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SIMSAFADIM-CLASTIC: A new approach to mathematical 3D forward simulation modelling for terrigenous and carbonate marine sedimentation

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ABSTRACT

Most sedimentary modelling programs developed in recent years focus on either terrigenous or carbonate marine sedimentation. Nevertheless, only a few programs have attempted to consider mixed terrigenous-carbonate sedimentation, and most of these are two-dimensional, which is a major restriction since geological processes take place in 3D. This paper presents the basic concepts of a new 3D mathematical forward simulation model for clastic sediments, which was developed from SIMSAFADIM, a previous 3D carbonate sedimentation model. The new extended model, SIMSAFADIM-CLASTIC, simulates processes of autochthonous marine carbonate production and accumulation, together with clastic transport and sedimentation in three dimensions of both carbonate and terrigenous sediments. Other models and modelling strategies may also provide realistic and efficient tools for prediction of stratigraphic architecture and facies distribution of sedimentary deposits. However, SIMSAFADIM-CLASTIC becomes an innovative model that attempts to simulate different sediment types using a process-based approach, therefore being a useful tool for 3D prediction of stratigraphic architecture and facies distribution in sedimentary basins. This model is applied to the neogene Vallès-Penedès half-graben (western Mediterranean, NE Spain) to show the capacity of the program when applied to a realistic geologic situation involving interactions between terrigenous clastics and carbonate sediments.

KEYWORDS **Forward modelling. Process-based. Diffusion. Advection. Sediment transport. Mixed terrigenous-carbonate sedimentation.**

INTRODUCTION

The advent of computers and computerised methods has led to the prediction of both sedimentary facies distribution and the geometric architecture of sedimentary basins by process-oriented numerical models, thus becoming an important tool in geological studies (Harbaugh and Bonham-Carter, 1970; Allen, 1978; Bitzer and Harbaugh, 1987; Hardy and Gawthorpe, 1998; Haupt et al., 1999; Bitzer and Salas, 2002). Computer-based simulation models predict the spatial distribution of physical, chemical and petrophysical characteristics within sedimentary deposits.

Various sedimentary modelling programs have been developed. Most of them consider either terrigenous clastics (Tetzlaff and Harbaugh, 1989; Lawrence et al., 1990; Martínez and Harbaugh, 1994; Flemings and Grotzinger, 1996a; Flemings et al., 1996b; Hardy and Gawthorpe, 1998) or marine carbonate sediments (Read et al., 1986; Goldhammer et al., 1987; Bosence and Waltham, 1990; Bice, 1991). Few models consider mixed carbonate-terrigenous sedimentation. Moreover, most of these programs work in two-dimensional space (Komar, 1973; Bridge and Leeder, 1979; Strobel et al., 1989; Bitzer and Harbaugh, 1987; Hardy et al., 1994; Bitzer, 1999; Syvitski and Hutton, 2001), a fact that is a major restriction since geologic processes take place in three-dimensional space and result in a great variety of sedimentary facies types with complex three-dimensional architecture. Lithological heterogeneity within sedimentary basins is better represented by three-dimensional models such as SIMSAFADIM (Bitzer and Salas, 2001, 2002), which is a 3D process-based simulation model, or CARBONATE 3D (Warrlich et al., 2002), a 3D "rule-based" model. Furthermore, the interaction between different types of sediments, such as terrigenous clastics and carbonate materials, needs to be represented in an integrated multiprocess model.

The three-dimensional mathematical forward simulation model for clastic sediment types presented here represents an extension to the three-dimensional carbonate sedimentation model, SIMSAFADIM, developed by Bitzer and Salas (2001, 2002). This new extended model called SIMSAFADIM-CLASTIC (Gratacós, 2004) simulates terrigenous sediment transport and sedimentation coupled with processes of carbonate production, transport and sedimentation in three dimensions. It is important to emphasise that SIMSAFADIM-CLASTIC is a process-based simulation model which attempts to simulate the physical processes that govern transport and sedimentation.

THE SIMSAFADIM-CLASTIC PROGRAM. CONCEPTUAL AND MATHEMATICAL MODEL

The main processes that are modelled by the program are fluid flow, transport and sedimentation (Fig. 1). The program can work with up to four different types of terrigenous sediments, including three siliciclastic grades and lithoclastic allochthonous carbonates. These clastic sediments are incorporated into the moving fluid, and they are transported and settle as a function of the corresponding fluid flow system.

Below, we describe the main characteristics of the conceptual and mathematical models used for different processes in the program (fluid flow, transport, and sedimentation, for both terrigenous and carbonate materials).

Fluid flow

The fluid flow model we use is identical to the model developed by Bitzer and Salas (2002) called SIMSAFADIM. This model assumes that:

- Flow can be considered as irrotational and the viscosity of water can be ignored;
- Variations of flow due to changes in density, temperature and salinity are negligible;
- The velocity of flow can be considered to be uniform over depth, leading to a 2D flow model;
- A 2D transient potential flow model can thus be applied (Equ. 1).

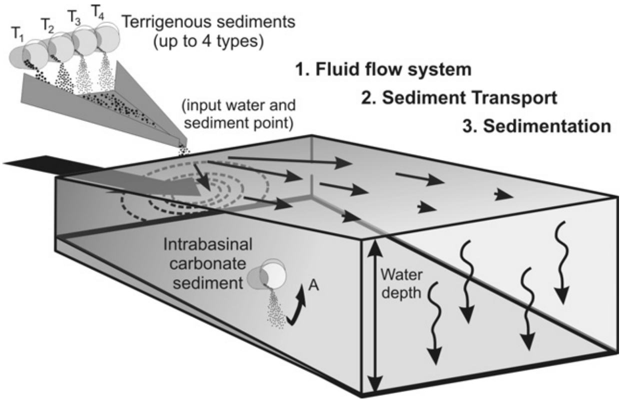

FIGURE 1 | **Simplified conceptual sketch of the principal processes incorporated into the SIMSAFADIM-CLASTIC program. Notice the program accepts up to four types of terrigenous extrabasinal sediment (one of them consisting of carbonate lithoclasts), which are added to the clastic carbonates that result from the reworking of the carbonates generated in the basin (A). The program also incorporates the interaction between the whole clastics (terrigenous sediments and reworked intrabasinal carbonate sediments) and the carbonate producing organisms. T_1-T_3: Silicilastic sediments. T_4: Lithoclastic carbonates.**

$$\frac{\delta}{\delta x}\left(\frac{\delta h}{\delta x}\right)+\frac{\delta}{\delta y}\left(\frac{\delta h}{\delta y}\right)=\frac{\delta h}{\delta t}+q \qquad (1)$$

where h is the potential head [L]; t is time [T]; q is a source fluid term [L^3/T]; and x and y are spatial coordinates [L].

Transport and sedimentation

To model the transport of clastic sediments, the following assumptions are made:

- All sediment particles are transported in suspension and suspended sediment is uniformly distributed within the water column (Fig. 2).
- Sediment is transported by diffusion, dispersion, and advection (Equ. 2),

$$\underbrace{\left[D^*\left(\frac{\delta^2 C}{\delta x^2}+\frac{\delta^2 C}{\delta y^2}\right)\right]}_{\textbf{diffusive term}}+\underbrace{\left[\alpha_x\left(\frac{\delta^2 C}{\delta x^2}\right)+\alpha_y\left(\frac{\delta^2 C}{\delta y^2}\right)\right]}_{\textbf{dispersive term}}$$

$$-\underbrace{\left[v_x\left(\frac{\delta C}{\delta x}\right)+v_y\left(\frac{\delta C}{\delta y}\right)\right]}_{\textbf{advective term}}=\left(\frac{\delta C}{\delta t}\right) \qquad (2)$$

where D^* is the diffusion coefficient [L^2/T]; C is the sediment mass concentration [M]; v_x and v_y [L/T] are the average linear fluid flow velocities in the X- and Y- directions; α_x and α_y [L^2/T] are the mechanical coefficients of dispersion in the X- and Y- directions and are functions of the average linear velocity: $\alpha_x = d_x * v_x$ and $\alpha_y = d_y * v_y$ (where d_x and d_y are the dispersivity [L] in the X- and Y- directions).

With regard to sedimentation, the model assumes that:

- Sedimentation depends primarily on the settling velocity of particles (Equ. 3),

$$\frac{\delta C_{di}}{\delta t}=f_{di}C_i \qquad (3)$$

where f_{di} is a deposition factor which is a function of the theoretical settling velocity (or settling velocity in the absence of fluid flow), water depth, and a velocity factor (scaled between 0 and 1, and which depends on fluid flow velocity and the critical velocity for deposition; Bitzer and Salas, 2002); C_i is the mass of sediment i in the water column [M]; C_{di} is the thickness of sediment deposited [L]; i is the index of the clastic sediment; and t is time [T]. This relationship was previously established (Hjulstrøm, 1935; Vanoni, 1975) and considered by other authors (Bitzer and Salas, 2002).

- Settling velocity depends on particle size and the shear forces imposed by turbulent flow. As SIMSAFADIM-CLASTIC does not consider turbulent flow, the program assumes a linear correlation between settling velocity and flow velocity (Fig. 3).

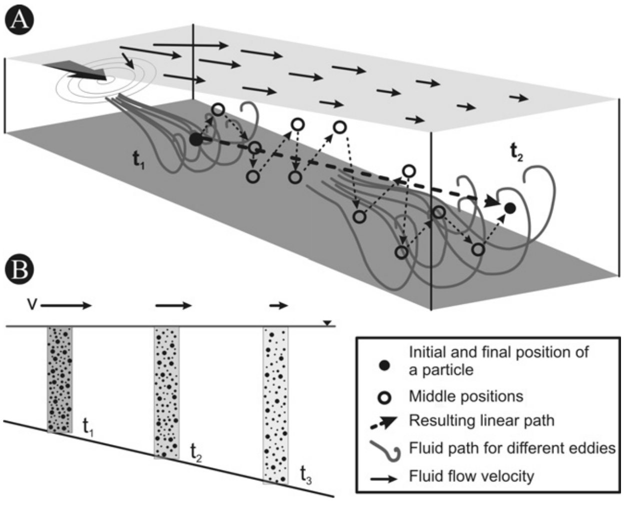

FIGURE 2 | **Conceptual model for sediment transport. A) Schematic diagram for transport of a particle in turbulent flow. The dashed arrow indicates the net transport for a particle between t_1 and t_2. B) Conceptual model of suspended sediment distribution in the water column. The sediment is homogeneously distributed within the water column due to turbulent flow. SIMSAFADIM-CLASTIC assumes that mixing processes distribute suspended particles homogeneously within the water column.**

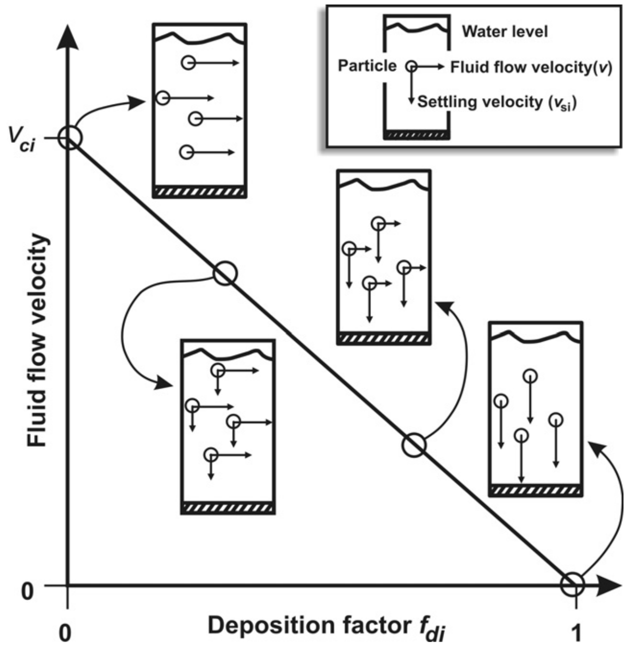

FIGURE 3 | **Relationship between deposition factor (f_{di}), theoretical settling velocity (v_{si}) and flow velocity (v). Note that settling velocity becomes zero as the flow velocity approaches critical deposition velocity (v_{ci}).**

- Small-scale transport and deposition processes (wave action, etc.) are considered to be diffusive and dispersive processes.

Carbonate sediments

As mentioned above, the model is able to consider up to four kinds of terrigenous clastics, i.e., three grades of siliciclastic sediments and a fraction of lithoclastic carbonates. This lithoclastic carbonate sediment may be added to a part of the previously deposited carbonates, which are reworked and redeposited. All these terrigenous and intrabasinal clastic sediments can interact with carbonate producing organisms. This part of the program is based on previous work by Bitzer (1999) and Bitzer and Salas (2001). Here, only the adapted equations are presented, for instance, the equation for the population density of carbonate-producing organisms (for species association 1 in this example) contemplates poisoning due to the presence of clastic sediments that may affect the carbonate producing organisms (Equ. 4).

$$\frac{\delta x_1}{\delta t} = \overbrace{\underbrace{a_1x_1 - b_1x_1^2}_{\text{Logistic growth}} - \underbrace{f_{12}x_1x_2 - f_{13}x_1x_3}_{\text{Competition or cooperation between species}} - \underbrace{g_1x_1x_5}_{\text{Influence of lime mud}} - j_{1C_4}x_1C_4}^{\text{Bitzer and Salas (2001)}}$$

$$\overbrace{- j_{1C_1}x_1C_1 - j_{1C_2}x_1C_2 - j_{1C_3}x_1C_3}^{\text{Present work}} \qquad (4)$$

Poisoning due to the presence of clastic-terrigenous (1,2 and 3) and clastic-carbonate sediments (4) in suspension

where J_{1C_1,C_2,C_3,C_4} is the poisoning factor from each clastic sediment type on specie association 1; $\boldsymbol{x_1}$ is the population of species 1; $\boldsymbol{C_{1,2,3,4}}$ are the mass concentrations of terrigenous and intrabasinal carbonate clastic sediments in suspension. We use the same indices and nomenclature as Bitzer and Salas (2001). The interaction between clastic sediments and carbonate producing organisms is based on the 2D model developed by Bitzer (1999) and extended to 3D in Bitzer and Salas (2001).

Solving the system equations

The transport-sedimentation equation

The flow equations are solved using a finite element model (Bitzer and Salas, 2002). The transport equation is solved for individual clastic sediment types using the same finite element scheme.

Initial and boundary conditions used to solve the equations for fluid flow are provided by: initial sea level; inflow and outflow rates; and fixed potential conditions. For the transport model, initial and boundary conditions are provided by fixed concentration nodes in the basin and sediment input rates.

Stability criteria

The sequential iteration approach (SIA) is used to solve the transport-sedimentation equation (Saaltink et al., 2000, 2004). Different stability criteria for spatial and temporal discretization are imposed to ensure the stability of the solution and to reduce numerical errors. Spatial criteria are imposed by the grid-Peclet number (Kinzelbach, 1986) and temporal stability is imposed by the Courant criteria (Steefel and MacQuarrie, 1996).

SAMPLE SIMULATION EXPERIMENT

In order to test the program, we performed an experiment involving the evolution of a carbonate depositional system interfered by the presence of terrigenous sedimentation, a situation that was comparable to a real geological situation. Our aim was to model the three-dimensional distribution of the different types of sediment (terrigenous and carbonate mixed deposits) that were deposited in the Vallès-Penedès basin (western Mediterranean, NE Spain) during a Langhian Middle Miocene depositional episode.

Geological setting

The Vallès-Penedès basin is a Neogene half-graben basin located within the central part of the Catalan coastal ranges (CCR, NE Spain, Fig. 4). This basin is oriented NE-SW, 10-14 km wide and up to 100 km long and is filled with more than 3500 m of continental to marine terrigenous deposits ranging from late Oligocene(?)-earliest Miocene to late Miocene (Fig. 5; Cabrera and Calvet, 1996; Roca et al., 1999; Bitzer, 2004; Cabrera et al., 2004; de Gibert and Robles, 2005). The half–graben is bounded on the NW by the SE–dipping ENE–WSW –trending Vallès–Penedès fault, which has a normal displacement of up to 4 km, and on the SE by a system of structural tilted highs (the Garraf-Montnegre horst).

The upper half of the sedimentary infill includes a complex transgressive-regressive Langhian sequence, which includes proximal to distal alluvial fan deposits, as well as shallow transitional (fan delta) and mixed terrigenous-carbonate marine deposits (terrigenous shelf and bay, and coralgal platform; Fig. 5). During deposition of these units, fault-related subsidence was mainly concentrated along the northwestern basin margin.

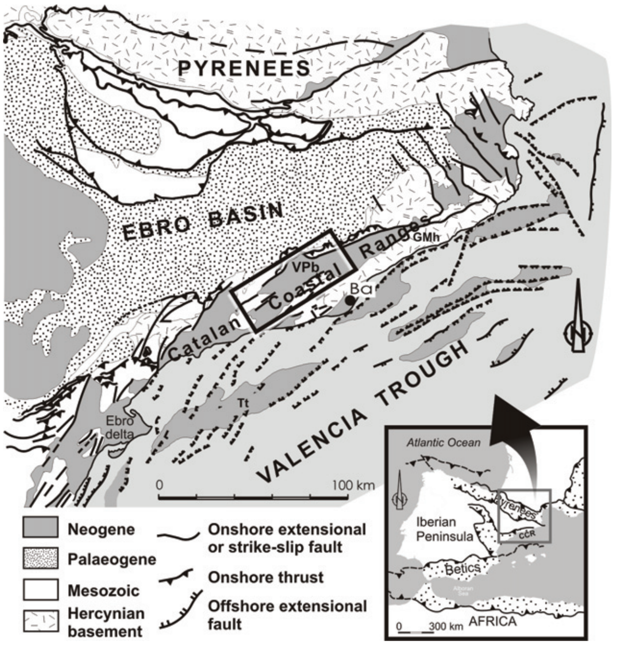

FIGURE 4 **Geographic and geological setting of the Vallès-Penedès basin (VPb, black rectangle) located in the central part of the Catalan coastal ranges (CCR, NE Spain). GMh: Garraf-Montnegre horst; Ba: Barcelona. Modified from Roca et al. (1999).**

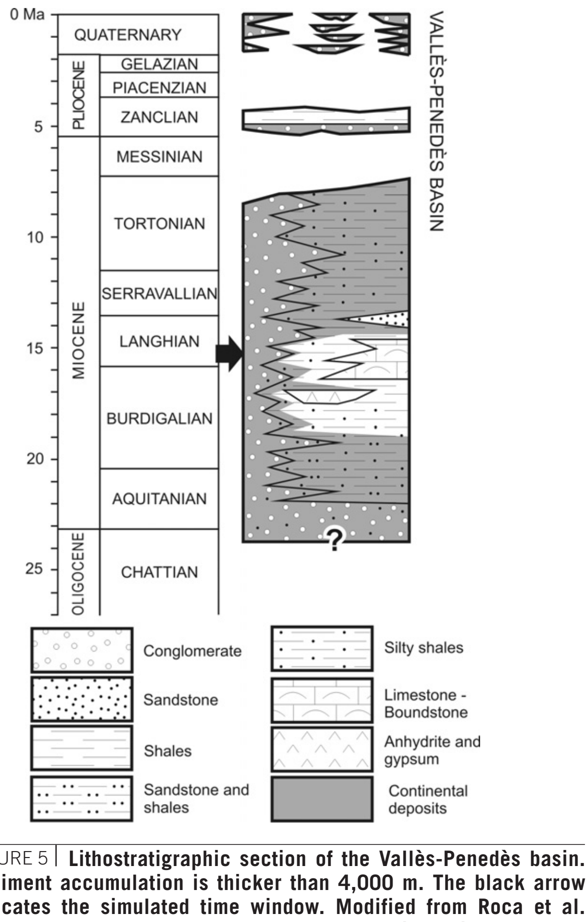

FIGURE 5 **Lithostratigraphic section of the Vallès-Penedès basin. Sediment accumulation is thicker than 4,000 m. The black arrow indicates the simulated time window. Modified from Roca et al. (1999) and Cabrera et al. (2004). Chronostratigraphic scale after Gradstein et al. (2004).**

Along the southeastern tilted basin margin the substratum was overlaid by the sedimentary units that prograded from the opposite margin and concealed formerly active southeastern margin faults (Cabrera and Calvet, 1996; Roca et al., 1999; Bitzer, 2004; Cabrera et al., 2004).

Specifically, during Langhian time (Fig. 6) a marine transgression gave rise to a complex mixed carbonate and terrigenous deposition pattern with the development of progradational terrigenous fan delta systems (which spread from the northwestern basin boundaries) and reefal build-ups that developed over the structural highs that fringed the southern basin areas (Permanyer, 1990; Cabrera and Calvet, 1996; Roca et al., 1999; Cabrera et al., 2004).

Initial configuration and parameters

The initial experimental set-up (Fig. 7) is defined by water depth, and the location of the alluvial inputs and of

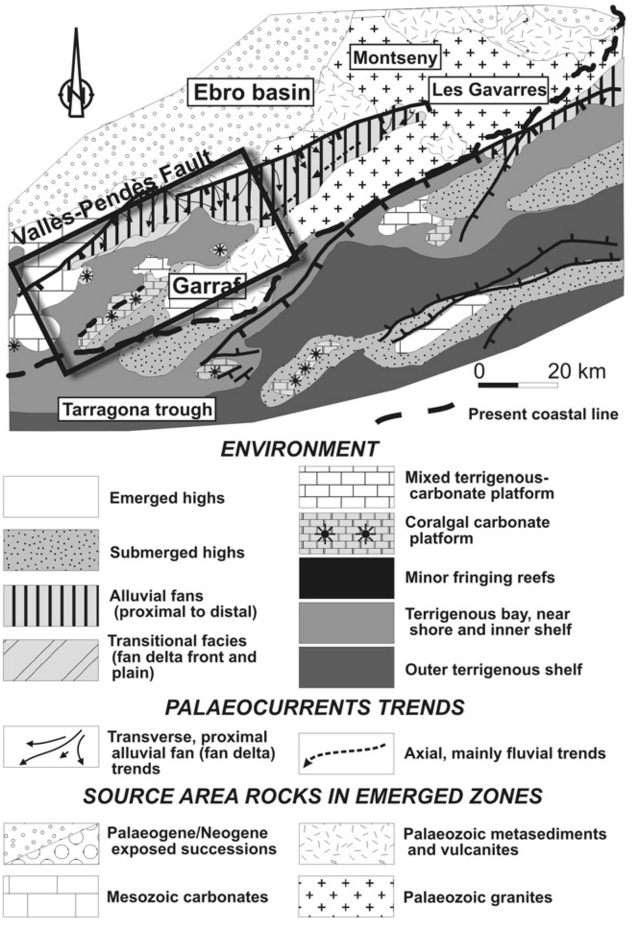

FIGURE 6 **Palaeogeographic sketch of the central part of the Catalan coastal ranges. The black rectangle indicates the area studied during early Langhian time (see also Fig. 7). Modified from Roca et al. (1999).**

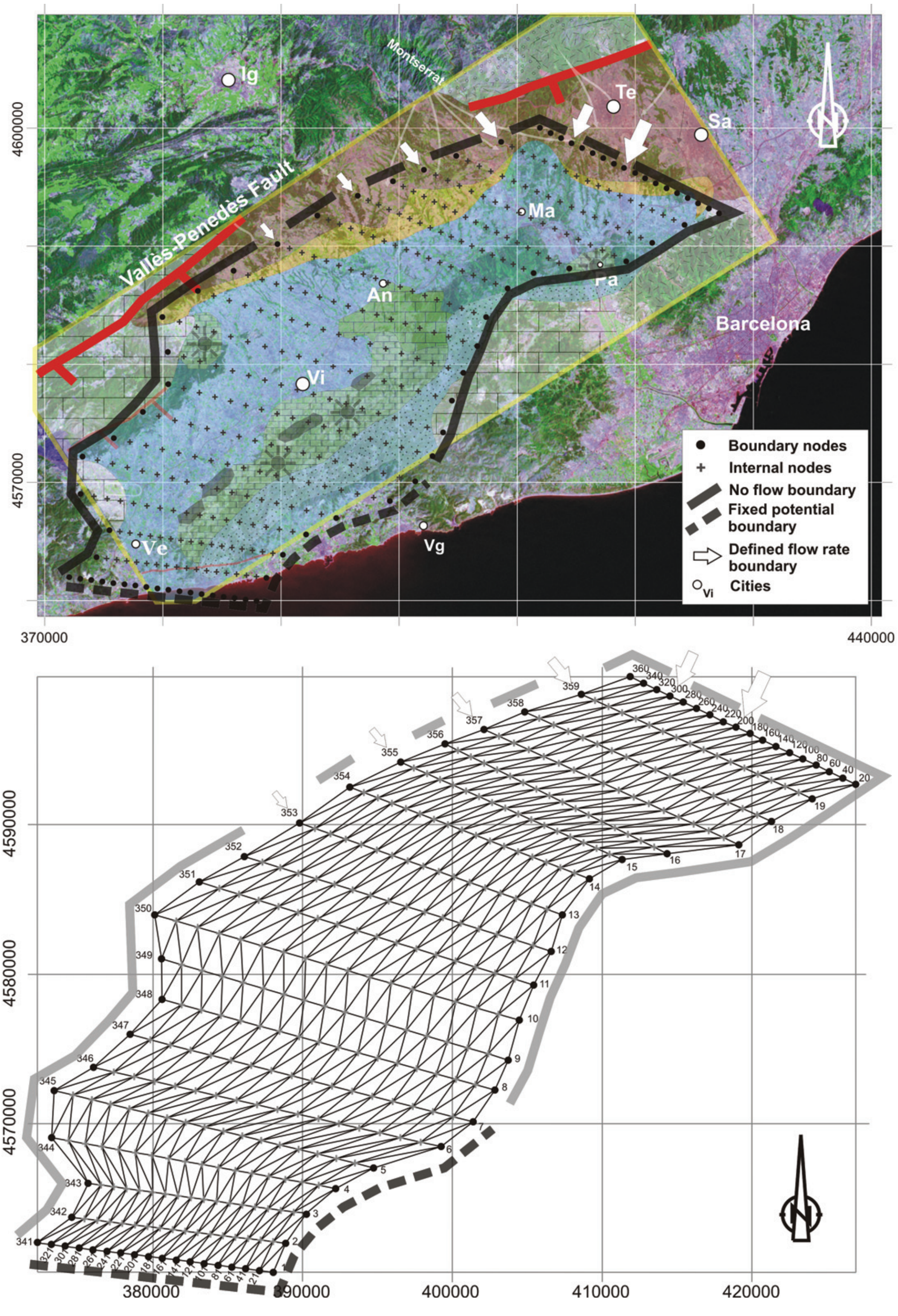

FIGURE 7 | **Spatial discretization of the studied area. The triangular elements of the finite mesh are represented in the lower part. The NW and NE boundaries are situated near the palaeocoastal line considering an HST situation. Arrow sizes indicate water and sediment volume supply. See legend of the geological data and location in Fig. 6. Localities: An. Sant Sadurní d'Anoia; Ig. Igualada; Ma. Martorell; Pa. El Papiol; Sa. Sabadell; Te. Terrassa; Ve. El Vendrell; Vi. Vilafranca; Vg. Vilanova i La Geltrú.**

TABLE 1 **Parameters introduced for the experiment defining sedimentation, transport and boundary conditions for the finite element mesh. The parameters defining the two associations of carbonate producing organisms considered are included.**

Terrigenous sediments

	Node	*Siliciclastic mud*	*Siliciclastic fine sand*	*Siliciclastic medium to coarse sand*	*Carbonate lithoclasts*
Inflowing sediment (Tn/s)	200	0.0042	0.0018	0.0015	Not considered
	300	0.0019	0.0012	0.00045	
	359	0.0002	0.0003	0.00039	
	357	0.00018	0.00028	0.00036	
	355	0.00016	0.00026	0.00034	
	353	0.00014	0.00015	0.00016	
Settling velocity (m/d)	-	0.026	0.049	0.067	0.03
Critical velocity for deposition (m/d)	-	8.25	20.35	70.5	25.25
Longitudinal dispersivity (m)	-	950	950	950	950
Transversal dispersivity (m)	-	950	950	950	950
Diffusion coefficients G_0 and G_1 (Kaufman et al., 1991)	-	10.09 0.1	6.87 0.1	6.87 0.1	6.87 0.1

Fluid flow

		Nodes
Inflowing water (m^3/s)	3.5	200
	2.8	300
	2.2	359
	2	357
	1.8	355
	1.6	353
Open Boundary	(fixed potential)	1, 2, 3, 4, 5, 6, 7, 21, 41, 61, 81, 101, 121, 141, 161, 181, 201, 221, 241

Carbonate parameters

	Type 1 carbonate producing organisms (ramp facies)	*Type 2 carbonate producing organisms (reefal facies)*
Birth	0.01	0.02
Death	0.01	0.02
Maximum depth (m)	55	30
Maximum production (m/y)	0.015	0.025
Poisoning due to carbonate mud	0.01	0.02
Poisoning due to clastic sediments (for each clastic sediment type)	0.06 0.09 0.11 0.03	0.09 0.11 0.21 0.04
Mud production	0.008	0.006

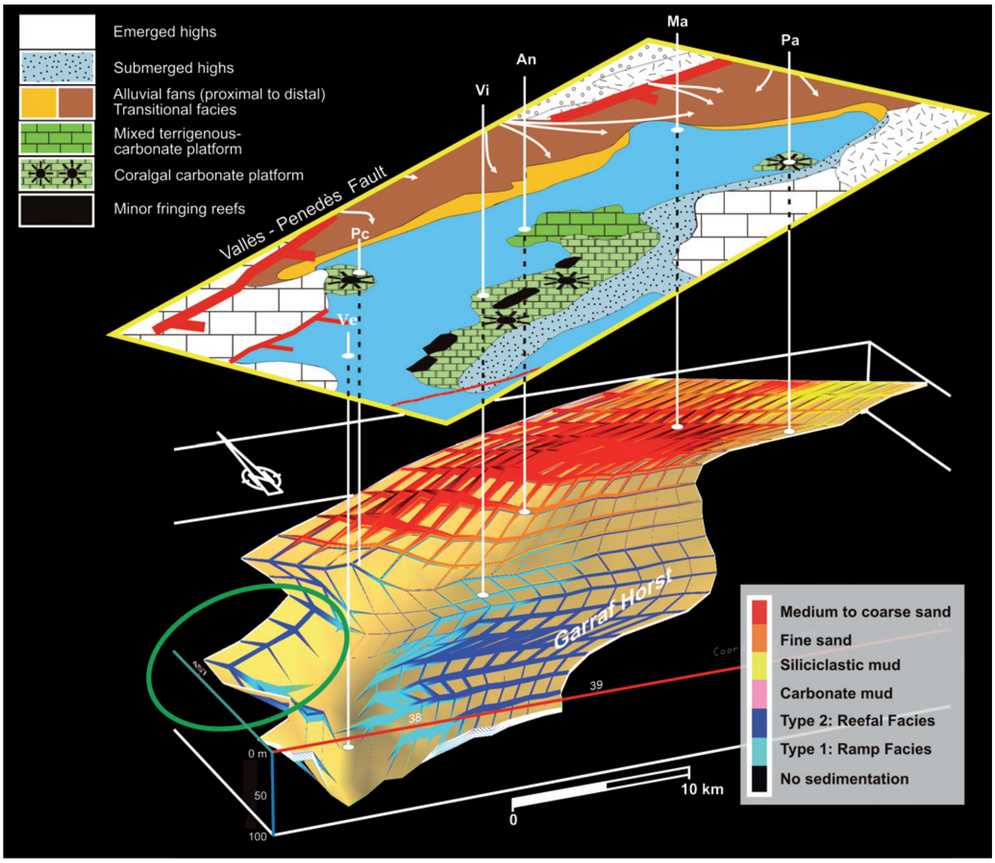

FIGURE 8 **Comparison of the results obtained with the SIMSAFADIM-CLASTIC program (lower part) and the palaeogeography established for early Langhian time. Notice that the modelled and the real basins are similar. Discrepancy only occurs in the SW area where carbonate sedimentation predicted by the model (green circle) is not observed in the field. This could be related to steep slopes caused by fault activity that did not provide a stable substrate for organism growth. Organisms association Type 1: ramp facies association (molluscs, algae, bryozoans, isolated hermatypic corals); Organisms association Type 2: reefal facies association (hermatypic coral reefs). Vertical exaggeration 100x. Localities: An. Sant Sadurní d'Anoia; Ma. Martorell; Pa. El Papiol; Pc. Pacs del Penedès; Ve. El Vendrell; Vi. Vilafranca.**

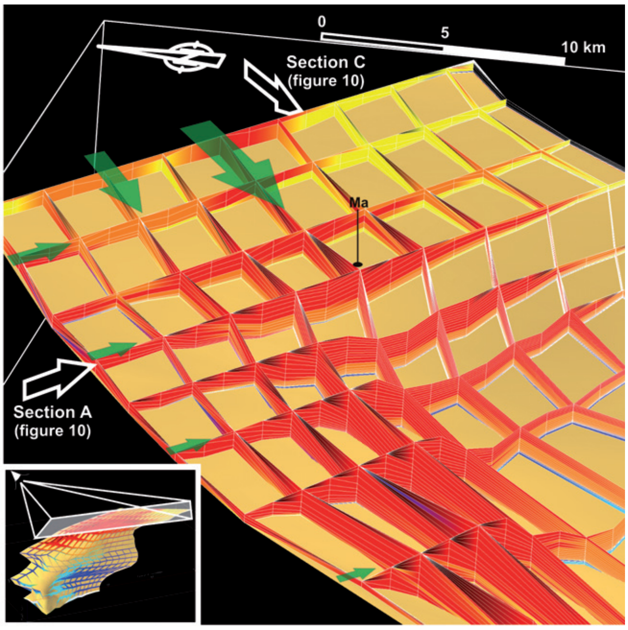

FIGURE 9 **Close-up view of the Northern basin region (see location in the lower image) characterized by terrigenous clastic fan-delta systems. Note the basinward progradation of these systems (green arrow) and the architectural complexity of the interfingered deposits resulting from the interaction between the different systems. Terrigenous clastic sediments overlaying previous carbonate deposits occur. See colour coded legend in Fig. 8. Vertical exaggeration 100x.**

the open sea boundary. Active alluvial axes are defined by a fixed inflow rate, and the open basin boundary by fixed potential. Discretization for the finite element scheme involves 18 columns and 20 rows; a total of 360 nodes that define 646 elements. Transport and mesh boundary conditions and sedimentation parameters are given in Table 1.

For the sake of simplicity, despite the overall varied depositional setting that resulted in the basin as a consequence of the Langhian transgression, in this sample experiment it was assumed a maximum sea level highstand situation, with negligible level oscillations. The time established for the simulation of this highstand stage was 20,000 years and it was split into 1,000 years time steps.

Three grades of siliciclastic sediment were introduced in the program to develop the sample experiment. Moreover, on the basis of sedimentological analysis of the carbonate dominated facies (Permanyer, 1990) two main types of carbonate producing organism associations were defined for this experiment: ramp facies association (type 1) with molluscs, algae, bryozoans and isolated hermatypic coral reefs; and reefal facies association (type 2) built up mainly by hermatypic corals.

Simulation Results

The facies distribution resulting from the Vallès-Penedès simulation experiment (Fig. 8) is similar to the distribution observed for the mixed terrigenous/carbonate Langhian successions. In the model, terrigenous sediments occur mostly in the NW area along the Vallès-Penedès fault, which bounds the main source area for the terrigenous sediments. Fan delta systems (in red and yellow) are restricted to the north and display a basinward progradational pattern. Reefal constructions (blue) dominate in the southern basin zones are also shown.

The fan delta successions in proximal basin zones are built up mainly by coarse-medium sand sediments (red) and grain size becomes finer basinward. The location of several source areas and the progradation of the related fan delta systems generate a complex pattern of facies interfingering (Figs. 9 and 10).

Carbonate sediments are deposited along the structural highs (the Garraf horst). Figure 11A is a detailed image of this southern zone. The basinward progradational architecture (blue arrow) of the mainly reefal deposits (type 2 association of carbonate producing organisms) can be observed. Deep down, this reefal facies assemblage becomes a ramp facies (type 1 association of carbonate producing organisms; Fig. 10). Field outcrops that show similar progradational architecture patterns have been reported in the Vallès-Penedès basin by Permanyer (1990; Fig. 11B). These progradational carbonates thin towards the NE where the proportion of terrigenous sediments increases (green arrow). These sediments prograded from NE to SE and overlaid the previously deposited carbonate sediments (see a more detailed view in Fig. 10, section C).

Simulation results do not match field data in the SW area (green circle, Fig. 8) where the model predicts carbonate sedimentation. This could be related to steep slopes caused by fault activity which do not provide a stable substrate for the growth of sessile carbonate producers.

Another simulation shows the simulated facies distribution and sedimentary architecture in the supposed absence of terrigenous sediment input (Fig. 12). This second experiment used the same parameters as the first one, except for the amount of terrigenous sediments entering the basin in the northern zones. The resulting carbonate distribution is similar to the previous one and shows a carbonate sediment zonation that depends on water depth and also a basinward progradational pattern. In this experiment, carbonates deposited in the NE basin zones are not affected by the impingement of clastic sediments.

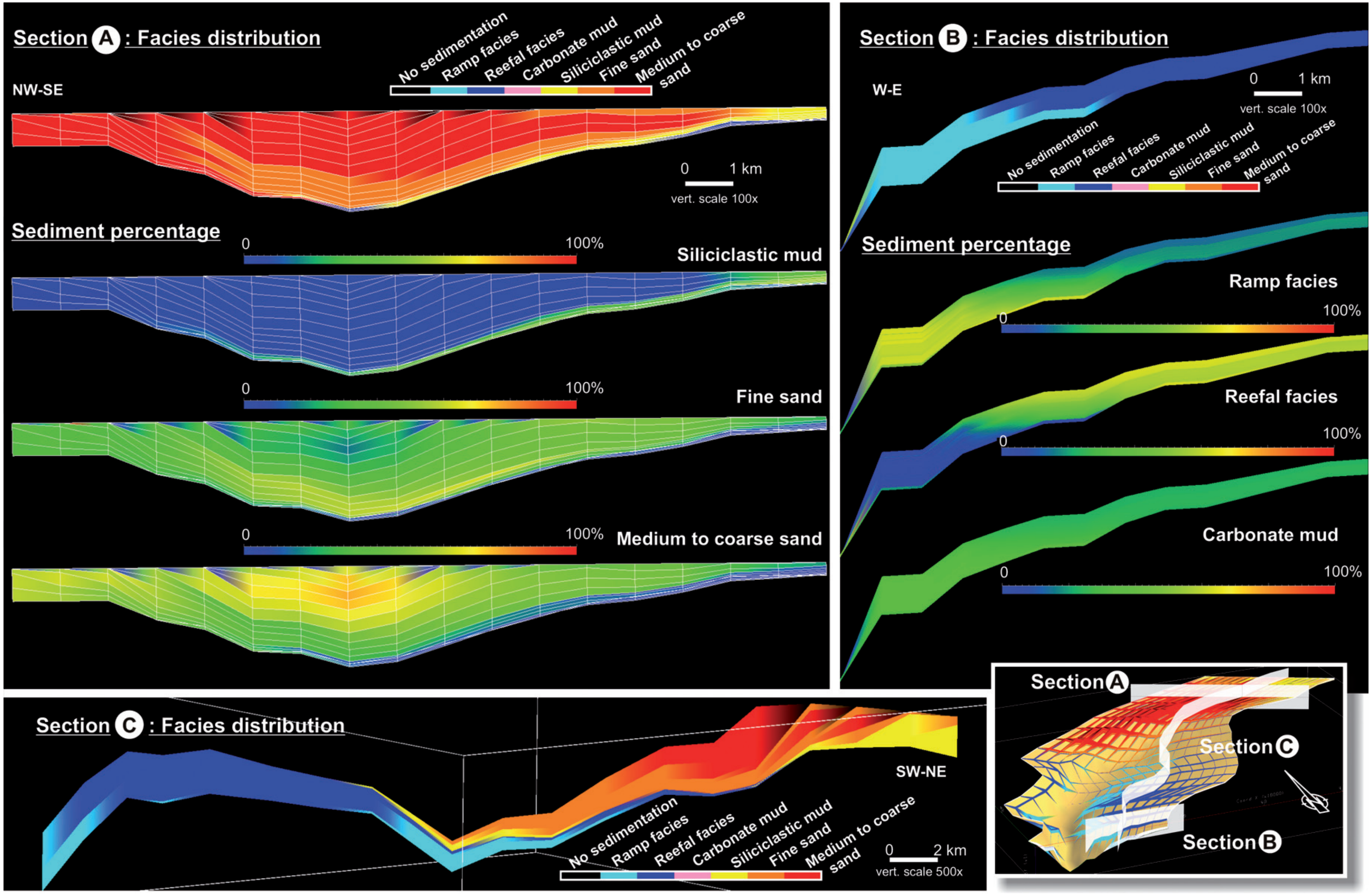

FIGURE 10 | **Detailed sections characterized A) by major terrigenous sediments and B) by carbonate deposits show the facies distribution and sediment percentages for each sediment type. Longitudinal section C) shows the sedimentary architecture as well as the interfingering between clastic and carbonate deposits. The complexity of facies distributions in section A) can be explained by the location of source areas and the progradation of the related fan-delta systems. Note the westward progradation (basinward) and the facies zonation along section B). See location in the lower right image and in Figs. 9 and 11.**

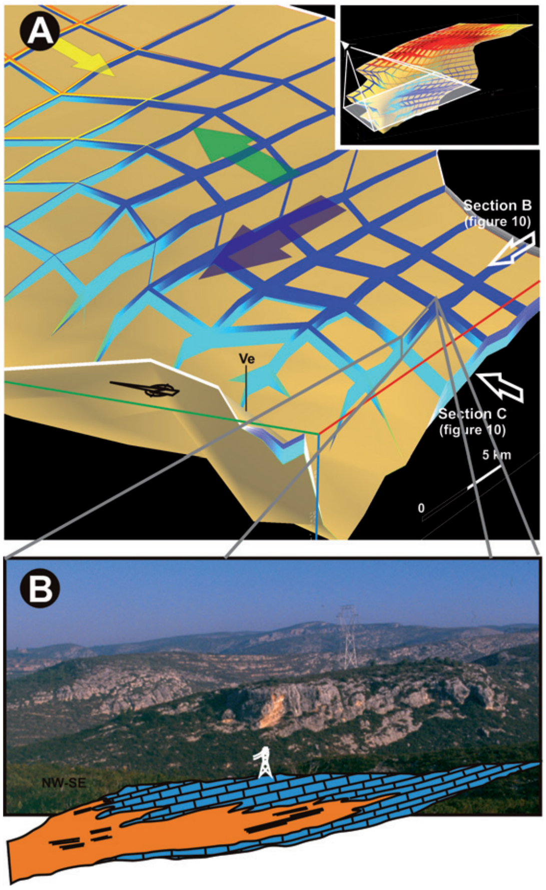

FIGURE 11 **A) Close-up view of the Southern basin region (see location in the upper right image) characterized by reef build-up. Note the basinward progradation of the carbonate platform. Carbonate thickness decreases towards the NE (violet arrows) while terrigenous clastic sediment percentage increases (yellow arrow). Vertical exaggeration 100x. B) Outcrop example near Castellet and scheme of the architecture patterns defined in reefal facies in the Vallès-Penedès basin. See colour coded legend in Fig. 8. Modified from Permanyer (1990).**

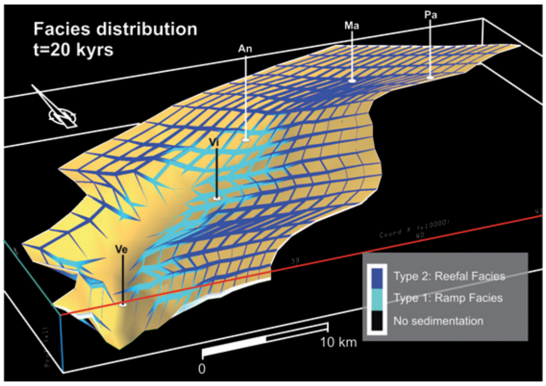

FIGURE 12 **Fence diagram with facies distribution on time step 020 (20,000 yr) for the experiment related to the Vallès-Penedès basin considering only carbonate sedimentation in the basin. Notice the dominance of only two facies corresponding to two kinds of associations of carbonate producing organisms. No terrigenous sediments are considered to influence the evolution of the carbonate systems. Vertical exaggeration 100x. See legend and abbreviations of localities in Fig. 8.**

CONCLUSIONS

The principle feature in SIMSAFADIM-CLASTIC is its capacity to represent the interaction between carbonate and clastic terrigenous sediments using a process-based numerical approximation. This leads to simulated facies distributions that are highly complex in geometry and facies patterns.

The results of the Vallès-Penedès simulation experiment show facies distributions and depositional architecture which are similar to patterns observed in the field. The poisoning effect of terrigenous sediments on carbonate producing organisms may explain the observed distribution of reefal deposits.

In spite of the good match for the example presented here, the model has several limitations:

- In its current form, the model does not include substratum erosion, which in some cases may be a very a significant sedimentary process in marine environments.

- Simulation of flow is reduced to a 2D potential flow, which is a major simplification, and tidal and wave action are excluded.

- The simulation of carbonate sedimentation using a predator-prey model might oversimplify the real interactions between carbonate producing species. Therefore, further parameters like brightness, nutrients or salinity should be included in the future in order to increase the predictive capabilities of the model.

In spite of these simplifications, computation time is considerable due to the stability criteria imposed by the numerical methods, which force the program to proceed in simulation steps of the order of days (or less).

Summing up, SIMSAFADIM-CLASTIC is a powerful process-based simulation code for 3D prediction of stratigraphic architecture and facies distribution in sedimentary basins. It may thus be applied to petroleum exploration including fluid flow modelling at the basin scale and prediction of petrophysical parameters.

Other modelling strategies may provide realistic and efficient tools for prediction of facies distribution and depositional architecture, nevertheless, SIMSAFADIM-CLASTIC is an innovative program which simulates different sedimentation types on the basis of a process-based model.

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