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Comparative analysis of calculation possibilities of MACCS and RODOS computer codes for tasks of emergency response and analysis of radiation consequences of severe accidents at NPPs

The paper provides a brief description of the Real-time On-line Decision Support system (RODOS) and MELCOR Accident Consequence Code System (MACCS) computer code and evaluates the application of these codes for assessment of radiation impact on the public and environment in case of a severe accident at NPPs in real time mode. The results of calculations performed using RODOS, WinMACCS and HotSpot codes are compared. In the framework of research, the chosen comparative criteria were assessed: total effective dose, thyroid equivalent dose, skin equivalent dose, I-131 and Cs-137 ground concentration at different distances up to 50 kilometers from the point of release.

Keywords: radiation consequences, MACCS, RODOS, emergency response, severe accident at NPP

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Порівняльний аналіз розрахункових можливостей комп'ютерних кодів MACCS та RODOS у застосуванні для задач аварійного реагування та аналізу радіаційних наслідків важких аварій на АЕС

Наведено стислий опис Європейської системи прогнозу радіаційних наслідків у режимі реального часу RODOS та розрахункового коду MELCOR Accident Consequence Code System (MACCS), розглянуто можливість застосування цих кодів для оцінки впливу радіаційного опромінення на населення та навколишнє середовище в умовах тяжкої аварії на АЕС у режимі реального часу. Виконано порівняльний аналіз результатів розрахунків, проведених з використанням кодів RODOS, WinMACCS та HotSpot. У рамках дослідження для розгляду обрано такі критерії: ефективна доза опромінення, еквівалентні дози опромінення щитоподібної залози та шкіри, поверхневі концентрації радіонуклідів I-131 та Cs-137 на відстанях до 50 км від джерела викиду.

Ключові слова: радіаційні наслідки, MACCS, RODOS, аварійне реагування, тяжка аварія на АЕС.

In order to improve the NPP safety, significant scientific and research resources are involved to expand the software base for evaluation of radiation consequences in case of a severe accident at NPP. For such purposes, many computer codes are widely used, such as COSYMA [1], HAVAR [2], PACE [3], HotSpot [4], etc. In recent years, there is the need for application of the existing computer codes for estimation of radiation consequences in real time. One of these codes, WinMACCS (MELCOR Accident Consequence Code System) [5], the product of Sandia National Laboratory (USA), has been used in SSTC NRS [6] since 2015 for the prognostic conservative estimates. The application of this computer code for real time calculations has not been studied very well. The objective of this work is to evaluate the possibilities of WinMACCS in the activities related to emergency response and analysis of radiation consequences of severe accidents on NPPs in comparison with European Real-time On-line Decision Support system (RODOS) [7].

Description of RODOS. RODOS is a Real-time On-line Decision Support system for off-site emergency management in case of a radiological release.

Models and databases can be customized to different site and plant characteristics and to the geographical, climatic and environmental variations. RODOS performs its calculation either with incoming online meteorological data and prognosticated meteorological fields or user defined meteorological information. All inputs and outputs of RODOS are provided via a graphical user interface [8].

After the input of initial meteorological data and release data, in conjunction with the RODOS database, the rapid assessment of radiation consequences is provided. The main goal is to determine the necessary countermeasures and their scope.

There are three dispersion models in RODOS:

RIMPUFF (RISU Mesoscale PUFF model) is a Lagrangian mesoscale atmospheric dispersion puff model designed for calculating the concentration and doses resulting from the dispersion of airborne materials. The model can cope well with the in-stationary and inhomogeneous meteorological situations, which are often of interest in connection with calculations used to estimate the consequences of short-term (accidental) release of airborne materials to the atmosphere (Fig. 1).

The model applies both to homogeneous and inhomogeneous terrains with moderate topography on a horizontal scale of up to 50 km, and responds to changing (in-stationary) meteorological conditions. It can simulate the time changing releases (emissions) of airborne materials by sequentially releasing a series of Gaussian shaped puffs at a fixed rate on a specified grid. The amount of airborne materials allocated to individual puffs equals the release rate times the time elapsed between puff releases [9].

ATSTEP is a Gaussian puff model for distances up to 50 km. ATSTEP can calculate real-time diagnoses of the radiological situation during or after a release and dispersion prognoses for 24 hours. The radiological situation is described by the following results calculated with ATSTEP: the concentration in the air near ground (instantaneous and time-integrated), the contamination of ground surface (dry and wet), and the gamma radiation from ground and from the radioactive cloud (Fig. 2). These results are presented as time dependent, nuclide specific fields in the whole calculation area in the environment of the release source. The following phenomena are considered in the modelling of atmospheric dispersion and the radiological situation in ATSTEP: time dependent meteorology (meteorological tower or SODAR data, forecast data, inhomogeneous wind fields), time dependent nuclide-group specific release rates, thermal energy and rise of the puffs released, dry and wet deposition

Fig. 1. Gaussian Puff Model RIMPUFF. Classical Puff Model: every 10 minutes a puff is released and then tracked with short time steps in between

Fig. 2. Gaussian Puff Model ATSTEP: Each puff treated as a separate cloud initially produced by an emission lasting 10 or 30 minutes transported along two trajectories

Fig. 3. Puff-Particle Model DIPCOT. Every 10 sec a particle is released, to each particle a 3D Gaussian kernel is added

and corresponding depletion of the cloud, gamma radiation from cloud and from ground, radioactive decay, and potential doses.

As distinct from classic puff models (RIMPUFF), no instantaneous puffs but time-integrated elongated puffs are released in ATSTEP, similar to the plume sections of a segmented Gaussian plume model. As distinct from a segmented plume model, in ATSTEP the transport of each elongated puff is achieved by two trajectories, which are fixed at both ends of the puff. As these pairs of trajectories follow the inhomogeneous and variable 2D-wind fields step by step, also the elongated puffs perform all the necessary changes in position, shape, and orientation, like stretching, rotations, shrinking, and sideways drift [10].

DIPCOT model (DIspersion over COMplex Terrain) is a computer code, which simulates the dispersion of air pollutants over complex terrain. The model has the ability to simulate atmospheric dispersion in both homogeneous and inhomogeneous conditions based on a Lagrangian particle model scheme. The mass of the pollutants is distributed to a certain number of fictitious puffs or particles that are displaced in the computational domain according to the wind velocity to which a random component is added to account for turbulent diffusion (Fig. 3).

DIPCOT uses topographical and meteorological information given on a 3D grid and is capable of simulating dispersion of multiple pollutants from multiple point sources.

In the case of buoyant point sources the model performs plume rise calculations. If applicable, the code also calculates dry and wet deposition on the ground and, in case of radioactive pollutants, the gamma radiation dose rates. Three types of input data, concerning the source characteristics, topography and meteorology, are necessary for the simulations. The emission characteristics (i.e., source location, release height, emission rate, stack diameter, gas exit velocity and temperature) are provided by the RODOS Source Term Module (or are calculated from the data provided by it), while 'gridded' topographical and meteorological information is provided by the RODOS Meteorological Pre-Processor (RMPP). **DIPCOT** uses 3-dimensional fields for the wind velocity, temperature, and pressure and 2-dimensional fields for topography, ground roughness, mixing layer height, friction velocity, convective velocity, category of atmospheric stability, precipitation

intensity and Monin-Obukhov length [11]. The model calculates instantaneous air concentrations, time integrated air concentrations, dry and wet deposition rates and deposition of pollutants, gamma radiation dose rates and time-integrated dose (cloud and ground) at the locations of the RODOS dispersion grid and at locations of detectors [12].

General input parameters [7]:

Delay between end of chain reaction (EOC) and beginning of the 1st release;

For up to 24 user defined time intervals;

Release height above ground (m);

Released thermal power (MW) (For calculating the vertical release velocity);

Vent area of the release to the atmosphere (m²) and Vertical volume flux released to the atmosphere (m³/sec);

Iodine fractions: Percentage of total amount of iodine released as elementary iodine, organically bound iodine, and iodine in aerosol form (e. g. CsJ).

Description of MACCS. MACCS models the transport and dispersion of plumes of radioactive material released to the atmosphere. As the plumes travel through the atmosphere, material may be deposited on the ground via wet and dry deposition processes. MACCS models seven pathways through which the general population can be exposed to radiation: cloudshine, groundshine, direct and resuspension inhalation, ingestion of contaminated food and water, and deposition on skin. Emergency response and protective action guides for both the short and long term are also considered as means to mitigate the extent of the exposures. As a final step, the economic costs that would result from the mitigative actions are estimated.

MACCS is organized into three modules. The ATMOS module (atmospheric transport and deposition) performs the atmospheric transport and deposition portion of the calculation. The EARLY module (emergency phase dose calculations) estimates the consequences of the accident immediately following the accident (usually within the first week) and the CHRONC module estimates the long term consequences of the accident

MACCS allows the release of radioactive materials to the atmosphere to be divided into successive plume segments, which can have different compositions, release times, durations, release heights, and amounts of sensible heat. The plume segment lengths are determined by the product of the segment's

release duration and the average wind speed during release. The initial vertical and horizontal dimensions of each plume segment are user specified.

During transport, dispersion of the plume in the vertical and horizontal directions is estimated using an empirical Gaussian plume model. In this model, dispersion depends on atmospheric stability and wind speed. Horizontal dispersion of the plume segments is unconstrained; however, vertical dispersion is bounded by the ground and by the mixing layer which are both modeled as totally reflecting layers. A single value for the mixing layer is specified by the user for each season of the year and is constant during a calculation. Eventually, the vertical distribution of each plume segment becomes uniform and is so modeled.

The MACCS dosimetry model consists of three interacting processes: the projection of individual exposures to radioactive contamination for each of the seven exposure pathways modeled over a user specified time period, mitigation of these exposures by protective measure actions, and calculation of the actual exposures incurred after mitigation by protective measure actions. For each exposure pathway, MACCS models the radiological burden for the pathway as reduced by the actions taken to mitigate that pathway dose. The total dose to an organ is obtained by summing the doses delivered by each of the individual pathways.

MACCS models seven exposure pathways: exposure to the passing plume (cloudshine), exposure to materials deposited on the ground (groundshine), exposure to materials deposited on skin, inhalation of materials directly from the passing plume (inhalation), inhalation of materials resuspended from the ground by natural and mechanical process (resuspension inhalation), ingestion of contaminated foodstuffs (food ingestion), and ingestion of contaminated water (water ingestion). Ingestion doses do not contribute to the doses calculated for the emergency phase of the accident. Only groundshine and inhalation of resuspended materials produce doses during the optional intermediate phase of the accident [5].

For the purpose of evaluating the Total Effective Dose (TED), only two modules are needed.

The ATMOS-module utilizes the Gaussian plume model to determine χ/Q (air concentration, Bq/m³ / source term rate, Bq/sec) release values, based on an input of the source term, release characteristics and deposition behavior.

Table 1. Recommended approaches for different scales and applications of atmospheric dispersion modeling

Application	<1 km	1–10 km	10–100 km	100–1000 km
Online risk management (short runtime is important)	—	Gaussian	Puff	Eulerian
Complex terrain	CFD*	Lagrangian	Lagrangian	Eulerian
Reactive materials	CFD	Eulerian	Eulerian	Eulerian
Source-receptor sensitivity	CFD	Lagrangian	Lagrangian	Lagrangian
Long-term average loads	—	Gaussian	Gaussian	Eulerian
Free atmosphere dispersion (volcanoes)	—	Lagrangian	Lagrangian	Lagrangian
Convective boundary layer	CFD	Lagrangian	Eulerian	Eulerian
Stable boundary layer	CFD	Lagrangian	Eulerian	Eulerian
Urban areas, street canyon	CFD	CFD	Eulerian	Eulerian

*CFD — Computational Fluid Dynamics models.

The γ/Q values are employed by the EARLY-module to calculate doses, accounting for dose conversion factors, sheltering factors and breathing rates [8].

Table 1 shows the recommended approaches for different scales and applications of atmospheric dispersion modeling [13].

Unlike MACCS atmosphere models, the RODOS models comply the necessary requirements for their applications for emergency response. The Gaussian model used for long distances can greatly inflate the dose indices and unreasonable high costs on the use of certain countermeasures to protect the public. At distances of 10 to 100 km it is recommended to use Puff-model. But for distances up to 20 km, the MACCS atmosphere model fully meets the requirements to use it in emergency response. In near future, the Sandia National Laboratory will develop an updated version of the atmospheric model, and MACCS can be fully used as a code for the purpose of prediction of radiation effects in real time and analysis of the radiation consequences of severe accidents at nuclear power plants.

Comparative calculations. For comparative calculation, possibilities of MACCS and RODOS radiation consequences for a severe accident were calculated. As an example, the scenario “total unit blackout without containment isolation” was chosen. The total activity of release was $5.8 \cdot 10^{19}$ Bq [14]. Release activity fractions are shown in Fig. 4.

Input data for calculation:

Height of release — 40 m;

Class of atmosphere stability (Pasquill-Gifford classification) — D [15];

Wind speed — 3.6 m/sec;

Distances for calculations — 0.5...50 km.

Additionally calculations were provided using HotSpot code [4].

Fig. 4. Release activity fractions according to MELCOR Groups [7]

Results. The results on effective dose are shown in Fig. 5. The most conservative results were obtained in HotSpot as its simplified models. As for MACCS and Rodos, the different Dose Conversion Factors files were used. FGR-13 was used in MACCS [15], and GSF-12/90 in RODOS [7]. The values of Dose Conversion Factors used in calculations are shown in Table 2.

Results for thyroid equivalent dose per 2 weeks (Fig. 6) obtained with MACCS and RODOS at near distances are similar. Difference in the results closer to 50 km is due to chemical forms of iodine. Unlike MACCS, RODOS has the possibility to set different forms of iodine (molecular, aerosol, organic). In this case, iodine form was used as 91 % molecular, 5 % aerosol and 4 % organic [7]. The molecular form of iodine has lower

Table 2. Dose conversion factors

Radionuclide	Submersion, (Sv/sec)/(Bq/m ³)		Groundshine, (Sv/sec)/(Bq/m ²)		Inhalation, Sv/Bq	
	RODOS	MACCS	RODOS	MACCS	RODOS	MACCS
Kr-87	3.89E-14	3.97E-14	-	8.38E-16	-	-
Kr-88	9.73E-14	9.71E-14	-	1.72E-15	-	-
Sr-89	3.89E-18	4.39E-16	5.28E-20	6.88E-17	3.99E-10	6.11E-09
Sr-90	0.00E+00	8.89E-16	0.00E+00	1.12E-16	4.13E-10	3.56E-08
Cs-134	7.23E-14	7.07E-14	1.00E-15	1.48E-15	5.05E-09	6.69E-09
Cs-136	1.00E-13	9.81E-14	1.36E-15	1.99E-15	5.70E-10	1.23E-09
Cs-137	2.59E-14	2.55E-14	3.61E-16	5.49E-16	2.98E-10	4.67E-09
Ba-140	7.78E-15	8.06E-15	1.53E-15	1.91E-16	8.18E-10	5.07E-09
I-131	1.67E-14	1.70E-14	2.47E-16	3.65E-16	3.43E-09	7.39E-09
I-133	2.72E-14	2.78E-14	3.89E-16	6.22E-16	1.46E-09	1.47E-09
Pu-238	-	-	-	-	8.63E-07	4.62E-05
Pu-239	-	-	-	-	7.69E-07	5.02E-05
Pu-240	-	-	-	-	7.71E-07	5.02E-05
Pu-241	-	-	-	-	3.61E-11	9.01E-07
Cm-242	-	-	-	-	9.53E-07	5.20E-06
Cm-244	-	-	-	-	8.65E-07	2.66E-05
Am-241	-	-	-	-	7.71E-07	4.17E-05

Fig. 5. Effective dose (14 days, adults), mSv

Fig. 8. Skin equivalent dose (14 days, adults), mSv

Fig. 6. Thyroid equivalent dose (14 days, adults), mSv

Fig. 9. Cs-137 ground concentration, Bq/m² Fig. 7. I-131 ground concentration, Bq/m²

deposition velocity than aerosol form, so dose in far distances will be higher than in case 100 % aerosol iodine release. The same effect is shown on the I-131 ground concentration graph (Fig. 7).

The closer results are obtained in calculation of skin equivalent dose (Fig. 8).

The most different results were obtained in calculations of Cs-137 ground concentration (difference is about 10 times) (Fig. 9).

All these codes use the same methodology for cloud shine dose and skin equivalent dose calculations. Unlike ground concentrations, air concentrations have similar values. Differences between the obtained ground concentrations are due to different aerosol deposition velocities. The value of aerosol deposition velocity is stable in RODOS, and equals approximately 5E-4 m/sec. In MACCS this value depends on aerosol aerodynamic diameter.

Conclusions

In the framework of evaluating the capabilities of MACCS application for emergency response tasks and analysis of the radiological consequences of severe accidents at NPPs, a comparative analysis of the MACCS computer code and Real-time On-line Decision Support System RODOS was carried out.

Unlike the MACCS atmosphere models, the RODOS models comply with the necessary requirements for their applications for emergency response. The Gaussian model used for long distances can greatly inflate the doses and nuclide concentrations, which leads to unreasonable high costs in the use of certain countermeasures to protect the public. At distances of 10 to 100 km, it is recommended to use the Puff-model. However, for distances up to 20 km, the MACCS atmosphere model fully meets the requirements for its use in emergency response.

Comparative analysis of the effective doses in codes MACCS, HotSpot and RODOS showed some differences associated with dose coefficients in MACCS and aerosol deposition rates. It is not a weakness, as MACCS interface allows the user to set dose coefficients according to required values.

Analysis of effective doses, thyroid doses and iodine concentration shows that problem with identification of chemical forms of iodine in MACCS may be essential for the adoption of countermeasures and boundaries of their application at distances exceeding 20–30 km.

It should be noted that with the new atmosphere dispersion model, MACCS will be fully used as a code for the purpose of predicting radiation effects in real time and analysis of the radiation consequences of severe accidents at nuclear power plants.

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