

Study on numerical models to evaluate atmospheric dispersion of radioactive materials on Vietnam territory

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Abstract: Atmospheric dispersion modeling is a challenging problem not only for environmental management, but also for predict the dispersion of radioactive materials. The key priority to promote an effective model for emergency response is making a balance between the accuracy and the computational cost. This research has made a brief review about the properties of several dispersion models as Gaussian, Eulerian, Lagrangian, and CFD (Computational Flux Dynamic). We also discussed their performance in parallel computing and proposed an approach for predict and fast nuclear accident response by using the WRF model (Weather Research and Forecasting) and the FLEXPART-WRF. For demonstration, we presented two examples by using FLEXPART-WRF for simulation of the dispersion of ¹³⁷Cs from the Fangchenggang nuclear power plant.

Keywords: Air dispersion modelling, Gaussian, Eulerian, Lagrangian, CFD, WRF, FLEXPART, FLEXPART-WRF.

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I. Introduction

Among lessons learned from the Fukushima Daiichi nuclear accident, emergency response planning plays a crucial role in preventing scenarios resulted after the accident. Vietnam is developing a national warning system for predicting the potential dispersion of nuclear accidents, in which the atmospheric dispersion modelling is aimed to be the main objective of this project. Choosing appropriate models is necessary and needs careful study.

Atmospheric pollution diffusion can be numerically simulated by several techniques, which are mainly divided into two categories:[1]

II. Lagrangian models

The basic difference between these two approaches is illustrated in Figure 1, in which the Eulerian coordinate is fixed in space and the concentration of the pollutant through a lattice is calculated by solving the mass conservation equation [2][3][4]. While the Lagrangian coordinate follows the motion of each individual species, the fluid flow of pollutants is assumed to be composed of a huge number of single particles, the total concentration is calculated by solving the motion of each individual particles. The Gaussian models are a consequence of the Lagrangian approach by normalize the probability density function.

This paper presents the pros and cons of each model to apply for simulating the dispersion of radioactive materials in mesoscale, we discussed their accuracy in calculation and their computational performance to make time-effective in emergency cases. The criteria to propose a model to be the most suitable for Vietnam is defined as has simulation time under 30 minutes and the model must have been validated with experimental results.

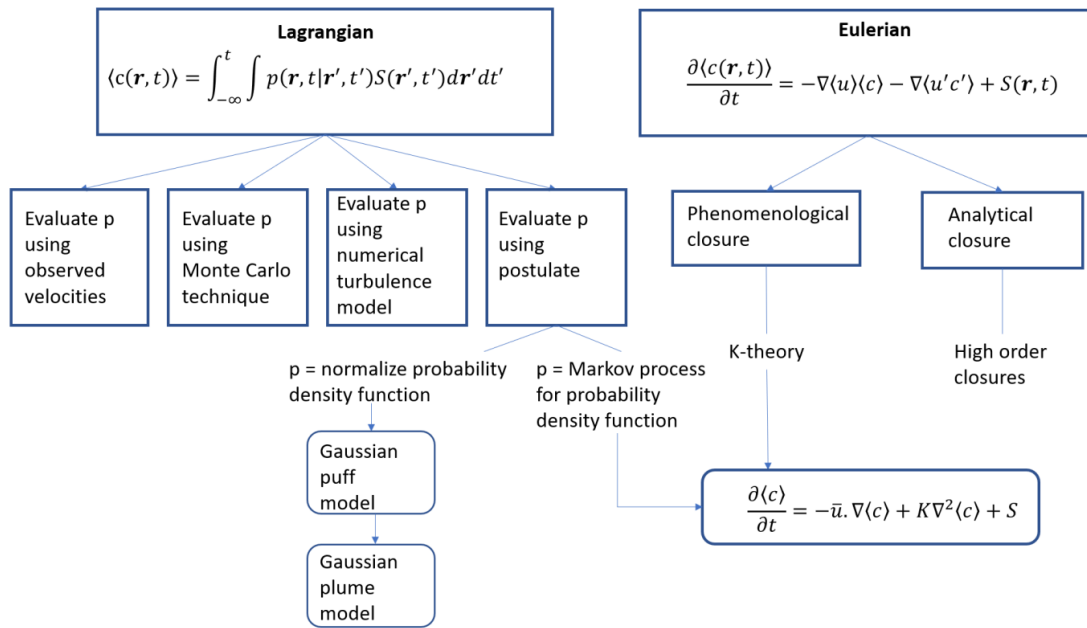


Fig. 1: Comparison of Lagrangian and Eulerian approach for atmospheric dispersion modelling. [1]

III. Gaussian dispersion models

The Gaussian dispersion models are the most simple and common model for air dispersion modeling. It assumes a homogeneous, steady-state emission rate, and under a stationary meteorological condition: wind speed and wind direction are constant in space and time [2][5][6]. Assume the plume is advected toward the positive x-axis, the concentration of the plume can be expressed by the Gaussian plume formula [5]:

$$c(x, y, z) = \frac{Q}{2\pi\sigma_y\sigma_z u} \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \left\{ \exp\left[-\frac{(z-h)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z+h)^2}{2\sigma_z^2}\right] \right\}$$

where $c(x, y, z)$ is the concentration at point (x, y, z) , (g/m^3)

Q is emission rate, (g/s)

u is wind speed, (m/s)

σ_y is dispersion parameter in the horizontal direction, (m)

σ_z is dispersion parameter in the vertical direction, (m)

In general, there are two types of Gaussian dispersion models: the plume model, and the puff model [5]. Fig. 1 shows the schematic of the Gaussian plume model, which is pollutant concentration profiles in y-axis and z-axis are results in a Gaussian distribution, centered at the plume centerline [1][5]. The terms σ_y and σ_z represent the affection of the weather conditions at the emission site to the dispersion of plume. These terms are semi-empirically calculated under stability classes based on Pasquill and Gifford criteria [5].

Gaussian models have the fastest calculation time by solving only one single formula, but they sacrifice accuracy for simplicity. It is widely applied for online risk management applications require fast response time [2].

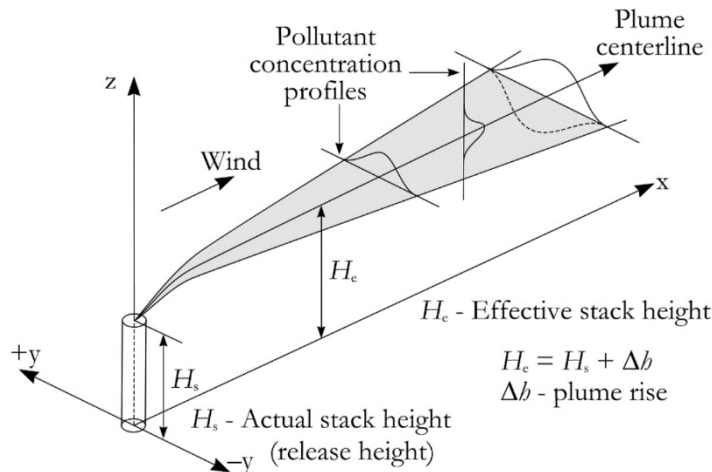


Fig. 2: Schematic of the Gaussian plume model.[2]

IV. Eulerian dispersion models

The Eulerian approach tracks the movement of pollution parcels in a fixed three-dimensional coordinate grid. The dispersion of the pollution parcels is solved numerically by the atmospheric transport equation [2][5][7]:

$$\frac{\partial c}{\partial t} = -\nabla \cdot (c\vec{v}) + S_c + \nabla \cdot (D_c \nabla c)$$

Where $\frac{\partial c}{\partial t}$ is the change of the local concentration in time.

$-\nabla \cdot (c\vec{v})$ is the transport term, \vec{v} is the wind vector.

S_c is the source term located in the given grid, including chemical production and loss, radioactive decay, dry and wet deposition.

D_c is the diffusion coefficient.

By considering a large number of particles as a pollution parcel, so Eulerian models can not track the movement of each individual particle. The accuracy of Eulerian models is largely depends on the resolution of the computation domain, the computational cost increases very rapidly with increasing resolution [2][1]. The main advantage of this type of model is able to handle complex chemical processes. Eulerian models are usually used for long-range applications (ranging from 100-1000km), such as long-term average loads, stable boundary layer, or reactive materials [2]. A typical model is the CMAQ (The Community Multi-scale Air Quality) used for predicting chemical and physical processes that are important in tropospheric ozone, toxics and acid deposition, and visibility degradation [2][4][5]. However, the computational cost of Eulerian models rapidly increases when increasing grid resolution.

V. Computational Fluid Dynamics (CFD) models

Similar to the approach of Eulerian models, CFD models calculate the motion of air packages on a computational grid (usually refer as the mesh) by solving the Navier-Stokes equation [2]:

$$\rho \left(\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} \right) = -\nabla P + \mu \nabla^2 \vec{v} + \vec{f}$$

Where $\frac{\partial \vec{v}}{\partial t}$ is the local acceleration.

$(\vec{v} \cdot \nabla) \vec{v}$ is the acceleration of convective term

∇P is the pressure gradient

$\mu \nabla^2 \vec{v}$ is the viscous term

\vec{f} is the body force term, including internal forces and external forces.

Obviously, the Navier-Stokes equation does not include the turbulence term [2][5], the only way to modelling the turbulence using Navier-Stokes equation directly calculates the turbulent kinetic energy on each scale where the energy is dissipated by viscous forces [2][5]. This requires the computational mesh cell must have 1mm-size to calculate atmospheric turbulence with acceptable accuracy, which results to need extremely high computational costs. Therefore, the turbulence has to be estimated by two common approaches: the $k - \epsilon$ approach, or Large Eddy Simulation (LES) approach [2][5]. The $k - \epsilon$ model uses the Reynolds-averaged Navier-Stokes (RANS) which gives more efficient than the LES, but least accurate [2][5]. The LES is a

state-of-the-art tool for turbulence modeling but requires high computational cost, its results are often used as a standard dataset for other models[2][5].

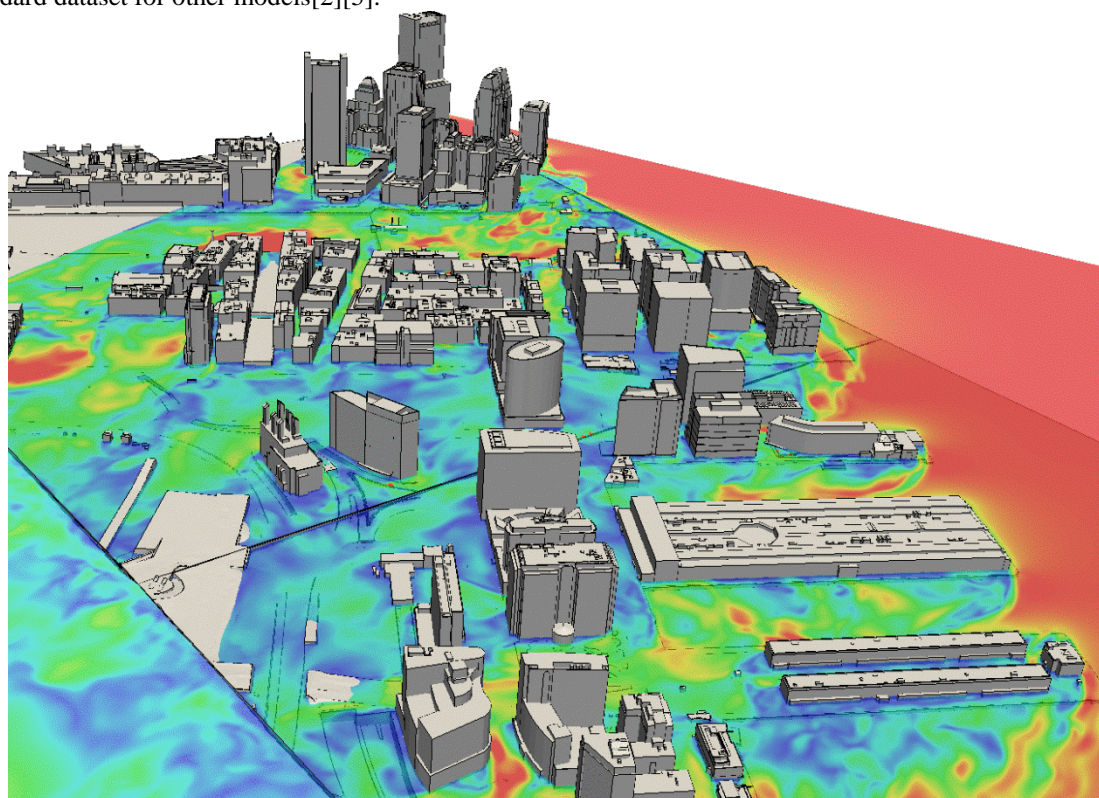


Fig. 3: An example of wind velocity simulation based CFD at Boston Seaport District using the SimScales software.[8]

Computational fluid dynamic is an intensive technique and costs extremely high performance computing, beside, it is required to construct all the buildings geometry, determine boundary conditions. The computational fluid dynamic is only feasible at small scales, ranging around 1-10 km[2].

VI. Lagrangian dispersion models

Unlike the approach of Eulerian models and CFD models, Lagrangian models solve the motion of each single particle as it moves away in the atmosphere (or also refer as air parcel)[2][4][5][6]. Over time, the position and characteristic of this air parcel are calculated by solving ordinary differential equations (ODEs) according to the mean wind field data[2]. In the Lagrangian particle models, the coordinate system of each particle is moving follow with its position. The key parameter of Lagrangian models is the probability density function $p(\mathbf{r}, t | \mathbf{r}', t')$ that an air parcel moves from \mathbf{r}' at t' to \mathbf{r} at t , where $t > t'$, this probability density function depends on the site-specific meteorology, particle size distribution, and particle density[2][5]. The velocity of the particle is calculated based on the Langevin stochastic differential equation[2]:

$$dw = -\left(\frac{w}{T_L}\right)dt + Xd\mu$$

where w is any component of particle velocity, T_L is the Lagrangian time scale, $\frac{w}{T_L}$ is the deterministic term, $Xd\mu$ is the stochastic term. By take into account for stochastic term in particle velocity calculation, therefore Lagrangian particle models is the better way for modelling the stochastic turbulence motion of particles.

Lagrangian particle models handle physics aspects that lay behind the air dispersion better than any other model and be more accurate at long distances (thousands of kilometers)[5]. The computational cost of Lagrangian models only depends on the number of particles, not depend on the output grid resolution, therefore Lagrangian models are exceptionally efficient for mesoscale simulation to compare to Eulerian gridded simulation with very fine resolution. Table 1 demonstrates recommended applications of several dispersion models by Leelosy et al.[2], therefore we proposed the Lagrangian models for atmospheric dispersion modelling that is suitable for the Vietnam territory scale.

Table 1: Recommended applications of numerical models for atmospheric dispersion modelling[2]

Application	< 1 km	1-10 km	10-100 km	100-1000 km
Online risk management	-	Gaussian	Puff	Eulerian
Complex terrain	CFD	Lagrangian	Lagrangian	Eulerian
Reactive materials	CFD	Eulerian	Eulerian	Eulerian
Source-receptor sensitivity	-	Lagrangian	Lagrangian	Lagrangian
Long-term average loads	-	Gaussian	Gaussian	Eulerian
Free atmosphere dispersion	-	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

VII. Proposed simulation models for Vietnam

There are several simulation programs based on Lagrangian models, such as AUSTAL2000 (Janicke, <http://www.austal2000.de/en/home.html>), FLEXPART (Stohl, <https://www.flexpart.eu/>), GRAL (The Graz Lagrangian Model), HYSPLIT (<https://www.ready.noaa.gov/HYSPLIT.php>). Especially with FLEXPART by Andreas Stohl, this program is good for simulation at the local and global scale, it contains advanced algorithms to describe particle transport and diffusion, dry/wet deposition, radioactive decay, OH reaction. FLEXPART has been comprehensively validated with experiments by using controlled tracer in intercontinental air pollution transport studies[9][10][11][12][13][14]. The study of Long et al. [15] showed good abilities of FLEXPART to be applied for simulation of long-range radioactive materials dispersion and good to deal with fast nuclear incident response on the whole Vietnam territory. FLEXPART takes data from the GFS (Global Forecast System) or the ECMWF (European Centre for Medium-Range Weather Forecasts) as meteorological input[16], however, the highest resolution of the GFS data is 0.25 degree resolution, which is grid resolution about 27km×27km, may need to ameliorate to higher resolution to get better accuracy. As far as our opinion, to improve the accuracy of the dispersion simulation, a meteorological module should be implemented to be used as an intermediary preprocessor. The intermediary meteorological module is expected to give better accuracy in terms of treating the coarse meteorological data for getting initial and boundary conditions. Here, we promoted the WRF-ARW (Weather Research and Forecasting) to be a meteorological preprocessor for this problem.

The ARW is a non-hydrostatic mesoscale model that is the most commonly used for weather prediction and atmospheric research, we simply invoke it as WRF. The WRF contains dozens of parameterization schemes for modelling in-depth all processes in the atmosphere, including microphysics, cumulus, short/long-wave radiation, planetary boundary layer, and surface layer. WRF has always been a free program ever since it was released, it is the most prestigious and powerful computational model for simulating atmospheric aspect, lots of institutions are using WRF for research and operational. Besides, WRF is flexible for nesting computational domains, defining geographical projection, and setting the grid resolution. Users can increase time-resolution or grid resolution in order to get higher accuracy. For running WRF requires initial and boundary conditions from GFS or ECMWF data[17]. The ECMWF dataset requires paying charges for license, but the GFS is provided for free by NCEP and users can freely access and download from NCEP server, therefore we proposed an approach for atmospheric dispersion simulation of radioactive material is that by using the WRF/GFS for meteorological simulation.

Besides the original version, FLEXPART has several branches which are bespoke for limited-area models, such as FLEXPART-WRF, FLEXPART-MM5, FLEXPART-AROME, FLEXPART-COSMO. These branches take input from meteorological module (WRF, MM5, AROME, COSMO) and use them as initial and boundary conditions. FLEXPART has always been a powerful tool for atmospheric dispersion modelling, but it is required for further development to be more comprehensive at small-scale, therefore the FLEXPART-WRF is developed and inherits the quintessence of FLEXPART. Some new highlight features are implemented into FLEXPART-WRF while keeping the strength of FLEXPART, which include new options for interpolating wind field data (instantaneous or time-averaged winds), parallelization computational (MPI, OMP, SERIAL), and improvement on skewed turbulence modelling based on the study of Cassiani et al.[17]. By new development, FLEXPART-WRF is expected to give insight into small-scale than FLEXPART can present[17].

VIII. Demonstration runs

We present two example runs in two different climate patterns in Vietnam by using the FLEXPART-WRF Lagrangian model for forwarding simulation of the dispersion of ¹³⁷Cs aerosol from the Fanchengang NPP. The first case took at the time when the winter northwesterly winds were striking the northern of Vietnam, and the second case was performed under heavy rainfall event from the Mun tropical storm. Both of two simulation runs are conducted on a High-Performance Computer (HPC) which has two Intel Xeon E5-2699 processors (44 cores, 88 threads, 2.2 GHz base frequency), 1 TB of RAM.

The WRF configuration for meteorological simulation and release properties in both two case are given in Table 2. The schemes used for WRF simulation are referenced based on the study of Tien et. al [18], that is tested on 32 different configurations for heavy rainfall forecast for the North Vietnam.

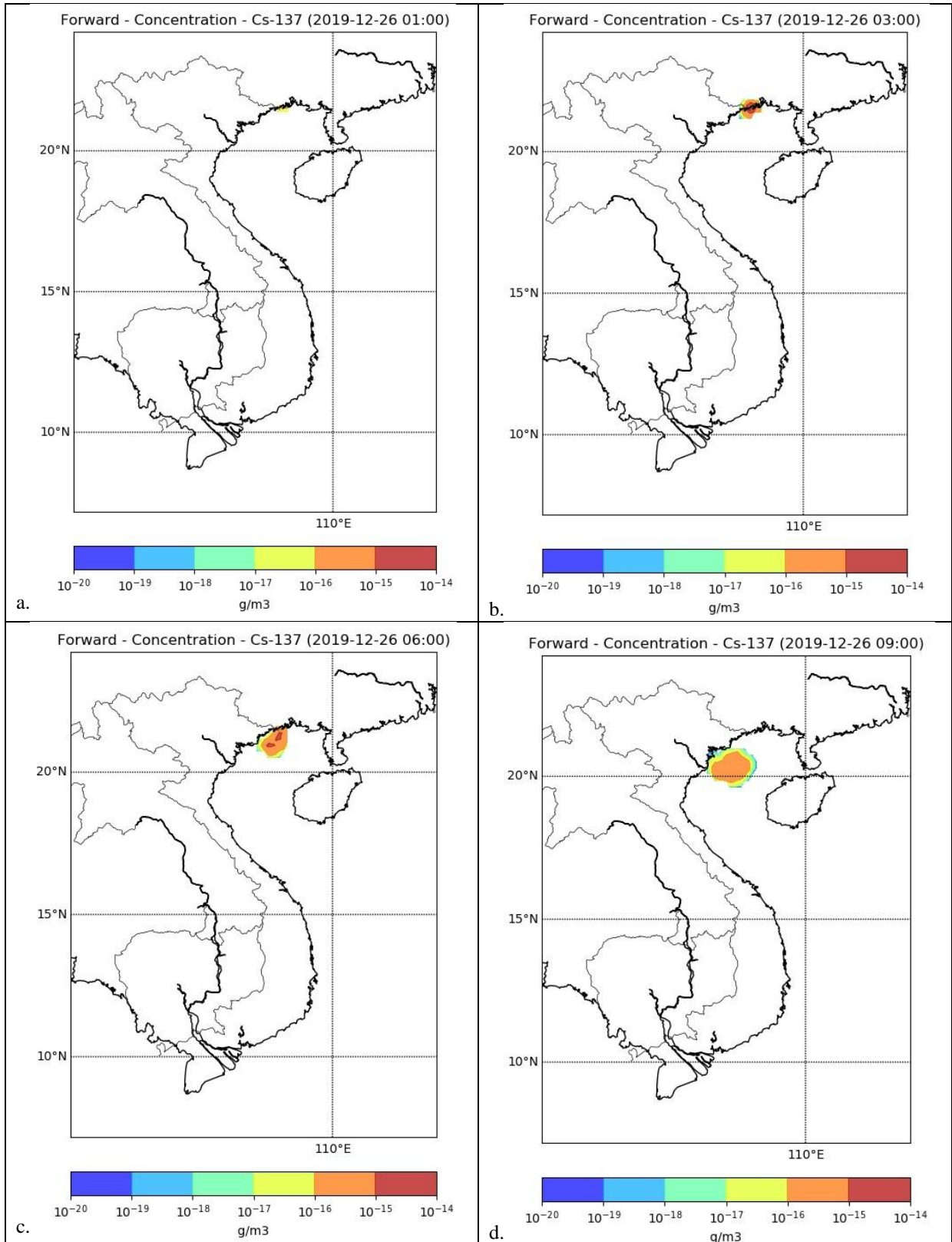
Table 2: Details on WRF schemes and release properties using for two demonstration runs

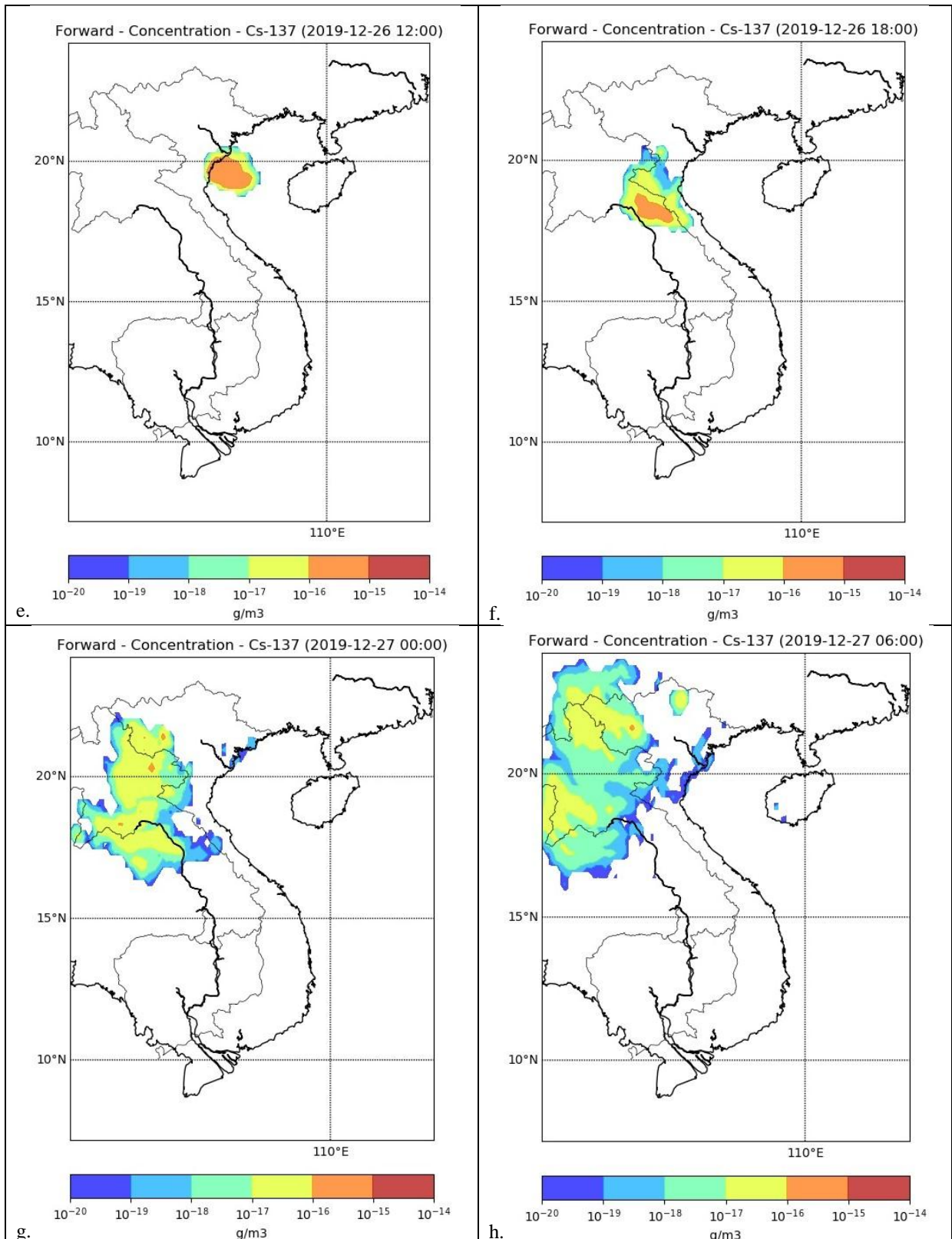
Parameter	Configuration scheme	Properties
Initial boundary data file	GFS final analysis.	Provide by NCEP for free.
Meteorological domain	214 grid point in West-East 316 grid point in South-North Centered at lat:16.17, long: 106.61	Cover all Vietnam territory and site of the Fangchenggang NPP.
Grid resolution	7 km	
Map projection	Mercator	Highly accurate for areas within tropical region.
Microphysics	WSM5	Replacement of the old version –NCEP5. Contains five categories of hydrometrics: water vapor, cloud vapor, cloud ice, rain and snow. [19]
Longwave radiation	Rapid Radiative Transfer Model scheme	A spectral-band scheme using the correlated-k method. It uses pre-set tables to accurately represent longwave processes due to water vapor, ozone, CO ₂ , and trace gases. Accounting for cloud optical depth in calculation. [19]
Shortwave radiation	Dudhia scheme	Contains simple downward integration of solar flux, accounting for clear-air scattering, water vapor absorption. account for terrain slope and shadowing effects on the surface solar flux. [19]
Surface layer	MM5 similarity scheme	Uses stability functions to compute surface exchange coefficients for heat, moisture, and momentum. [19]
Land surface	Noah Land-Surface Model	Developed jointly by NCAR and NCEP. Uses 4-layer soil temperature and moisture model with canopy moisture and snow cover prediction. Includes root zone, evapotranspiration, soil drainage, and runoff, taking into account vegetation categories, monthly vegetation fraction, and soil texture. [19]
Planetary boundary layer	Yonsei University scheme (YSU scheme)	First-order closure, non-local scheme, uses a parabolic K-profile in an unstable mixed layer. More accurately in simulation of buoyancy-driven PBLs with shallower mixing in strong-wind regimes. [20][21]
Cumulus Parameterization	Kain-Fritsch scheme	A simple cloud model with moist updrafts and downdrafts, including the effects of detrainment, entrainment, and relatively simple microphysics. [20]
Release location	Latitude: 21.64 Longitude: 108.50	At the Fangchenggang NPP.

8.1. Winter northwesterly winds

The trajectory of the plume is shown in Figure 4. This simulation took 23 minutes for running and about 9 Gb on disk storage. The simulation time was met our definition for fast nuclear response, which is under 30 minutes for running.

The simulation results showed that 3 hours after released (Fig. 4b), the radioactive material was beginning entered to the Vietnam territory, the main fraction of radioactive was remains stayed nearby the plant site. The dispersion direction towarded the South-West (Fig. 4c, 4d, 4e) led the radioactive material drifted to the North Central of Vietnam. After 12 hours (Fig. 4f), some province in the North Central of Vietnam was beginning affected by radioactive material. At 12 o'clock the next day (Fig. 4i), the impact area of radioactive material was including the whole North Central of Vietnam, some provinces in North-West of Vietnam, and Laos territory.





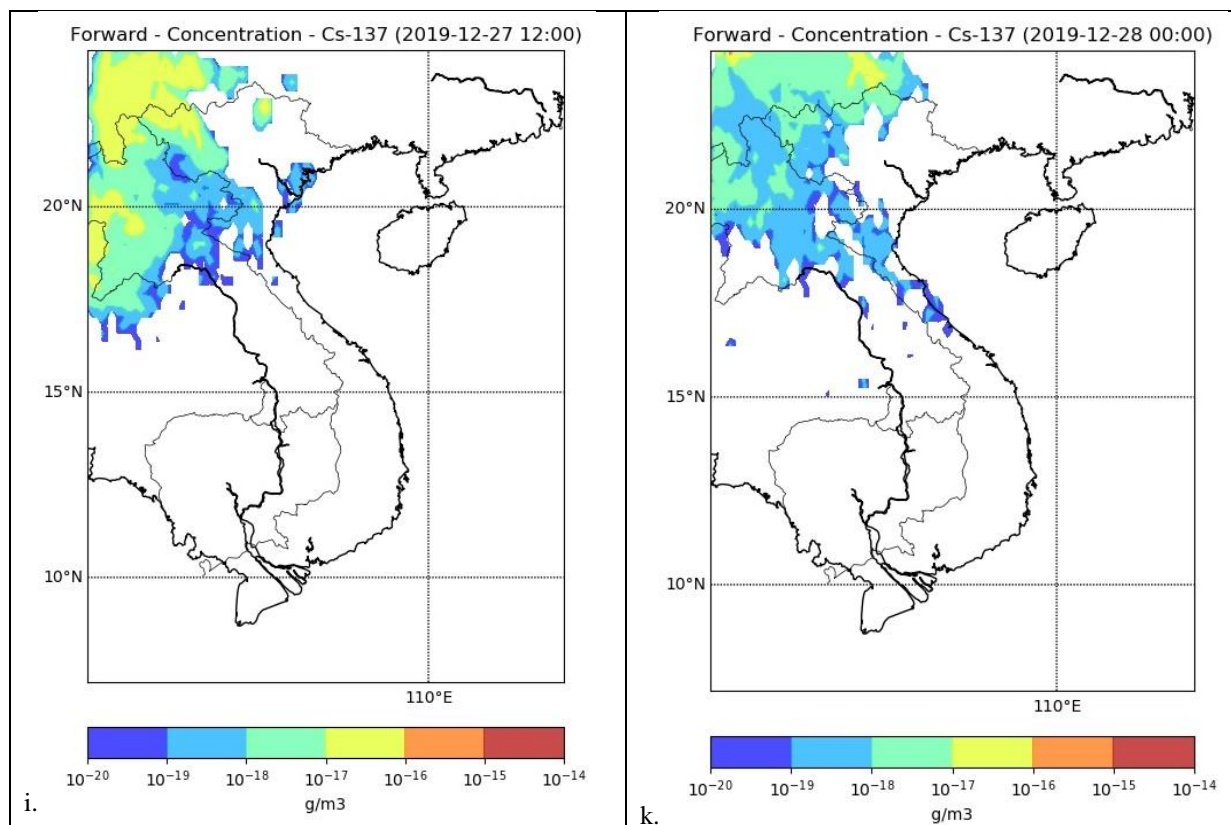
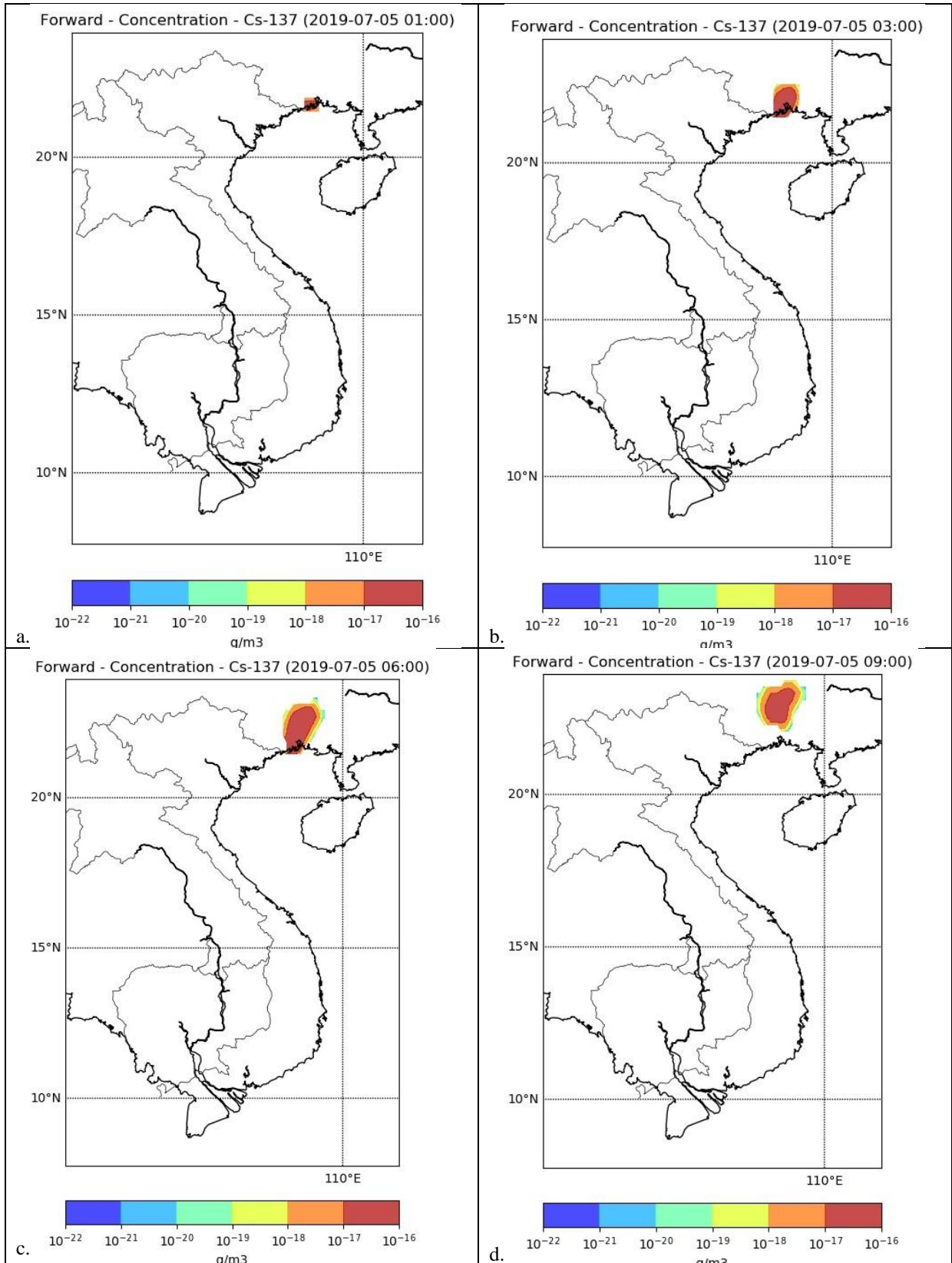


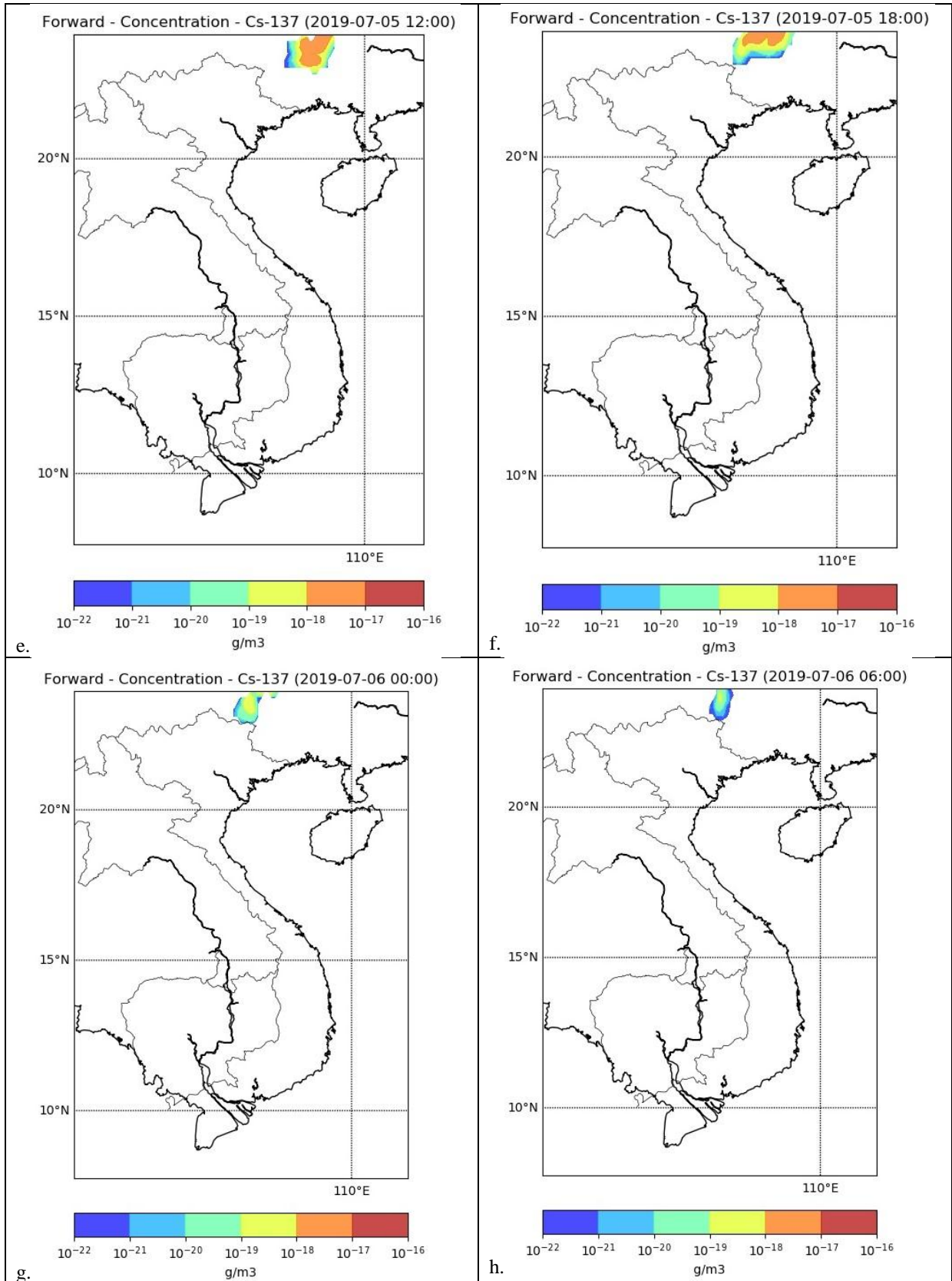
Figure 4: Trajectory of ¹³⁷Cs released from the Fangchenggang NPP from 26/12/2019 00:00:00 GMT to 28/12/2019 00:00:00 GMT.

8.2. Summer heavy rainfall

The trajectory of the plume is shown in Figure 5. This simulation took 19 minutes for running and about 7 Gb on disk storage. The simulation time was faster than the first demonstration run due to there was a large amount of the radioactive material dispersed to the out of bounds of the simulation domain after a short time from release.

The simulation results showed that Vietnam was not affected by radioactive material due to the southwestern monsoon from the South China Sea offered wind-action driving radioactive material away from the Vietnam territory, towards the North of the plant site and entered to China mainland.





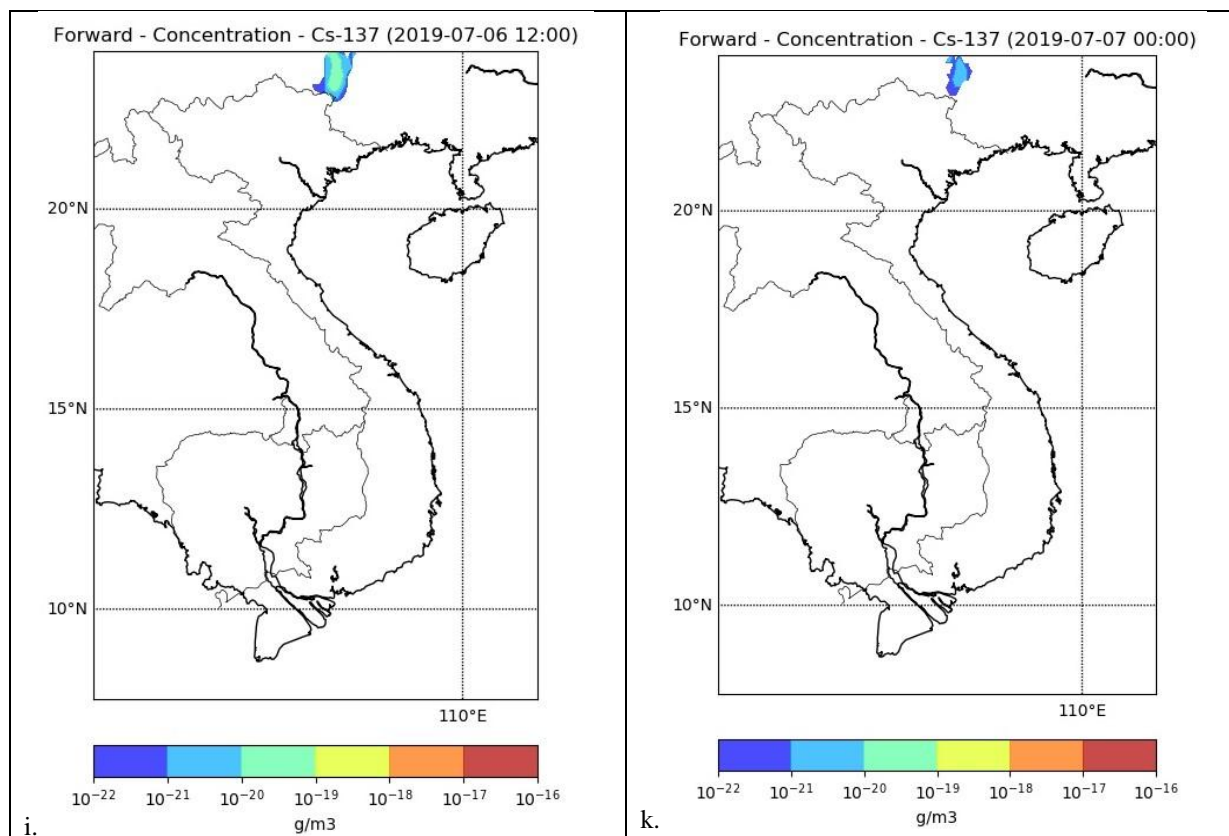


Figure 5: Trajectory of ^{137}Cs released from the Fangchenggang NPP from 05/07/2019 00:00:00 GMT to 07/07/2019 00:00:00 GMT.

IX. Conclusion

This research has made a discussion on atmospheric dispersion models and proposed a simulation approach by using the FLEXPART-WRF tool. Moreover, we demonstrated two case runs of two different climate patterns in Vietnam, the simulation time of each is fast sufficient for nuclear accident response.

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