (30 – 3000 km)
Features and capabilities	Eurad can be used in several political issues like: Ozone depletion Tropospheric ozone Acidification Summer smog Winter smog Air toxics Urban air quality Industrial pollutants Nuclear emergencies Chemical emergencies
Input data	The EURAD model consists of several modules which are developed at several institutions. Main modules are EEM EURAD Emission Module MM5 Meteorological Model Version 5 (http://www.mmm.ucar.edu/mm5/mm5-home.html) CTM Chemistry and Transport Model Meteorological data are calculated by MM5 which itself uses initial and boundary conditions from ECMWF-data. The actual CTM uses then the meterological input (wind, temperature, pressure etc.) and emission inventories from the

	EEM to predict the dynamic behaviour of air pollutants including aerosols in the model region.
Output data	Concentrations (e.g. NO, NO2, SO2, SO4, O3, CO, OH, HO2, several VOC) Deposition Fluxes Chemical Fluxes
Chemical reactions	Gas-Phase: RADM2-model, CBM4 in preparation. Aerosols with MADE/SORGAM
Model limitations	Source code not available for public in general. No experience yet with taifun, tornadoes

Table 22. MOCAGE model.

Name	MOCAGE (Modèle de Chimie Atmosphérique à Grande Echelle)
Version	2.0
Model developer	Core team at Meteo-France/CNRM - CERFACS - Laboratoire d'Aerologie
Web url	http://www.cnrm.meteo.fr/gmgec/spip.php?article76&lang=fr http://prevair.ineris.fr/en/modele.php http://macc-raq.gmes-atmosphere.eu/som_forecast.php
Description	MOCAGE is the Météo-France multi-scale Chemistry and Transport Model, that covers wide range of topical issues, ranging from chemical weather forecasting, tracking and backtracking of accidental point source releases, transboundary pollution assessment, assimilation of remote sensing measurements of atmospheric composition, to studies of the impact of anthropogenic emissions of pollutants on climate change.
Knowledge level	Basic
User community	developed for both research and operational applications in the field of atmospheric environment
Model code available?	Yes, freely in the framework of research collaborations (Memorandum of Understanding needed)
Computer requirements	Code is ported on Linux clusters. **Time needed for run**: Highly dependent on platform and model version: from ~10 minutes (simplified chemistry, low resolution) to 2 hours per 24h generally **Storage**: depends on domain, number of chemical variables and frequency of output...
Model scale	Meso and macroscale. MOCAGE considers up to 4 nested subdomains. The primary domain is global, hence the model provides its own time-dependent chemical boundary conditions. The downscale part is performed within the semi-lagrangian advection scheme.
Features and capabilities	MOCAGE provides a comprehensive physical and chemical package, in order to consider simultaneously the troposphere and stratosphere, for gases as well as for aerosols. Within GEMS FP6 project, MOCAGE was used in off-line mode, forced by ECMWF global analyses and forecasts. It is possible to zoom down to the regional scale over limited-area sub-domains, an option which is used within the Regional Air Quality subproject.
Input data	**meteorology**- ARPEGE/ALADIN operational numerical weather prediction analyses and forecasts (Météo-France) - IFS operational numerical weather prediction analyses and forecasts (ECMWF) - coupling with climate models (ARPEGE-Climat, ECHAM). **Concentrations** MOCAGE provides its own chemical initial and boundary conditions **emissions**- several available datasets at the

	global scale (EDGAR, GEIA, MOZART, RETRO,...). Several options for Europe (EMEP, GENEMIS). High-resolution emissions over some regions in France. Can be provided by the user. **Orography and land use**: Same as ARPEGE/ALADIN meteorological models
Output data	Outputs are user defined
Chemical reactions	The comprehensive version of MOCAGE merges the tropospheric RACM and stratospheric REPROBUS schemes for a total of 120 species / 350 reactions but several other schemes available.
Model limitations	ORILAM/ORISAM scheme for aerosol chemistry is currently tested within MOCAGE. Probably available in the next model release.

Table 23. NAME III model.

Name	NAME III (Numerical Atmospheric dispersion Modeling Environment)
Version	Version 5.4 (November 2009)
Model developer	UK's Met Office
Web url	http://www.metoffice.gov.uk/research/modelling-systems/dispersion-model http://gems.ecmwf.int/d/animate/gems/gems/raq/forecasts/plot_UKN
Description	NAME is used to model a wide range of atmospheric dispersion events. This includes nuclear accidents, volcanic eruptions, chemical accidents, smoke from fires, odours, airborne animal diseases as well as in the provision of routine air quality forecasts. The model is used for research activities and for emergency air pollution forecasts.
Knowledge level	Advanced
User community	The model can be made available to research users
Model code available?	NAME is available for external research use under licence. A number of UK Universities, UK government agencies and the South African Weather Service use NAME in collaboration with the Met Office to undertake dispersion based research.
Computer requirements	Runs on PCs (Linux or Windows) CPU time Dependent on many things. However a two-day dispersion run for a single point source, using 12 km resolution meteorology, typically takes 5 minutes on a modern (2007) desktop linux machine. A full air quality forecast for the whole of Europe out to 3 days takes between10 and 24 hours, depending on meteorological conditions. **Storage** Data is stored on local hard disk drives and retained in an archive.
Model scale	NAME is a flexible modelling environment able to predict dispersion over distances ranging from a few kilometres to the whole globe and for time periods of minutes to decades.
Features and capabilities	NAME III is an off-line Lagrangian air pollution dispersion model for short range to global range scales. In essence, NAME follows the 3-dimensional trajectories of parcels of the pollution plume and computes pollutant concentrations by Monte Carlo methods— that is, by direct simulation rather than solving equations. Summary of current capabilities: Met input as 3-D fields or, for short range problems, single site observations Use of radar rainfall data when available Dispersion and deposition using particles or puffs Building effects Small scale terrain effects (linear flow model) Fluctuations

	Radioactive decay Virus decay due to UV and humidity Chemistry The model can also be run 'backwards' to generate maps that locate possible plume originating sources. Source shape: cuboidal and elipsoidal. Source size: point to global. Number of sources only memory limited (> 10000 have been used)
Input data	Meteorological: from the Met Office NWP model (Unified Model). This is a well validated weather forecast model used operationally in the UK. Data is available for research purposes. Emissions:UK National Emissions Inventory and EMEP Orography and land use: From meteorological model
Output data	A wide range of output options can be specified, including concentrations in a cell at a given time, integrated columns, accumulated dose etc. etc.
Chemical reactions	40 advected tracers + 18 non-advected 140 reactions + 23 photolytic reactions 16 emitted species Gaseous and aqueous phase chemistry
Model limitations	As an off-line model the temporal resolution of the met data supplied (usually one or three hourly) is a limitation. - Computational constraints limit the number of Lagrangian particles which can be followed during an air quality simulation. This is a limiting factor in the case of widely dispersed secondary pollutants such as ozone and secondary particulates.

Table 24. MATCH model.

Name	MATCH (Multi-scale Atmospheric Transport and Chemistry model)
Version	5.0 (November 2009)
Model developer	SMHI - Swedish Meteorological and Hydrological Institute
Web url	http://www.smhi.se/en/Research/Research-departments/Air-quality/match-transport-and-chemistry-model-1.6831 http://macc-raq.gmes-atmosphere.eu/som_forecast.php
Description	MATCH models the basic processes of atmospheric transport, governing sources, sinks and transformation of atmospheric trace constituents in a three-dimensional framework. The model is Eulerian and can be configured with an arbitrary number of layers in the vertical and for different geographical areas with different resolution. Depending on application, specific modules describing physical or chemical transformation processes are added to the basic model.
Knowledge level	Intermediate - advanced
User community	Governmental organizations, regional networks, municipalities, cities, public
Model code available?	Yes, upon request and license agreement. The model is not a public domain programme.
Computer requirements	**Portability:** MATCH is portable to Linux, IBM, HP, SG, (Dec Alpha). The model could be compiled for parallel platforms (Linux, IBM, SG). **CPU time:** A setup for photochemistry with 72 compounds, a domain of 100x80x30 and over 3 days takes takes in total 18 hours on IBM. Distributed over 32 tasks the elaps time is 1.20 hours. In summary 15 min per simulated hour and 29 sec per task and simulated hour. **Storage:** Most often, results from MATCH are stored in WMO GRIB-format. However, other storage formats such as NetCDF and even ASCII have also been implemented and used in several applications.
Model scale	**Temporal resolution** Often used: 600 seconds. Simulated time period: several years. **Horizontal resolution** Grid cell size: down to 0.5 km. **Vertical resolution** Grid cell height: down to 15 m, typically for regional scale -lowest layer 60 m. Domain height: often used 8 km.
Features and capabilities	MATCH model is a three-dimensional, off-line Eulerian model developed at the Swedish Meteorological and Hydrological

	Institute (SMHI). It is used in a range of applications from urban scale studies on ca. 5km, or higher, resolution to regional/continental scale studies on acidifying/eutrophying deposition and photochemistry. MATCH is used for air pollution assessment in Sweden and the Baltic Sea region; the air pollution budgets of nitrogen and sulphur compounds for Sweden are calculated annually, using a system combining the MATCH model calculations and monitoring data from Sweden and the neighbouring countries. The model is also used operationally to provide forecasts of radioactivity in case of nuclear emergencies in Europe. Different set-ups of the model have been used in a variety of applications in Sweden, Europe, the Arctic, Africa, South America, Australia, South-, East- and Southeast Asia.
Input data	**Meteorology**: is taken from the three-dimensional dynamical meteorological model HIRLAM which is run operationally for weather forecasting at the Swedish Meteorological and Hydrological Institute (SMHI). Also data from ECMWF and from a regional climate model is used. **Concentrations** Measured data, e.g. from EMEP stations and/or data from large scale models **Emissions** EMEP, GEIA, SEI, Streets et al., Local emission inventories **Orography and land use**: from meteorological files
Output data	Hourly, daily, weekly, monthly and annual average, pollutant concentration and dry and wet deposition for each grid cell.
Chemical reactions	The total chemical scheme includes 110 thermal, 28 photochemical, 2 aqueous-phase, 5 aerosol reactions and 4 gas-phase aqueous-phase and aerosol equlibria between 60 chemical components. The gas-phase chemical mechanism used in MATCH is based on the EMEP MSC-W model chemistry but has been extended somewhat since the original implementation in 1998. Aqueous-phase oxidation of SO2 by ozone and H2O2 in cloud water is implemented in the model.
Model limitations	The model has been successfully used for simulations for a variety of applications within a range of scales and resolutions. Beyond a horizontal resolution of 500m though, no knowledge of its performance is available. Limitations resulting from the nature and current design of the model are a dependency of the vertical resolution on the vertical resolution of the driving meteorological model as well as the non-treatment of feedbacks of changes in chemical composition on physical meteorological variables due to MATCH design as offline-model.

Table 25. SILAM model.

Name	SILAM (Air quality and emergency modeling system)
Version	v.3.8.1 for emergency response, v 4.2 for other applications, v 4.5 pre-operational forecast (scientific use only)
Model developer	Finnish Meteorological Institute (FMI)
Web url	http://silam.fmi.fi/ http://macc-raq.gmes-atmosphere.eu/som_forecast.php
Description	The SILAM system is a universal framework built for a wide-range meso-to-continental-scale dispersion tasks including the emergency response, air quality assessment, scenario analysis, data assimilation and analysis, etc.
Knowledge level	Basic, intermediate or advanced. Largely depends on task. Via graphical interface (available for emergency tasks, restricted access via SILAM web portal), the model can be run with minor prior knowledge, while sophisticated setups might require extensive understanding of both theory and implementation of the specific processes.
User community	Emergency preparedness: operational dept. of FMI., Finnish Radiation Protection Authority Operational air quality forecasts: operational dept. of FMI. Research purposes: Finnish Met. Inst, University of Tartu (Estonia), University of Vilnius (Lithuania), Main Geophysical Observatory (Russia), over 15 downloads from various countries with unclear or non-specified current status of the installations.
Model code available?	The model is public. Well-tested operational version is available from the Web site. Additionally, registered users receive the crucial updates and, if subscribed, the information on new model versions. Research version of the model is available on request.
Computer requirements	workstation/server under UNIX/Windows/Linux **time needed for run:** from minutes to weeks depending on setup **storage** Strongly depends on the user request for the output. Typical feasible output with grid ~200 x 200 x 10 levels, hourly output for a month for 5 species or aerosol size classes ends up in ~10GB.
Model scale	**Temporal resolution** Maximum temporal resolution depends on the kernel: 15 minutes for Lagrangian and up to 2-5 minutes for Eulerian. Operational output time step is 1 hour to limit the amount of data. For Lagrangian kernel, it is also the recommended value. **Horizontal resolution** Depending on the kernel, the highest possible resolution is: 5km for Lagrangian and 1km (untested: 0.5km) for Eulerian. **Vertical resolution** Arbitrary. SILAM allows free selection of output vertical layers in several

	vertical types and generates the appropriate internal vertical used for actual computations to meet the user request.
Features and capabilities	SILAM v.4.0 and later contains two independent dynamic kernels - 3-D Lagrangian and 3-D Eulerian. The Lagrangian kernel incorporates a high-precision iterative advection algorithm and a Monte-Carlo random-walk representation of atmospheric diffusion. It is mainly used for the emergency-preparedness simulations. The Eulerian kernel is combines the SCD developed by M.Galperin and a complementary vertical scheme based on extended resistance-analogy approach. That model is used for the bulk of the applications, including air quality assessment and forecasting. SILAM includes a set of supplementary tools including a meteorological pre-processor, input-output converters, grid transformers, interpolation routines, etc. These ensure a high flexibility to the user requests, enabling in particular the usage of various NWP models as data sources, with dynamical determination of internal model parameters such as the computation grid, vertical structure and a list of meteorological quantities needed for computations.
Input data	The model requires the gridded basic meteorological data (routinely Hirlam and ECMWF, case studies: any NWP model capable of WMO GRIB format) and appropriate information on emission (depends on the computed species and type of the run), as well as the basic physiographical information.
Output data	Model output is performed in the user-requested grid (independently from the grids and projections of the input data) for the list of user-requested quantities, which can include both meteorological, physiographical and dispersion variables. Typically, concentrations, depositions, probability of the area to be affected by the accidental release (area of risk).
Chemical reactions	The 8 chemico-physical modules allow computations of radioactive pollutants (the model database includes 496 nuclides with decay chains, dose rates and doses targeting up to 23 organs of the human body); SOx-NOx-NHx-O3 (Eulerian kernel only), SOx-only, natural pollen, inert aerosol, toxic species, sea salt, and passive tracer (also used for probabilistic assessments).
Model limitations	The model was developed for meso-to-continental scales of dispersion simulations. Both Lagrangian and Eulerian advections provide near-analytical quality of solutions while the compromises are made in diffusion formulations. The main limiting factor for Lagrangian system is the well-mixed ABL assumption, which tends to over-mix the species for very high resolutions when short time steps are forced. For Eulerian model, the limit comes from the K-closure for the vertical and horizontal diffusion.

	The large-scale limitations come mainly from the simplified free-troposphere diffusion. Lagrangian kernel assumes fixed mixing coefficient, while Eulerian one takes 10% of the ABL max value. The model chemical schemes are so far kept independent with implicit assumption that interactions between species represented in different modules are negligible. A work is on-going to allow joint computations for some of the modules following the single-atmosphere principle.

Table 26. BOLCHEM model.

Name	BOLCHEM (Bologna limited area model for meteorology and chemistry)
Version	1.1.0
Model developer	Consiglio Nazionale delle Ricerche (CNR)- Instituto di Scienze dell'Atmosfera e del Clima (ISAC) Italy
Web url	http://bolchem.isac.cnr.it/projects:bolchem.do http://gems.ecmwf.int/d/products/raq/forecasts/
Description	The on-line modelling system BOLCHEM consists of a meteorological limited area hydrostatic model (BOLAM), developed at ISAC – CNR, coupled with different gas chemistry models (SAPRC90 and CB-IV chemical mechanisms), an aerosol model (aero3 module) and a Lagrangian dispersion model for computation of forward and backward trajectories.
Knowledge level	Intermediate – advanced. A suite of tools is under development for intermediate-knowledge users
Model code available?	available for scientific collaboration or for operational use
Computer requirements	depends on the resolution
Model scale	Mesoscale. Short and long term
Input data	**Meteorology:** IFS (ECMWF) , GFS (NCEP) **Concentrations:** EMEP , Mozart GEMS **Emissions:** EMEP GEMS/TNO ENEA (for italy) Cityzen/INERIS

Table 27. LOTOS-EUROS model.

Name	LOTOS – EUROS (LOng Term Ozone Simulation - EURopean Operational Smog model)
Version	Version 1.5
Model developer	TNO (Netherlands Organisation for Applied Scientific Research), RIVM (National Institute for Public Health and the Environment) Netherlands
Web url	http://www.lotos-euros.nl http://macc-raq.gmes-atmosphere.eu/som_forecast.php
Description	RIVM (EUROS model) and TNO (LOTOS model) have independently developed models to calculate the dispersion and chemical transformation of air pollutants in the lower troposphere over Europe. The LOTOS-EUROS model is a 3D eulerian chemistry transport model used for the assessment of photo-oxidants, aerosols, POPs and heavy metals.
Knowledge level	Basic-Intermediate
User community	Results are use by e.g. governmental or local authorities, scientists within national and international projects. The model can only be used properly by a skilled person.
Model code available?	No public availability
Computer requirements	**Type:** PC **CPU time** 4.5 CPU day on a PC for 1 year simulation.
Model scale	**Temporal resolution**: hourly **Horizontal resolution** Standard grid resolution is 0.5 x0.25 degrees lon-lat (approximately 25x25 km), zoom possible for regional/national applications generally up to 0.125x0.0625 degree lon-lat **Vertical resolution** 4 layers up to 3.5 km, surface layer of 25 meter, mixing height layer and 2 reservoir layers. Possible extension to 5 km with an extra top layer.
Input data	**Orography** from meteo **land use** PELINDA and CORINE/SMIATEK databases **meteorology** TRAMPER (Tropospheric Realtime applied meteorological procedures for Environmental Research) **concentrations** boundary conditions: from TM3 model or Logan climatology (ozone) or measurements **emissions** TNO or EMEP emission database
Output data	hourly 3-D concentration fields of O3, NOx, SIA (secondary inorganic aerosols), SOA (secondary organic aerosols), POPS (persistent organic pollutants), Na, Pb, Ld, primary aerosol (BC-black carbon, PM2.5 PM10, sea salt), hourly 2-D deposition fields, hourly 3-D budget fields per grid cell or larger units budgets are

	defined by the separate terms in the continuity equation (transport, chemistry, dry and wet deposition, emissions).
Chemical reactions	The LOTOS-EUROS model contains two chemical mechanisms, the TNO CBM-IV scheme and the CBM-IV by Adelman (CB99), the scheme includes 28 species and 66 reactions, including 12 photolytic reactions. Aerosol chemistry is represented using ISORROPIA and SORGAM.
Model limitations	Simple chemistry (a slightly adapted version of CBM-IV) does not allow accurate night time simulations coarse resolution, especially in the vertical direction. The mixing layer is treated as one layer. Ground level ouput is generated by assuming a vertical profile near the ground based on the deposition velocities.

Table 28. EMEP model.

Name	EMEP (EMEP Unified Model)
Version	rv3.0
Model developer	Meteorological Synthesizing Centre-West at Norwegian Meteorological Institute (MET.NO)
Web url	http://www.emep.int/ http://macc-raq.gmes-atmosphere.eu/som_forecast.php
Description	The Unified Eulerian EMEP model is an eulerian multi-layer atmospheric dispersion model for simulating the long-range transport of air pollution over several years. The air pollutants under consideration are those involved in ecosystem and health damages, in particular major acidifying and eutrophying pollutants (S,N), photo-oxidants and particulate matter (PM2.5, PM10).
Knowledge level	Advanced
User community	The EMEP models have been instrumental to the development of air quality policies in Europe since the late seventies, mainly through their support to the strategy work under the Convention on Long-range Transboundary Air Pollution. In the 1990's the EMEP models became also the reference atmospheric dispersion model for use in the Integrated Assessment Models supporting the development of air quality polices under the EU Commission.
Model code available?	Yes, The Unified EMEP model source code is publicly available under the GNU General Public License version 3 since the beginning of 2008, http://www.emep.int/OpenSource/index.html
Computer requirements	To compile the Unified EMEP model you need: Fortran 90/95 compiler NetCDF Library (>3.5.1) MPI Library (>1.) Time needed for run: It takes □ 4.5 hrs on 32 Opteron 246 (2GHz) for 1 year. Storage The code has been tested with 1 to 128 CPU, and scales well. If only one CPU is used 1-2 GB memory is required and if more than one for example 32 CPU are used, 200 MB of memory per CPU is enough (in the case of a 170X133 grid size).
Model scale	**Temporal resolution** 20 min **Horizontal resolution** 50x50 km2 **Vertical resolution** 20 layers up to 100hPa, varying height
Features and capabilities	The EMEP modelling system allows several options with regard to the chemical schemes used, and the possibility of

	including aerosol dynamics. In principal, the new modelling system can run any chemistry with relatively little effort, but we have two standard chemistries, UNI-ACID and UNI-OZONE, derived from the earlier acidification and oxidant applications of the model. Additionally, the model version with aerosol dynamics is labelled UNI-AERO. For current policy runs, the UNI-OZONE chemistry is used as standard.
Input data	The standard input files for the Unified EMEP model are provided in two different formats, netCDF or ASCII. The 3 hourly meteorological input data and the initial and boundary conditions data are in netCDF format, and all other input data are in ASCII. **Meteorology** Optional. Usually HIRLAM for regional model calculations. For Hemispheric transport of air pollution (HTAP) model calculations ECMWF **Orography** Dependant on model domain/meteorological input **Land use** EMEP for EMEP domain, else based on MM5 **Emissions** The emission input for the Unified EMEP model consists of gridded annual national emissions based on emission data reported every year to EMEP/MSCW (until 2005) and to CEIP (Centre on Emission Inventories and Projections) (from 2006) by each participating country. Outside EMEP domain combination of sources.
Output data	Output files from a model run are written out in either ASCII, or (for most data outputs) in netCDF format into the working directory. The user has the possibility to choose what kind of the output data will be written out in the different output data files. List of output files: Gridded daily, hourly, instantaneous, monthly, yearly values of a selection of compounds. (netCDF format) Surface, vertical daily values of a selection of stations and compounds per month (ascii format) Total emissions of different air pollutants per country (ascii format).
Chemical reactions	The chemical scheme couples the sulfur and nitrogen chemistry to the photochemistry using about 140 reactions between 70 species. The chemical equations are solved using the TWOSTEP algorithm.
Model limitations	Mainly 50x50km2 polarstereographic grid, extensions to hemispheric and 5x5km2 in progress.

Table 29. CAC model.

Name	CAC (tropospheric Chemistry Aerosol Cloud transport model)
Version	January 2001
Model developer	Atmospheric Environment Group, Danish Meteorological Institute (DMI)
Web url	http://gems.ecmwf.int/d/products/raq/forecasts/ http://gems.ecmwf.int/documents/workdescription/4_CAC_DMI.html
Description	The CAC modelling system is a highly flexible module based system. This makes it easy to perform changes of the chemistry (gas- and liquid-phase), add new aerosol distributions, and apply the model to another emission inventory and/or meteorological data. The model system is used for real-time regional scale forecasts of ground-level gas-phase air pollutants and regional scale modelling of historical ground-level gas-phase and aerosol air pollutant data.
Model code available?	No
Observations	DMI developed the on-line coupled ENVIRO-HIRLAM model, and has implemented CAC in the ENVIRO-HIRLAM model, as an aerosol mechanism. This implementation makes the inclusion of regional to urban scale feedbacks between CAC and DMI-HIRLAM possible.

4.3.2. Other European Models

Table 30. ENVIRO-HIRLAM model.

Name	ENVIRO-HIRLAM
Version	Version 7.2 (2009)
Model developer	Danish Meteorological Institute and HIRLAM community
Web url	http://hirlam.org/index.php?option=com_content&view=article&id=68:hirlam-chemical-branch-a-enviro-hirlam-online-integrated-nwp-actm-model&catid=119:mesoscale-modelling-harmonie&Itemid=123
Description	ENVIRO-HIRLAM is an on-line integrated system with a possibility of the off-line coupling as well.
Knowledge level	Advanced
User community	Hirlam community. For research purposes
Model code available?	No, question of negotiations with the HIRLAM consortium
Model scale	Meso and macroscale. Short term.
Chemical reactions	Gas-phase chemistry: RADM, RACM, CBMZ Photolysis: Madronich Cloud chemistry CAC-Aerosol mechanism, MOSAIC, MADE/SORGAM
Model limitations	An off-line version is not public available (suitable for emission scenarios analysis and air quality management)

Table 31. PHAST software.

Name	PHAST (Process Hazard Analysis Software Tool)
Version	v 6.6 (july 2010)
Model developer	Det Norske Veritas (DNV) company, Norway
Web url	http://www.dnv.com/services/software/products/safeti/safetiqra/phast.asp
Description	PHAST examines the progress of a potential incident from the initial release to far field dispersion, including modelling of pool spreading and evaporation, and flammable and toxic effects. PHAST is able to simulate various release scenarios such as leaks, line ruptures, long pipeline releases and tank roof collapse in pressurised / unpressurised vessels or pipes. This software contains models tailored for hazard analysis of offshore and onshore industrial installations. These include: • Discharge and dispersion models, including DNV's proprietary Unified Dispersion Model (UDM). • Flammable models, including resulting radiation effects, for jet fires, pool fires and BLEVEs. • Explosion models, to calculate overpressure and impulse effects. Available models include the Baker Strehlow, TNO Multi-Energy and TNT explosion models. • Models for the toxic hazards of a release including indoor toxic dose calculations.
Knowledge level	Level of knowledge needed to operate model: Basic - Intermediate. All configurations of Phast share the same Graphical User Interface and standard Windows look and feel. Compatible with popular office applications. Excel import and export facility. On-line electronic help and dedicated Helpdesk are available with the license agreement.
User community	Oil and gas industries, petrochemical companies, chemical manufacturers, governments and regulatory authorities, consultancy and design services, insurance companies, universities
Model code available?	No, the software developer doesn't distribute source code. Executables are available from DNV under commercial agreement. Phast is available in a number of modes, from consequence analysis only to full risk analysis, in order to match user requirements. Phast also comes with a number of extensions which increase the functionality available within each mode.
Computer requirements	PC Windows. GIS visualization tools.
Model scale	Microscale and short term releases.
Input data	Required Inputs ▪ Basic information about storage or process conditions and

	material properties in order to perform discharge calculations. The software comes with an integrated material property database containing more than 1,600 pre-defined pure component chemicals. ▪ Various discharge scenario options have been implemented to represent common process failures, and model their behaviour. These include: - Leaks and line ruptures from long & short pipelines - Catastrophic ruptures - Relief valves and disc ruptures - Tank roof collapse - Vent from vapour spaces - In building release effects ▪ Orographic conditions (surface roughness). ▪ Atmospheric information (wind speed, atm. temperature, atm. Pressure, atm. Humidity, wind profile, T/P profile, atm. Sp. heat).
Output data	Results in a graphical or report format (excel spreadsheets) Overlay results on Geographical Information System, maps, aerial photographs and CAD images **Dispersion** The dispersion models within PHAST are able to model the following phenomena: - Dispersion of gas, liquid and two-phase releases - Liquid droplet thermodynamics calculations and liquid droplet rainout - Pool spreading and vaporization - Building wake dispersion effects for vapour releases **Flammable Effects** For releases of flammable material PHAST calculates: - Radiation profiles and contours from a range of fire scenarios including pool fires, flash fires, jet fires and fire balls, including cross-wind effects on a jet fire - Vapour Cloud Explosion modelling using industry standards models including the TNO Multi-Energy, Baker Strehlow Tang and TNT Equivalence models - Overpressure contours from Boiling Liquid Expanding Vapour Explosions **Toxics effects** - Graphs of toxic concentration profile - Indoor and outdoor toxic dose prediction - Reporting of distance to specific dose and concentration - Calculated exposure time and use as "averaging time" for passive dispersion effects
Chemical	Not modeled

reactions	
Model limitations	Phast is quite flexible, allowing the user customize values for a wide range of model parameters. Users of the software have found that simulation results may depend quite strongly on the values chosen for some of these parameters. While this flexibility is useful, it can lead different users to calculate effect distances that vary considerably even when studying the same scenario.

Table 32. PERLE model.

Name	PERLE (Programme d'évaluation des rejets locaux d'effluents)
Version	Version 2 (april 2010)
Model developer	Centre Météorologique régional spécialisé (CMRS) Toulouse, Meteo France
Web url	http://www.meteorologie.eu.org/CMC/web_CMC_extranet_fixe/fr_doc_perle.html http://www.meteorologie.eu.org/CMC/web_CMC_extranet_fixe/index_fichiers/index_doc/WMO_TD778_Toulouse_10.pdf
Description	PERLE was developed to model the dispersion of a cloud of pollutant emmited accidentally at local and regional scales, in the vicinity of the radionuclide or chemical release. PERLE is based on the use, in first place of three meteorological models to model the fine structure of the boundary layer (Meso-NH coupled to ALADIN/ARPEGE or ALADIN/CEP or AROME), and secondly on a Lagrangian particle dispersion model (LPDM from Colorado State University), to represent the dispersion and ground deposition of the pollutant. The choice of meteorological model that best suits the situation is the result of the expertise of the forecaster.
User community	Meteo France. At present, PERLE is used only over the Metropolitan France in operations by using ALADIN forecasts for the initial and boundary conditions of Meso-NH.
Model code available?	Not known.
Computer requirements	Not known.
Model scale	For short range (from 10 to 100 km, up to 24 hours only). Meso-scale model.
Input data	Required inputs: Atmospheric conditions from one of three meteorological models available Basic scenario information (discharge amount, height of release, date, location, chemical compound discharged)
Output data	For a chemical accident in the output table will be added concentrations graphics (in ppmv) (level 10m) and duration (in minutes) of exposure to the thresholds set automatically. For a radiological accident, in addition, maps of integrated concentrations over time since the beginning of the issue (in Bq.h /m3) are presented. Dry and wet deposition at soil (g/m2)
Chemic	Not modelled

al reactions	
Model limitations	LPDM: - Possibility of "noisy" concentration zones when dispersion is high (amount of particles released to the plume not enough). Meteorological context: - Low wind: risk of significant error in plume direction. - Convective situations: high temporal variability of wind direction poorly represented by the model and likely underestimation of horizontal expansion and vertical plume. No possibility to initialize the model with a complex scenario of discharge: - Emission rate constant - Base and top of discharge constant - A single pollutant at once

4.4. International initiatives

Table 33. MOZART model.

Name	MOZART (Model of Ozone and Related Chemical Tracers)
Version	Version 4 (october 2009)
Model developer	NCAR, the Max-Planck-Institute for Meteorology (MPI-M), and NOAA Geophysical Fluid Dynamics Laboratory (GFDL).
Web url	http://gems.ecmwf.int/d/products/raq/forecasts/ http://www.acd.ucar.edu/acresp/forecast/
Description	Mozart is an off-line global chemical transport model designed to simulate the distribution of atmospheric ozone and other chemical compounds that affect its production and destruction. It is driven by standard meteorogical fields output from any number of meteorological centers (e.g. the National Centers for Environmental Prediction (NCEP), European Centre for Medium Range Weather Forecasts (ECMWF), or Global Modeling and Assimilation Office (GMAO)) or by fields generated from climate models.
Knowledge level	Intermediate
User community	The MOZART-4 source code is available to the scientific community to be used solely for educational, research, and not-for-profit purposes.
Model code available?	Yes, MOZART-4 is available from the NCAR website. Previous register required. http://cdp.ucar.edu/
Computer requirements	MOZART currently runs on a variety of platforms. For standard, multi-year simulations you will need access to a supercomputer with large amounts of disk space and/or tape storage (~200 GB). Short, or coarse-resolution, simulations or reduced-chemistry versions may be run on Linux workstations. On currently available 8-CPU linux workstations a year simulation of MOZART-4 takes 2-3 wall clock days. By comparison 64 IBM Power4 cpus will finish a year simulation in about 7.5 wall clock hours.
Model scale	Macroscale, long term
Features and capabilities	MOZART-4 is an "offline" model in that it requires dynamical and other data to be periodically input during a simulation. The standard dynamical datasets which drive MOZART-4 require about 6 gigabytes of disk storage for a simulation year. As supplied there is a standard output specification that results in about 25 gigabytes of output per simulation year. This is for the standard horizontal resolution of 128 x 64 and 28 vertical levels. Output is for variables that are output on a once a day and monthly basis. MOZART-4 has a preprocessor that among other

	capabilties allows the user to modify the "standard" output. Thus output could be considerably more than the "standard" 25 gigabyte per simulation year measure.
Chemical reactions	Mozart predicts the concentrations of approximately 100 chemical species from the surface up to the mesopause. The model includes approximately 200 chemical reactions including heterogeneous chemistry on aerosols and polar stratospheric cloud particles. It considers surface emissions of several chemical compounds (N_2O, CH_4, NMHCs, CO, NO_x, CH_2O, and acetone). The emissions due to fossil fuel combustion, agricultural burning and bio-fuel use follow the distribution of the EDGAR v2.0 inventory.
Model limitations	Not valid for short period simulations (less than one year)

Table 34. WRF-CHEM model.

Name	WRF-CHEM (Weather Research and Forecasting Chemistry model)
Version	Version 3.2 (April 2010)
Model developer	The development of WRF-Chem is a collaborative effort among the community: Department of Commerce / NOAA The Cooperative Institute for Research in Environmental Sciences (CIRES) The University Corporation for Atmospheric Research (UCAR) The National Center for Atmospheric Research (NCAR) The Max Plank Institute (MPI) The University of Chile
Web url	http://ruc.noaa.gov/wrf/WG11/
Description	WRF-Chem is a version of WRF that also simultaneously simulates the emission, turbulent mixing, transport, transformation, and fate of trace gases and aerosols with the meteorology. Applications of the current modeling system -Prediction and simulation of weather, or regional or local climate. -Coupled weather prediction/dispersion model to simulate release and transport of constituents. -Coupled weather/dispersion/air quality model with full interaction of chemical species with prediction of O_3 and UV radiation as well as particulate matter (PM). -Study of processes that are important for global climate change issues. These include, but are not restricted to the aerosol direct and indirect forcing.
Knowledge level	Advanced
User community	Community model Development (http://www.wrf-model.org/WG11), with significant number of developers and users. Currently about 250 users.
Model code available?	The WRF model and the chemistry code directory are available from the WRF model download web site http://www.mmm.ucar.edu/wrf/users
Computer requirements	The WRF/Chem model has been successfully ported to a number of Unix-based machines.
Model scale	Mesoscale. Short and long term.
Features and capabilities	**Photochemistry** • CBM-Z gas-phase mechanism • KPP version of CBM-Z • Compatibility of CBM-Z with the Model of Emissions of Gases and Aerosols from Nature (MEGAN) biogenic emission module (in collaboration with NCAR) • Fast-J photolysis

	Particulates • Model for Simulating Aerosol Interactions and Chemistry (MOSAIC) aerosol model • On-line treatments for sea-salt emissions module compatible with MOSAIC • Coupling GOCART dust emissions module to MOSAIC • MOSAIC modified to include treatment of secondary organic aerosols based on the volatility basis set approach • Coupled MOSAIC to SAPRC-99 photochemical mechanism • Generalized aerosol pointer array system that groups aerosols by composition, size bin, type (internal vs. external), and phase (interstitial, cloud water, ice, etc.) that can be employed by other aerosol models **Aerosol-radiation-cloud-chemistry feedbacks** • Through coupling with the Goddard shortwave radiation parameterization using aerosol optical depth, single scattering albedo, and asymmetry factor derived from MOSAIC particulates and Mie theory and the Lin et al. microphysics parameterization • Aerosol-radiative feedbacks extended to RRTMG shortwave and longwave radiation parameterization **Cloud-aerosol interactions** • Through coupling with the Lin et al. microphysics parameterization that include prognostic treatments of cloud droplet number and activated (cloud-phase) aerosol species, aerosol activation and resuspension, bulk cloud chemistry, and in-cloud and below-cloud wet removal of particulates and trace gases • Aerosol-cloud interactions extended to include MADE/SORGAM aerosol module • Extended aerosol-cloud interactions to include Morrison and Thompson microphysics parameterizations, in collaboration with NCAR
Chemical reactions	RADM2, CBM-Z, or KPP generated versions of RADM, RACM, and RACM-MIM
Model limitations	An off-line version is not public available (suitable for emission scenarios analysis and air quality management)

Table 35. HYSPLIT model.

Name	HYSPLIT (Hybrid Single Particle Lagrangian Integrated Trajectory model)
Version	Version 4.9 (july 2009)
Model developer	Joint effort between NOAA and Australia's Bureau of Meteorology. Recent upgrades include enhancements provided by a number of different contributors.
Web url	http://www.arl.noaa.gov/HYSPLIT_info.php http://www.ciecem.uhu.es/hysplit/ http://www.airquality.co.uk/uk_forecasting/forecast_is_made.php?view=HYSPLIT
Description	The HYSPLIT model is a complete system for computing simple air parcel trajectories to complex dispersion and deposition simulations. The model calculation method is a hybrid between Eulerian and Lagrangian approaches. The dispersion of a pollutant is calculated by assuming either puff or particle dispersion. In the puff model, puffs expand until they exceed the size of the meteorological grid cell (either horizontally or vertically) and then split into several new puffs, each with it's share of the pollutant mass. In the particle model, a fixed number of particles are advected about the model domain by the mean wind field and spread by a turbulent component. The model's default configuration assumes a 3-dimensiona particle distribution (horizontal and vertical).
Knowledge level	Basic- intermediate. The model can be run in batch mode with simulation parameters specified in a control file, or the control file can be configured interactively using a Graphical User Interface (GUI) written in tcl/tk. The GUI is available for both Windows 95/NT and Unix platforms.
Model code available?	The model can be run interactively on the Web through the READY system on our site or the code executable and meteorological data can be downloaded to a Windows or Mac PC.
Computer requirements	Computer operating system: UNIX, Windows **Disk space requirements**: less than 9 MB **Run execution time** (for a typical problem): about 1 to 3 min CPU time per simulation day.
Model scale	Designed to estimate long-range transport and dispersion
Features and capabilities	**Trajectories** -Single or multiple (space or time) simultaneous trajectories -Optional grid of initial starting locations -Computations forward or backward in time -Default vertical motion using omega field -Other motion options: isentropic, isosigma, isobaric, isopycnic -Trajectory ensemble option using meteorological variations -Output of meteorological variables along a trajectory -Integrated trajectory clustering option

	Air Concentrations -3D particle dispersion or splitting puffs (top-hat or Gaussian) -Instantaneous or continuous emissions, point or area sources -Multiple resolution concentration output grids -Fixed concentration grid or dynamic sampling -Wet and dry deposition, radioactive decay, and resuspension -Emission of multiple simultaneous pollutant species -Automated source-receptor matrix computation -Ensemble dispersion based on variations in meteorology, turbulence, or physics -Concentration probability output for multiple simulations -Integrated dust-storm emission algrorithm -Define rate constants to convert one species to another -Mass can be transferred to a Eulerian module for global-scale simulations
Input data	Gridded fields of meteorological variables are required at regular temporal intervals. The time interval between fields should be constant for each defined grid. The meteorological data file should consist of direct-access, fixed-length records, one record per variable per level. Meteorological data fields may be provided on one of four different vertical coordinate systems: pressure-sigma, pressure-absolute, terrain-sigma, or a hybrid absolute-pressure-sigma. At a minimum the model requires horizontal wind components, temperature, height or pressure, and the pressure at the surface. If wet deposition is to be included, the model also requires the rainfall field.
Output data	Two basic types of output are available: trajectories and air concentrations. Trajectories are output as ASCII files. Post-processing programs are available for graphical display of trajectories in Windows, or UNIX using NCAR graphics, Grads, or pc-wave. Air concentrations, or deposition are output as binary files. Contoured plots may be generated using similar postprocessing programs.
Chemical reactions	Not modeled
Model limitations	Primary limitation is that integration time steps less than 1 minute are not permitted, hence the spatial resolution and near-field calculations are limited to a domain of about 300 m. Meteorology is not directly coupled with the concentration grid, hence grid dependent (Eulerian) chemistry computations that are sensitive to meteorological parameters are difficult to code.

5. Discussion

As we said before, pollution caused by spillage of hazardous and noxious substances (HNS) is an extremely complicated issue that represents a severe threat to coastal regions. Hence releasing of some chemical substances evaporating under the weather conditions can generate vapour clouds that might be toxic or form an explosive mixture with air. Modelling of the spreading of airborne contaminants will help to forecast the movement and fate of the plume as it disperses, allowing the advisory of the public of potential dangerous zones or finding safety places.

Under these considerations, the most suitable model for the ARCOPOL project is selected among the models reviewed according to the following three criteria:

- ✓ Runtime (preferably less than one hour)
- ✓ Basic- intermediate level of difficulty
- ✓ Availability (better public model)
- ✓ Suitability (for emergency responders during an spillage of HNS)

Under these criteria, the most suitable models are the following:

1. **Aloha**:
   - ✓ Run time (1-2 minutes), ALOHA runs on Apple Macintosh computers and Microsoft Windows. It enjoys extremely good portability and can be used by a first responder at the scene of an emergency.
   - ✓ Knowledge level: Basic, ALOHA is designed to be extremely user friendly. It contains pull down menus with prompts and warning and caution messages. ALOHA's output is designed for easy use and interpretation.
   - ✓ Availability: Source code is available under commercial agreement with AICHE. Executables are available at U.S. EPA website. http://www.epa.gov/oem/content/cameo/aloha.htm
   - ✓ Suitability: Aloha model is suitable for use as a first step after the notice of a maritime accident because it is able to deliver results in a few minutes, and due

to its simplicity, this model allows to be used by emergency services without requiring a high knowledge on dispersion models of pollutants.

Intended users: First responders (such as fire and police services); State, local, and industry planners; Environmental organizations and academics.
ALOHA is used by thousands of people and organizations, and it has been introduced into about 50 countries.
CAMEO has been adopted by the United Nations Environment Programme's APELL (Awareness and Prevention of Emergencies at the Local Level) program, which promotes planning and preparedness for chemical accidents, especially in newly-industrializing countries. http://www.unepie.org/scp/sp/links/disasterprev.htm
The main features of the Aloha model are shown in table 19 of this report.

The implementation of the Aloha model was tested and implemented locally for a pilot experience in Galicia, northwestern Spain, where MeteoGalicia is responsible for the meteorological forecast.

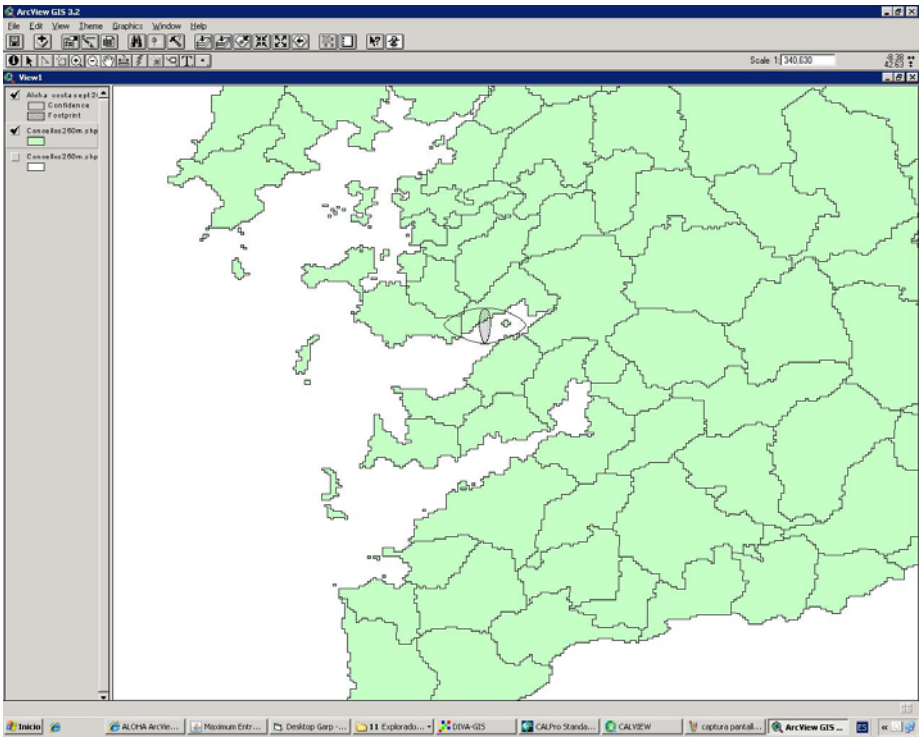

Figure 3: Threat zone simulated by Aloha model can be displayed on a GIS tool.

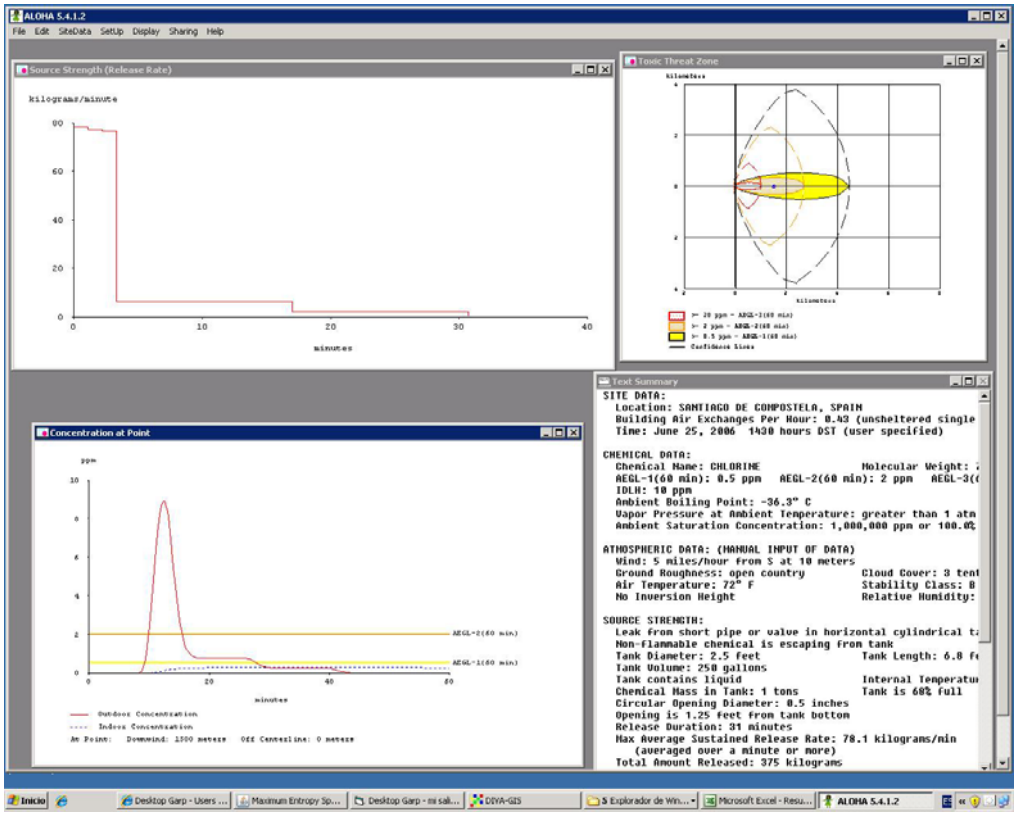

Figure 4: ALOHA displays hazard modeling results in four windows: threat zone, text summary, concentration at a point, and source strength.

2. **Calpuff**:

- ✓ Run time varies considerably depending on the model application, setup time required for experienced users varies from 10 to 15 minutes. Windows interface for CALPUFF, CALMET preprocessor, and CALPOST postprocessor. There is an input parameter error checking screen that lists all the errors detected by the CALPUFF GUI (graphic user interface). User interface and documentation are easy to use.
- ✓ Knowledge level needed to operate model: Intermediate – Advanced.
- ✓ Availability: Source code of EPA-approved version is free at developer website. http://www.src.com/calpuff/calpuff1.htm

  Improved versions are available from Lakes Environmental Inc under commercial agreement.

- ✓ Suitability: CALPUFF model is more suitable for use in more complex scenarios, as a second step in responding to emergencies, when the pollution episode can last several hours and requires a high degree of knowledge on weather and emission conditions.

Intended users: Consultants, industries, authorities, research and educational establishments.

The main features of the Calpuff model are shown in table 7 of this report.

The implementation of the Calpuff model was tested and implemented locally for a pilot experience in Galicia, northwestern Spain, where MeteoGalicia is responsible for the meteorological forecast.

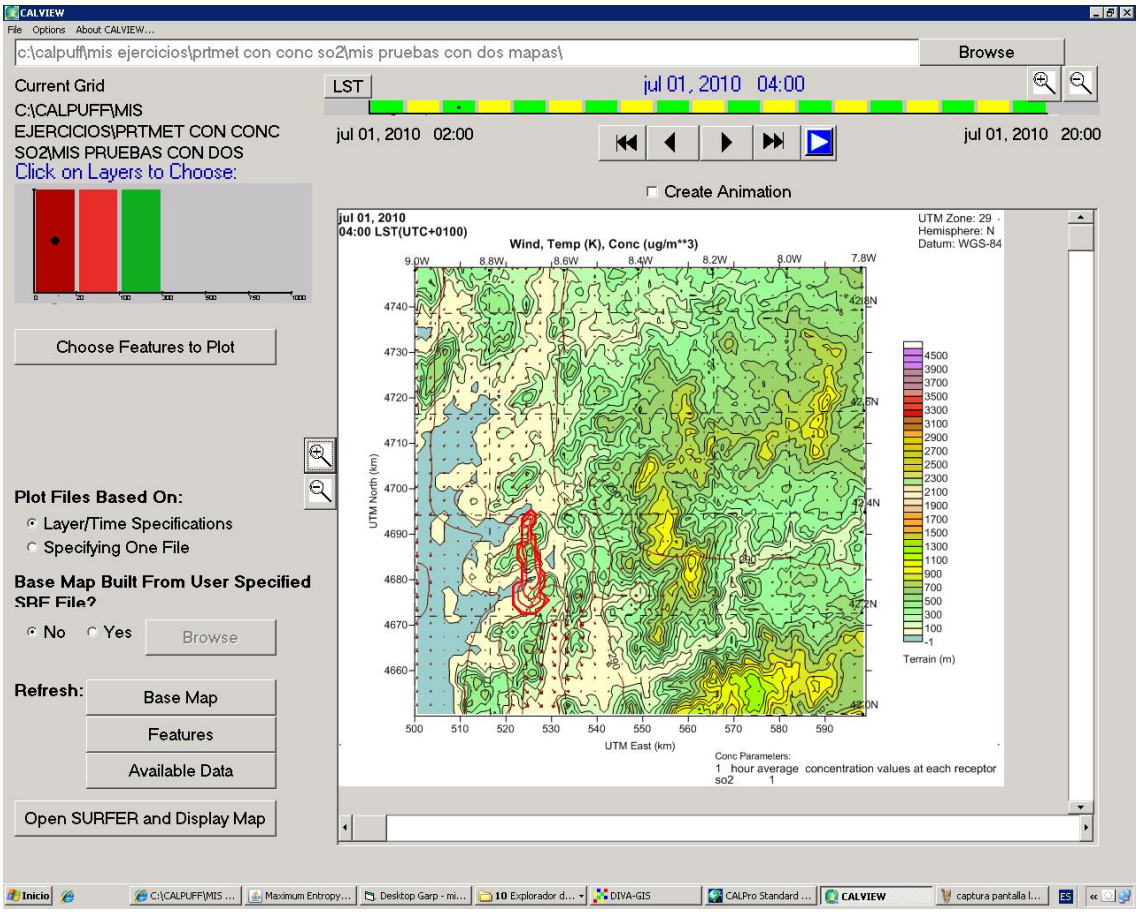

Figure 5: Wind field, isotherm and isoconcentration lines simulated by Calpuff model

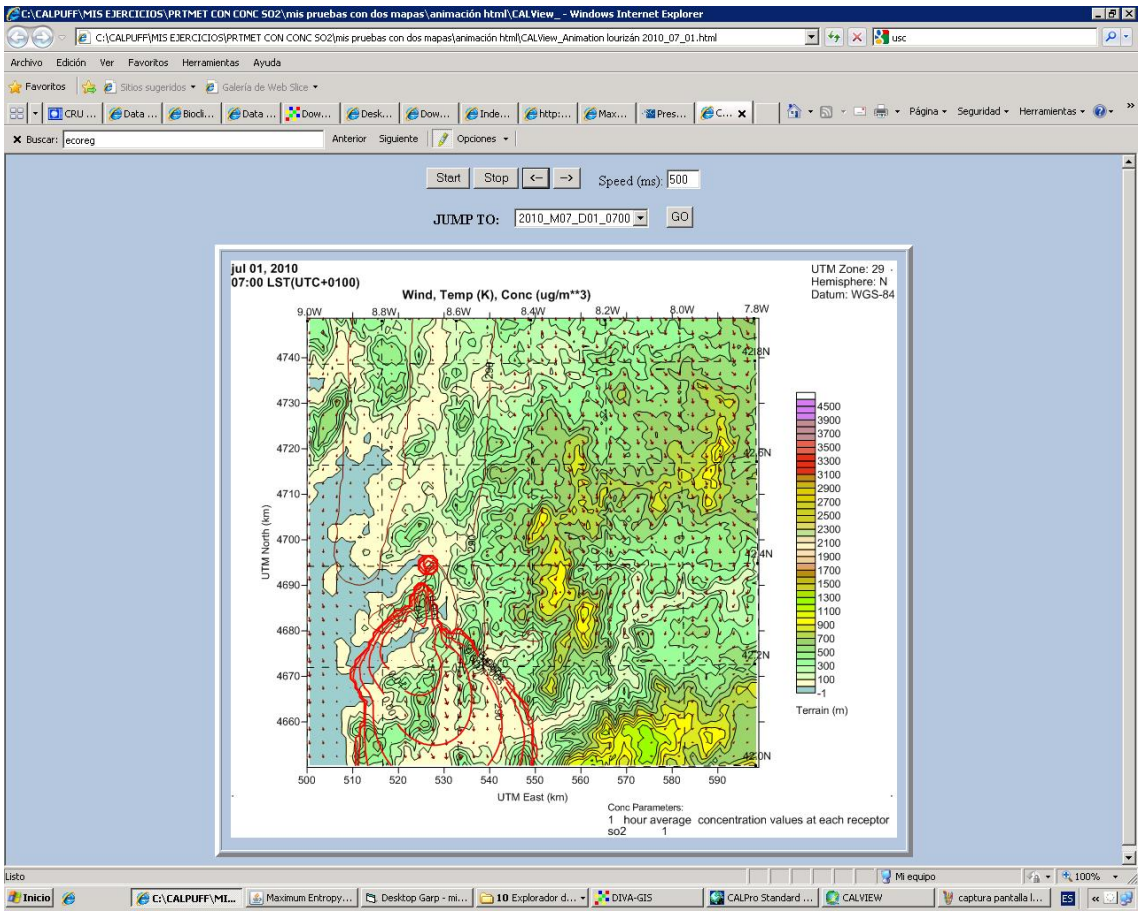

Figure 6: 24-hour animation created by Calpuff model and displayed in html

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