Journal of Physics: Conference Series

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To cite this article: M Giardina *et al* 2024 *J. Phys.: Conf. Ser.* **2685** 012047

A new dry deposition model implemented in CALPUFF code to simulate contamination of radionuclides released into atmospheric environment post-nuclear accidental event

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Abstract. Long-range transport and deposition analyses of 137Cs following a hypothetical incident at Gösgen nuclear power plant are studied by using CALMET-CALPUFF model system. Comparisons are performed with results obtained from a version modified of CALPUFF using a new dry deposition velocity model. This model is based on a combination of aerodynamic resistances and considers local features of the mutual influence of inertial impact and turbulent processes. The results show that the modified CALPUFF code seems to be an appropriate tool for performing impact assessments on long-range transport in complex terrain contexts or to support preparedness and response capabilities for nuclear and radiological accidents.

1. Introduction

As well known, CALMET/CALPUFF is an advanced non-steady state meteorological modelling system used to predict air quality and simulate meteorology [1, 2]. CALMET is a diagnostic meteorological model that reconstructs 3D wind and temperature fields starting from meteorological measurements, orography, land use data and CALPUFF assesses atmospheric pollution resulting from a wide number of species and a various range of emission sources. A new version of the CALPUFF tool allows for the assessment of particulate matter and the long-range transport of selected radionuclides and their decay products in several aerosol fractions.

In this paper, CALMET/CALPUFF system is used to study transport, dispersion, and deposition of radioactive particles released following a hypothetical accident at Gösgen nuclear power plant (in German Kernkraftwerk Gösgen, abbreviated in KKG), located in the canton of Solothurn, Switzerland. The analyses focus on the transport and dispersion of ^{137}Cs in Italian territory.

Meteorological data of European Centre for Medium-Range Weather Forecasts (ECMWF), surface stations measurements and data by upper-air stations, distributed throughout the domain of interest, are used.

In addition, comparisons are performed with results obtained from a modified CALPUFF version using a new dry deposition velocity model developed in [3].

Different physical processes interact to control the dry deposition of particles. Gravitational settling, turbulent diffusion, and surface collection are generally the most important, and their effects are usually accounted for by means of equivalent resistances (gravitational, aerodynamic, and surface collection resistances) that oppose to the deposition. The new model combines aerodynamic resistances that affect the particle flux in the quasi-laminar sub-layers and considers local features of the mutual influence of inertial impact processes and turbulent ones.

Results are compared to understand if the CALMET/CALPUFF tool has the capacity to provide data and recommendations in case of a post-nuclear accident in areas bordering with the Alps and beyond.

2. Dry deposition processes

The lifetime of particles in the atmosphere is determined by wet deposition, which removes particles by precipitation or in-cloud processing, and dry deposition, which directly uptakes particles to terrestrial surfaces.

Dry deposition remains a globally important first-order loss process that scales with concentration and is critical for estimating accurate spatial and temporal aerosol distributions in atmospheric models. The complexity of the fluid-dynamic processes that affect the deposition rate is governed by the following three main phenomena [4-6]:

- Atmospheric turbulence transport in the surface layer (SL). This process remains unaffected by the physical and chemical properties of the pollutant, relying solely on the degree of turbulence;
- Diffusion in the thin layer of air that overlooks the air-ground interface (i.e. quasi-laminar sublayer, QLS). It is molecular diffusion for gasses, Brownian motion for particles and gravity for heavier particles;
- Transfer to the ground (e.g. interception, impaction, and rebound) that is significantly influenced by surface characteristics such as urban context, grass, forest, etc.;
- Deposition process. For particles with intermediate diameters (dp) in the range of approximately 0.1÷1 μm, it strongly depends on atmospheric conditions, surface characteristics, and particle size. For dp above this range, deposition is primarily governed by the following interaction mechanisms;
  - Inertial impaction. It occurs when a particle has high inertia and is carried by the flow towards an obstacle. The particle becomes incapable of tracking the flow deviation, resulting in a collision with the obstacle;
  - Turbulent impaction. In this process, particles attain velocity high enough such that turbulent eddies can result in a transverse “free flight velocity”. Thus, particles can reach the surface.

A diverse set of parameterizations of dry deposition is available and used in different models and monitoring networks. The main difference lies on the schematisation of the surface resistances in QLS. However, there remains significant controversy regarding which mechanisms dominate for various particle sizes, atmospheric conditions, and surface characteristics due to limitations in both measurements and models.

2.1. A new resistance model to calculate the dry deposition velocity

The phenomena described in previous section are typically described using models based on resistances approach, and the interested reader is referred to [4] for further investigations.

In this context, a new approach is suggested in [3], where the electrical analogy method has been adapted to incorporate processes like particle rebound or resuspension.

The resistances, that affect the particle flux in SL and QLS, are combined as described in figure 1:

- aerodynamic resistance, r_a, in SL (i.e. contribution to the deposition due to the atmospheric turbulence) is connected in series with the resistance r_{ql} that takes into account mechanisms of diffusion by Brownian motions and impaction phenomena in QLS;
- quasi-laminar sublayer resistance, r_{ql}, is evaluated by considering a parallel circuit. The contribution of Brownian diffusion motions and the impaction phenomena can be considered as follows:
  - r_{db} assess the contribution of the Brownian diffusion;
  - r_{ii} considers the single effect of the inertial impaction regime for large particles;

- r_{ii} and r_{ti} are linked in a series arrangement to account the local characteristics of the mutual influence of inertial impact processes (represented by r_{ii}) and turbulent impact phenomena (represented by r_{ti}).

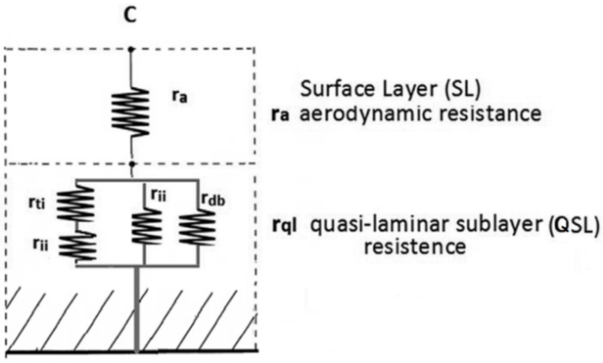

Figure 1. New resistances schematization for the particle deposition velocity calculation.

The total resistance r_t is evaluated using the following relationship:

$$r_t(z) = r_a + r_{ql} \tag{1}$$

where, r_{ql}, using the electric analogy, is evaluated as:

$$\frac{1}{r_{ql}} = \frac{1}{r_{bd}} + \frac{1}{r_{ii}} + \frac{1}{r_{ii} + r_{ti}} \tag{2}$$

The reader is referred to [3] for details on the calculation of resistances of eq. (2), not included here for the sake of brevity.

2.2. *Dry deposition velocity in CALPUFF*

CALPUFF is a multi-species non-steady-state puff dispersion model that simulates the effects of time and space varying meteorological conditions on pollutant transport, transformation, and removal [2].

It includes algorithms for near-field effects such as stack tip downwash, building downwash, transitional buoyant and momentum plume rise, rain cap effects, partial plume penetration, and coastal interactions effects as well as longer range effects such as pollutant removal due to wet scavenging and dry deposition.

- For dry deposition process, the technical algorithms are based on three options;
- Full treatment of space and time variations of deposition with a resistance model;
- User-specified diurnal cycles for each pollutant;
- No dry deposition.

The first option allows the computation of dry deposition of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutant species.

The resistance across the QLS is evaluated according to the following relationship:

$$r_{ql} = \frac{1}{u_*(Sc^{-2/3} + 10^{-3/St})} \tag{3}$$

where u_* is the friction velocity, St is the Stokes number and Sc is the Smith number [3, 4].

The second option allows user-specified, diurnally varying deposition velocities to be used for one pollutant instead of the resistance model. This option allows a "typical" time dependence of deposition to be incorporated but it does not include any spatial dependency. The last option bypasses the dry deposition model completely.

The CALPUFF deposition module has been modified to incorporate a fourth option that utilizes the resistance model described in [3].

DRY, DRYI, VDCOMP subroutines, that read data and process geophysical parameters and meteorological conditions, and a new VDPG subroutine, which allows the application of the new model, have been modified and incorporated in CALPUFF code.

3. Brief description of the Gösgen reactor

Gösgen KKG is a pressurized water nuclear reactor that generates about 15% of the Switzerland's electricity consumption, producing 8 TWh of electricity every year.

The main components of the reactor coolant system include the reactor itself, the pressuriser system, and three identical parallel circulation loops, each characterized by the presence of a steam generator (SG). The coolant enters the reactor at a temperature of 565 (K) and then moves downward through the annular gap, which is the space between the core barrel and the reactor pressure vessel. When the coolant reaches the semi-spherical base of the reactor vessel, it undergoes a 180-degree redirection, flowing through the reactor core and heating up to 598 K.

The thermal energy of the primary coolant in the SGs is transferred to the water on the secondary side of the SGs, resulting in the production of steam. This steam is then utilized in the turbine and subsequently passes through the condenser, where it condenses into liquid water. The heat from the condenser is released into the environment through a natural-draught cooling mechanism within the cooling tower, a reinforced concrete structure with a hyperbolic design, reaching a height of approximately 140 m.

4. CALMET-CALPUFF simulations

In this work, the computing domain for the CALMET simulation covers an area of 1.315.108 km^2 extended to a territory comprising the Switzerland and Italy countries, with cell resolution of 15x15 km.

The CALMET wind field module uses the following two-step approach:

- ***step 1***, involves refining the initial estimated wind field to account for the kinematic impacts of terrain, slope flows, and terrain blocking effects, resulting in an initial wind field;
- ***step 2***, an objective analysis procedure is employed to incorporate user-specified observational data from surface and upper air measurements into the wind field obtained in step 1, yielding the final wind field.

Meteorological conditions, with time step of 1 hour, are calculated by using meteorological data from 94 surface stations and measurements of 10 upper air sounding stations, for 5 days starting from the 2011-12-16 at 01:00 up to 2011-12-21 at 12:00.

Location of surface and upper-air stations, used in this study, are reported in figure 2. Surface stations are shown as white square points, upper-air stations as red circle points.

ERA5 reanalysis datasets, conducted by ECMWF, were acquired for the examined time frame and then processed with the FORCAL software [7] to enable their utilization in step 1 of the CALMET wind field module. FORCAL tool allows the reduction of grid cell sizes of the computational domain compared to the data initially supplied by ECMWF, enhancing the resolution of the meteorological information.

CALPUFF analyses have been performed by using CALMET results, and the input conditions reported in table 1 to schematize the emission source.

Radioactive emission has been hypothesized to occur at the exit of the cooling tower. The release is set to be of only a single isotope ^{137}Cs with a value of 10^{16} Bq over 1 hour (puff emission). This is a typical release for a PWR under severe accident conditions [8].

In the following, results of three different CALPUFF simulations, obtained by using the following options for the dry deposition process, are compared:

- CALPUFF default option for the dry deposition resistance eq. (3), that we call in the following section default option (DO);
- new option to use dry deposition resistance model of [3], referred as new option (NO);
- imposed deposition velocity of 0.005 m/s as suggested in [9], referred as imposed deposition velocity (IDV).

In [9] the constant for the deposition velocity of ^{137}Cs aerosol particles was taken from [10, 11] and it comes from the assessments made during the Chernobyl Nuclear Power Plant (CNPP) accident.

It is worth noting that the IDV approach does not account for phenomena such as eddy diffusion due to turbulent air movements or interception/impaction with the surface element structures. Additionally, near the surface, retention or rebound is influenced by a combination of surface and impact properties as described in section 2.

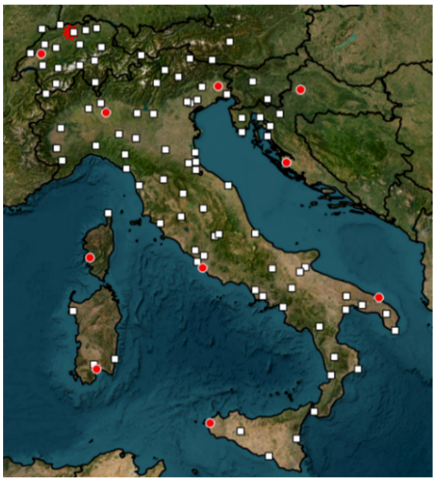

Figure 2. Surface stations (white square points) and upper-air stations (red circle points.

Table 1. Input data used for CALPUFF simulations.

Input data	
Source of ^{137}Cs	10^{16} Bq
Particle diameter of ^{137}Cs	1 μm
Time emission	2011/12/16 h=19:30
Duration of emission	1 h
Temperature of emission	423 K
Cooling tower height	140 m
Cooling tower diameter	70 m

4.1. Results

Figures 3 and 4 report results of wind field maps at 10 m above the ground.

For the day 2011-12-16 at 01:00 and 12:00, the northern part of Italy is characterized by low-intensity wind fields (figure 3), and cloudy weather. In the Tyrrhenian Sea, high-intensity wind blows from west toward south-east at the time 01:00. Over the next 24 hours, the wind direction changes, shifting from the west towards north-east (figure 3, 2011-12-16 at time 12:00).

This wind field behaviour takes places again the next days 2011-12-17 and 2011-12-18, and the low-intensity wind situation persists in the northern regions of Italy. However, the formation of wind fields characterized by vortical motions is predicted, initially affecting the central regions of Italy, and subsequently extending to the southern regions.

In the day 2011-12-21, a circular wind field forms at the center of the Tyrrhenian Sea at 00:00 and gradually moves towards the Calabria region by 12:00 (figure 4).

Note that, during the simulation period, no significant precipitation is observed in any region of Italy, indicating the prevalence of dry deposition processes.

Significant attention has been given to studying the evolution of atmospheric stability conditions during the simulated period. In CALMET, the Pasquill-Gifford-Turner (PGT) stability scheme is used to classify atmospheric conditions in the boundary layer. The classes range from unstable (Classes 1, 2, and 3) to neutral (Class 4) and stable (Classes 5 and 6). Unstable conditions typically occur during the day due to ground-level heating, leading to thermal turbulence in the boundary layer. Stable conditions, on the other hand, are associated with night-time cooling, resulting in reduced turbulence levels and the presence of temperature inversion at lower levels. Neutral conditions are often observed during high wind speeds or overcast sky conditions.

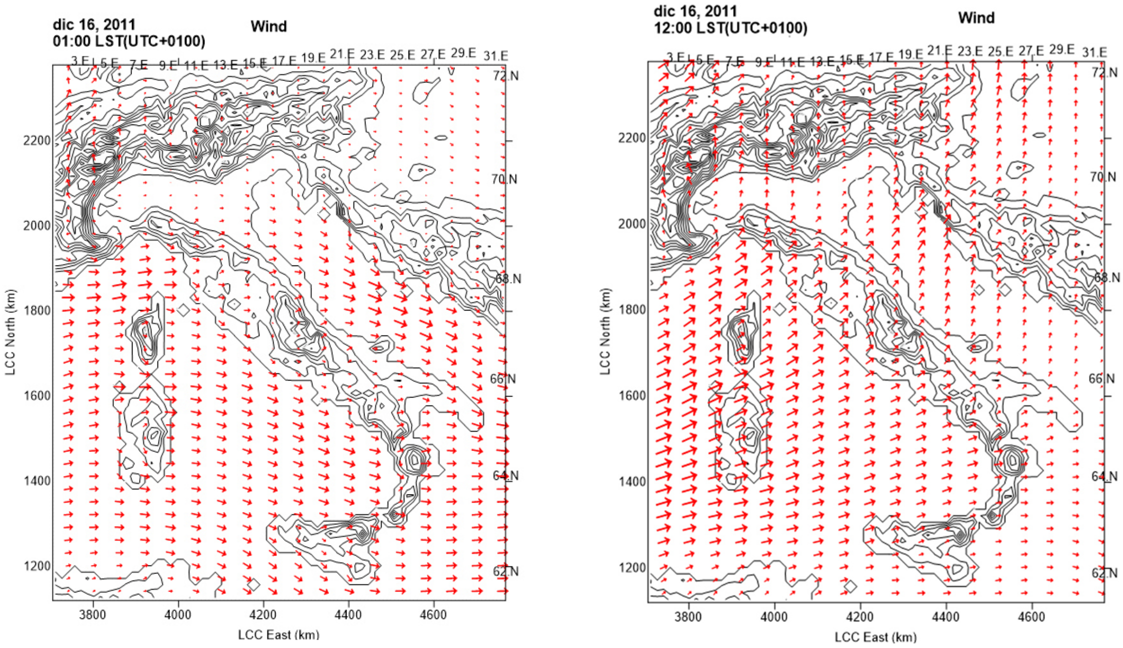

Figure 3. Wind field at 10 m on the 2011-12-16 at 01:00 and 12:00.

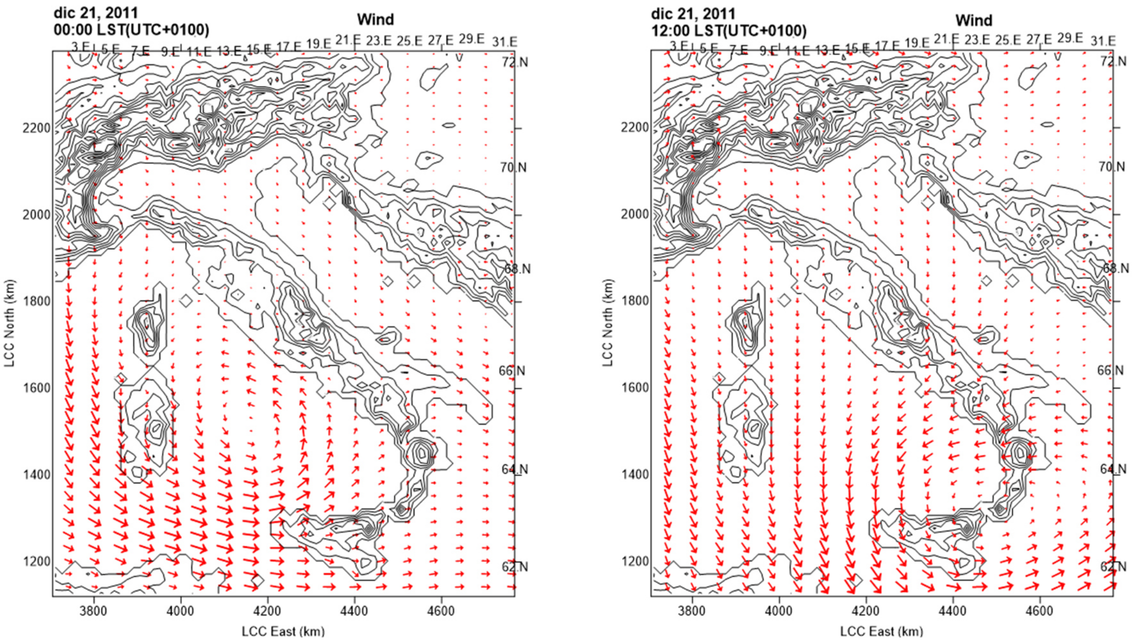

Figure 4. Wind field at 10 m on the 2011-12-21 at 00:00 and 12:00.

Analysing the temporal distribution of PTG, except for the first day of simulation that is characterized by class 5 (moderately unstable) and 4 (slightly unstable) conditions for almost the entire Italy, it can be observed that, classes 2 (slightly stable) and 3 (neutral condition) occur with high frequency in the northern regions. Class 4 is predominantly observed in Tyrrhenian Sea, Adriatic Sea and major islands.

Extended periods of atmospheric stability or low stability during winter, characterized by a lack of precipitation, do not favour the dispersion of pollutants in the air and promote their accumulation.

Figures 5 through 7 show the maps of cumulative dry deposition distribution of ^{137}Cs predicted by CALPUFF for the entire simulation period, applying DO (figure 5), NO (figure 6), and IDV (figure 7) options, respectively.

 doi:10.1088/1742-6596/2685/1/012047

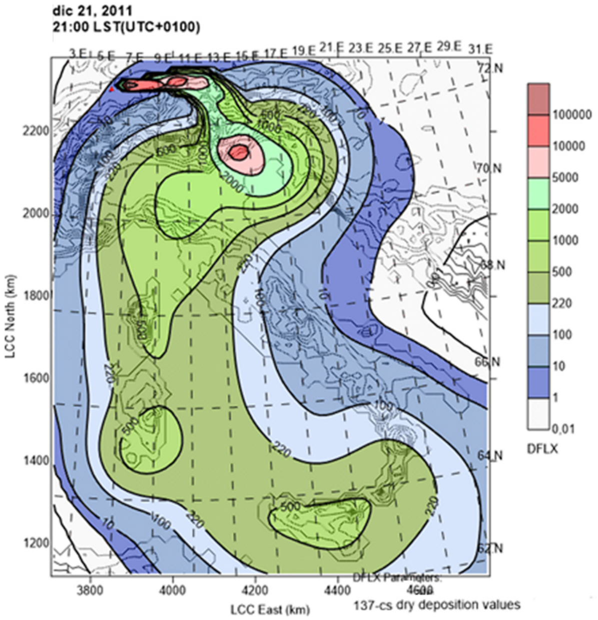

Figure 5. Cumulative dry deposition of ^{137}Cs obtained by using default resistance model of CALPUFF.

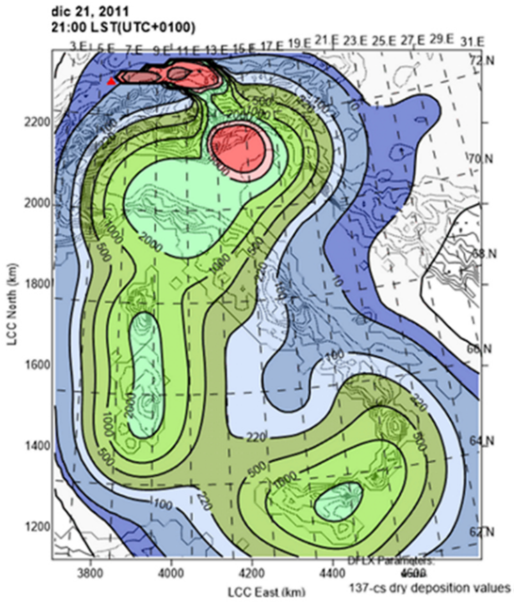

Figure 6. Cumulative dry deposition of ^{137}Cs obtained by using new resistance model.

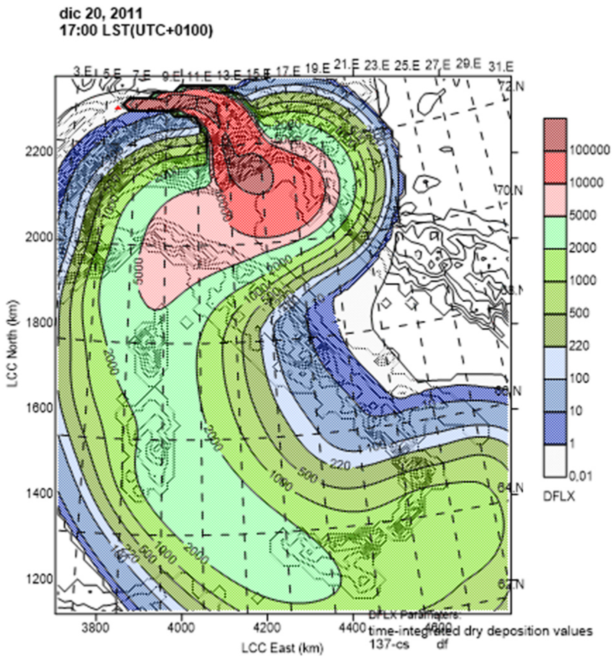

Figure 7. Cumulative dry deposition of ^{137}Cs obtained by using imposed deposition velocity.

All simulations highlight that the most critical condition takes place in the same regions of Italy with the following differences:

- The results obtained using DO option (figure 5) identify Lombardy, the eastern part of Liguria and Piemonte, Toscana, and western zone of Emilia-Romagna as the territories with the deposition in range 1.000÷10.000 Bq/m^2 and values higher than 5.000 Bq/m^2 in Veneto.
  Deposition of about 500 Bq/m^2 is predicted in the southern area of Sardinia and in the central zone of Sicily. Some territories of Switzerland, regions of Italy not listed before, and Mediterranean Sea are characterized by a pollutant deposition lower than 220 Bq/m^2;
- The results obtained by using NO option (figure 6) extend the areas with high pollution to Veneto, Friuli Venezia Giulia and northern area of Trentino Alto Adige. These areas experience deposition in the range 1.000÷10.000 Bq/m^2. ^{137}Cs deposition involves the regions of Sardinia and Sicily but with the difference that it is in the range of 1.000÷2.000 Bq/m^2. It is worth noting that there is an area to east of Gösgen KKG affected by a deposition exceeding 100.000 Bq/m^2.
- The analysis carried out by using IDV option (figure 7) highlights an extension of territories at east of the Gösgen KKG where the ^{137}Cs deposition exceeds 100.000 Bq/m^2. The comparison with the NO simulation shows that in this case the deposition is relatively uniform in the Tyrrhenian Sea with depositions in the range 1.000÷2.000 Bq/m^2.

In summary, the use of default resistance model, compared to the other two cases, predicts lower dry deposition and, consequently, underestimates health consequences for the population.

On the other hand, the use of the new model yields results that are more consistent with those obtained by setting the deposition velocity to 0.005 m/s. CALPUFF simulations with NO and IDV options results in an estimated deposition velocity that is at least one order of magnitude higher than the values calculated with DO option. However, NO and IDV options also yield significantly different deposition maps, particularly regarding the spatial coverage across the territory.

It is worth highlighting that, the result of CALPUFF simulations of Chernobyl nuclear accident reported in [9] with the default resistant model for the dry deposition velocity of ^{137}Cs aerosol particles have shown substantial underestimation in comparison with the measured data. Moreover, the Authors in [9] highlight that the magnitude of the deposition velocity is an order of magnitude smaller than in other previously published assessments performed for particle sizes ranging from approximately 0.1 up to1.0 μm [10, 11].

5. Conclusions

Research activities have concerned transport and dispersion analyses of ^{137}Cs radioactive particles released after a hypothetical severe accident in the Gösgen nuclear power plant by using CALMET/CALPUFF modelling system. Comparisons are performed by three different CALPUFF simulations. The most unfavourable conditions are predicted by CALPUFF results that use an imposed dry deposition velocity, while the least severe conditions are associated with the simulation that uses the default model of CALPUFF for dry deposition. The use of the new dry deposition model led to results falling into an intermediate condition. In future research activities, there are plans to further validate the model by simulating events such as the Chernobyl accident.

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Acknowledgments

Acknowledgement is made for the use of ECMWF's computing and archive facilities in this research.