



Numerical modeling of brine discharge: commercial models, MEDVSA online simulation tools and advanced computational fluid dynamics

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ABSTRACT

Numerical modeling is a prediction tool useful for the design of brine discharge configurations and for environmental impact assessments, to prevent the potential impacts of brine in marine environments. Among the existing approaches of governing equations, dimensional analysis formulas and integration models are usually applied to brine discharge simulations, as is the case of the most used commercial tools for modeling brine discharges. Simulation with computational fluid mechanics (CFDs) advanced models has not yet been implemented and only some research studies are available in the literature. In order to improve the knowledge related to the use and degree of feasibility and reliability of these approaches for the modeling of brine discharges, an exhaustive investigation has been carried out, also including validation with high-quality experimental data. An analysis of the most used *commercial models*—CORMIX, VISUAL PLUMES, and VISJET—has been carried out focusing on brine discharges. As a result, Technical Specification Cards have been developed for each model (Cormix1, Cormix2, Corjet, UM3, and JetLag), including: theoretical basis, capabilities, limitations, sensitivity analysis, and degree of feasibility and reliability, based on its validation with published experimental data. Faced with the commercial model limitations, alternative *MEDVSA simulation tools* have been developed and are available on the MEDVSA webpage. They are simple models, based mainly on dimensional analysis and integration formulas, which model the behavior of brine in the near and far field region. Codes have been programmed in Matlab and include tools for modeling different discharge configurations and ambient scenarios. An improvement of the interface and results report and recalibration with new experimental data has been carried out in order to provide alternative higher-quality tools for the commercial models. The following tools have been developed and will be explained in this conference: MEDVSA-IJETG, MEDVSA-MJETS, MEDVSA-JET-SPREADING, MEDVSA-JET-PLUME2D, MEDVSA-PLUME2D, and MEDVSA-PLUMED3D. This global investigation on the numerical modeling of brine discharges has been carried out within the MEDVSA project. The R&D project (2009–2011), financed by the Spanish Ministry of the Environment and Rural and Marine Affairs, aims to develop and implement a methodology to reduce the environmental impact of brine discharges. The information, compiled into a methodological guide, and the numerical tools developed are available on the web site of the project (www.medvsa.es).

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Keywords: Brine discharge; Numerical modeling; Commercial models; Integral models; CFDs

1. Introduction

Desalination is a rainfall independent source of water for the security of long-term water supplies. Seawater desalination has gained importance in coastal countries where conventional water sources are insufficient or overexploited. It can be considered an inexhaustible natural source that generates a high-quality product and guarantees demand supply while at the same time being expensive (due to high-energy consumption) and which can cause negative effects on important marine ecosystems.

The term desalination refers to any of the several processes involved in removing dissolved minerals (especially salt) from seawater, brackish water, or treated wastewater. At present, seawater reverse osmosis (SWRO) has gained importance over other desalination technologies, and is expected to be the most important desalination technology in the future. SWRO plants usually work with 40–50% conversion rates.

The main environmental impacts of SWRO desalination plants are those associated with [1]: marine structure construction, water intake, energy consumption and brine discharge into seawaters (anoxia at the sea bottom, impacts on larvae or younger individuals of fish fauna [2], impacts on seagrass due the presence of hypersaline effluents [3]). The waste effluent or brine has no chemical or thermal pollution; however, the salt concentration is very high, making it denser than seawater and thus increasing the risk of negative effects on benthic ecosystems.

When studying the behavior of a brine discharge into a receiving water body, two regions with different effluent behavior should be considered: the near and the far field.

The *near field region* is located in the vicinity of the discharge point and is characterized by initial mixing, which depends on the brine discharge configuration design and the effluent and ambient properties. Higher dilution rates are reached in the near field.

The *far field region* is located further away from the discharge point, where the brine turns into a gravity current that flows down the seabed. Mixing depends on the ambient conditions (bathymetry, currents, waves, etc.) and the differences in density between the hypersaline plume and the environment.

Fig. 1 shows a diagram of the different behavior areas of a brine jet discharge.

There are different types of configurations for brine discharges. Previous studies, concluded that the system generating the greatest dilution is the submerged jet with an initial discharge angle around 60° . Overall, the jet discharge configuration is the only one that most commercial models can simulate.

To design the discharge configuration, numerical models are required to predict the behavior of the effluent discharged into the sea and the performance of water-quality standards. Depending on the simplifications assumed, there are different approaches for modeling this phenomenon. For all cases, experimental tests are necessary to calibrate the numerical tools.

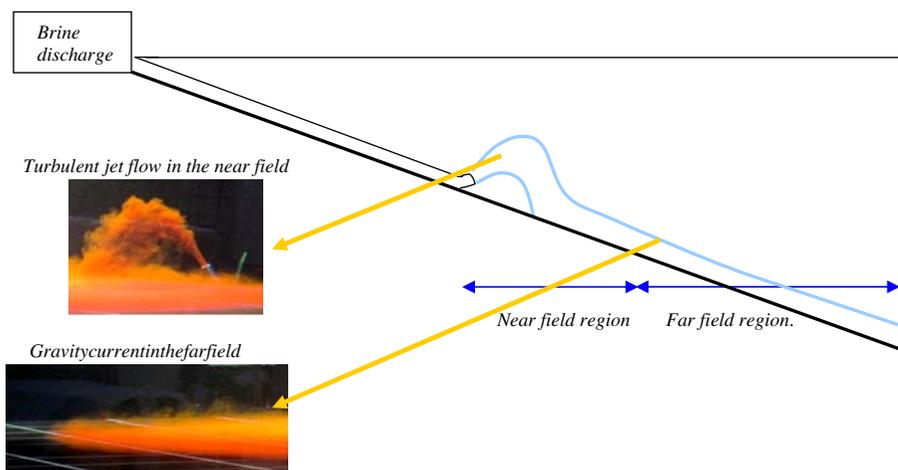


Fig. 1. Near and far field regions in a jet discharge.

2. Modeling as a predictive tool

From an environmental point of view, the design of a brine discharge device must guarantee the performance of quality standards beyond the mixing zone while at the same time guaranteeing that critical salinity limits will not be exceeded in the area of protected sensitive ecosystems.

In order to predict the behavior of the brine in the seawater, a simulation model can be applied as an essential prediction tool in the environmental assessment of desalination projects. Considering effluent brine properties and the discharge configuration, the model predicts the brine behavior under different ambient conditions.

Two types of modeling techniques can be utilized: experimental and numerical.

Numerical modeling applied to brine discharges solves the hydrodynamics and transport equations adapted to a negatively buoyant effluent, which can be set up by a Lagrangian or Eulerian system. The governing equations of brine discharge phenomenon are: equation of continuity, equation of momentum conservation, transport equation, and equation of state.

Regarding the basic approaches for solving the equations according to the hypothesis and simplifications assumed that there are three types of physical models: those based on dimensional analysis; those based on the integration of differential equations, and hydrodynamic models.

3. Formulas based on dimensional (for commercial models validation)

3.1. Stagnant ambient

Dimensional analysis for round jets into a stagnant and homogeneous ambient, assuming full turbulent flow and Boussinesq hypothesis for gravity terms, concludes that, for a specific initial discharge angle (θ), jet geometric features (Z_i, X_i) and dilution rates (S_i) depend mainly on port diameter (D) and the Den-simetric Froude number (F_{rd}) [4].

For a single-port dense negatively buoyant jet, the following nondimensional parameters are commonly calibrated to characterize the flow at some specific points (i.e. maximum rise height and impact point):

$$\frac{Z_t}{DF_{rd}}; \frac{Z_m}{DF_{rd}}; \frac{X_m}{DF_{rd}}; \frac{X_i}{DF_{rd}}; \frac{S_i}{F_{rd}} \quad (1)$$

where Z_t : maximum rise height (maximum height of the top boundary or upper edge of the jet), Z_m : vertical location of the centerline peak, X_m : Horizontal location of the centerline peak, X_i : horizontal location

of the impact point; and S_i : minimum centerline dilution at the impact point.

In this study, we have used the terms “impact point” and “return point” interchangeably.

F_{rd} : densimetric Froude number. $F_{rd} = \frac{U_0}{\sqrt{g'_0 R}}$, being: U_0 : initial discharge velocity, g'_0 : reduced gravity; $g'_0 = g \frac{\rho_0 - \rho_A}{\rho_A}$; ρ_0, ρ_A : effluent and ambient density, and R : jet radius.

Figs. 2 and 3 show the main geometric characteristics of an inclined dense jet.

Regarding the case of a single-port dense inclined jet discharged into an unlimited, homogeneous, and stagnant environment, multiple experimental studies have been developed in recent years [5–13] among others. Table 1 [14] shows the experimental coefficients for dimensional analysis formulas obtained by some of these authors, showing the measurement technique used by each one.

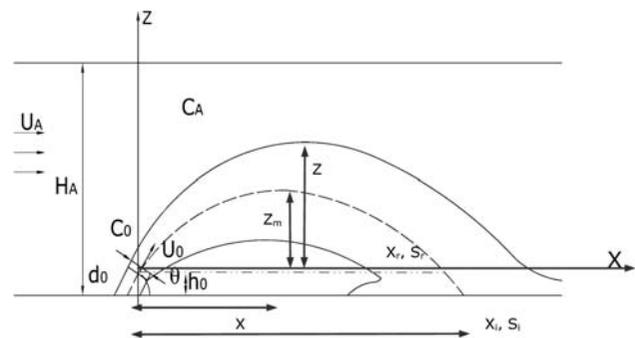


Fig. 2. Profile view of an inclined dense jet. Where H_A : average depth at discharge point; U_A : ambient velocity; C_A : ambient salinity; ρ_A : Ambient density; σ : horizontal angle between jet and current; ϕ : angle of crossflow to the vertical plane containing the nozzle axis $\phi = 180^\circ - \sigma$; U_0 : initial discharge velocity; ρ_0 : effluent density; C_0 : effluent salinity concentration; h_0 : port height; $d_0 = D$: port diameter; and θ : jet discharge angle (vertical angle with respect to the bottom).

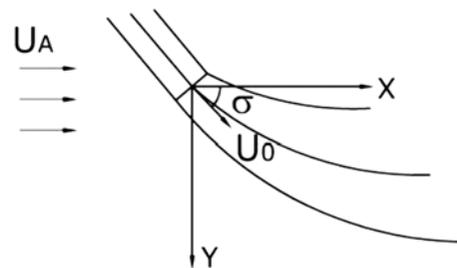


Fig. 3. Plan view of an inclined dense jet.

Table 1

Experimental coefficients for dimensional analysis formulas for inclined dense jets into a stagnant ambient

Experimental studies							
Single-port dense jet into a <i>stagnant environment</i>							
Research	F_{rd}	θ	$\frac{Z_t}{DF_{rd}}$	$\frac{Z_m}{DF_{rd}}$	$\frac{X_m}{DF_{rd}}$	$\frac{X_i}{DF_{rd}}$	$\frac{S_i}{F_{rd}}$
Roberts et al. [13] LIF	19–36	60°	2.2	–	–	2.4	1.6 ± 0.12
Cipollina et al. [16]	16–216	30°	1.08	0.79	1.95	3.03	–
Conventional techniques		45°	1.61	1.17	1.8	2.82	–
		60°	2.32	1.77	1.42	2.25	–
Kikkert et al. [17]	14–99	30°	1.0	0.56	1.75	3.14	1.51
LA (Laser Attenuation)		45°	1.6	1.06	1.84	3.26	1.71
		60°	2.27	1.6	1.6	2.72	1.81
		45°	1.58 ± 0.03	1.17	2.1 ± 0.1	3.16	1.55 ± 0.14
Papakonstantis et al. [9,18]	7.5–58.3	60°	2.14 ± 0.03	1.68	1.8 ± 0.08	2.75	1.68 ± 0.1
Digital picture analysis		60°					
Shao et al. [20]	8–32	30°	1.05	0.66	1.54	3.0	1.45
PIV-LIF		45°	1.47	1.14	1.69	2.83	1.26

3.2. Dynamic environment

Dimensional analysis for negatively buoyant round jets into a dynamic environment [14], assuming fully turbulent flow and Boussinesq hypothesis for gravity terms, concludes that, for a specific initial discharge angle (θ), jet geometric features, and dilution rates mainly depend on the port diameter (D), Densimetric Froude number (F_{rd}), ambient crossflow velocity (U_A), discharge velocity (U_o) and the horizontal angle of the jet with respect to the ambient current (σ), as is given by the following expression:

Geometric features and dilution

$$= f_i(D, F_{rd}, \theta, \sigma, U_r), \quad \text{where } U_r = \frac{U_A}{U_o} \quad (2)$$

Different formulas have been proposed by authors [15,16]. We have selected here those of Roberts and Toms [17] and Gungor and Roberts [18], which have the following expressions:

$$\frac{Z_t}{DF_{rd}} = K_i \text{ for } 0.2 < U_r F_{rd} < 0.8 \quad (3A)$$

$$\frac{Z_t}{DF_{rd}} = K_i (U_r F_{rd})^{-1/3} \text{ for } U_r F_{rd} > 0.8 \quad (3B)$$

$$\frac{S_t}{DF_{rd}} = A_i (U_r F_{rd})^{1/2} \quad (4)$$

$$\frac{S_i}{DF_{rd}} = B_i (U_r F_{rd})^{1/2} \quad (5)$$

where A_i, B_i, K_i are the experimental coefficients obtained by fitting experimental data.

Gungor and Roberts [18] also includes an expression for the horizontal location at the impact point:

$$\frac{X_i}{DF_{rd}} = J_i \quad (6)$$

To calibrate these formulas, Roberts and Toms [17], carried out different tests of 60° hyperdense jets discharged into a uniform crossflow of various speeds and directions, in the range $0 < U_r F_{rd} < 1.87$, taking measurements of the following geometrical features and dilution rates:

- Z_t : terminal rise height,
- S_t : minimum dilution (centerline) at the terminal rise height, and
- S_r : minimum dilution (centerline) at the return (identified with the impact point).

Although Roberts and Toms [17] only published formulas for 90° and 60° inclined jets perpendicular to the crossflow ($\phi = 90^\circ$), their experiments were carried out for a huge variety of crossflow directions, including: $\phi = 180^\circ, 150^\circ, 120^\circ, 90^\circ, 60^\circ, 30^\circ, 0^\circ$. With the aim of making the most of Roberts and Toms [17] experiments, all their data have been used, using the

Table 2
Experimental coefficients for the dimensional analysis formulas of a dense jet discharged into a dynamic environment

Experimental coefficients for dimensional analysis formulas Single-port dense jet into a <i>dynamic environment</i>								
	θ	ϕ	σ	A_i	B_i	K_i Range: $0.2 < U_r F_{rd} < 0.8$	K_i Range: $U_r F_{rd} > 0.8$	J_i
Roberts and Toms [25]	60°,90°	90°	90°	0.80	2.00	2.80	2.50	–
Gungor and Roberts [26]	90°	–	–	0.87	2.3	2.8	2.5	5.6
Best-fitting of Roberts and Toms [25] rough data carried out in the present work	60°	180°	0°	1.06	2.09	2.24	2.10	–
		90°	90°	0.77	1.84	2.23	2.07	
		0°	180°	0.61	1.36	1.83	2.06	

Table 3
Commercial models applicable to single-port negatively buoyant effluent discharges

CORMIX software	VISUAL PLUMES software	VISJET software
CORMIX 1: submerged and emerged single port jet		
CORMIX 2: submerged multiport jets	UM3: submerged jets single and multi-port	JetLag: submerged jets single and multi-port
D-CORMIX: Direct surface discharge		
CORJET: submerged single and multi-port jets		

following protocols: the rough data values of Z_t , S_t , and S_i variables were extracted from Roberts and Toms [17] and for each combination of θ and ϕ , the A_i, B_i, K_i coefficient values have been calculated by best fitting rough experimental data in logarithmic graphs, using the same laws proposed by Roberts and Toms.

Table 2 shows the coefficients proposed by Roberts and Toms [17] and Gungor and Roberts [18] for expressions (3A, 3B), (4)–(6), together with the coefficients obtained in the present work by the best-fitting of rough data.

4. Analysis of commercial brine discharge models: cormix, visual plumes, and jetlag

The most noteworthy commercial software used for brine discharge modeling are: CORMIX [19], VISUAL PLUMES [20], and VISJET [21].

CORMIX software was developed in the 1980s at Cornell University as a project subsidized by the Environmental Protection Agency (EPA). CORMIX is defined as a hydrodynamic mixing zone model and decision support system for the analysis, prediction, and design of aqueous toxic or conventional pollutant

discharges into diverse water bodies. CORMIX includes the subsystems CORMIX1 [22] and CORMIX2 [23], based on dimensional analysis, and the CORJET [24,25] model, based on the integration of differential equations, applicable to positive and also negative buoyancy effluent discharges.

VISUAL PLUMES is free-access software developed by the EPA, which includes the model UM3, applicable to negatively buoyant jets.

VISJET software is a commercial model developed by the University of Hong Kong which can simulate positively and negatively buoyant discharges.

Table 3 shows the models included in these software which are applicable to negatively buoyant effluents:

To obtain a better knowledge of the theoretical basis and the use of the tools applied by the promoters and environmental authorities, the software simulation models have been studied and analyzed in depth.

4.1. CORMIX 1 and CORMIX 2 dimensional analysis models

See Table 4.

Table 4
Summarize of CORMIX1 and CORMIX2 commercial models

Commercial models for brine discharge simulation			
Based on dimensional analysis	Based on the integration of differential equations		
CORMIX 1 (CORMIX)	CORJET (CORMIX)	UM3 (VISUAL PLUMES)	JETLAG (VISJET)
Positively and negatively buoyant effluents Single port jet discharge Mainly applicable to the near field region. The subsystem yields a rough approximation of the spreading layer and the far field region by coupling modules Steady state model Stagnant and dynamic environment	Positively and negatively buoyant effluents Single and multiport submerged jet discharges Unlimited environment. Boundary interaction is not considered Simulation is limited to the near field region. The jet behavior is modeled before it impacts the bottom Self-similarity cross-sectional profiles. Round section for jets Simple entrainment models based on the eddy viscosity concept Steady state models Stagnant and dynamic environment		

4.2. CORJET, UM3, and JETLAG integration models

The analysis carried out includes [26]: theoretical basis, simplifying assumptions, components and modeling options, possibilities and limitations, initial data sensitivity analysis, and validation by authors. A synthesis of this information is shown in the following paragraphs:

4.2.1. Application

They are applied in positively and negatively buoyant effluents. single and multiport submerged jet discharges, three-dimensional, near field models.

4.2.2. Modeling approach

CORJET and *UM3*: The models are based on the integration of the motion and transport differential equations through the cross section, transforming them into ordinary equation systems, which can be resolved using a simple numerical method (Runge Kutta fourth order).

JetLag: The mathematical governing equations are not strictly solved but make an approximation of the physical processes, considering entrainment.

4.2.3. Main assumptions

The assumption are unlimited environment, self-similarity cross-sectional profiles, round section for jets, Cartesian coordinates. stationary state, and simple entrainment models based on the eddy viscosity concept.

CORJET: Gaussian profiles. The results refer to the jet centerline. A term for inclination effects is included. For merging between jets, the hypothesis of an equivalent slot diffuser is applied, conserving the fluxes. *CORJET* is strictly valid only for the five asymptotic self-similar regimes (pure jet, pure plume, pure wake, advected pluff, and advected thermal). For other cases, such as inclined buoyant effluents, it is an approximation.

UM3: Top Hat (uniform) jet profiles. The results refer to the average values of the cross section. The generalized (three dimensional) 3D projected area-entrainment (PAE) hypothesis, quantifying the mass incorporated into the plume in the presence of a current including the effect of a cross current.

Dilution from diffusers parallel to the current is estimated by limiting the effective spacing to correspond to a cross-diffuser flow angle of 20°. Merged plumes are simulated by distributing the cross-current entrainment over all plumes.

JetLag: Top Hat (uniform) jet profiles. The results refer to the average values of the cross section. The 3D jet is divided into independent slices, following the jet path increasing the mass by entrainment. The “entrainment” is based on the PAE hypothesis and includes terms for the effect of the jet excess of velocity and the presence of a cross (transverse) ambient current [18]. Origin (x₀,y₀,z₀) at the jet nozzle.

4.2.4. Limitations

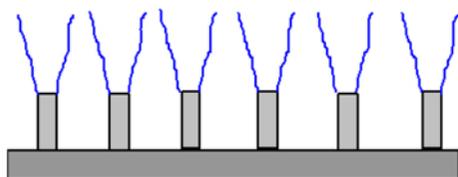
Interaction with boundaries is not modeled since an unlimited environment is assumed. The simulation is thus limited to the near field region, to the zone

before the jets impact the bottom and far field cannot be modeled. COANDA effect and re-entrainment are not modeled. Wave effects are not taken into account.

The interaction of the upper edge with the surface is not detected, although this case also invalidates the unlimited environment hypothesis and hence the results of these models.

Only submerged jets near the bottom can be modeled.

CORJET: The diffuser design is limited to unidirectional jets perpendicular to the diffuser, with the same diameter and port height jets, flow rate, initial discharge angle, and equal space.



No graphics are available for the evolution of variables. Time series data files cannot be introduced for sequential modeling.

UM3: The diffuser design is limited to unidirectional jets perpendicular to the diffuser, with the same diameter and port height jets, flow rate, initial discharge angle, and equal space. *UM3* does not detect the impact of the jet centerline with the surface or bottom. The graphics have a low quality.

JetLag: No graphics are available for the evolution of variables. Time series data files cannot be introduced for sequential modeling. Merging between jets is not modeled by *Jetlag*, although it seems to do this. Thus, the choice of diffuser type is irrelevant since

JetLag always calculates each jet individually as a single port.

4.2.5. Sensitivity analysis

Considering the range of real data on ambient conditions in the Western Mediterranean and the range of realistic values for brine discharge design, all the results from these models are especially sensitivity to the variables:

- Initial Discharge angle with respect to the bottom (θ) and discharge velocity (U_o).
- Ambient current intensity: faster and higher dilution.

However, the results in these ranges are less sensitive to density differences. Results are in all models no sensitive to the water column depth if the jets do not impact the surface and insensitive to the separation between jets if there is no merging.

CORJET: Maximum dilutions at the impact point for initial discharge angles between 45° and 60° . Not very sensitive to port height. With respect to ambient current direction, *CORJET* dilution results are almost insensitive to this parameter. If merging occurs, sensitivity to the separation between nozzles remains very small.

UM3: Maximum dilution at the impact point for a 60° initial discharge angle. Insensitive to port height. Low sensitivity to ambient current directions with respect to the jet. Slightly higher dilutions are obtained for cross (transverse) currents. If merging occurs, sensitivity to the separation between nozzles remains very small.

Table 5
Experimental results selected for commercial numerical model validation

C_A psu	C_o psu	T $^\circ\text{C}$	ρ_o kg/m^3	ρ_A kg/m^3	g'_o m/s^2	D m	H_A m	h_o m	θ	F_{rd}	U_o m/s	Q m^3/s
37.5	68	21	1,050.2	1,026.4	0.2228	0.2	15	0	30°	20	4.22	0.1326
										30		
										40		
									45°	20		
										30		
										40		
									60°	20		
										30		
										40		

Notes: C_A : ambient salinity; C_o : effluent saline concentration; T : ambient and effluent temperature, supposed to be almost the same; ρ_A : ambient density; ρ_o : effluent density; H_A : water column depth; h_o : port height; F_{rd} : densimetric Froude number; U_o : discharge jet velocity; and Q : effluent flow rate.

JetLag: Maximum dilution at the impact point for an initial discharge angle of 60°. Insensitive to port height. With respect to ambient current direction, higher dilution is obtained for transverse currents and lower dilution rates for counterflow (opposing) and coflowing (parallel) currents. Insensitive to the separation between ports, as each jet is modeled independently.

CORJET: Hypotheses considered for the merging process have not been validated for inclined hyperdense jets. Validation limited to a stagnant and homogeneous environment. Validation limited to the jet path, with very few data for dilution rates.

UM3: Hypotheses considered for the merging process have not been validated for inclined hyperdense jets. No validation data have been found for negatively buoyant effluents.

JetLag: Validation limited to the jet path and only for the case of a vertical jet discharging into a dynamic and homogeneous environment.

4.2.6. Validation by software authors

There is a lack of validation studies presented by the software authors for negatively buoyant jets.

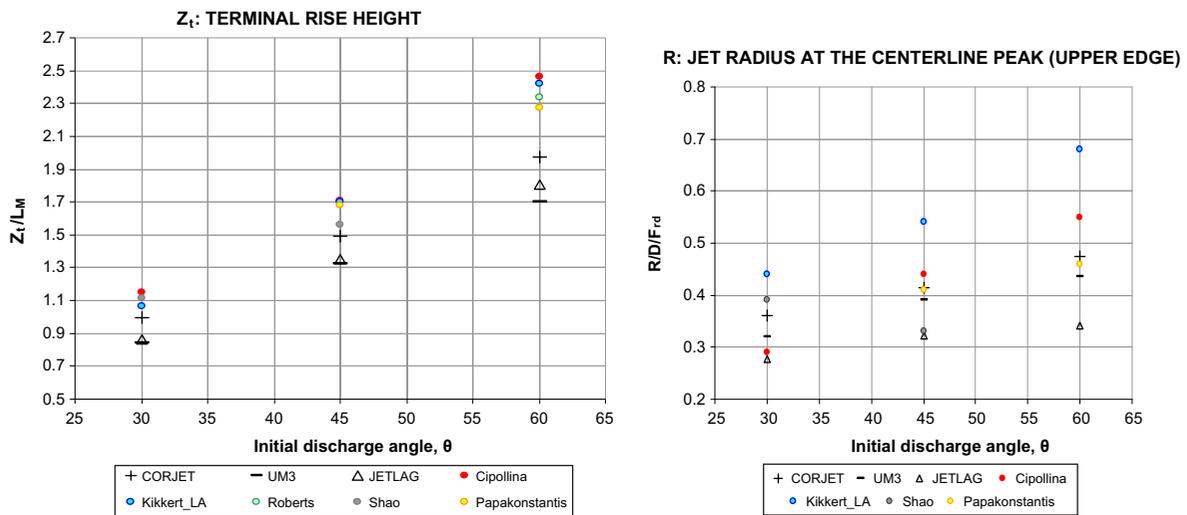


Fig. 4. Validation of the terminal rise height and the location of the return point of inclined hyperdense jets (stagnant ambient).

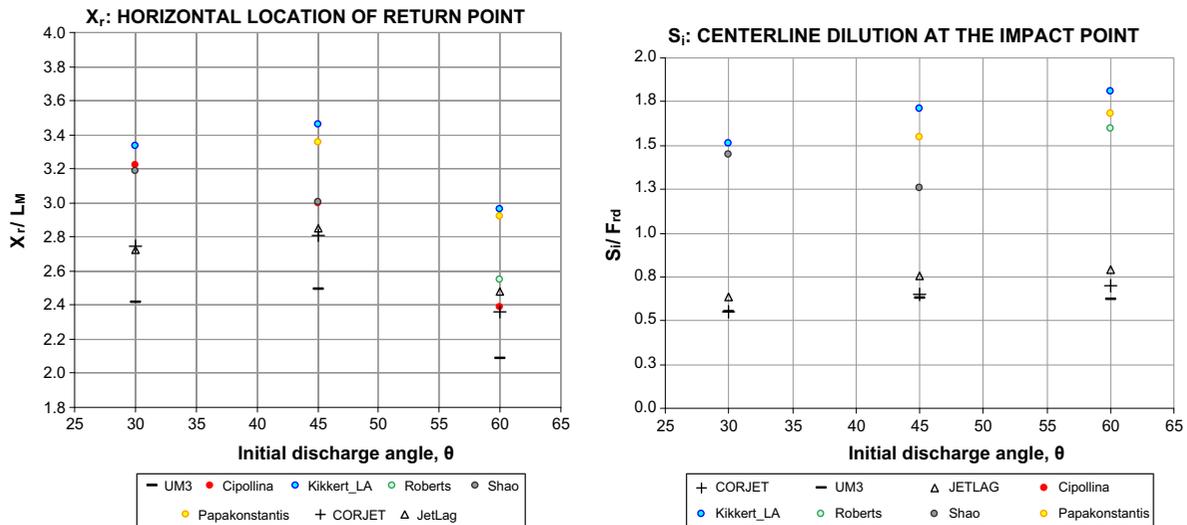


Fig. 5. Validation of return point dilution for inclined dense jets (stagnant ambient).

5. Validation of the commercial models with experimental data

One of the most important shortcomings of commercial models related to brine simulation is the significant lack of validation by the software authors for negatively buoyant jets.

To overcome this deficiency, experimental results published by different authors have been used [14] for commercial models validation related to brine discharges into a stagnant or dynamic environment.

5.1. Stagnant ambient

With the aim of validating commercial models, CORJET, UM3, and JETLAG numerical results have been compared with experimental data obtained by Roberts et al. [6], Cipollina et al. [9], Kikkert et al. [10], Shao and Law [13], and Papakonstantis et al. (2011) [11,12].

To validate the models, the brine is considered to be the subproduct of a SWRO desalination plant with a 45% conversion rate. A realistic and optimized brine jet discharge configuration has been considered taking into account [14]. The Western Mediterranean Sea has been considered as the discharge zone.

Table 5 shows the input data considered for the validation. The jet modeled could perfectly be one of the ports of a diffuser with sufficient port space to prevent the jets from merging.

The geometry magnitudes were adimensionalised in the figures using the L_M length scale, related to the “ DF_{rd} ” term using the formula: $L_M = (\frac{\pi}{4})^{0.25} D * F_{rd}$. The dilution rate was adimensionalised by the densimetric Froude number.

For values of the densimetric Froude number of 20, 30, and 40, the commercial models were run in this work for all the cases on the Table 5, calculating the average of the results obtained with different F_{rd} as the representative final result. These results were compared with the semi-empirical formulae presented in the section 3, for the specific points: Z_t , X_r , S_r .

The upper edge position was calculated with formula: $Z_t = Z_m + R * \cos \theta$. The radius considered for CORJET results is: $R = 2b$.

Fig. 4 [14] shows the validation of the terminal rise height and the jet radius at the centerline peak.

For the terminal rise height, commercial models significantly underestimate the real value, CORJET being the model with the best agreement and UM3 the model with the poorest estimation.

Fig. 5 shows the adimensionalised impact point location and minimum dilution at the impact point for different discharge angles.

For the horizontal location of the return point (identifiable with the bottom impact point), the values are underestimated by all the models, with JetLag

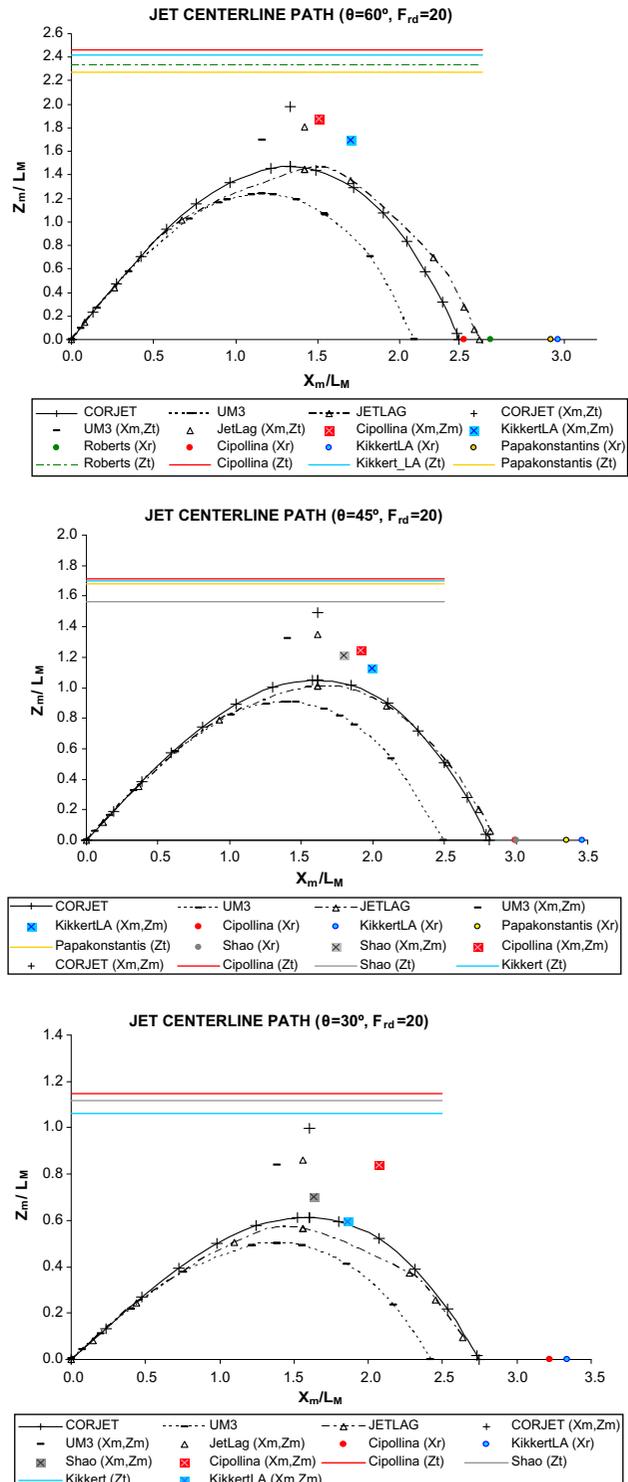


Fig. 6. Horizontal location and minimum dilution at the impact point.

Table 6
Input data for commercial models validation in the case of an inclined jet discharged into a dynamic environment

C_A	C_o	T	ρ_0	ρ_A	D	H_A	h_o	F_{rd}	θ	U_0	Q	U_A	$U_r F_{rd}$
Fpsu	psu	°C	kg/m ³	kg/m ³	m	m	m			m/s	m ³ /s	m/s	
37.5	68	21	1,050	1,026.4	0.18	15	0.2	20	60°			0.06	0.3
									90°	4	0.1018	0.25	1.25
												0.374	1.87

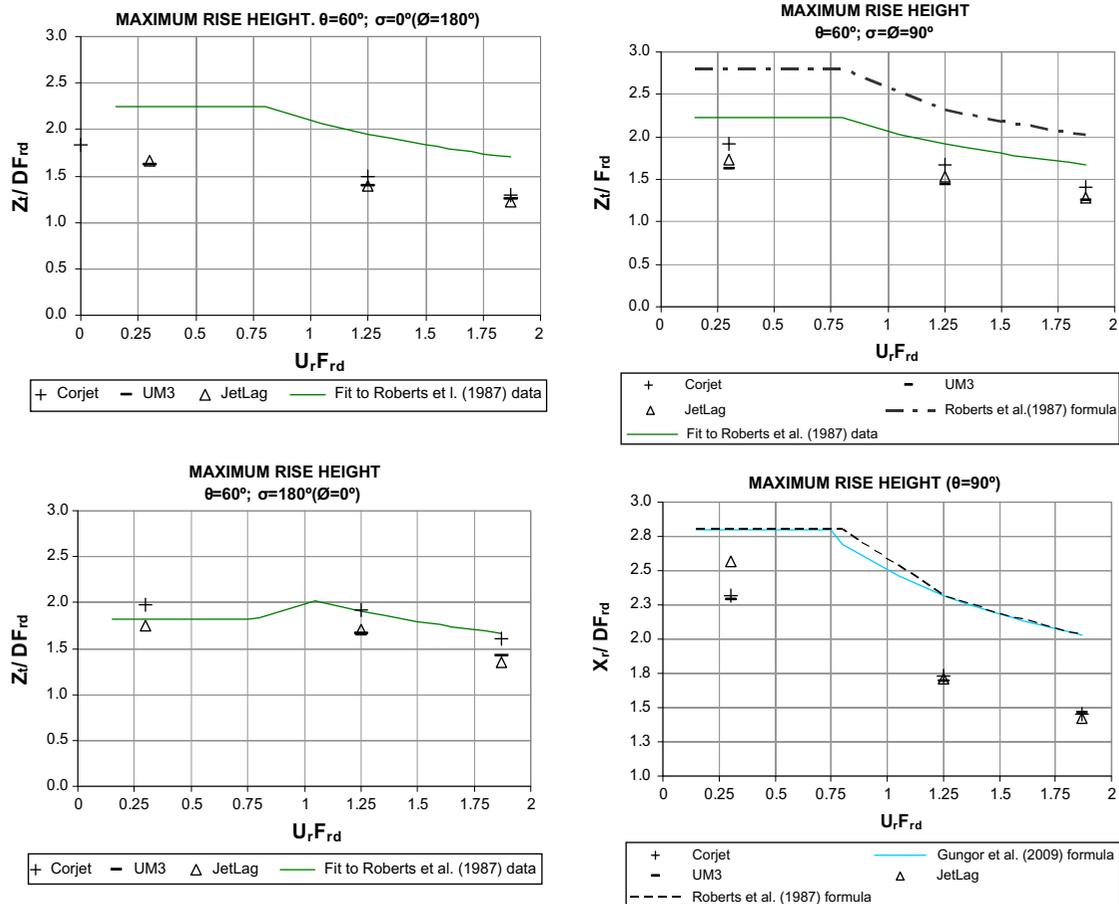


Fig. 7. Validation of maximum rise height for dense jets, for different $\theta - \phi$ combinations (dynamic environment).

providing the best estimation, and UM3 the poorest one. It is seen that dilution is greatly underestimated.

Fig. 6 [14] shows the validation of the jet centerline path for jets with different initial discharge angle.

The following conclusions [14] are derived from the validation study carried out in this section:

- Commercial models in general correctly follow the trend of real data (increasing or decreasing the magnitude with the initial jet discharge angles).
- CORJET, UM3, and JetLag commercial models correctly achieve the trend of experimental data, but underestimate the geometric features and dilution of the brine jet in all cases. The 60° inclined jet is the case worst estimated by the commercial models.
- CORJET gives, in general, better agreement for geometry variables, with deviations around 10-20%, while UM3 provides the greatest differences (around 20–30%).

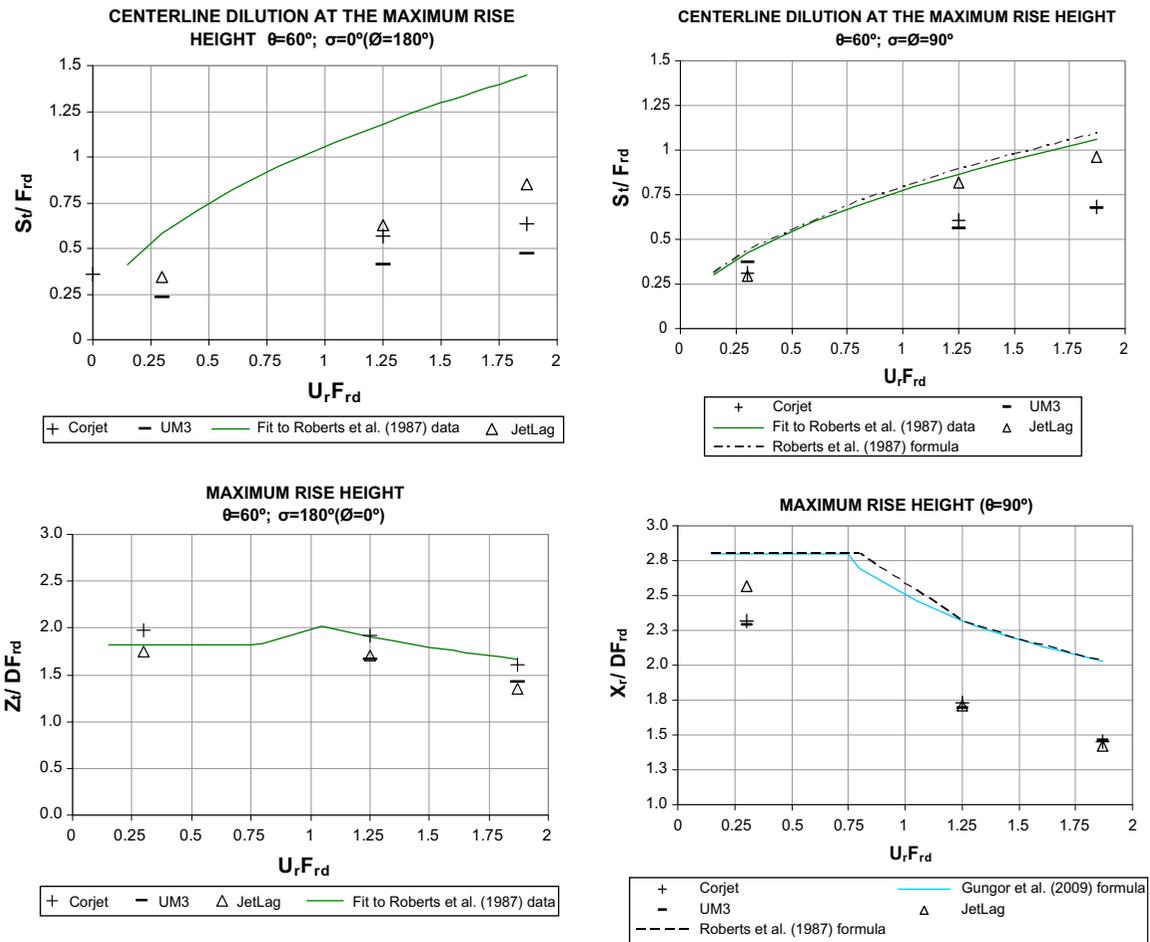


Fig. 8. Validation of centerline dilution at the maximum height for dense jets, for different $\theta - \phi$ combinations (dynamic environment).

- Dilution at the impact point is greatly underestimated by all the models in all cases presented in this work, with deviations ranging between 50 and 65%. In this regard, JetLag reaches the best agreement.

CORMIX1 has been observed to provide the same results as CORJET when no impact with the surface is detected. However, in some cases, important discrepancies are obtained in the flow classification. For example, for $\theta=30^\circ, 45^\circ$ and $F_{rd}=30, 40$ and for $\theta=60^\circ$ and $F_{rd}=40$, CORMIX1 classifies an unstable near field and flux mixing over the full layer depth, while experimental tests show a jet behavior.

5.2. Dynamic environment

CORJET, UM3, and JetLag integrated models have been validated in the present work with the experimental data shown in Table 6, considering the Roberts

and Toms [17] formulas. Table 5 shows the input data for commercial model validation:

For the input values shown on Table 6, CORJET, UM3, and JetLag commercial models have been used, obtaining the numerical results at the specific points and comparing them with the experimental solutions.

Fig. 7 shows the predictions of adimensionalised terminal rise height for different $U_r F_{rd}$ values.

As can be seen in Fig. 7, the commercial models in general follow the trend, decreasing the rise height with the crossflow speed. However, rise height in most cases is significantly underestimated, especially in cases of transverse current ($\phi=90^\circ$) affecting to a 60° inclined jet. CORJET seems to be the model which gives a better agreement, but results of all models are quite similar.

Fig. 8 shows the predictions of dimensionless dilution at the maximum height point for different $U_r F_{rd}$ values.

Fig. 9 shows the predictions of adimensionalised dilution at the return point for different $U_r F_{rd}$ values.

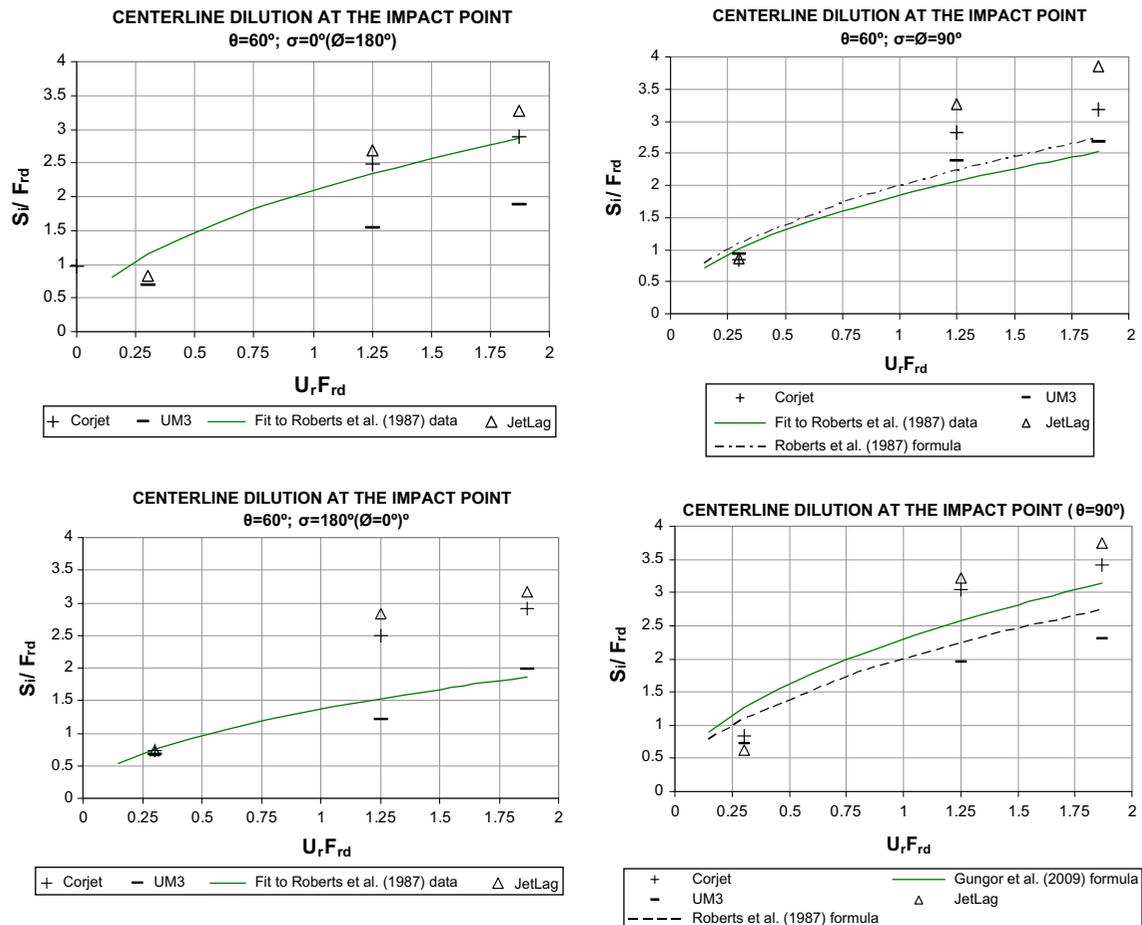


Fig. 9. Validation of centerline dilution at the return point for dense jets, for different $\theta - \phi$ combinations (dynamic environment).

As can be seen in the graphics, commercial models follow the trend of increasing dilution with the crossflow speed but in general significantly underestimate this magnitude, especially in the case of co-flowing. JetLag is the commercial model which better agrees this magnitude.

As can be seen in the graphs, commercial models follow the trend of increasing dilution with the crossflow speed but in general overestimate the value of this magnitude, especially for larger crossflow speeds. UM3 provides in this case the best agreement, while JetLag the poorest.

5.3. Summarizing table

Table 7 [14] summarizes the estimated deviations from the selected experiments made by the commercial models when modeling a brine dense jet discharged into a stagnant and dynamic environment. Best agreement is indicated in gray.

5.4. Conclusions

Three of the most notable commercial tools for brine discharge modeling have been analyzed in detail in order to obtain a better knowledge of the theoretical basis and the use of the tools applied by the promoters and environmental authorities. Validation of the models for different cases, including stagnant and dynamic environments, has also been carried out in the present work to obtain conclusions regarding the feasibility of the models in brine discharge modeling.

The following conclusions and recommendations [14,26] for the use of commercial tools for brine discharge modeling are derived from this manuscript:

- For single-port jet discharges, the use of integrated models, such as CORJET, UM3, and JetLag is recommended. An alternative is the use of the length scale formulas calibrated and validated in the literature, with experimental data for hyperdense

Table 7

Summary table of commercial tools validation [14]. Estimated errors for brine dense jet modelling

Estimated errors made by commercial tools when modeling brine discharges										
Stagnant ambient	Variable	$\theta = 30^\circ$ inclined jet			$\theta = 45^\circ$ inclined jet			$\theta = 60^\circ$ inclined jet		
		Corjet	UM3	JetLag	Corjet	UM3	JetLag	Corjet	UM3	JetLag
	Z_t	~10%↓	~25%↓	0%	~10%↓	~20%↓	~20%↓	~15%↓	~30%↓	~25%↓
	S_i	~60%↓			~60%↓	~60%↓	~50%↓	~60%↓	~60%↓	~50%↓
	X_r	~15%↓	~25%↓	~15%↓	~10%↓	~25%↓	~10%↓	~15%↓	~25%↓	~10%↓
All variables are underestimated by the commercial models, especially dilution rates										
Dynamic ambient 60° inclined jet	Variable	Coflowing case $\theta = 60^\circ, \phi = 180^\circ$			Counter-flowing case $\theta = 60^\circ, \phi = 0^\circ$			Transverse current case $\theta = 60^\circ, \phi = 90^\circ$		
		Corjet	UM3	JetLag	Corjet	UM3	JetLag	Corjet	UM3	JetLag
	Z_i	~25%↓	~30%↓	~30%↓	10%↑– 5%↓	~5%↓– 15%↓	~5%↓– 20%↓	~30%↓	~40%↓	~40%↓
	S_i	15%↓– 1%↑	~30%↓	30%↓– 15%↑	2%↓– 60%↑	10%↓– 10%↑	5%↓– 70%↑	25%↓– 25%↑	15%↓– 2%↓	20%↓– 45%↑
For values $U_r F_{rd} > 0.75$, commercial models tend to overestimate variables, especially dilution at the impact point and jets opposing the crossflow										

Notes: ↓: underestimation; ↑: overestimation.

Table 8

MEDVSA online modeling tools

Discharge configuration	“MEDVSA” tool	Scope of the modeling	Mathematical approach	BASE code
Single port submerged jet discharge	MEDVSA-IJETG	From the nozzle to the impact point with the bottom	Models based on the integration of the differential equations	CORJET [24]
Multi-port submerged jets discharge (including jets merging)	MEDVSA-MJETS			CORJET [25]
Single port submerged jet discharge (inclined 60°)	MEDVSA-JET-SPREADING	From the nozzle to the end of the near field region (including jet path and spreading layer)	Dimensional analysis	Roberts et al. [6]
Single port submerged jet discharge (inclined 60°)	MEDVSA-JET-PLUME2D	From the nozzle to the far field region (jet path, spreading layer and plume)	Dimensional analysis and integration of differential equations	Roberts et al. [6] and García [27]

inclined jets; however, these formulas only characterize geometry and dilution at specific control points.

- Models based on the integration of differential equations are not recommended for initial discharge angles (relative to the bottom) over 75° and under 30°, since re-entrainment and COANDA phenomena, respectively, are not taken into account.

For a *stagnant ambient*, validation carried out in the present work shows that CORJET, UM3, and JetLag

models underestimate jet dimensions in all cases. With respect to dilution at the impact point, all models significantly underestimate the values.

For a *dynamic environment*:

- 60° inclined jet perpendicular to the crossflow (transverse): dilution models at the rise height are underestimated by commercial models. Dilution at the impact point is in general overestimated by commercial models, with best agreement for the UM3 model.

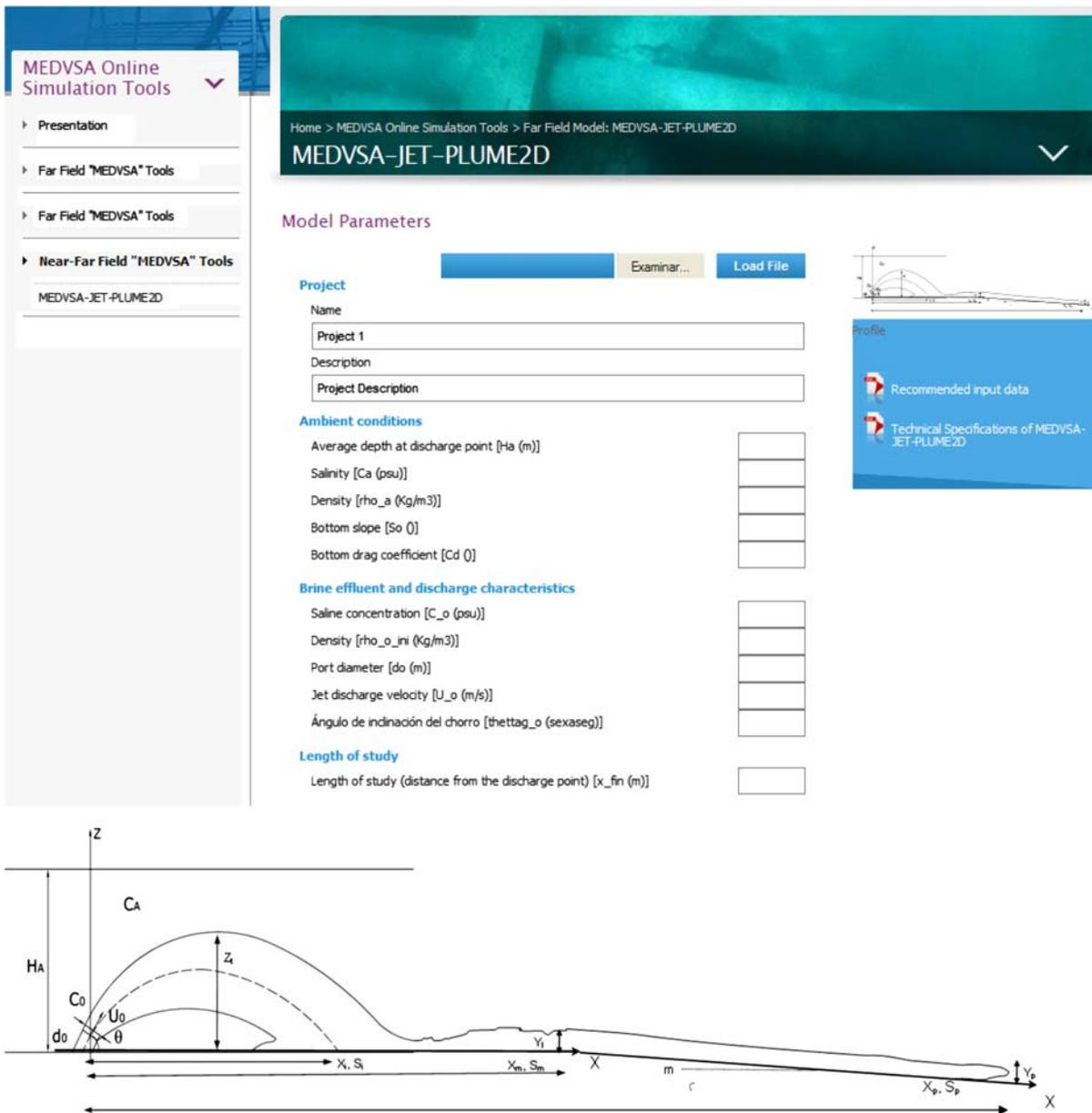


Fig. 10. Interface of the model MEDVSA-JET-PLUME2D and scheme of the jet path, spreading layer and hypersaline plume modeled.

- Vertical jets: dilution at the maximum rise height is underestimated by commercial models, with the best agreement for JetLag and the poorest for UM3 model. Dilution at the impact point is underestimated by UM3 while it is underestimated for CORJET and JetLag for lower $U_r F_{rd}$ values but overestimated for higher $U_r F_{rd}$ values. The best estimation for this magnitude is achieved by CORJET. Regarding maximum rise height, commercial models underestimate the value in all cases.

6. MEDVSA online simulation tools

MEDVSA online simulation tools have been programmed, in MATLAB language, in order to have freely accessible online tools, with codes similar to those of the most reliable commercial software for brine discharge modeling, while optimizing the interface and results report. MEDVSA models have been validated with experimental data published in scientific magazines and are now being re-calibrated with new experimental data, based on LIF-PIV techniques, developed within the framework of the MEDVSA project [28].

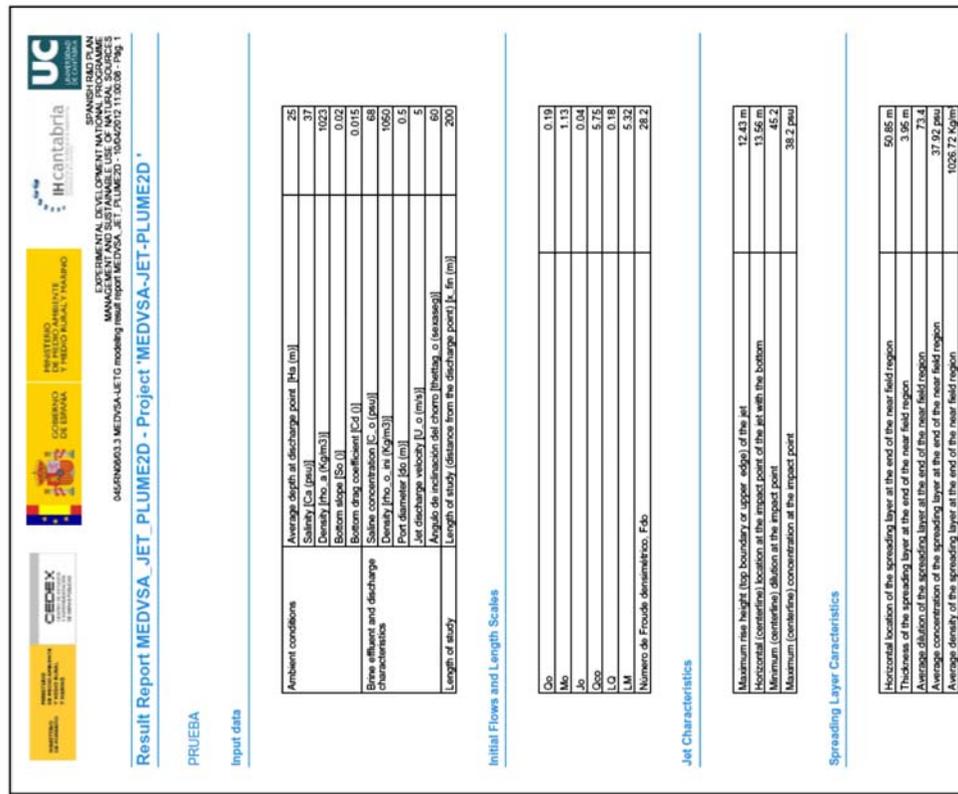
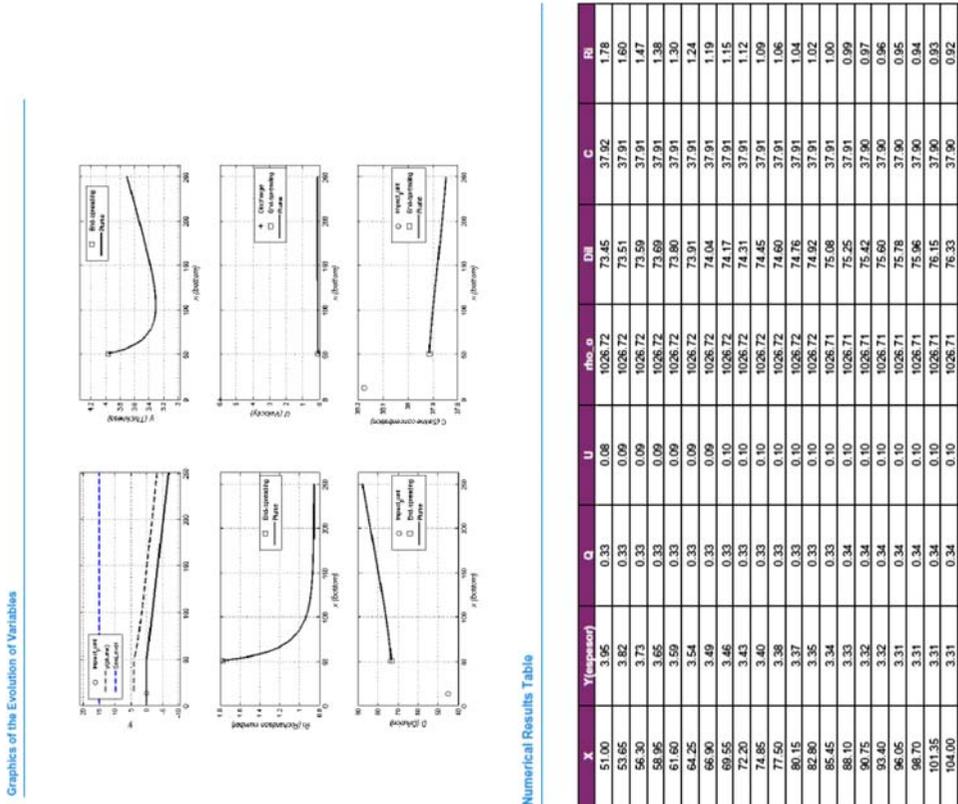


Fig. 11. Result report obtained from the MEDVSA-JET-PLUME2D online run.



MEDVSA models can run online from the website and provide a report with analytic and graphic data results as well as file with rough data. Every model includes the following information:

- Summary table of the model *Technical Specifications*.
- Table of *recommended input data values* for the model, focusing on brine discharge design.
- *Validation report* (against experimental data), including the approximate error made for the tool for the case modeled.

MEDVSA tools include different models for the near and far field regions, all of them available online.

6.1. Near field “MEDVSA” tools

The near field region is located in the vicinity of the discharge point and is characterized by initial mixing, which mainly depends on the brine discharge configuration design, and the effluent and ambient properties. Higher dilution rates are reached at the near field, due to the turbulence effects created by the shear layer because of the differences in velocity between the jet and the ambient body. Flow and mixing characteristics are dominated by small scales (\sim meters and \sim minutes). Normally, the brine discharge system is designed to maximize dilution in the near field region. Among others, the most common discharge systems are: submerged single and multiport jets and direct surface discharges.

The design of the discharge system determines the degree of brine dilution in the near field region, where density differences (between brine and seawater) and momentum (depending on the discharge system) control the geometry and mixing processes of the brine effluent. This dilution influences the salinity of the gravity current in the far field region and, consequently increases the risk of impact on benthic communities located far from the discharge point.

MEDVSA models programmed for near field brine discharge modelling are summarized in Table 8. Every model includes technical specifications and recommended input data values.

The graphics and results report have been optimized with respect to those of the commercial models and a table of realistic and recommended values for the initial data of brine discharge has been included.

The results report includes the kinematic fluxes and length scale values and the jet characteristics (dimensions and dilution) are indicated for some specific control points (maximum rise height, bottom

impingement point, etc.). The graphic and analytical evolution of the variables characterizing the jet (x , y , z trajectory, velocity, vertical angle, concentration, dilution, etc.) are also obtained from the model.

The models and the information are now available and can be run online in the project website www.medvsa.es, in Spanish and English.

As an example, Figs. 10 and 11 show the interface and results report of the MEDVSA-JET-PLUME2d online model.

7. Future lines of research

The following research lines have been proposed and will be developed in the future:

- *Validation* of the MEDVSA online simulation tools with experimental data carried out with optical techniques PIV (Particle image Velocimetry) and LIF (Laser Induced Fluorescence). Calculation of the numerical error with respect to the experimental results for each case.
- *Re-calibration* of the MEDVSA tools to obtain a better agreement with the experimental results.
- *Development* of new MEDVSA tools, for different discharge configurations, including the modeling of the near field and the far field region, and stagnant and dynamic environment.

Acknowledgments

The commercial software analysis and the validation of the numerical results were developed within the framework of the R&D project MEDVSA: A Methodology for the design of brine discharges into the seawater [28].

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