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3.3.2 Model of dispersion of floating waste

Model identification PART 1

Activity 3.3

WP 3

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Model of dispersion of floating waste

Activity Deliverable (3.3.2)

PART 1

Model Identification

WP3

Activity 3.3

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Introduction

The deliverable D3.3.2 is composed by three parts; the first describes the process followed to identify the numerical model that is used for simulating the dispersion of floating waste. This document reports this process and the sources of information considered to achieve the deliverable targets. The second part deals with the model implementation while the third focuses on the model features; both those parts are included in one document that is going to be released after this one.

In the following, the surveyed dispersion models are going to be presented. There are two complementary approaches that can be used to simulate litter transport in the sea: the Eulerian and the Lagrangian frameworks. There are advantages and disadvantages on both Eulerian and Lagrangian approaches and they mostly complement each other.

The Lagrangian formulation focuses on an individual particle's trajectory which is driven by the mean fluid flow and the turbulence needs to be represented by ad hoc random motions. The Eulerian framework describes particles in terms of their mass or volume concentrations, that are advected by the ocean's velocity field and diffused by parameterized and resolved turbulence [1].

The Lagrangian simulations use (pre-computed) Eulerian velocity data, which are derived from observations or hydrodynamic models, to compute the pathways of particles, by integrating the velocity field in time.

These models' applications to nearshore systems, with complicated geometry, are less mature with respect to the Eulerian ones. Recently, it has been shown that the Lagrangian connectivity of nearshore flows depends strongly on the horizontal resolution of the underlying Eulerian hydrodynamic data [2].

On the other hand, the effort required by Eulerian simulations, in particular for application in complex coastal areas, is huge with respect to the Lagrangian approach.

Presentation of considered models

Here below, the models that have been considered for the purposes of the MARLESS project, are described in summary and the main advantages and shortcomings are presented, with respect to their application to the marine litter transport and dispersion simulations.

Delft3D model

Delft3D model is an Eulerian one. It is developed by Deltares company and consists of a number of well-tested and validated programs, such as Delft3D-PART.

In Delft3D-PART two type of models are available: Tracer model and Oil model. In the Tracer model, particles are not allowed to be subjected to additional advection due to wind drag. Instead, with the Oil model, neglecting all oil specific processes in the module, the transport simulation of plastic litter of different types is possible. [3]

Advantages

- It includes sediment transport [2]

Disadvantages

- It does not resolve adequately surface processes such as wave breaking [2]

This model is accessible from: <https://www.deltares.nl/en/software/delft3d-flexible-mesh-suite/#service-packages>

X-Beach model

X-Beach model is an Eulerian model and it is developed by Deltares. No more considerations are needed since those reported on Delft3D suit also to this model.

Advantages

- It includes sediment transport [2]

Disadvantages

- It does not resolve adequately surface processes such as wave breaking [2]

This model is accessible from: <https://oss.deltares.nl/web/xbeach/downloads>

OpenFOAM model

OpenFOAM model is an Eulerian one and it is developed primarily by OpenCFD Ltd.

Advantages

- It resolves wave breaking and particle-flow interaction (so it could potentially give insight in the small-scale processes) [2]

Disadvantages

- Its computational efficiency is still too limited to solve flow on a time scale longer than a few single wave events [2]

This model is accessible from: <https://www.openfoam.com/news/main-news/openfoam-v2106>

DualSPHysics model

DualSPHysics model is an Eulerian one.

Advantages

- It resolves wave breaking and particle-flow interaction (so it could potentially give insight in the small-scale processes) [2]

Disadvantages

- Its computational efficiency is still too limited to solve flow on a time scale longer than a few single wave events [2]

This model is accessible from: <https://dual.sphysics.org/downloads/>

SCUD model

The (Surface CUrrents from Diagnostic) SCUD model was developed by the International Pacific Research Center (IPRC). The project goal was to model near-surface currents forced by satellite sea level height and wind data currents consistent with trajectories of Lagrangian drifters [4].

The model uses satellite sea level data (provided by satellite altimeters and distributed by AVISO) and wind data (provided by scatterometers QuikSCAT and ASCAT) to estimate on a quasi-global $1/4^\circ$ grid near-real time near-surface currents, consistent with historical trajectories of satellite-tracked drifting buoys of the Global Drifter Program.

The spatial grid of SCUD ($1/4^\circ$) adequately resolves important ocean scales (i.e. the deformation radius and size of mesoscale eddies). However, such resolution may be too coarse for simulations in coastal areas and those around islands. To increase the resolution of drift in coastal areas and its accumulation on shorelines, the SCUD model can be blended with HYCOM3 data, then increasing the original $1/4^\circ$ grid of SCUD to $1/12^\circ$. [5]

Advantages

- Tracers sensitive to windage [4]

Disadvantages

- The accuracy of the model deteriorates near shore due to higher errors in satellite data and increased complexity of dynamics.
- It does not include nearshore processes, and, as it is a daily product, it does not account for differences in mixed, semi-diurnal tidal state [6]

OSCURS model

Ocean Surface CURrent Simulations (OSCURS) model is a Lagrangian particle tracking one.

Advantages

- It allows hindcasts [4]
- It includes the adjustments for windage with two factors: a drag coefficient and an angle of deflection [7]

Disadvantages

- Available only in a limited area in the North Pacific Ocean

The website to run the model is: <https://oceanview.pfeg.noaa.gov/oscurs/>

GNOME model

The General NOAA Operational Modeling Environment (GNOME) model is a Lagrangian one.

It is an interactive environmental simulation system designed for the rapid modeling of pollutant trajectories in the marine environment.

GNOME is a modular and integrated software system that accepts input in the form of maps, bathymetry, numerical circulation models, location and type of spilled substance, oceanographic and meteorological observations and other environmental data. Spilled substances are modeled in GNOME as point masses, or particles, whose trajectories depend on “movers” (winds, currents and horizontal diffusion).

Moreover, there is a set of python bindings (and utilities) called pyGNOME, that can be used to write customized models using the GNOME code base.

Advantages

- It allows hindcast [4]
- It includes adjustments for windage [4]
- It includes turbulent diffusive processes that spread particles horizontally which are simulated by a random walk [5]

Disadvantages

- No spatial variability in the horizontal diffusion, resulting in a uniform spreading of the particles over time [5]

The desktop version of the model is accessible from: <https://response.restoration.noaa.gov/oil-and-chemical-spills/oil-spills/response-tools/downloading-installing-and-running-gnome.html>

NEMO model

Nucleus for European Modelling of the Ocean (NEMO) model is an Eulerian one; the version 3.6, configuration ORCA2-LIM3, simulates the 3-dimensional dispersion of plastics in the global ocean.

Advantages

- It allows hindcasts and forecasts

Disadvantages

- Its is computationally consuming and requires initial and boundary conditions

The model is accessible from:

<https://forge.ipsl.jussieu.fr/nemo/chrome/site/doc/NEMO/guide/html/install.html#>

Parcels model

Parcels (“Probably A Really Computationally Efficient Lagrangian Simulator”) model is an offline 3D Lagrangian one and it is developed by the MIT (Massachusetts Institute of Technology).

It is a framework for computing Lagrangian particle trajectories, whose main goal is to process the continuously increasing amount of data generated by the contemporary and future generations of ocean general circulation models (OGCMs).

The user interface is written in python, while the computational intensive integration is Just-In-Time (JIT) compiled into C. The code is formed around a flexible and customizable API that allows rapid model development, based on discrete time-stepping algorithms. It has a high-level abstraction that hides complexities from the user (field sampling, efficient loop scheduling, file I/O, etc.). [8]

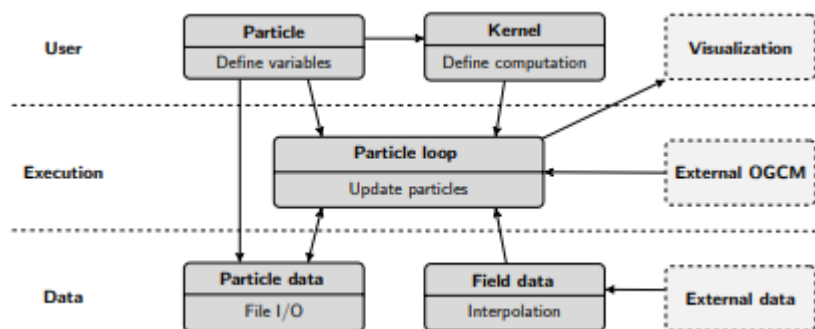


Figure 1 Taken from [9]

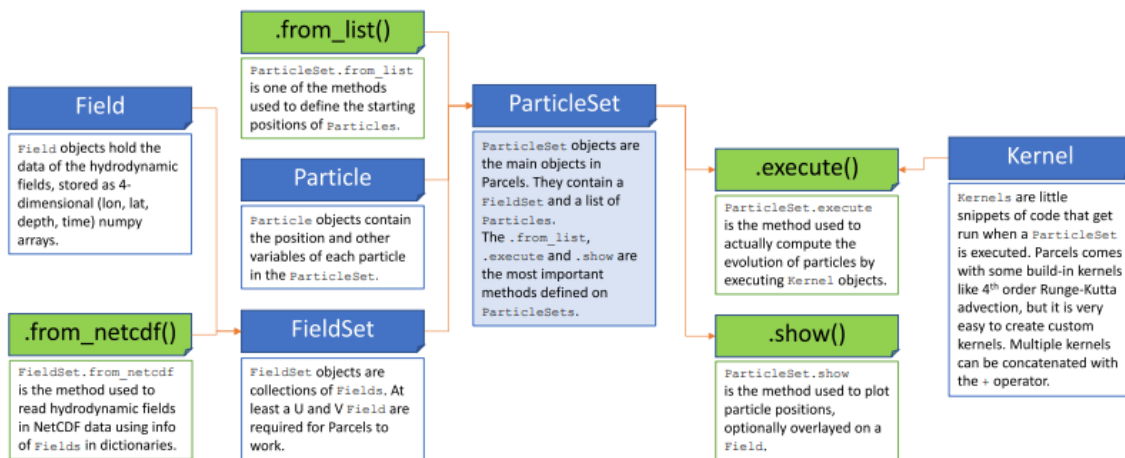


Figure 2. Class diagram of the Parcels v0.9 prototype implementation. Classes are depicted in blue, methods in green. Note that not all methods and classes are shown in this diagram.

Figure 2 Taken from [9]

Advantages

- Time-forward and -backward mode
- It supports external field data from NetCDF files, with a configurable interface to describe the input data and variable structure [9]
- It reads data from multiple fields discretized on different grids and grid types [10]
- Allowed A-, B- and C- variable distributions, rectilinear and curvilinear horizontal grids and z- and s-vertical levels [10]

This model is accessible from: <https://oceanparcels.org/#installing>

TRACMASS model

TRACMASS model is an offline 3D Lagrangian one.

It can be used to calculate trajectories using velocity and tracer fields from a variety of ocean models and it can handle a wide variety of vertical grids and data formats.

Advantages

- trajectories are unique and if a trajectory is calculated forward and then backward the solution will be the same up to numerical noise due to round-off errors [8]

Disadvantages

- Comparing the simulated drifter trajectories with observed surface-drifter trajectories has showed coarse-resolution ocean models lack variability in the surface currents, which is very likely due to the omission of stochastic noise to mimic sub-grid scale diffusion [8]

This model is accessible from:

<https://www.tracmass.org/docs/configuration/installation/index.html>

CMS model

Connectivity Modelling System (CMS) model is an offline 3D Lagrangian one.

It is an open-source Fortran toolbox, created at the University of Miami. The tool is multiscale, allowing for the seamless moving of particles between grids at different resolutions.

The CMS uses RK4 (Runge-Kutta 4) time-stepping and tri-cubic interpolation and it is designed to be modular and probabilistic, thus it is relatively easy to add additional behaviors.

Advantages

- Modules including random walk diffusion, mortality, vertical migration, mixed layer mixing, and a seascape module designed to generate a connectivity matrix output from the source to the final destination of the particles. [8]

Disadvantages

- The model is mainly oriented for biological applications

This model is accessible from: <https://github.com/beatrixparis/connectivity-modeling-system>

MITgcm

The Massachusetts Institute of Technology general circulation model is a Lagrangian one.

Advantages

- It allows hindcasts and forecasts

Disadvantages

- Its is computationally consuming and requires initial and boundary conditions
- It is poorly documented [8]

This model can be downloaded following the guidelines in:

https://mitgcm.readthedocs.io/en/latest/getting_started/getting_started.html

HYCOM model

The HYbrid Coordinate Ocean Model is an online Lagrangian one. [8]

It is a generalized (hybrid) vertical coordinate ocean model (isopycnal, bottom following, and/or pressure). It includes online code designed to follow numerical particles during model run time and has the ability to follow a fluid particle in three dimensions.

Advantages

- It has the possibility to release both isobaric and isopycnic floats [8]

Disadvantages

- Its is computationally consuming and requires initial and boundary conditions

This model is accessible from: [http://ccrm.vims.edu/w/index.php/How to download HYCOM](http://ccrm.vims.edu/w/index.php/How_to_download_HYCOM)

ROMS

The Regional Ocean Model System (ROMS) is an Eulerian one with online Lagrangian extensions. [8]

It includes a module called *floats*, which allows the release and tracking of numerical particles during model run time. Passive floats can be of three different types: neutral density 3D Lagrangian, isobaric or geopotential. [8]

This model is developed and supported by researchers at the Rutgers University, University of California Los Angeles and contributors worldwide.

Advantages

- possibility to add a random walk to simulate sub-grid scale vertical diffusion [8]
- clusters of floats with user defined distributions can be released at specified locations [8]
- possibility to release particles multiple times, at defined time intervals throughout the run [8]

Disadvantages

- Its is computationally consuming and requires initial and boundary conditions

This model is accessible from: <https://www.myroms.org/index.php?page=RomsPackages>

MEDSLIK-II Model

MEDSLIK-II model is a Lagrangian one.

It is applicable to surface passive tracers that simulates the behavior of floating plastic debris at a first approximation.

As outputs, it provides the particle concentrations in two states: at the surface and on the coast. Particle concentrations at the surface and coastline are calculated on a finer grid in respect to the one used in the hydrodynamic model. [11]

Advantages

- capability to simulate the adsorption of particles into the coastal environment, taking into account a probability that particles may be washed back into the water [11]
- turbulent fluctuation parametrized with random walk scheme [11]
- particles can change due to various physical and chemical processes (evaporation, emulsification, dispersion in water column, adhesion to coast) [11]
- the Markov chain allows the forward-in-time simulation and allows to perform correctly the backwards-in-time simulation [11]

Disadvantages

- Its requires significant customization on the code before to apply it to specific realities

This model is accessible on request from: <http://www.medslik-ii.org/users/login.php>

PELETS-2D

PELETS-2D model is an offline Lagrangian one.

Particle trajectories on the sea surface are calculated on a 2-dimensional triangular grid.

Advantages

- It allows forward and backward in time simulations

Disadvantages

- the trajectories simulated close to shorelines involve much uncertainty arising from limited resolution of coastline details and from difficulties to model the subscale process of beaching and potential resuspension [12]
- vertical transport (e.g. sinking of particles) is not included. [12]

Tables with some summarized information

Table 1
Summary of the specifications of the offline Lagrangian codes discussed Appendix A

Code name	Ariane	TRACMASS	Octopus	LAMTA	CMS	Parcels
Website	www.univ-brest.fr/lpo/ariane	tracmass.org	github.com/jinbow/Octopus	bitbucket.org/f_nencio/spasso/overview	github.com/beatrixparis/connectivity-modeling-system	oceanparcels.org
License	CeCILL (http://www.cecill.info)	open source	MIT	GNU General Public License	GNU GPL v3	MIT
Key citation	Blanke and Raynaud (1997); Blanke et al. (1999)	Dóos et al. (2017)	Wang et al. (2016)	d'Ovidio et al. (2015)	Paris et al. (2013b)	Lange and van Schille (2017)
OGCMs supported	NEMO/OPA, ROMS, Symphonie and any C-grid	NEMO, IFS (AGCM), MOM, MICOM, POM, HYCOM	MITgcm; any C-grid	AVISO satellite velocities; any velocity field on A-grids (euclidean or spherical)	HYCOM, OFES, NEMO, SOSE, MOM, MITgcm	NEMO, OFES, GlobCurrent; customizable to any OGCM with NetCDF data format
Language(s)	Fortran 90/95; Matlab (IDL on request) for visualisation	Fortran	Fortran	GNU/Octave and C++	Fortran	Python user interface, auto-generated C
Primary use	Offline calculation of 3D streamlines in the velocity field at any scale (regional, basin, global); volume transport calculations	3D water mass pathways, particle/tracer dispersion	3D watermass pathway, particle/tracer dispersion, cross-frontal transport, Argo float simulation	Compute satellite based Lagrangian diagnostics to optimize sampling strategy of mesoscale-based field campaign and support interpretation of in-situ observations	Dispersion, connectivity, fate of pollutants; Individual Based Modelling	Large scale oceanography; Individual Based Modelling; teaching (via customizable interface)
Advection method	Analytic	Analytic	RK4	RK4	RK4	RK4, RK45, Explicit Euler; extensible interface for custom advection methods
Diffusion method	No diffusion (purely kinematic method)	Brownian motion for background diffusion with random displacement or randomly added velocities	Brownian motion for background diffusion, random displacement within the mixed layer	Random walk optional	Brownian motion for background diffusion, random displacement within the mixed layer	Extensible interface for Random Walk and custom behaviour
Grids supported	Arakawa C, also tested with Arakawa B interpolated on C-grid, partial cells supported	Arakawa A, B, C. Spatially and temporally varying vertical grids supported (partial cells, z*, sigma, hybrid) including those for AGCMs	Arakawa C	Arakawa A	Orthogonal (rectangular) Arakawa A, B and C	Arakawa A, B and C; unstructured meshes planned
Key strengths	Almost 25 years of experience with core of the code; easy-to-install, easy-to-use; fast analytical solution; no coast crash; qualitative mode (full details of selected trajectories) and quantitative mode (volume transport calculations); compatible with the conservation laws of the OGCM	Volume conserving, fast analytical solutions without intermediate time steps, works with both OGCMs and AGCMs	Fast using Fortran, supports openMP	Designed to work out-of-the-box with AVISO surface geostrophic velocities. Already configured to compute a broad range of Lagrangian diagnostics (i.e. Finite Time/Size Lyapunov Exponents; longitudinal and latitudinal origin of particles; time of particle retention within mesoscale eddies etc.)	Modular, fast, parallel; Multi-grid support; Used in a wide variety of contexts, from marine ecology to physical oceanography	Ease-of-use, customizable extension interface and automated performance optimization
Shortcomings	No parallel mode; trajectory scheme is somewhat crude beyond the context of 3D water mass tracing	Need of improving the diffusion method	Non-scalable parallelization, not very efficient in reading large model output	Particle advection only 2D; cannot be run in parallel.	No support for non-orthogonal grids; parallel implementation is heavy on I/O	Not yet parallel; support for unstructured meshes in progress

Figure 3 Taken from [8]

Table 2
Summary of the specifications of the online Lagrangian codes discussed Appendix A

Code name	LIGHT in MPAS-O	NEMO online floats and icebergs	MITgcm	HYCOM Float Package	ROMS online floats
Website	mpas-dev.github.io	nemo-ocean.eu/About-NEMO/Reference-manuals	mitgcm.org	hycom.org	myroms.org/wiki/floats.in
License	Copyright (c) 2013, Los Alamos National Security, LLC (LANS) and the University Corporation for Atmospheric Research (UCAR).	CeCILL (http://www.cecill.info)	None	None	Open source MIT/X
Key citation	Wolfram et al. (2015)	Madec and NEMO team (2016) for floats; Marsh et al. (2015) for icebergs	Marshall et al. (1997a)	Halliwel and Garraffo (2002), Garraffo et al. (2001a); 2001b)	Piñones et al. (2011), Narvaez et al. (2012b)
OGCMs supported	Model for Prediction Across Scales Ocean (MPAS-O) (Ringler et al., 2013)	NEMO	MITgcm	Hybrid Coordinate Ocean Model (HYCOM) (Bleck, 2002; Chassignet et al., 2003; 2006)	ROMS
Language(s)	Fortran (post-processing in python)	Fortran	Fortran	Fortran	Fortran
Primary use	Large scale oceanography, diagnosing ocean mixing	Floats: large-scale, eddy ocean circulation. Icebergs: coupling of iceberg fluxes with ocean physics and dynamics and sea ice, via heat, freshwater and momentum fluxes; evaluating/forecasting iceberg hazard	Ocean modelling at all scales, offline advection	Large scale and coastal oceanography, biology	Coastal and mesoscale oceanography, Individual Based modelling for biophysical applications
Advection method	Sub-stepped generalized RK for time integration; Wachspress and RBF horizontal interpolation; linear vertical and temporal interpolation	Floats: Ariane method or RK4. Icebergs: RK4	RK4	RK4	4th-order Milne predictor and 4th-order Hamming corrector
Diffusion method	None	None	Brownian motion optional	Brownian motion optional	Vertical random walk optional
Grids supported	Unstructured C-grid	Arakawa C	Arakawa C	Arakawa C	Arakawa C
Key strengths	Fast (minimal cost to OGCM), high temporal and spatial fidelity, computes isopycnal advection by construction, extensible within Fortran framework	Floats: Analytical advection on model timestep resolution. Icebergs: freshwater flux due to melting icebergs	Works well with archived MITgcm velocity fields, scales to very large sizes using MPI and domain tiling	Stable and relatively easy to use and understand	Reliable since trajectories are coherent with ocean circulation, parallel, easy to set up
Shortcomings	Currently no explicit offline mode, tied to MPAS framework and presently embedded in MPAS-O	Floats: limited use/publications to date. Icebergs: physics and dynamics subject to several uncertain parameters; giant tabular icebergs not yet represented; interactions with sea ice currently limited	Complicated to set up	No parallel mode	Computationally expensive since no offline model is available; Large output files for long runs or many particles.

Figure 4 Taken from [8]

Table 1. Existing modelling packages for simulation of pollutant dispersion processes.

Example models	Corresponding mathematical approaches for pollutant dispersion	Availability	Major functionalities and (or) capabilities related to pollutant dispersion
Jet and plume models			
CORMIX (Doneker and Jirka 2007)	Empirical solutions; Eulerian jet integral method	Commercial model	Prediction of jet and (or) plume geometry and dilution in the near field; single or multiple jets
VISJET (Lee and Cheung 1990; Lee and Chu 2003)	Lagrangian jet integral method	Commercial model	
Visual PLUMES (Frick et al. 2003)	Empirical solutions; Eulerian and Lagrangian jet integral methods	Free package	
Sophisticated multidisciplinary models			
MIKE 21/3 (DHI 2007)	FVM; RWPT method	Commercial package	Predictions of ocean hydrodynamics; pollutant fate and transport in the far field; water quality; sediment processes
Delft3D (Delft3D 2009)	FDM; RWPT method	Commercial package	
EFDC-Hydro (Hamrick 1992; USEPA 2002)	FDM; RWPT method	Free package	Predictions of ocean hydrodynamics; Pollutant dispersion in the far field; near-field processes using the embedded jet model JETLAG; suspended sediment transport
HydroQual-ECOMSED (Hydroqual 2002)	FDM; RWPT method	Free package	Predictions of ocean hydrodynamics; pollutant fate and transport in the far field; sediment processes
Specialized model – produced water modelling			
DREAM (Reed et al. 2001)	Coupled jet integral method and RWPT method	Not available	Predictions of pollutant fate and transport in both near field and far field; single or multiple sources
PROTEUS (Sabeur et al. 2000)	RWPT method	Not available	

Note: FVM, finite volume method; FDM, finite difference method; RWPT, random walk particle tracking.

Figure 5 Taken from [13]

Table 2. Summary of modelling techniques for wastewater dispersion from offshore outfalls.

Methods	Formulation	Advantages	Limitations	Utilization	References
Empirical solutions	Dimensionless analysis	Easy to evaluate and implement; includes physical effects	Limited applications; Discontinuous problems under certain flow conditions	Near field mixing processes; simple steady flow conditions	Jirka et al. 1996; Davis 1999; Bleninger 2006
Analytical solutions	Closed form solution	Very simple formulations; useful for validating numerical solutions;	Limited applications; requires assumptions for flow, geometry, and water quality situations	Simple steady flow conditions; validating other methods and models	McCutcheon 1990; Martín and McCutcheon 1998
Numerical solutions for directly solving the advection-diffusion equation	FDMs, FEMs, FVMs	Simulation of complex geometry, larger domain, long-term simulations; easily describes higher-order chemical kinetics; assures conservation of mass, momentum, and energy	Complicated formulations and computations; stability problems; excessive numerical dispersion	Far-field modelling; complex flow and geometry conditions; time series results	Westerink and Shea 1989; Zhang and Adams 1999; Chung 2002; Li and Hodgins 2004; Ilyina et al. 2006
RWPT method	Lagrangian-based particle tracking	Free of numerical dispersion; maintains physical dispersion processes; easy implementation of multicomponent effluents; assures conservation of mass	Accuracy depends on the particle density per grid cell; time consuming, especially for long term and large domain simulations; difficulty incorporating higher-order chemical reactions	Near-field or intermediate-field modelling; variable time and flow conditions	Abulaban et al. 1998; Periañez and Elliott 2002; Israelsson 2006; Salamon et al. 2006; Suh 2006
Jet integral methods	Eulerian formulation or Lagrangian formulation	Good approximation of plume behaviour; simple formulations and easy to implement	Requires assumptions for distribution profiles; spatial restrictions for applications; Requires termination conditions	Near-field simulation; unbounded ambient conditions	Davis 1999; Lee and Chu 2003; Jirka 2004; Li and Hodgins 2004

Note: RWPT, random walk particle tracking; FDMs, finite difference methods; FEMs, finite element methods; FVMs, finite volume methods.

Figure 6 Taken from [13]

Conclusions

Looking at the overall advantages and disadvantages of the considered models, for our purpose the Lagrangian framework is preferable. We will consider the GNOME and the pyGNOME models as the most suitable candidates to achieve the MARLESS objectives. The MEDSLIK-II model is a tool that could improve the results obtained by means of the GNOME and pyGNOME implementation and runs, but it needs a customization that requires a longer implementation time with respect to the GNOME and pyGNOME. Moreover, the Parcels model is considered the best code on which to develop new features for trajectory and back trajectory marine litter computations, as it is a new tool for the Lagrangian particle trajectories framework which offers the opportunity to exploit the high computational efficiency of the code.

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