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TESI DI LAUREA MAGISTRALE IN
GEOLOGIA E GEOLOGIA TECNICA

INFLUENCE OF RELATIVE SEA-LEVEL VARIATIONS ON VEGETAL-RELATED ORGANIC MATTER DISTRIBUTION WITHIN ALLUVIAL ENVIRONMENTS: A NUMERICAL MODELLING APPROACH

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1. Abstract

DionisosFlow is a numerical stratigraphic model which predicts the facies distribution in response to a given basin history. Recently, a new R&D project dedicated to organic-rich facies in DionisosFlow was created. The aim is to reproduce the main organic matter depositional environments. This work presents the first results associated to the terrestrial organic matter module. First a literature review is proposed to fix the context and the objective to achieve. Then, the methodology of the model is presented. Finally, several case-studies are used to enlighten the behaviour of the model.

2. Introduction

This work has been developed as part of an industrial project named Dionisos-Organic-Rich-Sediment (DORS), funded by REPSOL, TOTAL, ENGIE, ENI and CHEVRON. The overall objective is to provide an appraisal of source rock characteristics based on a quantitative estimation of the TOC_0 (total organic carbon) / HI (hydrogen index) properties. The proposed methodology consists in an evaluation of the organic matter production and preservation on marine, lacustrine and terrestrial environments. The aims of this project are to contribute to the development of the terrestrial organic matter module (TOM) on DionisosFlow. In particular, this work was mainly focused on in-situ TOM accumulation. It means that all the processes controlling the exported TOM in a marine realm are beyond the scope of this study. To achieve this goal, a literature review was first conducted. Several possible conceptual models have been discussed. Finally, this report presents the most adapted model, illustrated by different synthetic case studies, including 2D and 3D simulations. The main steps of this work are briefly described below.

2.1 Contexts and objectives

Peat is a predominantly organic material deposit derived from decayed plants in certain types of ecosystem associated to wetland conditions. Indeed, water-saturated ground and flooding events decrease the decomposition rate by minimizing the contact between oxygen and the in-situ preserved organic matters. This specific condition allows a positive balance of organic material accumulation (Moore, 1989). When a sufficient amount of peat is accumulated the area is called "Peatland" (at least 30cm, following the definition of Bozkurt, 2000). In the end "Peat" is sedentary accumulated material consisting of at least 30% of dead organic matter (Hans Joosten, 2002). The in-situ organic matter accumulation is the main difference between peat and other terrestrial sedimentary bodies bearing organic matter like pollen and planktonic material. However, it is current to observe a mixture between allochtonous and autochtonous materials in a peatland (Pakarinen, 1984; Succow and Stegmann, 2001).

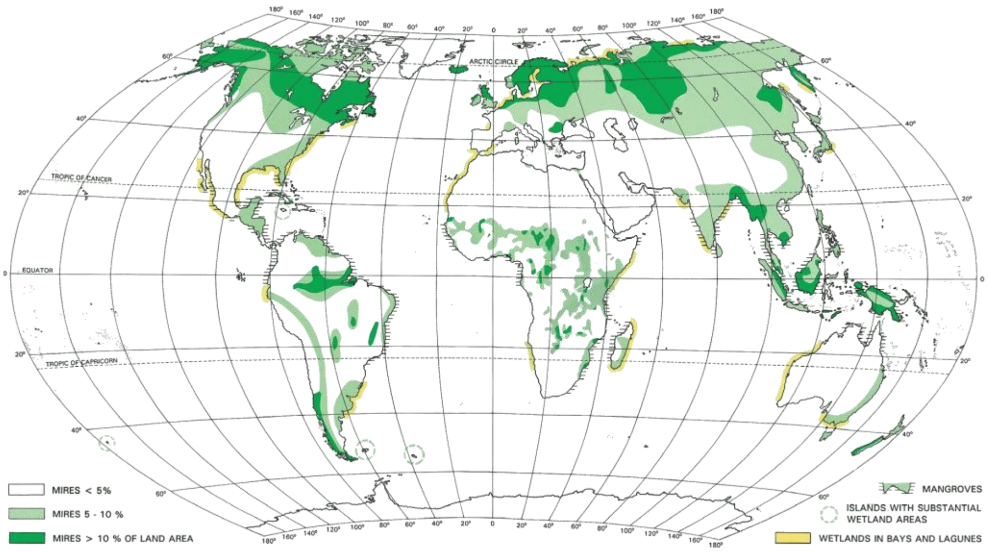

Figure 1 Distribution of mires. Extent and location of global mires and peatlands, from Lapaillanen, 1996

The worldwide mires location does not show a strong control of the climatic ring (Figure 1). This observation can be explained by the impact of the temperature on the peatland system. In one hand, a low temperature favours the preservation but prevent high peat production rate. On the other hand, high temperature increases the degradation rate but favours high peat production rates. In term of net accumulation however, it seems that warm and humid climates are the more optimal conditions. Recent studies in areas where peat is currently being produced show a range of values roughly between 0.1 and 7 mm/y with an average value of 1.5 mm/y (Diessel, 1994, Bohacs, 1997). However, a few sites show a peak of peat production rate 13 mm/y (Neuzil, 1997).

Two main types of peat can be identified depending on the hydrological conditions. The first peat-class is associated with an ombotrophic context, which means that the vegetation receives its water and nutrients mainly from rain-fall. The second category refers to the rheotrophic mires, i.e. all peatland that are deeply attached to the groundwater flow (Figure 2). If the ombotrophic mires are directly link the evaporation-precipitation regimes, the rheotrophic mires are link to the nature of the ground and to the topography. From stratigraphic modelling point of view, it means that the distribution of the ombotrophic mires are directly linked to climatic conditions, which are user-imposed, whereas the distribution of the rheotrophic mires are coupled to the dynamic of sediment transport, which is more a result of the simulation. For this reason, the main objective of our work was to build and evaluate a methodology including the rheotrophic mires accumulation during the history filling of a sedimentary basin. This method relied on a new groundwater flow module that is currently included in the IFPEN stratigraphic model (DionisosFlow) as a prototype.

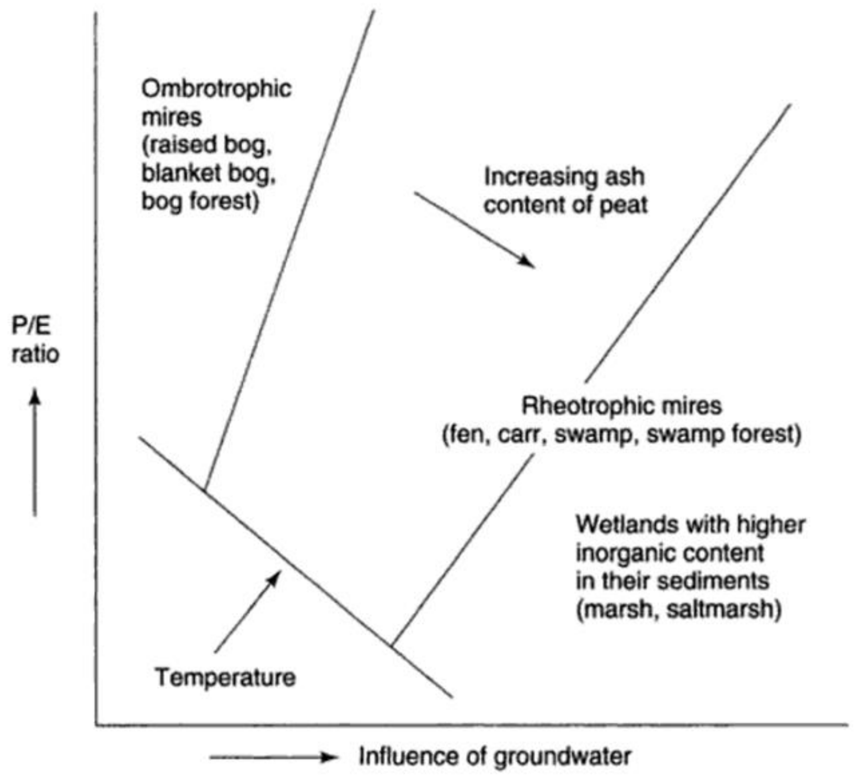

Figure 2 Regime diagram illustrating the main differences between the ombotrophic and the rheotrophic mires (Moore, 1987)

Our purpose is not to model the peat production but more the accumulation of coals resulting from the preserved peats. Coal is currently defined as a rock which contains at least 50 percent of terrestrial organic material by weight.

Coalification (Figure 3) is the process during which TOM undergoes several chemical and physical changes due to anaerobic bacteria, heat, compaction and time (adapted from AGI's "Glossary of Geology"). The peat-to-coal transition is commonly assumed to be accompanied by compaction that decreases the thickness of the organic deposit to values of 10% or less of the original peat thickness (Nadon, 1998).

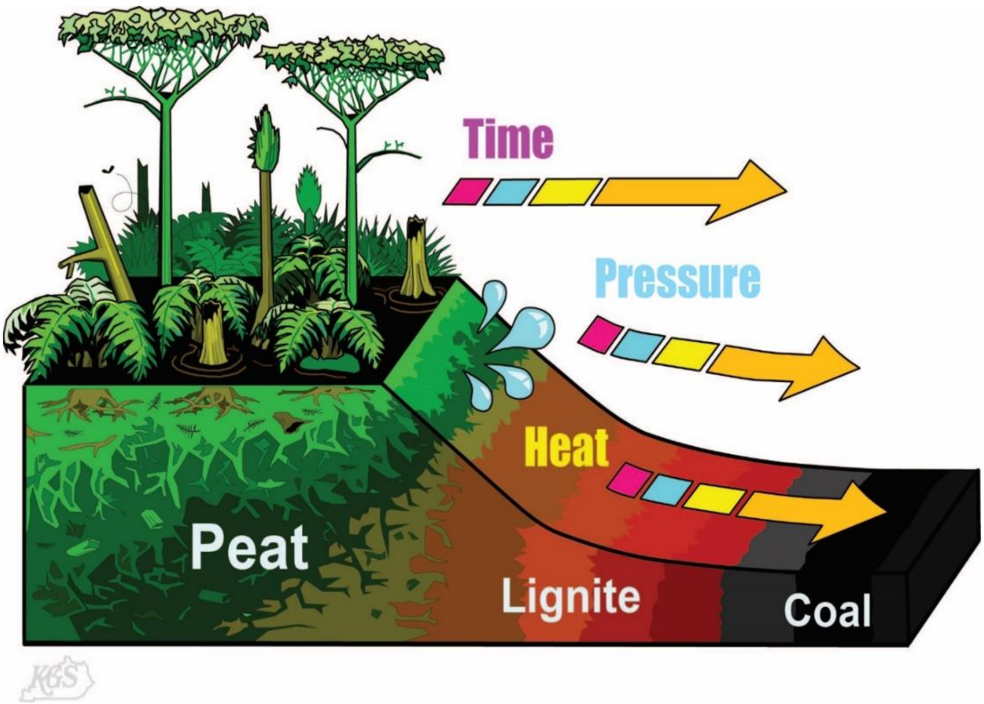

Figure 3 Peat-to-coal process due to time, pressure and heat. Stephen Greb, Kentucky Geological Survey, University of Kentucky.

The development and the validation of a terrestrial organic matter module were done in part in the scope of this work. This project can be decomposed in four phases:

I. Selection of a conceptual model for the simulation of the TOM in-situ accumulation. As the module was not ready at the starting point, the first objective for the student (D. Carraro) was to closely interact with the numerical developer (B. Chauveau) to select the most appropriate methodology.

II. Calibration of the model under several different simple accommodation regimes. Calibration done with 2D synthetic models.

III. Calibration of the model under several more complex different accommodation regimes. Calibration done with 2D synthetic models.

IV. Building of 3D stratigraphic models.

3. Peat Production & Accumulation

3.1 Introduction

The accumulation of terrigenous coaly organic-rich rocks depends on the production and preservation of terrigenous organic matter from freshwater and land plants (Bohacs, 1997). Non-saline wetlands in which peat accumulates are called mires (McCabe, 1992; Joosten, 2002; Moore, 1989) and the organic-rich deposits, founded in these areas, are named peats (Bohacs, 1997; Moore, 1989; Joosten, 2002).Variation in sedimentation and accommodation space, vegetation, peat-forming type at the surface and hydrologic properties of the site (groundwater level, sea-level fluctuations and the water quality itself) are interconnected and peat-to-coal processes are firmly subordinated to these factors (Joosten, 2002; Bohacs, 1997, McCabe, 1992). The so called mires end up with a positive carbon balance because plant production exceeds the organic decay, thus a carbon surplus is accumulated as peat (Joosten, 2002). Peat preservation (and the following conversion into coal) leans on a relatively rapid burial and anoxic condition (Bless 1989). Coal seams are found in a great number of different environments, from alluvial fans to lagoons (Wadsworth, 2010; Wang, 2010; Holz, 2002).

3.2 Structure and Classification

Analysis of peat structure revealed the presence of four distinct layers, mainly controlled by the water table (Clymo, 1992):

- the euphotic layer, at the top, where photosynthetic plants live.
- the aerobic layer, up to 50cm from the top, contains most of the dead material. Aerobic decay is the controlling processes.
- the collapse layer, 10cm below the aerobic one, is characterized by an increase of the bulk density. Hydraulic conductivity is drastically reduced.

- the lower peat layer, up to several meters, is characterized by anoxic conditions.

A simplification could be made taking into account just the water table position: the vadose zone, above the ground water table, is called acrotelm whereas the anaerobic layer is named catotelm (Clymo, 1992; Bozkurt, 2000). Peatlands are also described according with their placement on top of the topography: bogs or rising-mires, elevated above the surrounding landscape and fens, or low-lying mires, situated into depression. (Joosen, 2002; Flint, 1995)

3.3 Major Control Factors …

In order to obtain a deposit of terrigenous organic-rich rocks, a balance between peat production and accommodation rate must be achieved (McCabe 1992, Bohacs, 1997, Wust, 2007). Here below, the major control factors to enhance peat accumulation and preservation are listed: organic matter production versus degradation, clastic sediment input, ground water table dynamics and subsidence rate (Wust, 2007; Holz, 2002; Koster, 2000; Bohacs, 1997). From the literature review, the conditions allowing terrestrial organic matter accumulation can be discussed in terms of accommodation regimes or in terms of physical processes.

… from considerations based on the accommodation space

The accommodation space is related to the principle of base level. However, the definition of this theoretical surface is still a subject of to debate. Moreover, its definition depends first on the studied geological object. In the case of peat, it is now well accepted that the base level and the piezometric surface can be represented by the same surface. When the piezometric surface is below the ground surface, no space is available for peat accumulation as preservation conditions are very poor. When the piezometric surface is at or above the ground surface, conditions for peat preservation are optimal. Several previous studies reported the main geological factors that will act on the relative location of the piezometric surface in comparison with the topography. These factors are the subsidence, the eustatic variation, the inorganic sediment supply and the rainfall/evaporation ratio (Moore, 1989; Bohacs, 1997; Davies, 2004; Joosten, 2002; Wadswoth, 2010; McCabe, 1992; Flint, 1995; Diessel 2007). In affecting the relative location of a surface compared to the other, it modifies the accommodation space.

A large part of the accommodation space created is located in the paralic zone (Freeze, 1979; deMarsily 1986; Wadswoth, 2010). First because the sea level variation impacts mainly the piezometric surface at proximity to the shoreline, but also because the sea level fall creates fluvial incision. These incise valleys, depending on the magnitude of the base level negative fluctuation, are up to 100m and tens kilometers wide (Van Wagoner, 1990). Thus, these areas are an adapt environments to thrive and initiate mires growth as at the bottom of the valley the vadose zone is usually narrower (Staub, 1994; Aitken, 1995; Bohacs, 1997). The extent of the paralic zone is itself deeply linked to the topography. In paralic settings, the vadose zone thickness is controlled by the sea level and by the ratio between precipitation and evaporation (Freeze, 1979; deMarsily 1986; Wadswoth, 2010). Furthermore, a flat topography can favour a paralic zone spreading over more than 150 km inland (Wadsworth, 2010).

The subsidence (tectonic or thermic) is the second control factor of the accommodation rate and it's mainly dependent from the basin type, plate-tectonic setting, loading and compaction processes (Pigott, 1993). As base level is moving faster than the subsidence rate, Bohacs and Suter (1997) describe it as the main long term control of accommodation in non-marine settings. However, subsidence is not constant through time and it varies depending on the type of basin considered. Strike and slip basins are characterized by a high subsidence rate and peat production cannot keep up with such a huge subsidence rate. Passive margins show a slow subsidence rate which is easily overcome by processes like sea level fluctuation, river avulsion and climate changes: these mechanisms are much more rapid and effective in this particular setting, preventing TOM accumulation. In foreland basins, instead, subsidence rates closely match rates of peat production.

Indeed, these types of basins are the optimal site for coal accumulation (McCabe 1992, McCabe 1991).

As stated by Bohacs and Suter (1997) when the increase of accommodation is greater than the peat production rate, mires can be either inundated by clastic debris or drowned by the sea. Conversely if the accommodation is much less than the peat production, organic matter is more likely to be exposed and eroded by migrating channel and oxidized. Changes in composition and pattern of peat accumulation are due to variation in accommodation creation and peat production in a narrow "coal window", Figure 4 (Bohacs, 1997; Davies, 2005).

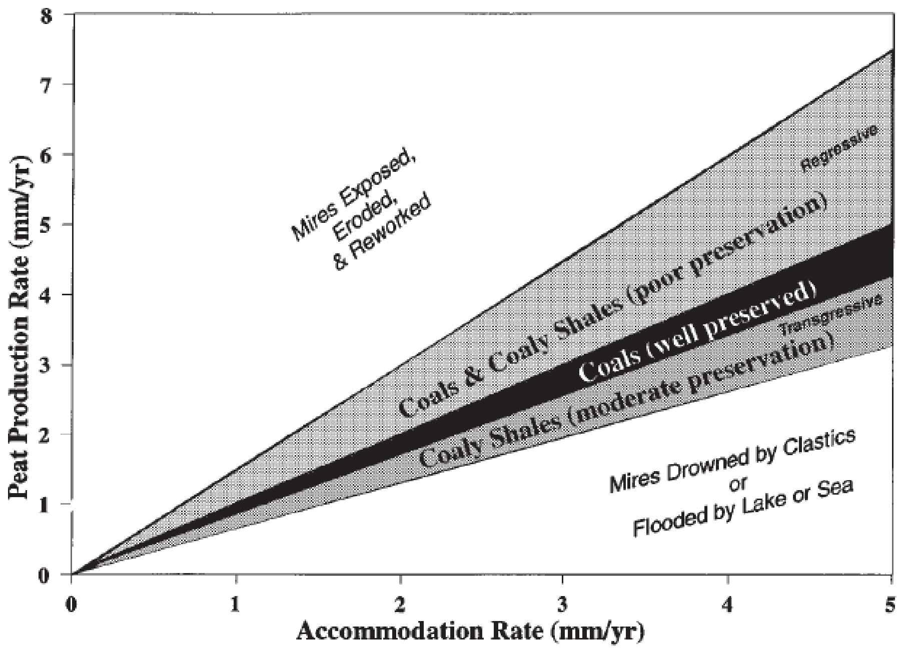

Figure 4 Peat accumulation regimes in relation with the accommodation rate (from Bohacs and Suter, 1997)

…from identified physical processes

Having a representation of the areas allowing peat (and then coal) accumulation from base-level consideration implies to work with the theoretical piezometric surface. Another approach would consist in using the water table as the starting point for peat accumulation. This description will be useful for building a numerical model based on the groundwater flow mode dedicated to free aquifer as the main result is a water table and not a piezometric surface.

The water table, defined as the top-surface of the free aquifer, is always below or at the ground surface. Its presence next to the surface is fundamental for peat deposit to be preserved and turned into coal (Diessel, 1992). By definition, the catotelm is always below the water table, thus saturated by water (Ingram, 1984; Bozkurt, 2000, Clymo, 1992). Such a waterlogged area is in a perdurable anoxic state and it is required in order to have organic matter preservation as oxygen cannot move freely in this condition and biogenic activities are inhibited or strongly slow down (McCabe, 1992; Bohacs, 1997; Bozkurt, 2000). Furthermore, an organic rich environment is easily under anoxic condition because the oxygen resupply cannot keep up with the oxygen request by the organic decay processes (McCabe, 1992). Moreover, low pH, induced by organic molecules breakdown, inhibits organic decay and supports coal accumulation (Teichmuller, 1982; McCabe, 1992; Wust, 2007).

The important factor for understanding the peat accumulation with the water table is also the dynamic of the groundwater flow and thus the evolution through time of this water table. If peat production can start when the vadose zone is narrow (i.e. the water table is closed to the ground surface), the production will be maintained only if the water table follows the topography modification due to peat accumulation. When peat growth is overcome by the rise of the groundwater table, mires are drowned and peat production stops; in the other hand, largely above the groundwater table, peat production is inhibited by oxidation and erosion. (Bohacs, 1997; Banarjee, 1996).

Water table fluctuations are directly impacted by climate (Beerbower, 1984; Flint, 1995.McCabe, 1992, Cecil, 2003). First because the sea level variations are controlled by the temperature fluctuation at global scale (McCabe, 1992). This effect has indirect consequence on the extension of the paralic zones. Precipitation/evaporation plays also a major role as it contributes to modulate the quantity of water inflow in the groundwater system (Booth, 2009; Bohacs, 1997; Wust, 2007; Bozkurt, 2000; Hans Joosten, 2002 and McCabe, 1992). Climate also controls the rate of peat production and preservation. Generally speaking, cold settings help organic matter preservation; conversely the peat production is greatly reduced by high latitude temperature (Wust, 2007). Thus it is clear that the prediction of the peat accumulation zone is a complex objective. Moreover, the climatic effects are modulated through time as it is affected by astronomical cycles. Milankovitch theory describes in detail all the collective variations affecting climate due to earth movements: eccentricity, axial tilt, and precession of the Earth's orbit fluctuate periodically with period respectively of 100kys, 26kys and 22kys (Tuenter 1975, Jansson 2002, Clement, 1999). Talking about peat production, one of the major effect of Milankovitch cycles is the seasonal cycle of solar radiations (Kutzbach, 1985; Clement, 1999). Climate also affects organic matter preservation/decay rates, flora composition, evapotranspiration, rainfall and thus the sediment flux (Beerbower, 1984; Flint, 1995.McCabe, 1992, Cecil, 2003). Clastic sediment supply represents another important control factor on peat accumulation as it can either provide nutrients supply necessary to the peat to grow or dilute the organic matter and obliterate the vegetation (Boachs, 1997; McCabe, 1992). Considering organic production ability to fill the available space intended for inorganic sediments, clastic sediments and peat compete for the same accommodation space, specifically, a high clastic supply reduce the available space for TOM sedimentation (Bohacs and Suter, 1997). As stated by Schumm (1997), sediment flux is related with the total amount of precipitation per year, hence it’s deeply connected with the climate. Interaction between mires and sediments is also influenced by the mire-type itself: low lying mire is easily flooded by a clastic influx and such type of mires must be excluded as a potential peat formation site; in the other hand, rising mire type, in force of its height, can accumulate low-ash peat deposits even in areas characterized by active deltas and rivers (McCabe, 1992; McCabe, 1989; McCabe, 1984; Bohacs, 1992, Diessel, 1992). Indeed, low inorganic matter content of rising mires prove their capability of self-exclude clastic material (Flint, 1995).

4. Coal Stratigraphy

In this section, factors previously described like peat production, climatic fluctuation, tectonic and eustasy oscillation are used to describe coal deposits location within a stratigraphic framework. Additionally, the relation between regressive-transgressive shoreline cycles and coal formation is emphasized. As a matter of fact, many authors have recognized a sort of pattern in coal seams shape and distribution mainly linked with sea level – base level fluctuation (Flint, 1995; Bohacs, 1997; Davies, 2005; Wust, 2007 among the others). A new stratigraphic model and thus justification of coal formation, introduced during the 1990s, expresses a new concept to explain coal framework into a depositional sequence: the most important variable in coal accumulation is not the total amount of accommodation but instead the rate of change in accommodation (Holz, 2002; Diessel, 1992). The same concept has been reiterated by Bohacs (1997), illustrating different peat – coal seams geometry and thickness all along a sedimentary cycle, from low to high and from high to low accommodation rate, Figure 5. The author expected a symmetrical couplet of coal layer in thickness and geometry, as a matter of fact, mires should respond to the rate of change and not to the direction of the change itself. In the further detailed description of a coaly-rock formation, the keys controls factors remain accommodation rate and peat production rate, assuming that an active clastic depositional system is able to full fill any residual accommodation space (Cross, 1988; Bohacs, 1997; Holz, 2002).

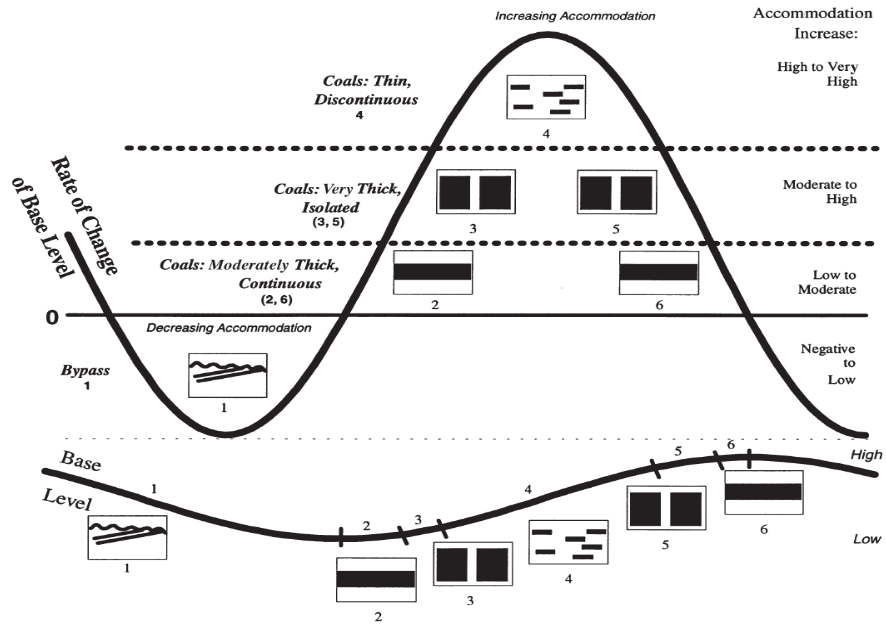

Figure 5 Relation of rate of change of base level to coal thickness and geometry for a given peat production rate, from Bohacs and Suter, 1997

4.1 Coal Seams Within A Stratigraphic Framework

Thanks to this chart (Bohacs, 1997), it is easy to see how, throughout the sea level fluctuations, mires / coal accumulation responds to the rate of these changes (Bohacs, 1997; Holz, 2002):

1. Late Highstand / Falling Stage / Early Lowstand System Tract - The strong retrograding movement of the sea level does not allow organic matter preservation. Therefore, the sedimentary surface is interested by oxidation, subaerial exposure and erosion. Bypass surface might develop. Fluvial channels try to reach the base level, hence extensive erosive phenomena (e.g. incise valley) take place due to fluvial erosion. Strictly speaking, a sequence boundary is now forming. Figure 6A.

2. Middle to Late Lowstand System Tract – In this tract, the sea level fall gently slows down, it standstills and eventually it starts to rise.

Peat production is now able to match it. Thin widespread continuous coal layers are here produced. Figure 6B.

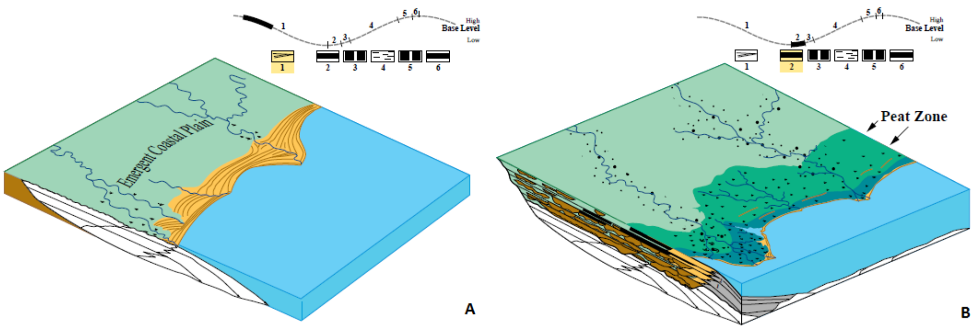

Figure 6 A: Bohacs' illustration of the distribution of paralic TOM during the late highstand system tract. B: Bohacs' illustration of the distribution of paralic TOM during the middle lowstand system tract

3. Late Lowstand to Early Transgressive System Tract - Thanks to the steady / slightly rising sea level, fluvial channels are stabilized and mires are now able to expand vertically and very thick and scattered coal seams are produced. As well, the rising water table allows excellent coal preservation. Figure 7C.

4. Middle Transgressive System Tract – Rate of sea level change is now high, the shore line is moving landwards and flooding events are frequent: if coal seams are forming, they will contain a large quantity of mineral matter. As mires are forced to constantly move toward the land, organic matter deposit pattern is scattered and isolated. Poor coal preservation. Figure 7D.

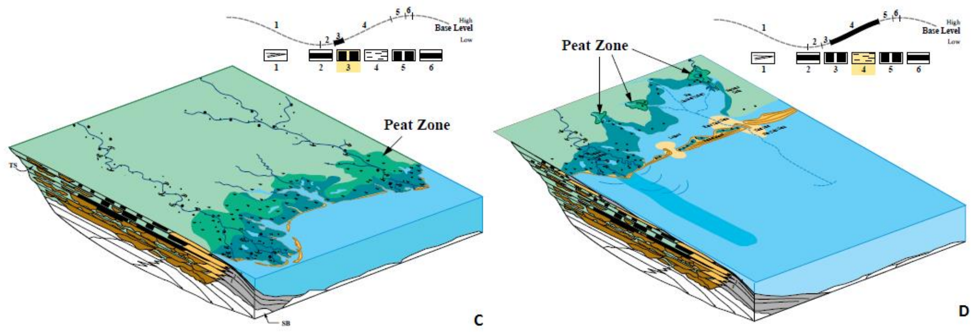

Figure 7 C: Bohacs' illustration of the distribution of paralic TOM during the late lowstand system tract. D: Bohacs' illustration of the distribution of paralic TOM during the transgressive system tract.

5. Late Transgressive to Early Highstand System Tract – Sea level rise starts here to slow down, mires are thriving, expanding vertically. Thick and isolated coal seams are formed. Very good preservation of the organic matter. Figure 8E.

6. Early to Middle Highstand System Tract – Rate of sea level change reach the minimum, stable conditions allow peat production in large areas. Moderately thick, continuous and well preserved coal seams are produced thanks to very high and steady water table. Figure 8F.

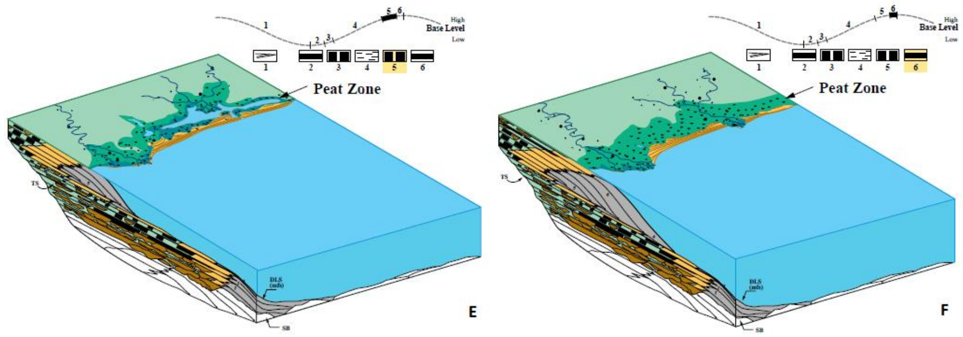

Figure 8 E: Bohacs' model of the distribution of paralic TOM during the early highstand system tract. F: Bohacs' model of the distribution of paralic TOM during the middle highstand system tract.

To sum up: thickest coal seams correspond to best condition of organic preservation: as a matter of fact, a slow rising of the water table forces mires to expand vertically and, at the same time, it protect the organic matter produced underneath them from microbial activity. One of the main messages from Bohacs and Suter (1997) is that, both in low stand and high stand, a slow accommodation rate favours mires initiation, whereas high rate either forces mires to move landward (transgression system tract), not giving them the possibility to create a suitable deposit for coal accumulation, or even hinder their formation thanks to the erosive action of fluvial system (falling stage system tract). However, these sketches give us just a broad idea of the coal signatures within an optimal stratigraphic cycle: we must not exclude that other accommodation regimes could provide the correct equilibrium (between peat production and accommodation space creation e.n.) even in other system tract.

4.2 Diversification on the proposed model

As stated before, peat flourish and coaly organic-rich rock accumulation are the results of several nonlinear parameters, interacting all together to create an elaborate system. Results might diversify even due to the slightest changes of this framework. During the depositional sequence development, magnitude and the rate of these processes vary (e.g. nonlinear fluvial system evolution, described by Wescott (1993) due to the sea level fluctuations). Not mentioning that local peculiar condition could affect the coal deposition.

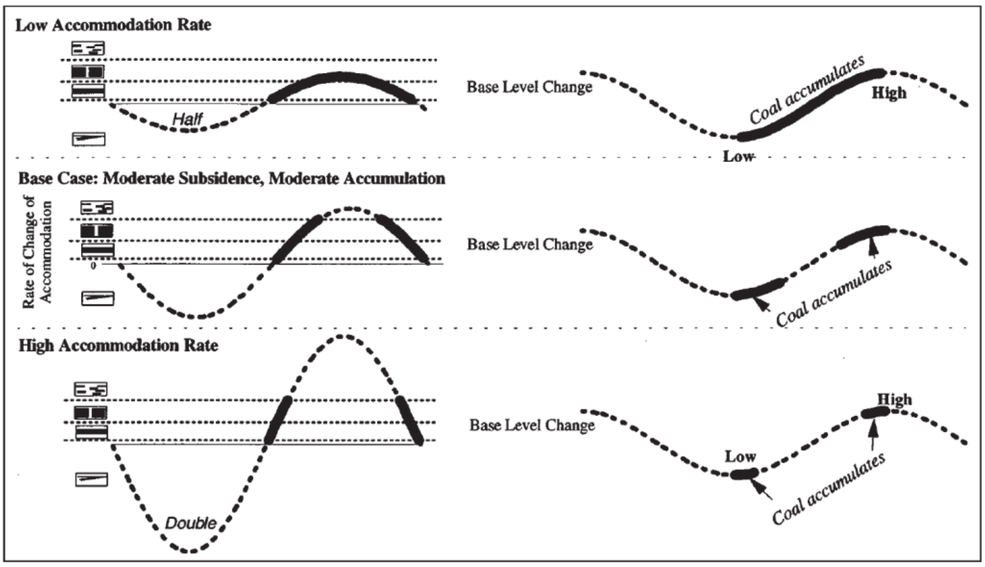

Figure 9 Distribution of coaly-rock within stratigraphic frameworks controlled by different accommodation regimes, from Bohacs and Suter, 1997

Figure 9 illustrates, for a given peat production rate, coaly rock up-growth, highlighting the fact that it is strongly dependent on the local changes of accommodation rate. According to Bohacs & Suter (1997), due to the compulsory balance between accommodation and peat production, low subsidence rates trig mires formation earlier in the lowstand systems tract and late termination of those in the highstand systems tract. Following the same illation, high accommodation-creation rates have as consequences a delay in mires initiation starting point and a high rate rise of sea level may prevent peat production even during the transgressive systems tract as result of a high accommodation rate which cannot be balanced by peat production, that is such a fast sea water transgression might generate drowning areas or flooding events.

In contrast with that, combined effects of subsidence and sediment supply, concurrently with peat production, might selectively preserve certain system tracts during the sequence deposition: highstand coals are easily affect by post depositional modification from both falling of groundwater table and erosion by rivers, due to sea level fall.

Another important allocyclic mechanism which controls (and affect) the coaly-rich rock distribution is the climate: sequences with appropriate accommodation rate and shoreline stacking patterns might show a deficit in coal by cause of an adverse climate condition. In the other hand, the proper climate ring -tropical areas- are able to enhance a huge and unusual peat production, capable to overcome even a high accommodation space creation. In truth, entire depositional sequences may be completely coal (Diessel, 1995).

4.3 Occurrence of Paralic Peats within Sequence Set and Supersequences

All the stratigraphic units are pervaded by several sedimentary cycles, characterized by different frequencies. High wave period reflect

Milankovitch cycles whereas lower frequency cycles are linked to tectonic movements. Furthermore, low order cycles (parasequences) are the building blocks of higher order sequences. (Mitchum, 1991). The same mechanisms that control the occurrence and distribution of peat at a sequence scale, are supposed to operate even at the larger stratigraphic scale, such as composite sequences or supersequences (Bohacs, 1997; Mitchum, 1991). That is the concept of accommodation balanced by peat production is applied to all the depositional sequences order. Figure 10 shows, in the upper part, an eustatic cycle built up by a lower order sequences, within peat production areas are highlighted. The lower part instead displays the rate of sea-level changes, superimposed onto the zone of peat accumulation thus the area in which accommodation is balanced by peat production (Bohacs, 1997).

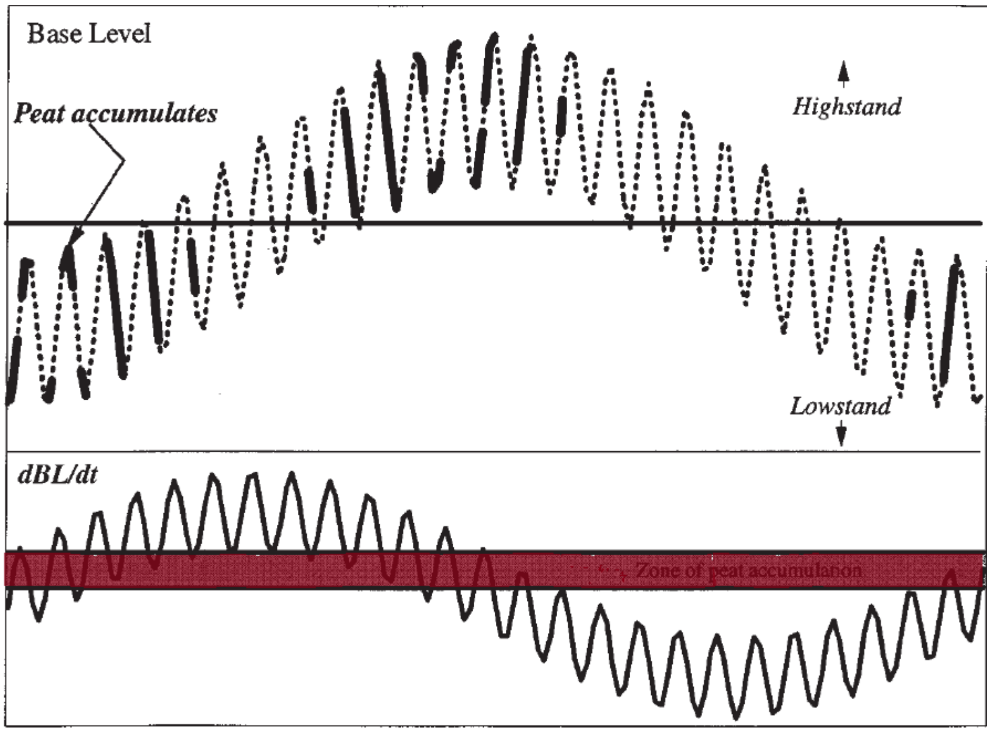

Figure 10 Sea-level variation and rate of changes of sea-level. The two curves are to be compared in order to define the peat production areas through several parasequences set, forming the so called composite sequences (modified from Bohacs, 1997)

4.4 Coal seam splits and transgressive-regressive coal couplets

Based on the study of the coal-bearing Lower Cretaceous Mannville Group of Canada Western Basin, several coal seams showing a progressive splitting pattern moving basinward have been recognized (Banerjee, 1996). The model proposed describes this stacking pattern as the results of an overall sea-level regression, affected by several lower order sequences (Diessel, 1992; Banerjee, 1996 above all). Regionally thick coal seams might form on top of a prograding platform by amalgamation of several low order sequences; afterwards they tend to split moving basinward. However, a marine sediments wedge is expected to separate the transgressive-regressive coal couplet. Similar behaviours have been spotted in plenty of coal-bearing rock successions such as in the Westphalian of England and in the Cretaceous coals of Utah (Fielding, 1987; Flint, 1995). Figure 11 illustrates the progressive formation of a regional coal seam splitting.

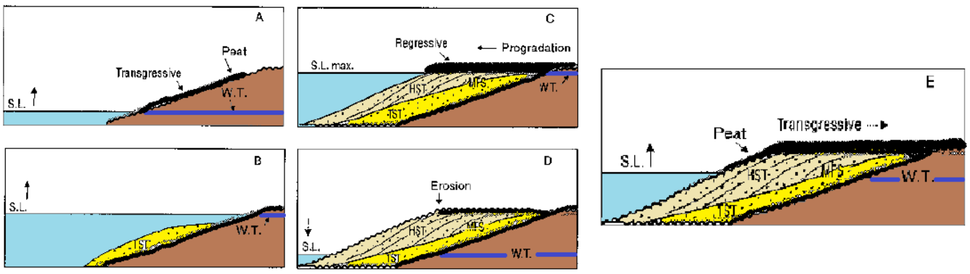

Figure 11 Genesis of a coal couplets from a 4th order eustatic cycle. A: Sea-level (S.L.) and the groundwater table (W.T.), controlled by it are both rising; peat production takes place in the area just above this wet-front. B: Mire is drowned by the sea and peat production is inhibited; the peat deposit is buried down a marine sediment wedge forming during the TST. C: Maximum flooding surface (MFS) is formed, progradation/aggradation sequences are deposited. Peat might be produced on the top. D: Erosion occurs due to sea-level fall, forming an unconformity which can be considered as a 4th sequences boundary. E: Another eustatic cycle starts. (modified from Banerjee et al 1996)

Furthermore, there is another detail we can capture from Figure 11: all the fourth order sequence boundaries fuse landward into an unconformity which is meant to be the boundary of a higher eustatic cycle (3^{rd}, ndr). Unusual thick coal seams could be justified by these stacking patterns creating an amalgamation of high-frequency sequences (Shearer, 1994; Banerjee, 1996).

5. DionisosFlow

The main objective of this work was to develop a terrestrial organic matter module (TOM) able to simulate the in-situ accumulation of the terrestrial organic matter during the filling of a sedimentary basin through geological time-scale. To achieve this goal, a module embedded into the IFPEN Home-made stratigraphic model, DionisosFlow, has been developed by the IFPEN team. This module reproduces a basin-scale steady state groundwater flow and includes production and degradation laws for terrestrial organic matter. Even if the GWF model has been already validated, his behaviour has never been studied since it is coupled with DionisosFlow. This work consists in finalising the validation of the GWF model and in improving these TOM production and preservation laws.

DionisosFlow is the software produced by IFP which has been largely used during the entire length of this work. Its main function is to provide the stratigraphic models of sedimentary basins: the stratigraphic framework is thus put in a digital formal and the geology of the area is integrated as a numerical model. The model is based on fluid-flow mechanic laws and a generalized diffusion equation that takes into account water discharge and simulates fluvial- and gravity- dominated sediment transport. Sediment load carried by water is proportional to the basin slope (moving force), water discharge (water transport capacity), lithology fraction (sediment availability) and diffusivity coefficient (transport efficiency), (Granjeon and Joseph, 1999).

DionisosFlow reproduces the stratigraphic architecture and the facies distribution during the basin filling history. The model simulates the sediment transport from source to sink. The sources (sediment and water fluxes and their locations), the transport properties (diffusion coefficients and grain sizes) and the deformation of the basin (total subsidence maps) are mandatory to build a stratigraphic modelling (Figure 12).

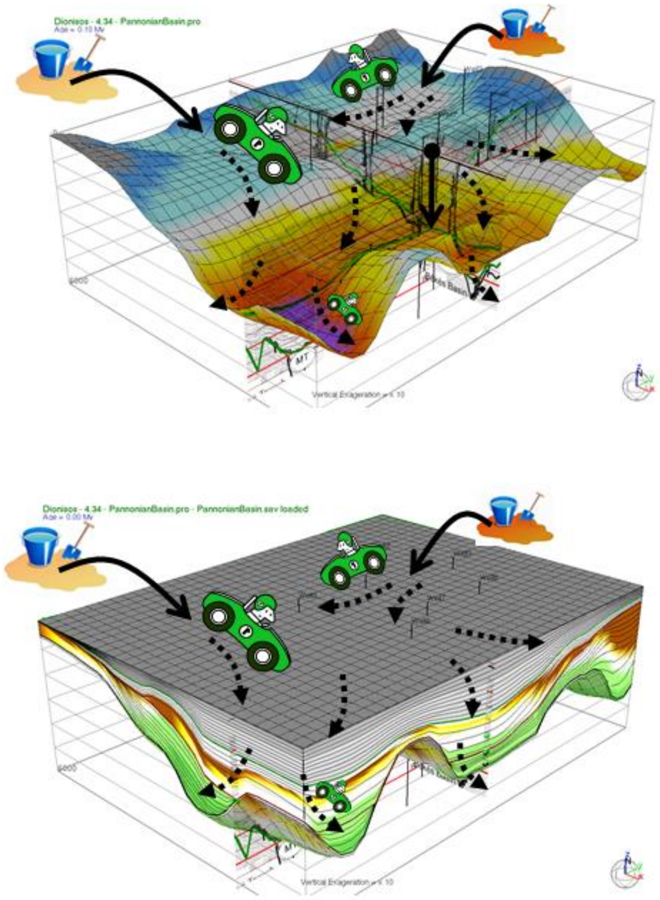

Figure 12 Schematic illustration of a Dionisos Simulation

DionisosFlow relies on the principle of stratigraphic forward models, it specifically constructs a sedimentary basin by modelling processes. Tectonics and sedimentary processes from source to sink are simulated in a forward way (from the past to the present) as illustrate in Figure13. Either weathering processes and sediment sources might be chosen as sediment supply.

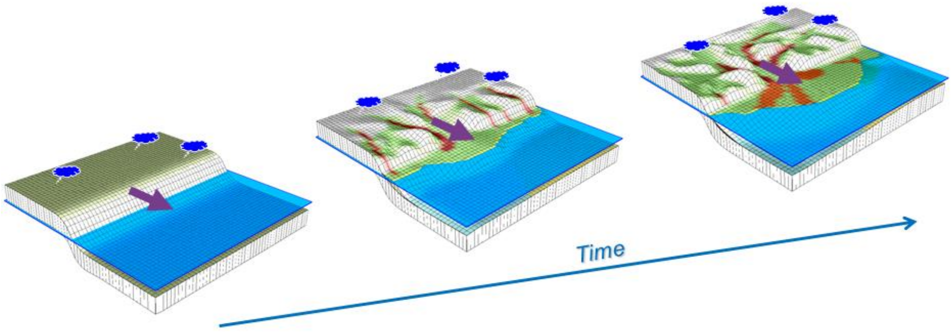

Figure 13 Example of a DionisosFlow simulation: land area is affected by intense weathering and therefore riverine and delta system develop through time.

The entity gathering all the required data to build and analyse a model is called stratigraphic model and it is the central element of DionisosFlow. Several step need to be followed in order to create a proper stratigraphic model. Different editor tabs are available and allow users to define some specific aspects of their models such as sediment types, structural history, sea level variations, clastic & carbonate supply among others. The following list describes the main editors used during the simulation performed for the purpose of this work.

- Domain Definition editor: domain area, grid sized and geo-referencing are a defined in this tab.
- Sediment editor: the list of sediments used is displayed here. Grain size, permeability of sediment and infiltration ratio can also be edited through this editor.
- Structural Evolution editor: initial bathymetry map, subsidence map, basement characteristics and geological relevant events are items linked in the basin history, described by users in this editor.
- Eustasy Variation: sea level variations are described by different curves; however, the final composite eustatic curve is the data sent to the calculator.
- Sediment Supply: rainfall occurring through ages, clastic sediments influx and the sediment proportion of sediments arriving at the basin are defined by this editor.

- Transport Parameters: this editor allows the users to define the transport law, the diffusive transport coefficients, slope failure model and above all, the weathering model.
- Simulation Parameters: editor in which we defined starting and ending ages of the model and also the associated time step. Saving option are available in this tab.

This 3D diffusive model helps to determine an average geometry of sedimentary units and to characterize the facies content (depositional water depth and sand:shale:carbonate ratio) inside each of them: The software also provides a quantitative tool for better understanding the 3D stratigraphy of a sedimentary basins (Granjeon and Joseph, 1999).

The water table is deduced from the groundwater flow at each numerical time step of the simulation. This groundwater flow is controlled by the boundary conditions (water divides where the limit of the domain is a continental area and imposed head at the shoreline location), by the precipitation/evaporations input maps and by the facies distribution (result of a Dionisos simulation) as it controls the infiltration ratio.

Thanks to these information (hydric balance, sediment influx/outflux, precipitation, subsidence), the main goal was to propose at a conceptual model allowing to reproduce or to mimic the main physical processes that control the distribution of the TOM at a basin-scale.

6. Model for the TOM accumulation

6.1 Philosophy of the model

In this workflow, groundwater table position and fluctuations are considered as a golden spike: swamp and peat cannot take place in dry environments. For the purpose of this approach, we define, for each time step of a DionisosFlow's simulation, a wet area as an area where the vadose zone thickness is below five meters. As consequence, no terrestrial organic matter production will occur in cells where the vadose zone is equal or thicker than five 5 meters (this value is at this stage empirical, but its calibration could be adjusted). By this way, our objective is to capture the main distribution of the wet and dry zones during the whole modelled geological period. However, having the mean level of the water table is not sufficient enough for characterizing the TOM depositional environment. Indeed, we also need to know the stability of the wet conditions through time. For estimating that, we propose a link between the water table evolution and the topography evolution, controlled by subsidence, clastic deposition/erosion, and sea-level variation. This approach will allow us to estimate the residence time of a given surface in a wet environment, thus this parameter will mainly control the effective TOM accumulation.

6.2 Detailed description

Peat production is only triggered in the so called wet environment under the assumption that for a given climate, humidity of soil is controlled by the water table location. To achieve our target and correctly evaluate the distribution through space and time of areas that might allow TOM accumulation, a link between the thickness of the vadose zone and the TOM production/preservation laws is proposed. As such, the terrestrial organic matter module allows us to predict the hydrodynamic regime of the study area and to estimate the in situ production/degradation of the terrestrial organic matter based on the groundwater flow at any given time. Wet and dry areas are controlled only by the groundwater table location. Moreover, a wet environment is defined by a vadose zone thinner than 5 meters and, on the other hand, a dry environment is described by a vadose zone thicker than 5 meters. Figure 14 illustrates the connection between sea-level and groundwater table and how its location defines a wetland. In the presented model, effective TOM accumulation rate (TOMacc) is supposed to be linked to the thickness of the vadose zone (V^{th}). Maximum TOM accumulation is obtained for $V^{th} = 0$ (burial efficiency, which corresponds to a preservation percentage, is BE = 100 %, Figure 15). No accumulation is possible for $V^{th} > 0$. A linear interpolation is imposed between TOMacc ($V^{th} = 0$) and TOMacc ($V^{th} = 5$) (Figure 15).

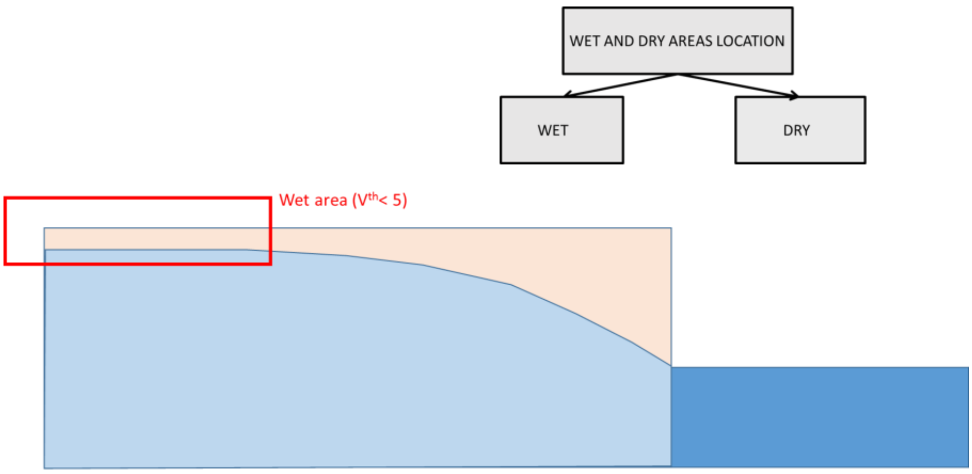

Figure 14 Simple draft to illustrate the water table (WT) location, its connection with the sea-level and the so called wet area, defined by a vadose zone thinner than 5 meters

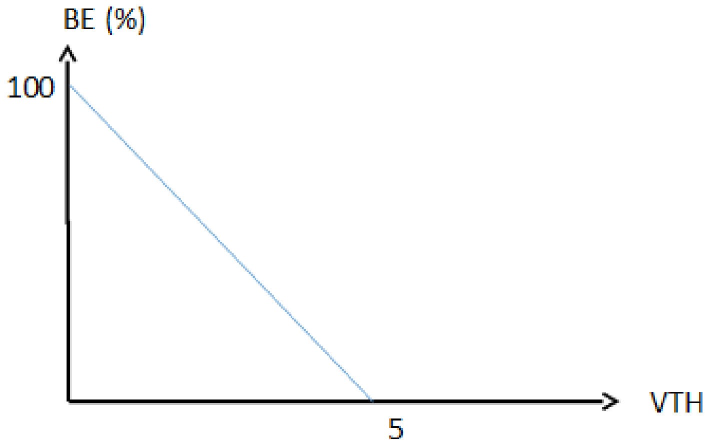

Figure 15 Burial efficiency affected by the thickness of the vadose zone

Once the location of the potential TOM accumulation sites is determined, the next step consists in regarding the expected evolution of the vadose zone during the considered time-interval. For that, an estimation of the water table variation is proposed, based on the evolution trends of the eustasy and the subsidence, and in considering a topography evolution according to the deposition/erosion regime of the inorganic sediments and to the TOM accumulation. Several examples are illustrated below. Figure 16 & Figure 17 show a case where a sea level rise is observed between t_0 and t_2. In these sketches, the sea level rise is higher than the topography elevation rate when only clastic sediments are considered. Between t_0 and t_1, the vadose zone thickness decreases but it achieves a steady state position in the TOM production zone simply because there is a given vadose zone thickness for which the TOM accumulation rate is equal to the water table rise. Between t_1 and t_2, the sea level rise increases and it is above the maximum TOM accumulation rate (TOMacc (V_{th} = 0)). Consequently, the water table is at the ground surface and "it would like to be above it". In other terms, the piezometric surface is above the ground surface. In this situation, we consider that the potential peat production zone identified at t_1 is regularly flooded, preventing TOM production.

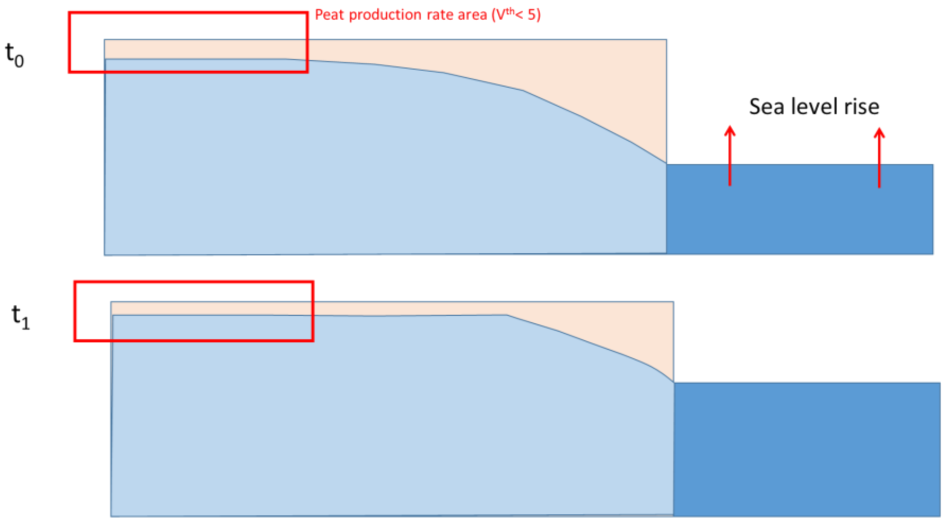

Figure 16 Simple draft to illustrate the groundwater table evolution during a marine transgression from t_0 to t_1

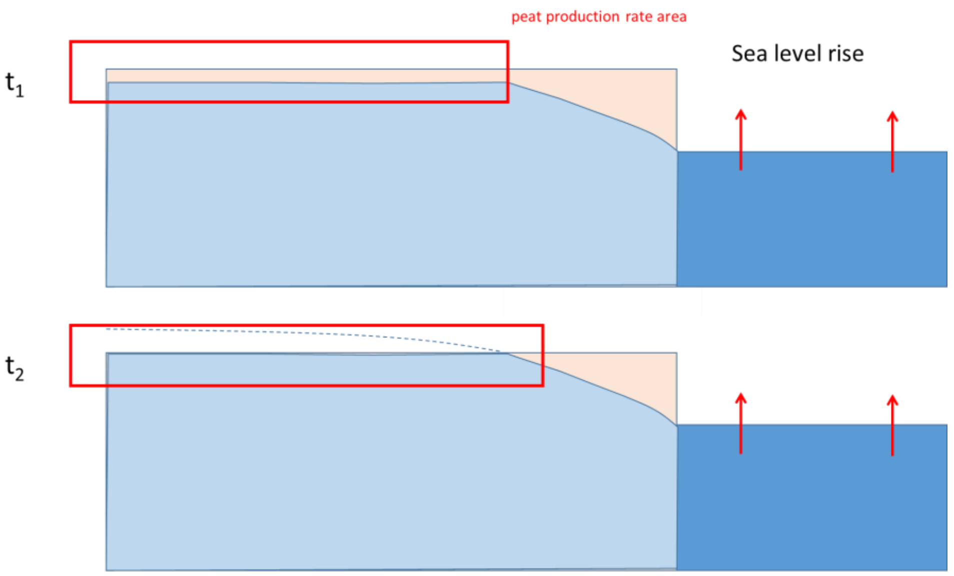

Figure 17 Simple draft to illustrate the groundwater table evolution during a marine transgression from t_1 to t_2

Case scenario in Figure 18 simulates a marine regression. During a sea-level fall, due to the link between the base level and the groundwater table, the vadose zone gets thicker.

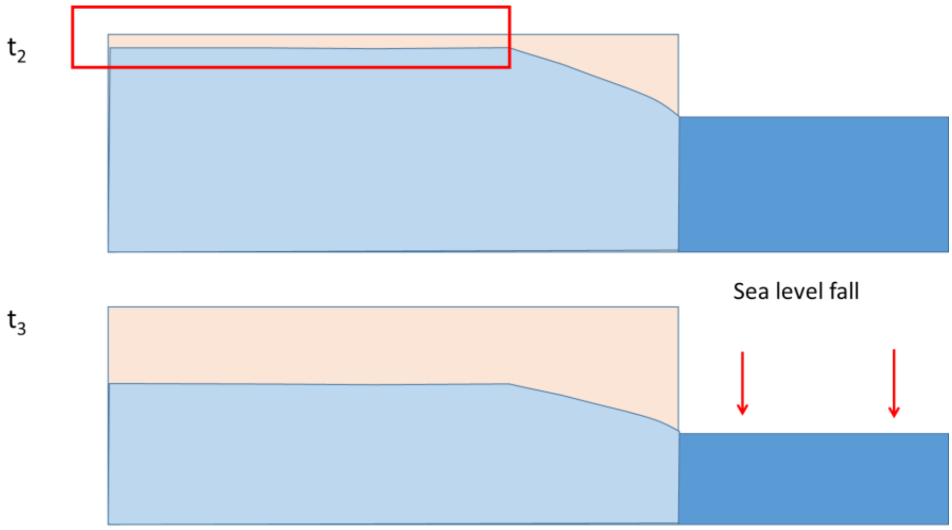

Figure 18 Simple draft to illustrate the groundwater table evolution during a marine regression from t_2 to t_3

As it can be deduced from Figure 18, the wet environment described at t_2 is expected to be substituted by a dry zone during Δt_3. In such conditions, peat production is prevented.

What we described is a “static” computation of the water table dynamics: as a matter of fact, between two simulated time step of DionisosFlow there is no a direct calculation of the groundwater table evolution. However, we are implicitly estimating its behaviour during all the simulated delta-time: strictly speaking, during each time step, the groundwater location is calculated and it give us the humidity content of the soil, in this way we define the presence of a wet or dry environment that is the potential peat productivity. The next step is the evaluation of this condition through time until the next groundwater table calculation: if a wet condition is expected to be maintained, peat starts to accumulate at a given rate until the subsequent numerical time step.

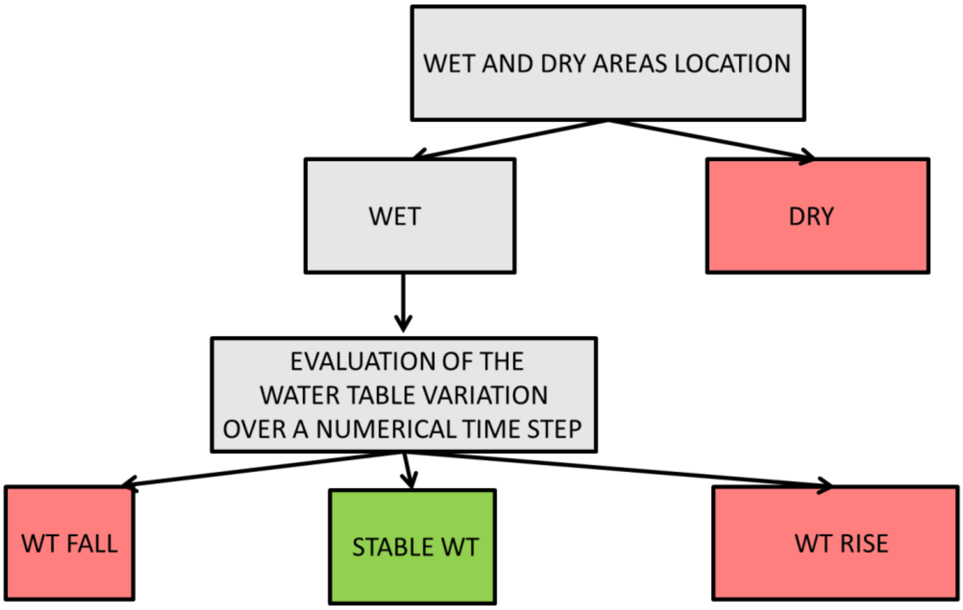

Figure 19 Abstract of the philosophy of the proposed model

This is the key point of the whole workflow, what is measured here is the accommodation space available for organic (and inorganic) sedimentation. Whenever a wetland is identified, peat production has to deal with the hydrodynamic regime: if the peat production rate is equal to the accommodation creation rate, defined by the fluctuation of the groundwater table, an organic matter deposit can be produced. Thick and widespread TOM deposits are the product of a water table which rises at a rate equal or close to the peat production one. As can be seen, groundwater table fluctuations (due to accommodation changes) and peat production rate are the two keys parameters to enhance the production of an evaluable TOM deposit. This concept workflow is summarised in Figure 19.

The first step was to describe from a hydrological point of view the distribution of the TOM accumulation areas. The second step to complete the model is to quantify the net accumulation rate of these TOM, as peats can create thick deposits that significantly modify the morphology of the area. This topography increase has to be taken into account because it directly affects the vadose zone thickness. Potential peat zones are determined by vadose zone thickness but effective peat production will occur only if the water table is stable through a reasonably amount of time, that is if the water table rise is balanced by the peat production rate.

Peat production rate depends mainly from the climate regime of the peatland. Figure 20 illustrates 3 different peat production rates, expressed in millimetres per year, as function of the temperature (Boyd and Diessel, 1995).

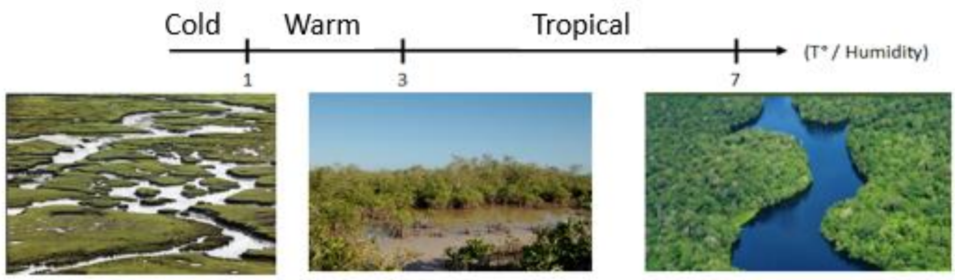

Figure 20 Peat production according with the climate regime

Nevertheless, geological records show that well preserved TOM accumulates in areas associated with “apparent subsidence rates” between 1 and 177~m/Ma (Bohacs and Suter, 1997), which corresponds, from 0.001 to 0.177 mm/y. Compared to the peat production rate, the gap of one or two order of magnitude is observed. This discrepancy can be explained considering the time-scale dependant nature of the subsidence rate and all the processes that take place during geological times: peat production is reported in mm/y whereas the rate of accommodation space creation reflects primarily a long-term rate, reported usually in m/Ma.

Under those circumstances, a conversion factor is needed as we compare processes acting in different time intervals. Gardner et al. (1987) already analysed the numerical components of diverse geomorphic and tectonic processes rates and indicated that processes rates were not independent of measure time interval (Gardner et al, 1987). A scaling function is built, allowing to convert a measured subsidence rate at a given time-interval to another time-interval.

For the purpose of this work, we use

[TOM Accumulation Rate - m/Ma] = [Peat Production Rate - mm/y] x [Gardner Coefficient]

with Gardner Coefficient = 25-30 to have a good correspondence with the peat production range in mm/yr and the peat production range in m/My that would be expected to reproduce the optimal conditions of TOM preservation associated with arrange of subsidence from 1 to 177 m/My.

6.3 Comparison with the Bohacs and Suter conceptual model

The Bohacs and Suter (1997) model deals with the concept of accommodation space. They proposed to define the optimal conditions for TOM accumulation based on the ratio between the accommodation space and the peat production rate. Figure 21 (Bohacs and Suter (1997)) shows the main context for TOM preservation and the expected TOM distribution in stratigraphic sequence associated with a regressive-transgressive event.

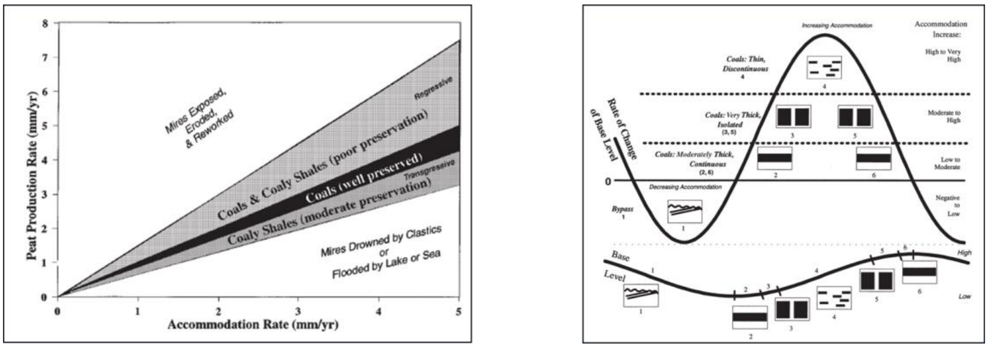

Figure 21 TOM preservations according to the accommodation rate and geometry of coal seams as function of the sequential stratigraphic framework. From Bohacs and Suter, 1997

According with Bohacs (1997), accommodation creation rate has to closely match the organic production in the interest of forming peat and concentrating terrigenous organic matter, indeed accommodation has to balance peat formation in order to obtain peat accumulation. Areas in Figure 21 (left part) represent condition of accumulation for terrigenous organic-rich rocks. In particular, the black area in the middle represents an equilibrium between accommodation rate and peat production rate. Another case scenario describes an increase in accommodation that largely exceeds the peat production rate: as results, mires are contaminated by clastic sediment or drowned by water. At last, when the increase of accommodation is much lower than peat production, mires are more likely oxidized or eroded by rivers (Bohacs and Suter, 1997). Figure 21 (right part) gives us another prospective about how changes in accommodation rates during an eustatic cycle affect the peat architecture. As reported by Bohacs and Suter, mires should respond mainly on the rate of changes instead of the direction of the base level variation and in according with that assumption, they predict symmetrical pairs of thickness-geometry attributes throughout the whole cycle.

Furthermore, Bohacs and Suter described the accommodation space as result of the interaction between sea-level variation and tectonic activity, both of which are able to make the ground water table fluctuating. According to their model, as long as the vadose zone has zero thickness, peats flourish. During the whole process, inorganic sediment flux is not taken into account: clastic sedimentation takes place only when peat production is no more thrived and it fulfils the accommodation space left, if any.

6.4 New properties associated with the TOM module

In order to facilitate the comparison between the Bohacs and Suter model and the TOM module in Dionisos, a new output property has been created: the A/P ratio property map (accommodation over peat production). With reference to Figure 22, the accommodation is estimated from the eustatic curve, the subsidence maps and the sedimentation rate of transported sediments.

This property can be analysed directly based on the three following regimes

- A/P > 1 → Accommodation space exceeds peat accumulation rate, normally a flooded environment is formed and no peat is produced under these condition.
- 0 < A/P < 1 → Peat production now balances the accommodation creation rate, enhancing terrestrial organic sedimentation at a given rate.
- A/P < 0 → Negative accommodation space value means that the ground water table is moving far beneath the surface and peat do not flourish in the so called dry environment.

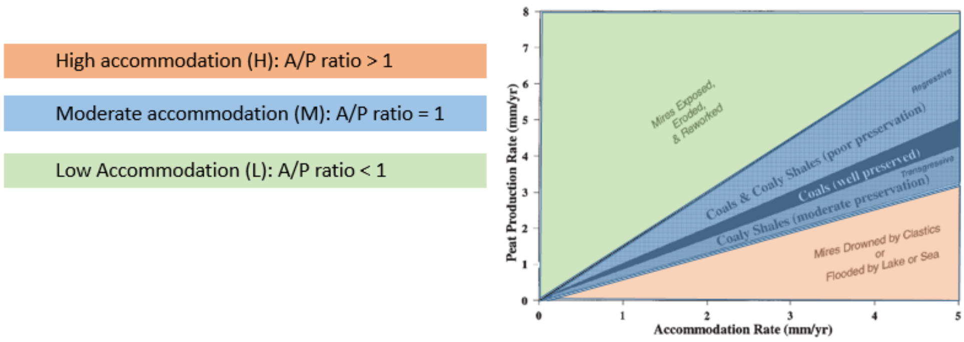

Figure 22 Different accommodation regimes defined by the A/P ratio; end members are also plotted in the chart proposed by Bohacs and Suter (1997)

In the interest of delineate a TOM accumulation model which works in the framework simulated by DionisosFlow, a slightly different interpretation of accommodation space is given: the net accommodation space has to take into account also the sedimentation rate, to correctly represent what actually is simulated by the software. Total accommodation space is thus defined by the summation of sea level variation, tectonic activity and sediment rate.

A water table fall is always linked to a negative accommodation regimes and no peat production occurs. When the accommodation space creation is positive but it does not exceed the peat production rate, a stable water table is created. The best case scenario is achieved when the accommodation rate is close or equal to the peat production rate: this equilibrium enhances the maximum peat production rate. Finally, if accommodation rate is higher than the peat production rate, peat formation is prevented and a flooding area is created instead.

So far, peat production has been described as a process mainly controlled by the vadose zone thickness and the theoretical evolution of the base level but accumulation rates might vary as well. Starting from the assumption that organic matter preservation requires a water-table at or very near the surface to retard oxygen diffusion and prevent any form of decay (Frenzel, 1983; Diessel, 1992; Moore, 1989; Bohacs, 1997), a simple law is given to define the peat degradation rate. All things considered, burial efficiency is determined by the groundwater table, hence the vadose zone thickness, determining the net TOM accumulation. The burial efficiency is so defined:

$$BE = (1 - \frac{Vth}{5}) * 100$$

As such, a zero thickness vadose zone guarantees a total TOM preservation whereas a groundwater table 5 meters or more below the surface indicates a dry environment in which organic matter cannot be either produced or preserved. Figure 23 simply illustrates the relation between burial efficiency and groundwater table position.

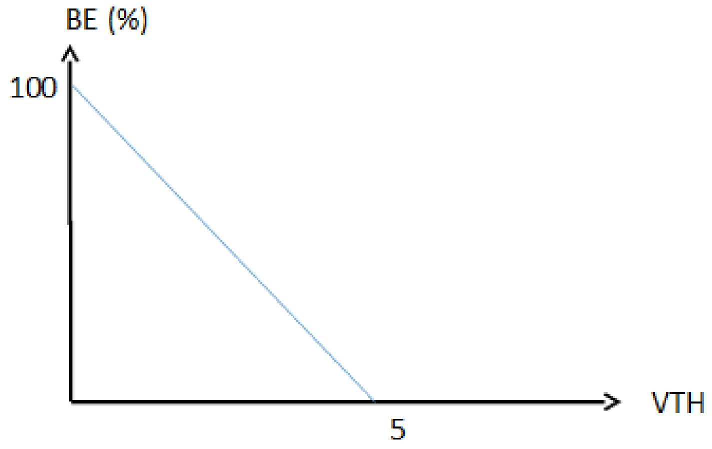

Figure 23 Graphic relation between burial efficiency (BE) and vadose zone thickness (VTH)

To summarise, the TOM concept model we described is able to simulate in-situ TOM deposition. Accumulation rates depend on the initial vadose zone thickness, fluctuations of the groundwater table and the initial peat production rate, controlled by the climate regime. TOM can be either preserved or eroded after its initial deposition. Vadose zone thickness and A/P ratio are the new output properties introduced in this module to correct display and correlate the results obtained from DionisosFlow's simulations.

7. Results

All the simulation tests that were made are distributed between 4 major projects. Each single project has its own objective and they were accomplished using different parameters combinations such as 2D or 3D topography and either with and without sediment supply. The purpose of each project and its peculiar characteristics are displayed in Table 1. All the simulations have been done using a Gardner coefficient equal to 33 and with a peat production rate of 1 mm/yr.

Project	Purpose	Main Features
1	Validating and testing peat production in relation with the groundwater table oscillation.	One single 3rd order eustatic cycle is used.
2	Validating and testing the organic matter module in 2D synthetic scenarios.	Different combination of subsidence maps and/or sea-level variations.
3	Validating and testing the organic matter module in one 2D complex scenario.	Subsidence map and eustatic curves (3rd and 4th cycle).
4	Validating and testing the organic matter module in one 3D scenario	3D setting in which a complex riverine system is able to develop.

Table 1 List of projects with purpose and description.

7.1 Project 1 – Water Table Dynamics and Peat Production

Groundwater flow is a key point of our organic matter module as TOM accumulation rate is a function of the humidity index that is directly controlled by the groundwater table position. Peat can flourish only if the vadose zone is thinner than 5meters. Therefore, the stationary groundwater system is solved at each Dionisos numerical time step.

The 2D synthetic case presented here is depositional context controlled by a 3rd order eustatic cycle on an extreme simplified 2D topography. The purpose of this simulation is to study how the groundwater table moves in respond of a sea-level fluctuation and, as a consequence, how the vadose zone thickness affects peat production. The initial bathymetry does not reproduce a realistic environment. However, such a simple layout worked as a test to highlight the purpose of the model. A single sediment source was selected and positioned at the top-left of the model; transport of sediment is limited by transport parameters. The gradient in the terrestrial part of the profile is about 3 meters per kilometer. The topography is illustrated in Figure 24 together with the sea-level (S.L.) position at t_0.

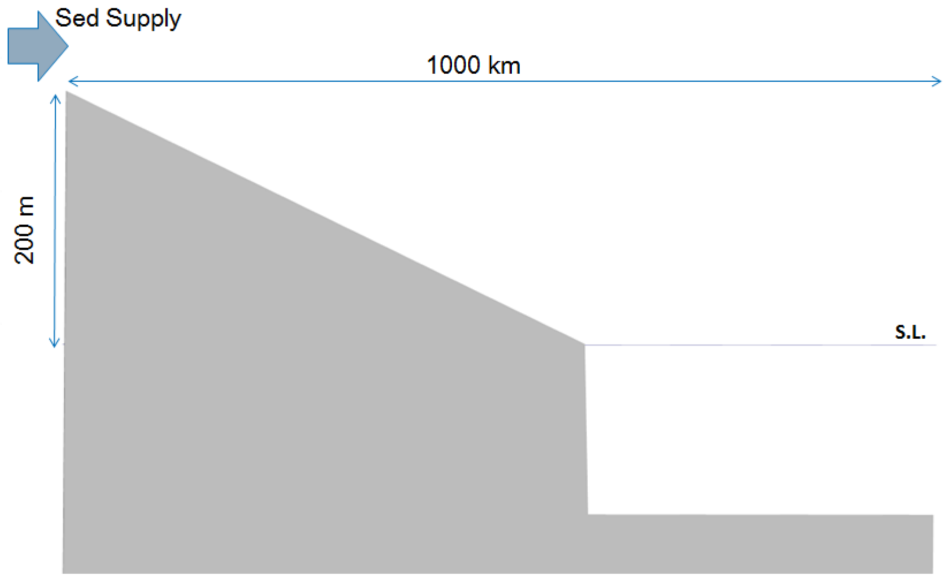

Figure 24 Topography and sea-level at t_0. Sediment supply source is displayed as well

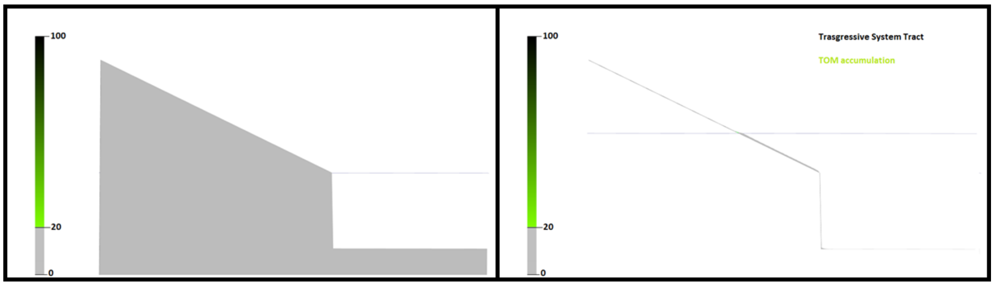

Figure 25 Figure 25 Model's evolution, from t0 to the middle TST. The colour palette displays the TOM (sediment proportion)

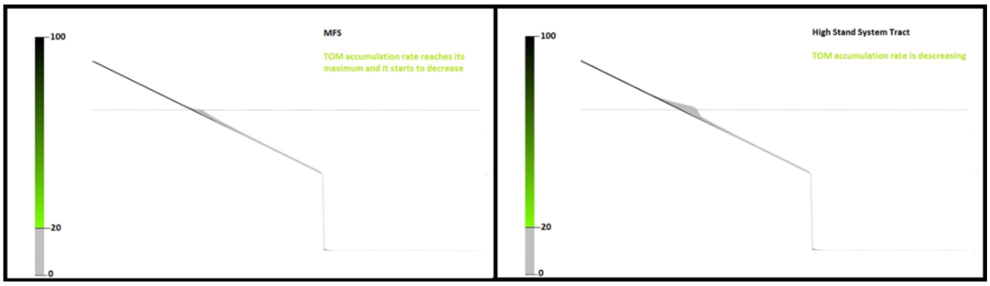

Figure 26 Model's evolution, from the end of the TST (MFS formation) to the HST. The colour palette displays the TOM (sediment proportion)

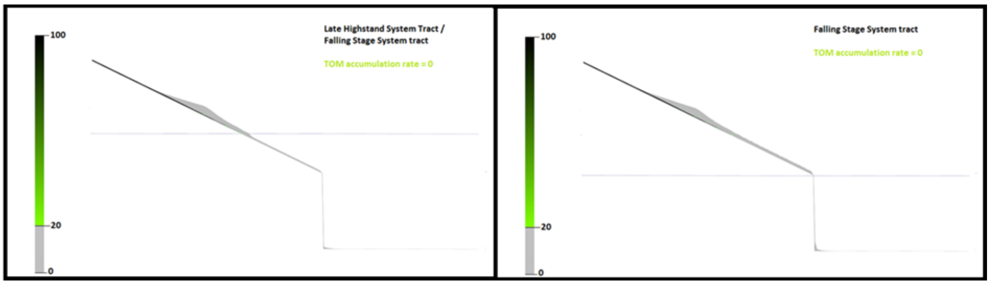

Figure 27 Model's evolution, from HST to the FSST. The colour palette displays the TOM (sediment proportion)

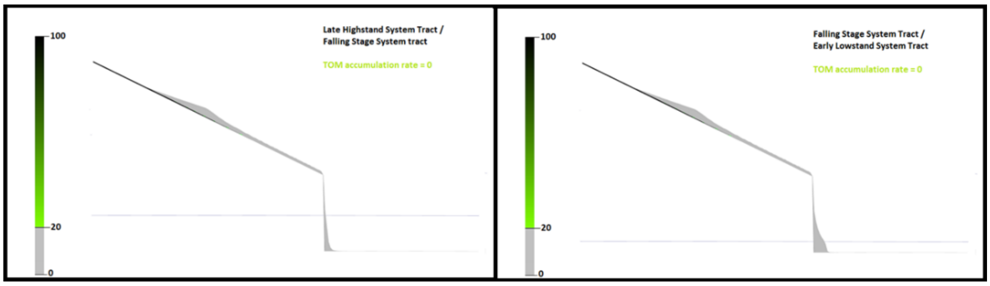

Figure 28 Model's evolution, from the late FSST to the early LST. The colour palette displays the TOM (sediment proportion)

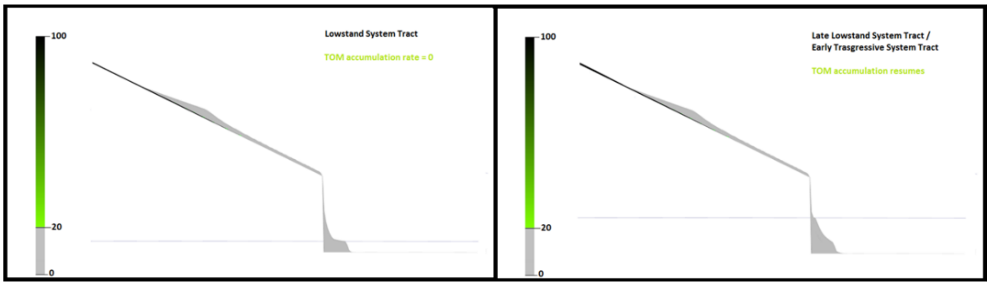

Figure 29 Model's evolution, from the LST to the beginning of the marine transgression. The colour palette displays the TOM (sediment proportion)

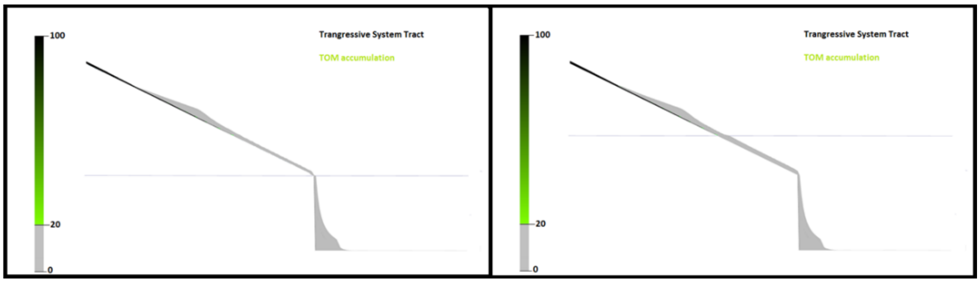

Figure 30 Model's evolution, TST. It marks the end of the first eustatic cycle. The colour palette displays the TOM (sediment proportion)

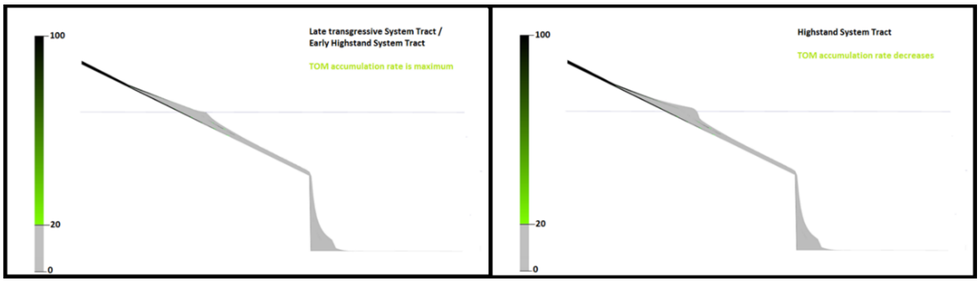

Figure 31 Model's evolution, from the TST to the HST of the second eustatic cycle. The colour palette displays the TOM (sediment proportion)

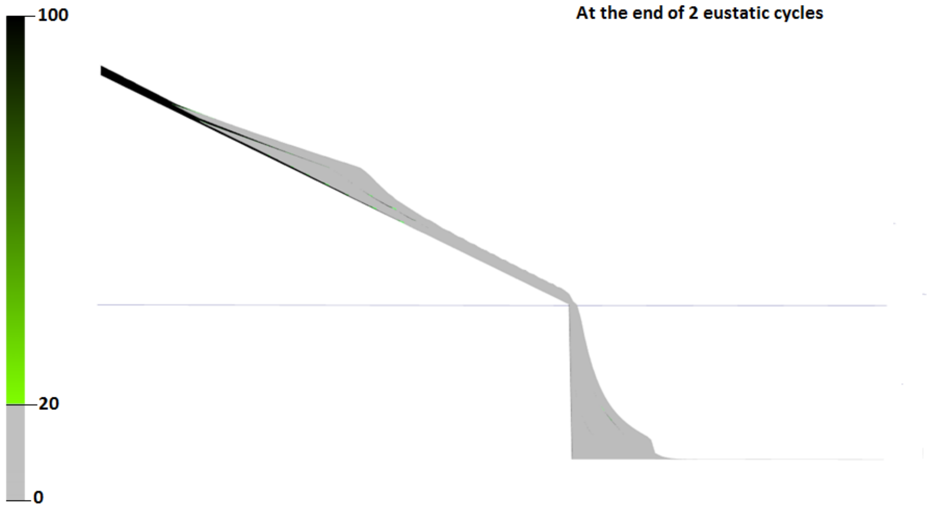

Figure 32 Model's evolution after the end of the second eustatic cycle. The colour palette displays the TOM (sediment proportion)

Each step of the simulation shows the evolution of the sedimentation regime while the chosen source provides constantly inorganic supply (sand e.n.) through time. The basement has been hidden after the first step in order to have a better view of the deposited sediment. Figure 25 & Figure 26 show the transgressive system tract (TST) deposit until the early highstand system tract (HST); sea-level transgression pushes the groundwater masses landwards, modifying the regional vadose zone thickness. Prograding sediment wedge is forming during the HST. Organic sedimentation occurs whereas possible. Figure 27 & Figure 28 show the whole transgressive system tract (TST) and the early lowstand system tract (LST); sea-level regression has an important influence in the regional water table position, which is drastically lowered down. TOM production is inhibited and the inorganic sedimentation depocenter is shifted basinward. Figure 29 displays the LST and the beginning of marine transgression. This specific moment is crucial in our simulation: sea-level rising moves the shoreline position landwards and, moreover, the groundwater table is forced to follow this transition. Wet conditions are settled next to the shore and peat production restarts. However, the beginning of the sea-level rise does not guarantee homogeneous TOM accumulation all along the profile. Further eustatic positive variation will accomplish this objective, such as the situation observed in Figure 30. The end of the eustatic cycle is shown in Figure 31: another MFS is created and an aggradation stacking pattern, characteristic of the HST, is forming.

Figure 32 displays the sedimentation pattern after two eustatic cycles. As a matter of fact, our workflow is correctly "producing" organic sediment in wet environment and, as soon as the groundwater table is dragged down by sea-level fall, it prevents peat production, accordingly with the static water flow dynamic applied by DionisosFlow in regressive cycles

7.2 Project 2 – Synthetic Case 2D

The previous chapter underlined the correct respond of the peat production to groundwater table variations. The second project moved one step forward to validate the terrestrial organic matter module and to test the sensitivity of the factors that are able to affect the TOM distribution. Furthermore, an estimation of peat accumulation rate is given accordingly with the vadose zone thickness: the thinner the vadose zone, the bigger the TOM accumulation rate. Only one single stratigraphic model was built but several calibrations for eustasy, subsidence map and the sedimentation rate are proposed. Our main goal in this study was to observe the responds of peat production rate under different accommodation regimes. Table 2 summarizes the main input parameters used in each simulation.

SCENARIO	AMPLITUDE OF THE EUSTATIC CURVE	SUBSIDENCE MAP	SEDIMENTATION RATE
Su_H_nosediment	No eustasy variations	75 m/Ma	None
Su_H			Sediment source applied
Su_M_nosediment		30 m/Ma	None
Su_M			Sediment source applied
Su_L_nosediment		10 m/Ma	None
Su_L			Sediment source applied
Eu_H_nosediment	200 m	No tectonic subsidence	None
Eu_H			Sediment source applied
Eu_M_nosediment	170 m		None
Eu_M			Sediment source applied
Eu_L_nosediment	80 m		None
Eu_L			Sediment source applied

Table 2 Major input parameters used in Project 2

All the three accommodation regimes described by Bohacs and Souter (1997) are achieved either with different subsidence rates and eustatic variations. Ultimately, at each calibration models, a clastic sediment source has been applied: the result is an overall mitigation of each result due to the occurrence of clastic sedimentation. Nevertheless, the accommodation space shows a positive variation as inorganic sediment is now competing for the same space with the TOM. It is important to remind that most of the applied input parameters work quite good in the simulated framework but they might result geologically inappropriate if considered standing-alone.

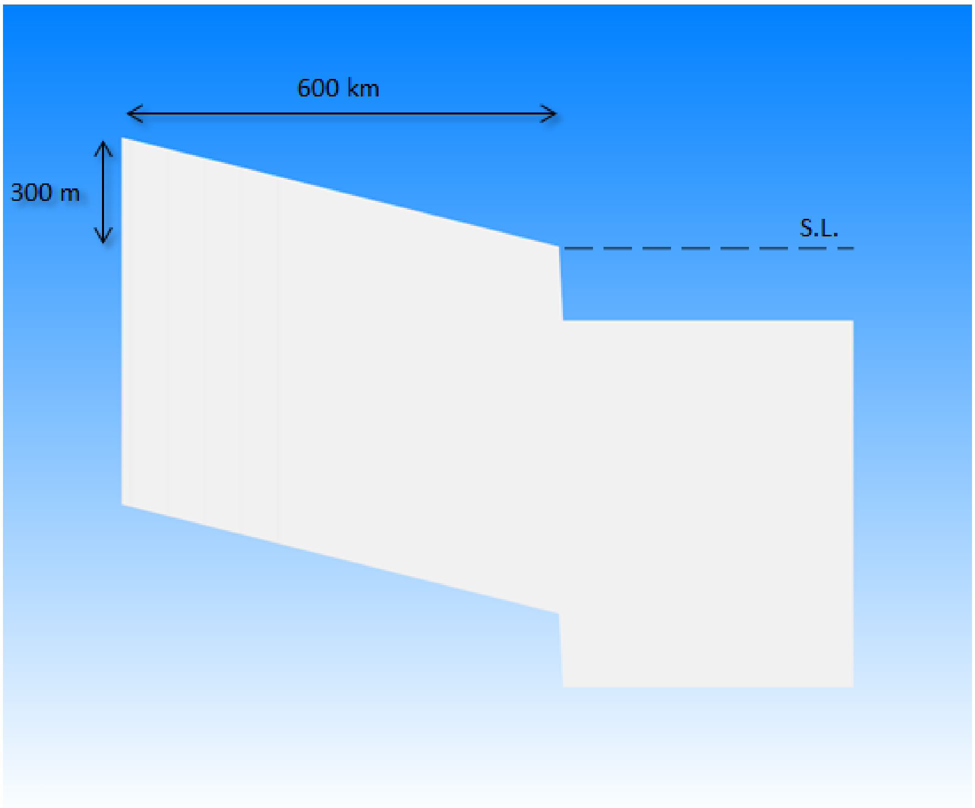

Figure 33 Initial Paleobathymetry, base-topography used for each simulations in project2. Vertical scale exaggeration x500

As an example, Figure 33 illustrates the selected synthetic topography with a moderate continental slope-gradient that help us to isolate the impact of every input parameter. Once the main accommodation regimes are defined, other possible sub-scenario are evaluated combining the previous simulation all together. These new models associate different subsidence rate and eustatic curves, either with or without sedimentation rate. A briefly summary is given by Table 3.

Due to the large number of models that have been built in this project (30 n.e.) only a relevant selection, that gives a representative illustration of the behaviour of the model, is presented.

SCENARIO	SUBSIDENCE MAP	EUSTATIC AMPLITUDE	SEDIMENTATION RATE
Su_M_Eu_L_nosediment	30 m/Ma	80 m	None
Su_M_Eu_L			Sediment source
Su_M_Eu_M_nosediment		170 m	None
Su_M_Eu_M			Sediment source
Su_M_Eu_H_nosediment		200 m	None
Su_M_Eu_H			Sediment source
Su_L_Eu_L_nosediment	10 m/Ma	80 m	None
Su_L_Eu_L			Sediment source
Su_L_Eu_M_nosediment		170 m	None
Su_L_Eu_M			Sediment source
Su_L_Eu_H_nosediment		200 m	None
Su_L_Eu_H			Sediment source
Su_H_Eu_L_nosediment	75 m/Ma	80 m	None
Su_H_Eu_L			Sediment source
Su_H_Eu_M_nosediment		170 m	None
Su_H_Eu_M			Sediment source
Su_H_Eu_H_nosediment		200 m	None
Su_H_Eu_H			Sediment source

Table 3 Major input parameters used in Project 2

Moderate Subsidence Rate (no sediment input)

The first synthetic case we illustrate is built *ad hoc* to recreate an equilibrium between accommodation rate, controlled only by subsidence rate, and peat production rate.

Table 4 summarises the main input parameters used to build the model.

Eustatic Curve	Subsidence Rate	Inorganic Sediment Supply / Erosion	Time Length
None	30 m/Ma	None	2 Ma

Table 4 Main input parameters in the model Su_M without sediment supply

Peat production rate has been set as default at 1mm/y and, thanks to the Gardner coefficient, it is possible to define the maximum peat accumulation rate at 33m/Ma. As such, the chosen subsidence rate is supposed to guarantee the equilibrium required to enhance the formation of a thick peat deposit.

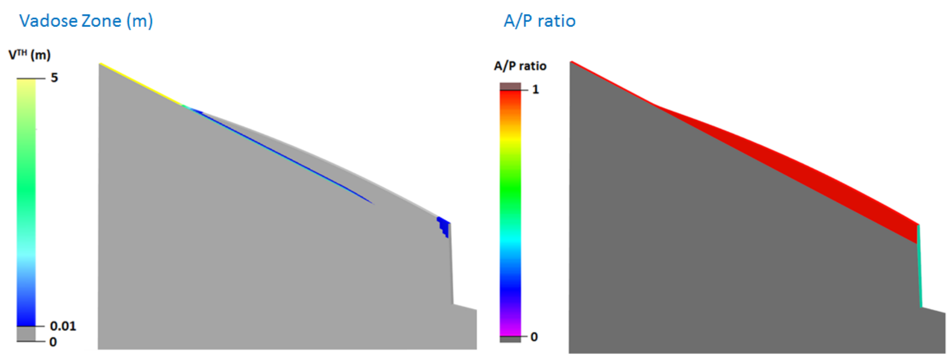

Figure 34 Vadose zone and A/P ratio output properties from model Su_M without sediment supply. Vertical scale exaggeration x500

According with the two properties maps illustrated in Figure 34, we are dealing with a wet area and this condition is maintained through time as the A/P ratio is between 0 and 1. Furthermore, because this ratio is equal to one, a vertical peat deposit is expected to be formed.

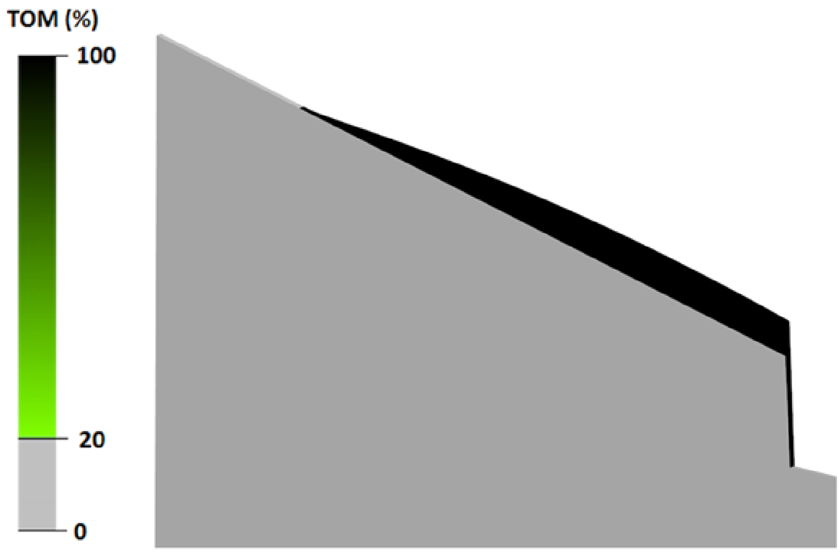

Figure 35 TOM (sediment proportion) output property from model Su_M without sediment supply. Vertical scale exaggeration x500

Whereas the vadose zone thickness is below 5 meters and the A/P ratio is equal to 1, we observe the formation of a thick TOM deposit. The black colour of the sediment body highlighted in Figure 35 indicates that inorganic sediment supply is prevented, thus the organic sediment is not diluted. However, the groundwater table dynamics does not allow the settlement of a wet environment all along the profile: whereas the vadose zone is thicker than 5 meters (landward part of the section) peat accumulation is prevented, even within the most favourable accommodation regime.

Furthermore, it is important to point out the deep connection between vadose zone thickness and peat accumulation rate.

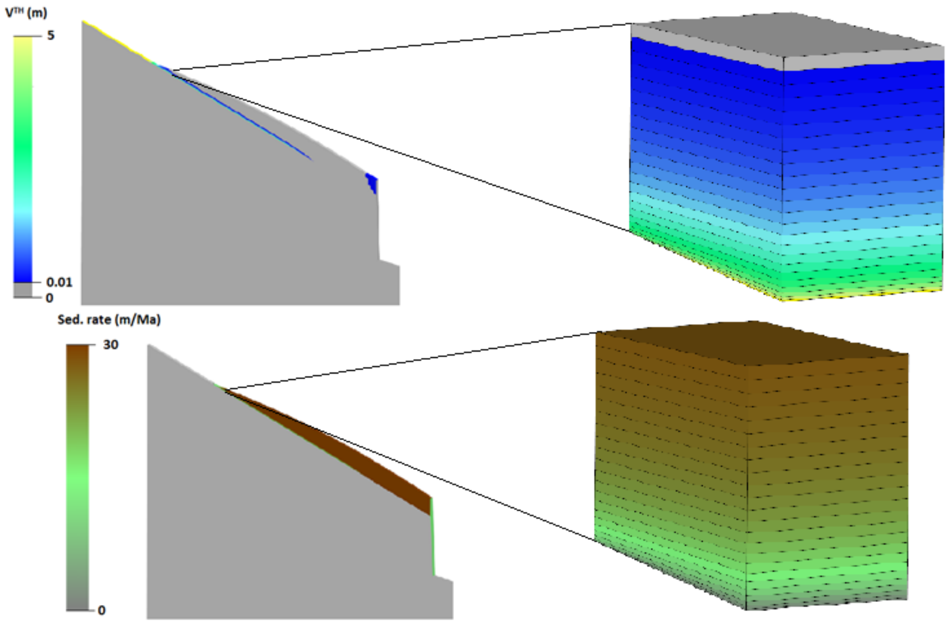

Figure 36 Comparison between sedimentation rate and vadose zone thickness. Vertical scale exaggeration x500

Figure 36 illustrate two details from two different property maps: vadose zone thickness and sedimentation rate. Please notice that, as inorganic sedimentation has been excluded, this last output property is referring exclusively to the organic sedimentation rate. What we could easily infer by a closer look is that the thinner the vadose zone, the greater the accumulation rate of peat.

High Eustatic Variation (no sediment supply)

We are now introducing another synthetic which is also built without selecting a sediment source but, instead, the accommodation regime is controlled only by eustasy. Table 5 summarises the main input parameters of this model.

Eustatic Curve	Subsidence Rate	Inorganic Sediment Supply / Erosion	Time Length
200 m	None	None	2 Ma

Table 5 Main input parameters in the model Eu_H without sediment supply

In order to give a clear representation of the result we obtained, this case is going to be illustrated with the so called Wheeler Diagram, useful stratigraphic chart in which the vertical scale represent the time and the horizontal one shows the distance across the study area. Results are also filtered by the continental area to better follow variation of the shoreline through time.

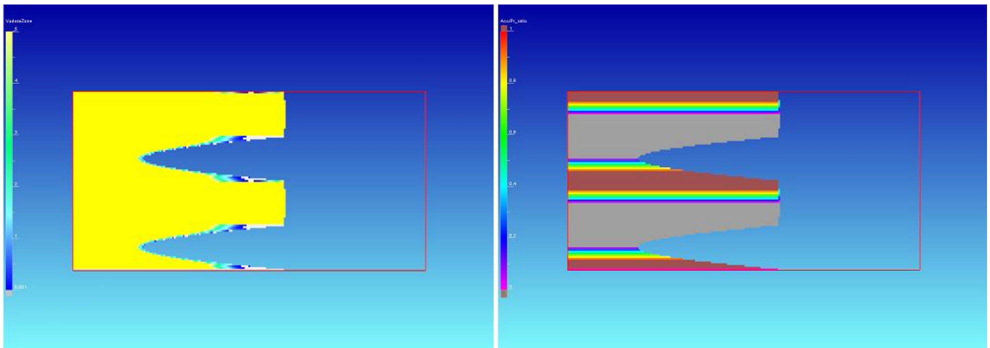

Figure 37 Vadose zone and A/P ratio output properties from model Eu_H without sediment supply

The two output properties illustrated in Figure 37 represent respectively the vadose zone thickness and the A/P ratio through two eustatic cycles with an amplitude of 200 meters. The squared border drawn by the shoreline oscillation is due to the high slope gradient of the paleo-bathymetry.

According to high sea level variation, the distance between the coastline (east boundary condition) and the water divide (west boundary condition) varies. However, the water divide condition can influence the spreading of the paralic zone. When this distance is long enough, the water table is not impacted by the water divide and the spreading of the paralic zone is mainly controlled by the topography. Nonetheless, when the distance between the water divide and the coastline is reduced, the rising of the water table is limited by the water divide condition, as highlighted in Figure 38, limiting the expansion of the paralic zone

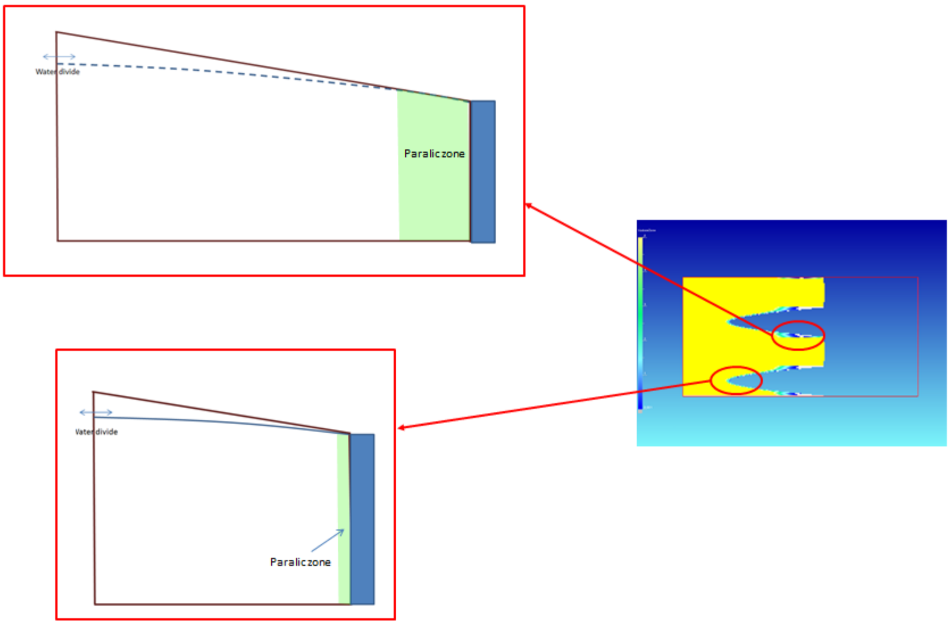

Figure 38 Water table trajectory from the paralic zone to the edge of the model (water divide condition is highlighted). Emphasis is given to two different time step of the previously described simulation

Additionally, the A/P ratio indicates a symmetric behaviour through the eustatic cycle. A negative ratio (grey areas) represents dry zone characterized by a falling groundwater table. Brown colour areas describe A/P ratio above one, most likely due to the marine transgression and the flooding events associated. Moreover, each eustatic cycle highlight two narrow areas where the A/P ratio oscillates between 0 and 1 value, meaning that there, the wet environments, if any, are preserved. The observed A/P ratio indicates possible TOM production during the early highstand system tract and the late lowstand system tract. However, due to the very low extension of the vadose zone areas below 5 meters, a very thin and poorly preserved TOM deposit is expected to be formed.

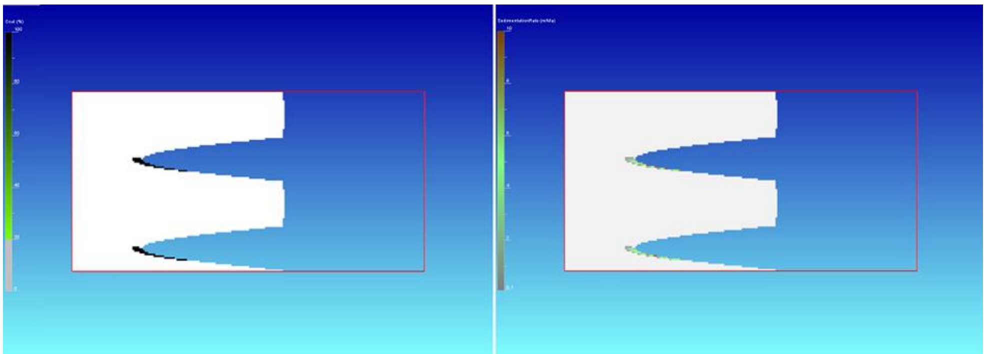

Figure 39 TOM (sediment proportion) and sedimentation rate output properties from model Eu_H without sediment supply

As anticipated, Figure 39 shows TOM accumulation occurs in a very narrow area with a low sedimentation rate.

Low Eustatic Variation & Moderate Subsidence Rate (no sediment input)

The study case described below is part of the set of model built using both eustatic variation and tectonic subsidence as the main input features affecting the accommodation regime. Table 6 summarises the principal input parameters used to build this stratigraphic framework.

Eustatic Curve	Subsidence Rate	Inorganic Sediment Supply / Erosion	Time Length
80 m	75 m/Ma	None	2 Ma

Table 6 Main input parameters in the model Su_M_Eu_L without sediment supply

Once again, due to the complexity of the data obtained, results are given through the Wheeler diagram.

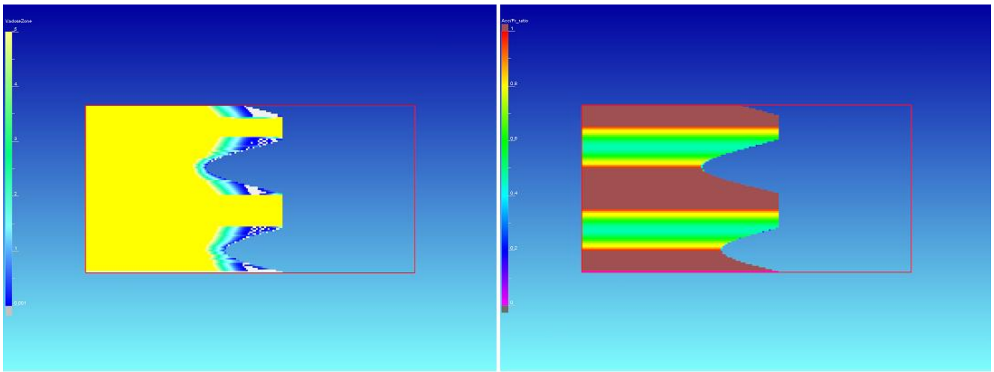

Figure 40 Vadose zone and A/P ratio output properties from model Su_M_Eu_L without sediment supply

Figure 40 shows, once again, the same squared profile, due to the high slope gradient of the break shelf (see Figure 24 as a reference). Eustasy variations modify the location of the vadose zone in a narrow area due to the low amplitude of the eustatic cycle. However, the main characteristic of this stratigraphic model is highlighted by the A/P ratio: indeed, the observed variation of this ratio indicates possible TOM accumulation during the whole regressive system tract. Such result is mainly due to the two parameters that affect the accommodation regime of the model: as the moderate subsidence map guarantees an equal proportion between tectonic subsidence and potential peat accumulation through time, each marine transgression involves an overall increase of the accommodation space. In other words, the water table rise is too rapid compared with the potential topography modification by peat production and no peat is produced, as represented by the A/P ratio greater than one (brown areas). Furthermore, during marine regression, the groundwater table fall is balanced by the subsidence rate. This leads to a vadose zone thickness below 5 meters and an A/P ratio between 0 and 1, which allows peat accumulation. However, because A/P ratio is oscillating around 0.5, accumulation rate is low-moderate, as illustrated in Figure 40.

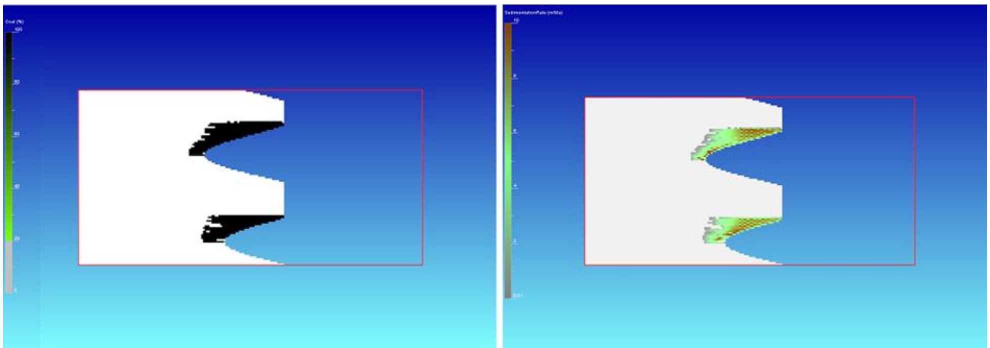

Figure 41 TOM (sediment proportion) and sedimentation rate output properties from model Su_M_Eu_L without sediment supply

As inferred in the previous discussion, TOM accumulation occurs during the regressive system tract due to this particular accommodation regime. As the inorganic sedimentation is excluded, the sediment body does not show any dilution (Figure 41).

7.3 Project 3 – 2D Case Study: 3rd and 4th order eustatic cycles

The 3rd project collected another interesting information: the stacking pattern of TOM deposits within a stratigraphic framework controlled by two different order eustatic cycle. As a matter of fact, this model has been built to study the impact of sea level variations on the available accommodation space. Table 7 summarises the main input parameters used during this simulation.

<table>
<tr><th colspan="4">Eustatic Curve</th><th>Subsidence Rate</th><th>Inorganic Sediment Supply / Erosion</th><th>Time Length</th></tr>
<tr><td colspan="2">3rd Order Cycle</td><td colspan="2">4th Order Cycle</td><td rowspan="3">50 m/Ma</td><td rowspan="3">Rainfall
480 mm/y</td><td rowspan="3">10 Ma</td></tr>
<tr><td>Amplitude</td><td>Period</td><td>Amplitude</td><td>Period</td></tr>
<tr><td>50 m</td><td>4 Ma</td><td>20 m</td><td>0.6 Ma</td></tr>
</table>

Table 7 Main input parameters in the model out of project 3.

It is important to notice that here erosion takes place thanks to the rainfall rate, set at 480 mm/y. Ultimately, the eustatic curve is now built up by two different order cycles. Figure 42 illustrates the composite curve built by DionisosFlow: high and low frequency eustatic cycles are illustrated.

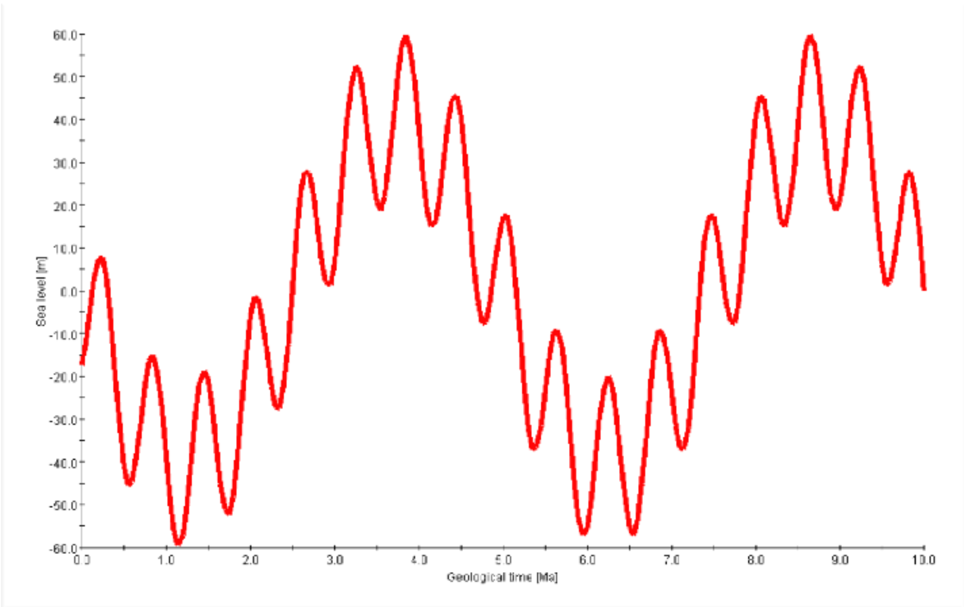

Figure 42 Eustatic variation from DionisosFlow, 3rd and 4th cycles are displayed altogether in a composite curve

Vadose zone thickness property map defines wet and dry areas whereas the A/P ratio highlights the favourable zones for peat accumulation (Figure 43).

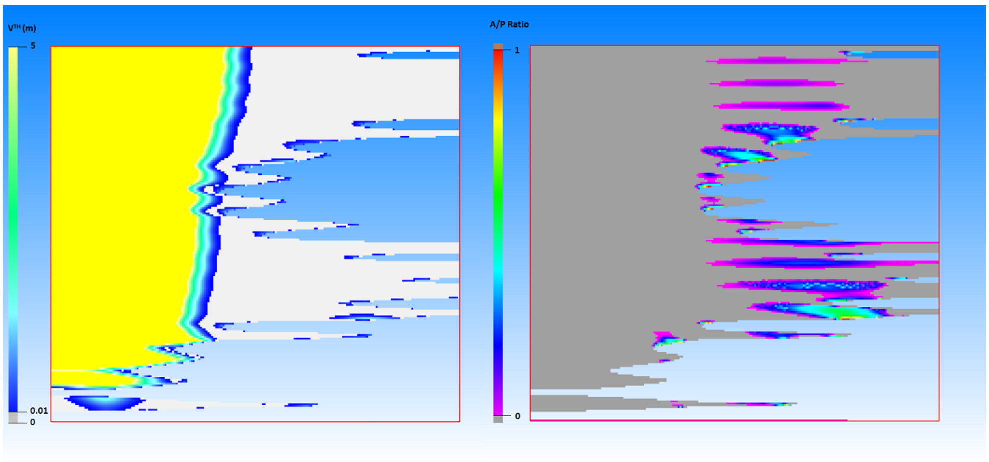

Figure 43 Vadose zone and A/P ratio output properties of the model out from project 3

Result presented in Figure 44 shows the formation of several isolated coal seams, distributed with some sort of order through time. In the first place, it is easy to notice that all the TOM deposits are formed during the marine transgression controlled by the 4th order cycles. However, such regular distribution does not appear during the 3rd order cycles: tectonic subsidence, eustasy variation, erosion and subsequent inorganic sedimentation are now controlling the accommodation regime, thus the signature of TOM accumulation as well. The TOM (sediment proportion) property map is deeply linked and co-dependent with other two output properties: the vadose zone thickness and the A/P ratio (Figure 43). In accordance with the philosophy of the model, organic sediment accumulation is guaranteed only in the portion of the profile where the following condition are both respected: wet environment and an A/P ratio between 0 and 1. Nevertheless, erosion might occur afterwards and the organic deposits could not be as homogeneous as the optimum area defined by the two previous output properties.

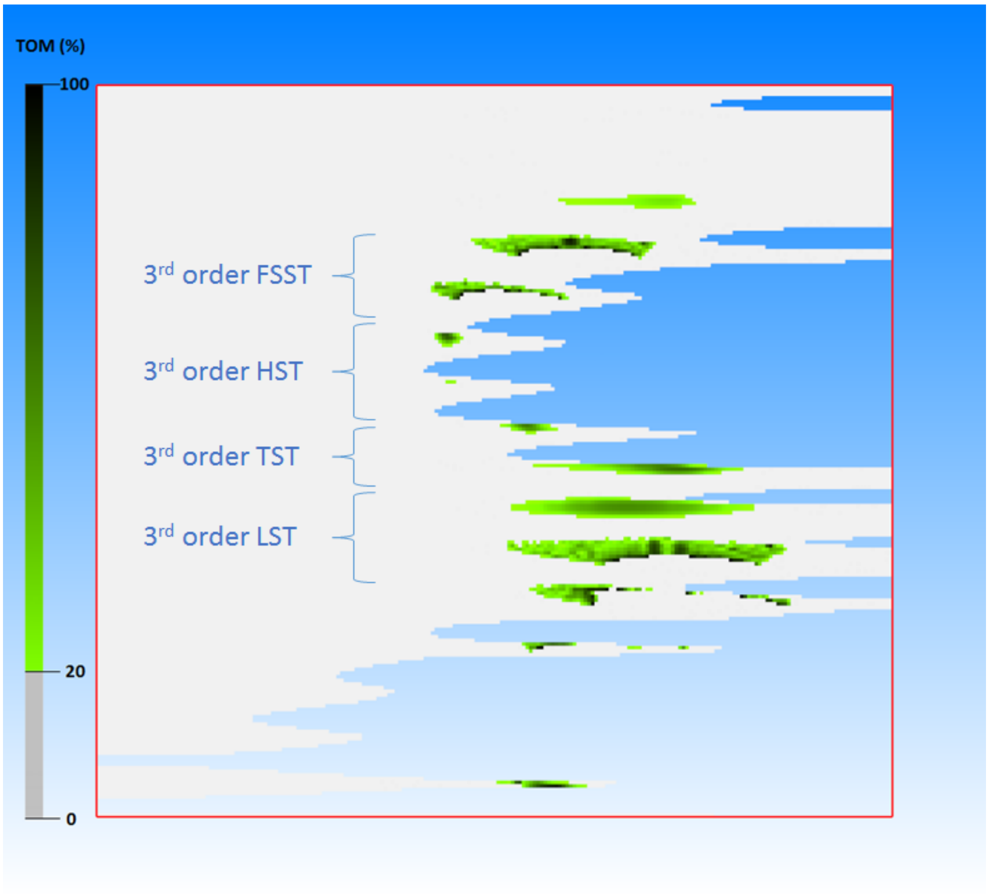

Figure 44 TOM (sediment proportion) output properties of the model out from project 3

The result above displayed is to be interpreted and compared with the peat accumulation model from Bohacs and Suter (1997), illustrated in Figure 45. As a matter of fact, peat production is not permanently linked with any system tract: in such particular scenario, TOM is accumulated accordingly with amplitude and frequency of different order cycles which build up the composite eustatic curve.

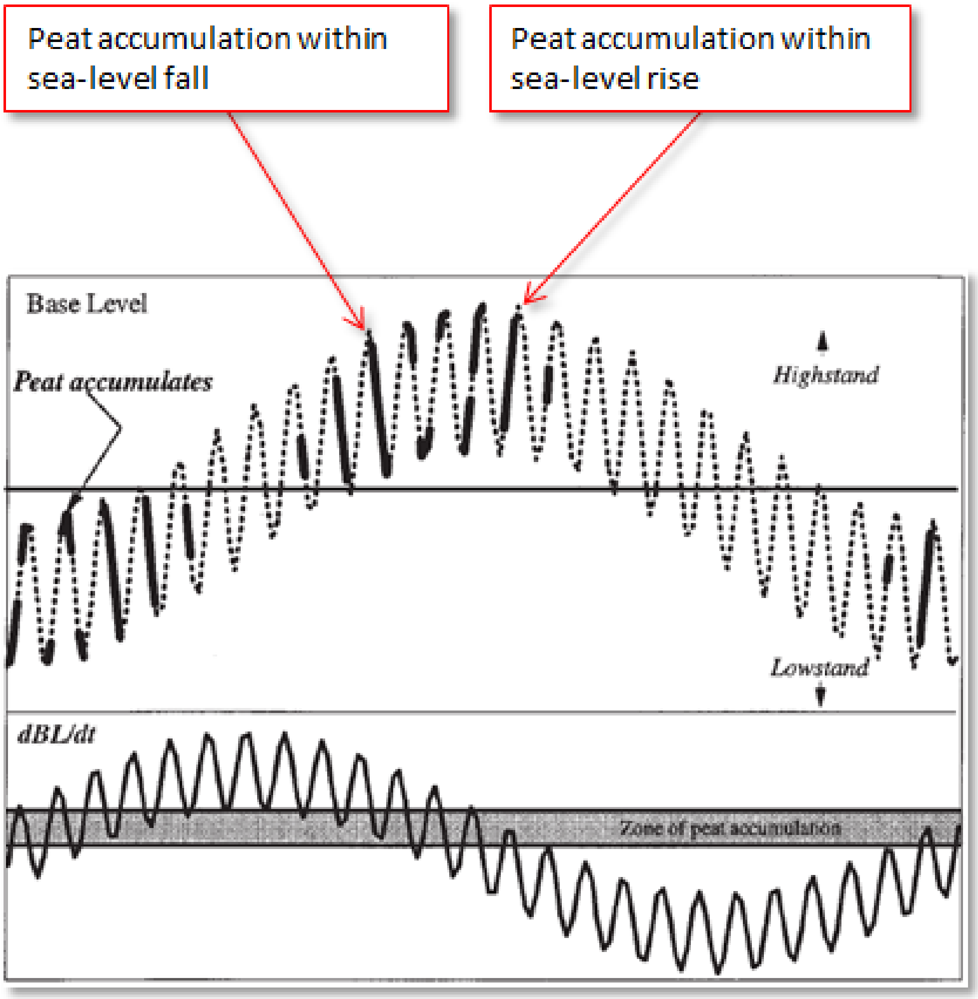

Figure 45 Sketch illustrating the connection between base level fluctuations, rate of sea level changes and peat window (defined by A/P ratio). Modified from eat production/accumulation model, Bohacs and Suter 1997

7.4 Project 4 – 3D scenario: a geologically reliable study-case

All the information collected during all of the previous surveys now converge in this project, which aims to demonstrate the connection between TOM deposits/coal seams and the stratigraphic framework.

Eustatic Curve				Subsidence Rate	Inorganic Sediment Supply / Erosion	Time Length
3rd Order Cycle		4th Order Cycle		30 m/Ma	Rainfall 480 mm/y	6 Ma
Amplitude	Period	Amplitude	Period			
20 m	3 Ma	10 m	0.8 Ma			

Table 8 Main input parameters in the model out of project 4

As it is displayed in Table 8, 2 eustatic curves were used to build the stratigraphic model, in addition to a moderate subsidence map and weathering processes. In addition, the RunOff option has been selected from DionisosFlow' sediment (TOM) tab, in order to prevent peat accumulation on rivers.

Bathymetry is displayed as property map in Figure 46. The shoreline transition, due to eustatic cycles, can be followed from the lateral section of the same output. It is also possible to appreciate the formation of a riverine delta, which demonstrates the validity of the result proposed. Sub-marine canyons are present as well. Figure 46 illustrates also another output property, the WaterFlow (superficial), to better visualize the riverine system and the submarine flows developed by the model.

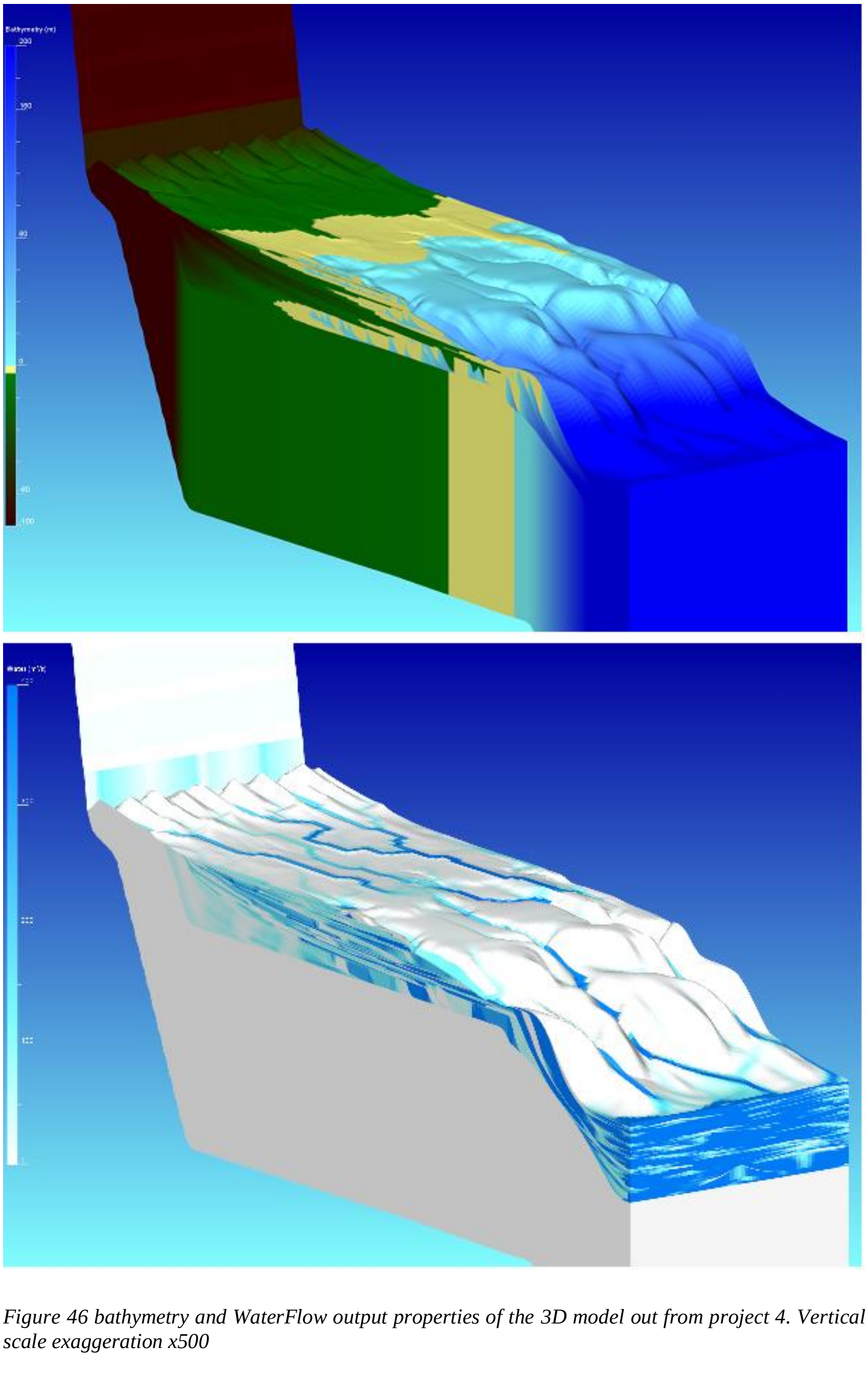

Figure 46 bathymetry and WaterFlow output properties of the 3D model out from project 4. Vertical scale exaggeration x500

A/P ratio and Vadose zone property maps are given in Figure 47. It is interesting to notice how the A/P ratio allows TOM accumulation all over on the continental area, whereas the vadose zone thickness restricts the potential peat accumulation area only in a narrower zone next to the shoreline.

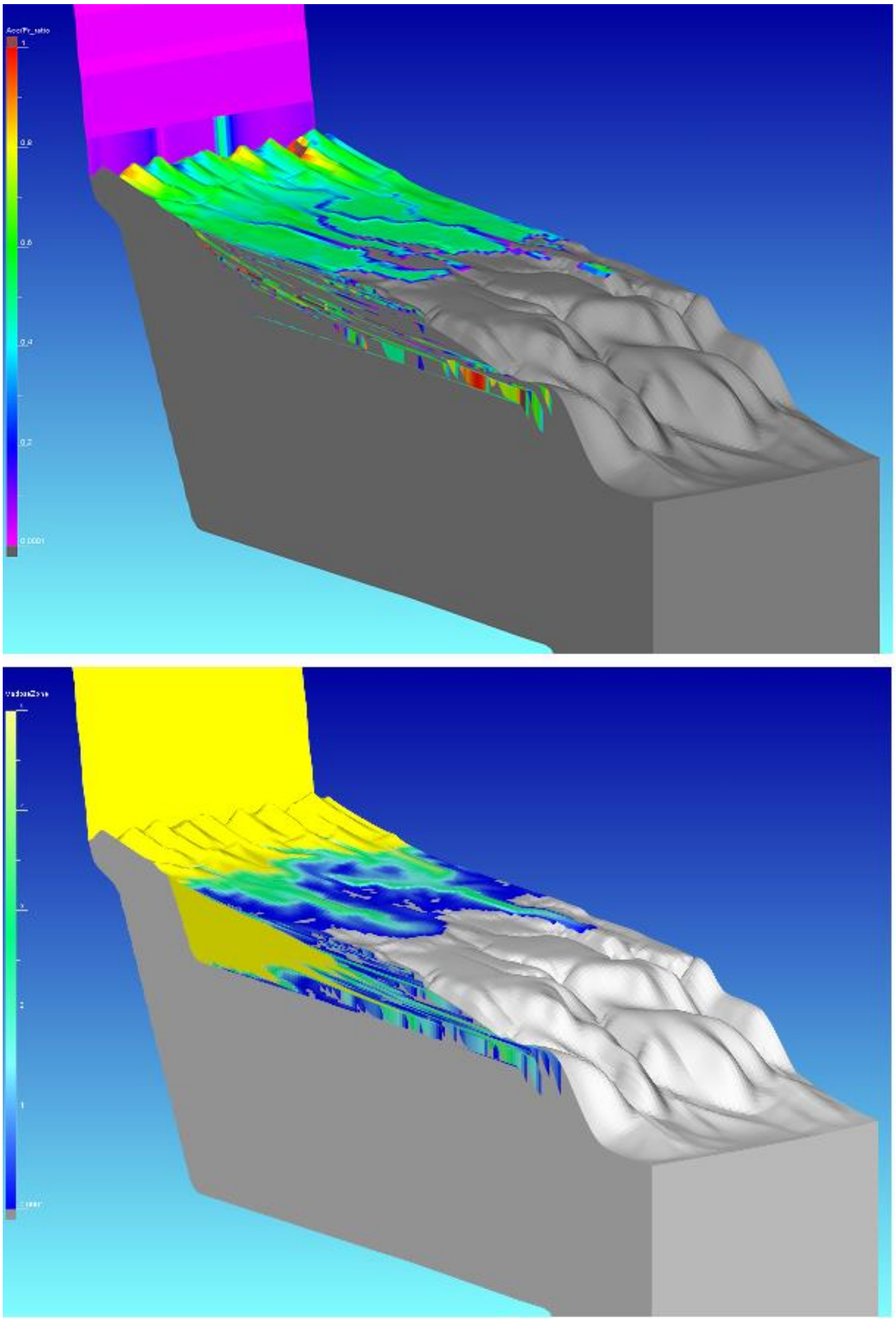

Figure 47 A/P ratio and Vadose Zone output properties of the 3D model out from project 4. Vertical scale exaggeration x500

The sedimentation rate is displayed as output property in Figure 48. This property map highlight in red the cells with a negative value, which means they are under an erosional regime: source areas of sediment supply and incise submarine valleys are distinguished by this reddish colour. Grey-green areas describe a part of the model where the sedimentation rate is very low. Furthermore, because we are dealing with a low gradient profile, this particular area might be described as a paralic zone. The last property map is the TOM percentage included within the sediment, illustrated as well in Figure 48.

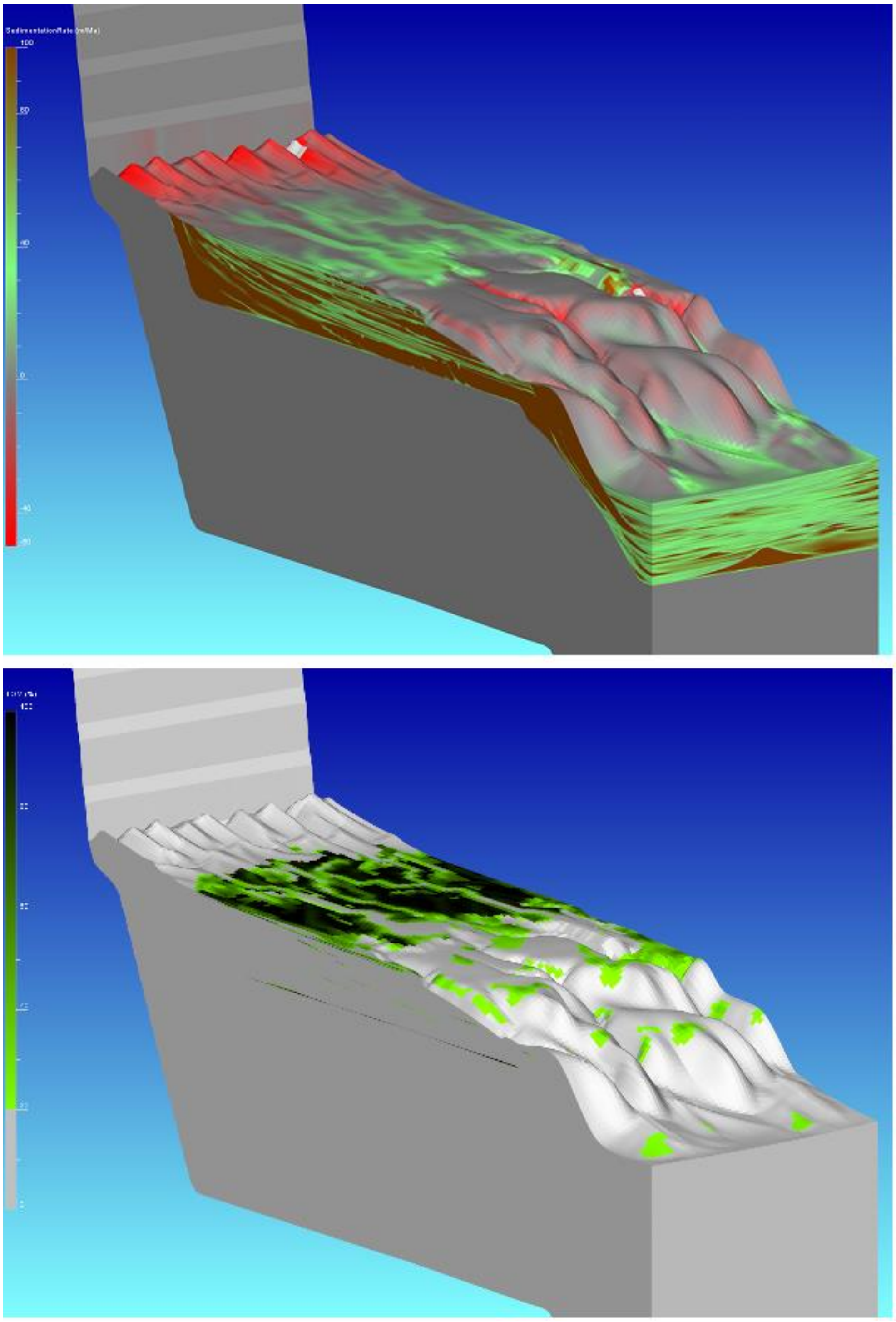

Figure 48 Sediment rate and TOM (sediment proportion) output properties of the 3D model out from project 4. Vertical scale exaggeration x500

According to what we have described so far, TOM accumulation occurs in those areas of the model characterized by a low runoff value (thus organic sedimentation in rivers is excluded), an A/P ratio between 0 and 1, a vadose zone thickness below 5 meters and a positive sediment rate (no TOM accumulation takes place in erosion zone. Figure 49 represent the TOM property map but in this case, we applied a filter to put in evidence those cells which contain at least 70% of TOM, hence, on first approximation, coal.

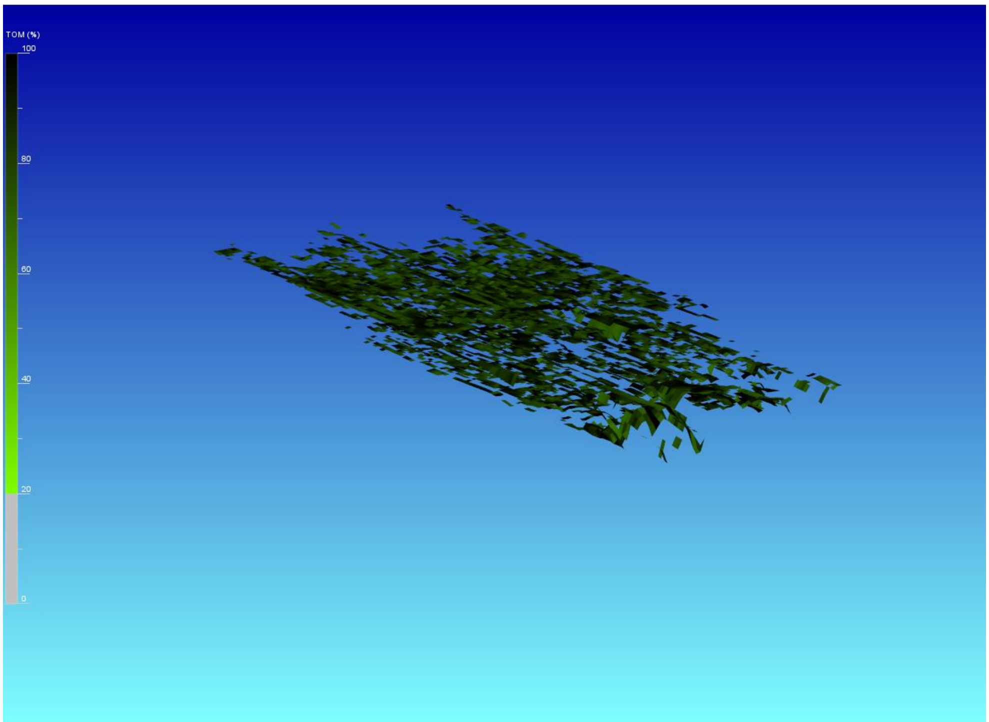

Figure 49 TOM (sediment proportion) property map, filtered by TOM > 70%. Vertical scale exaggeration x500

The same data has been then subdivided in the 4 system tract that composes a stratigraphic sequence (Figure 50), with the purpose of studying the coal signature along the simulated framework. As we were expecting, no significant coal deposits are formed during a marine regression, although relatively thin and widespread coal seams are preserved during the lowstand system tract. Isolated deposits appear during the subsequent sea level rise but it is during the highstand system tract that widespread and continuous thick coal seams are produced.

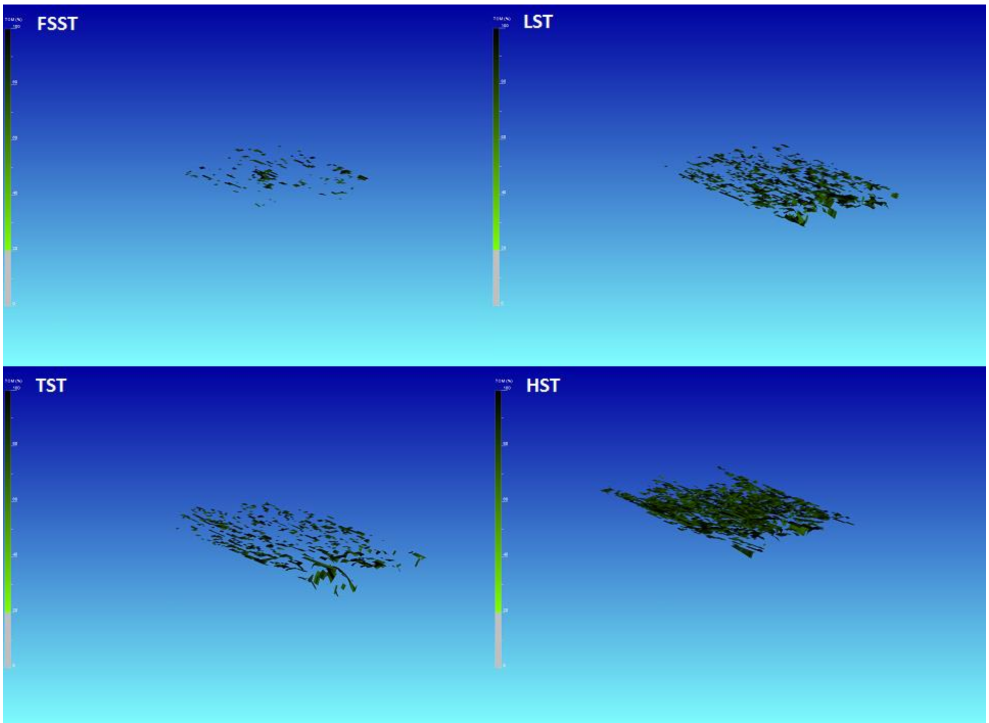

Figure 50 TOM (sediment proportion) subdivided in the system tracts that compose a stratigraphic sequence

8. Conclusions

This study used geological information available from literature to recreate, through DionisosFlow simulations, a properly sedimentation environment for terrestrial organic matter. The focus was to identify and describe the main control parameters that affect the accommodation regime in which peat accumulation takes place. The conceptual model proposed by Bohacs and Suter (1997) was used to construct the methodology of a numerical model dedicated to terrestrial organic matter production and preservation. This model, still under construction at the beginning of this work, was modified and finally validated thanks to the numerous discussions and to the numerical tests presented in this report. In particular, one of the main difficulties was to build a model controlled by real physical parameters whereas the Bohacs and Suter model was built on the concept of accommodation space, which is more a geological parameter than a physical one.

In the model used for this work, the hydrodynamic regime is now the golden spike for the correct evaluation of potential organic matter deposit. Furthermore, the water table dynamics allow us to infer about the preservation of the TOM, as a wet environment (nearly or totally water-saturated soil) must be maintained through time to enhance the formation of a thick deposit of organic sediment. All the sub-depositional environments proposed by Bohacs and Suter (1997) have been successfully represented in both synthetic and more complex stratigraphic models. Different subsidence maps, 3rd & 4th order cycles and weathering processes have been properly used to recreate an ideal depositional framework in which coal accumulation takes place.

Normally the formation of TOM deposits is observed in environments characterized by a static or slightly rising water table. The most evident geological situations which reflect such condition are the late-LST and the early-HST of a stratigraphic sequence. Nevertheless, this specific stratigraphic framework is not a constrain: as we observed thanks to the simulations we performed, the accommodation regime that allows the accumulation of TOM sediment bodies is related to several control parameters: the groundwater table fall driven by a marine regression might be compensated by a high subsidence rate and TOM accumulation could take place.

TOM deposits are thus correctly displayed within a stratigraphic framework where the organic sediment preservation required is guaranteed by the accommodation creation regime which is controlled, in turn, by eustasy variations, tectonic subsidence and inorganic sedimentation rate. Ultimately, TOM deposits are developed when the accumulation rate is balanced by the accommodation space creation rate.

9. Future Perspective

This work presents the validation of a method which simulates the in-situ accumulation of the terrestrial organic matter. The validation has been done qualitatively and semi-quantitatively based on synthetic case studies. Future investigations could consist in building a real case study. A preliminary work has already been done at IFPEN on the Mannville Group (Canadian). Another field of improvement would be to validate the exported terrestrial organic flux in the marine realm. In particular, it would be interesting to know if this model reproduces also correctly the exported terrestrial organic flux, taking into account the net accumulation and then the transport, or if we need to de-correlate the production from the degradation to model the production-transport-degradation sequence.

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12. Appendix – Project 2 Results

This chapter gathers all the results obtained from project 2. The most relevant output properties are Vadose Zone (thickness), A/P Ratio, TOM (sediment proportion) and Sediment Rate and they are all displayed for each calibration. Details in regard to the various input parameters are available in Table 3 (Chapter 7.2).

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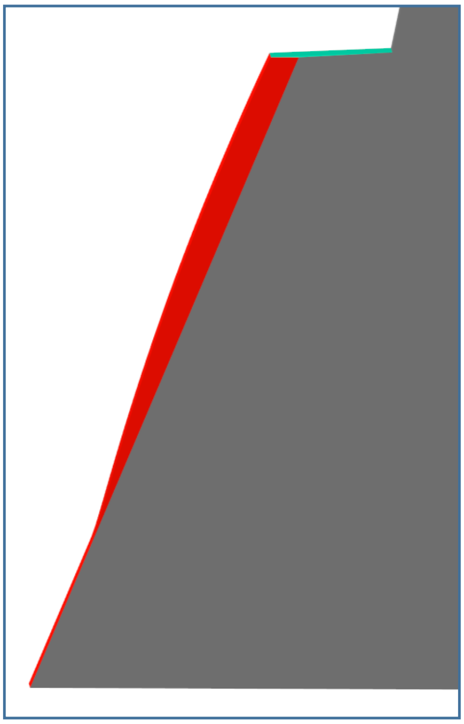

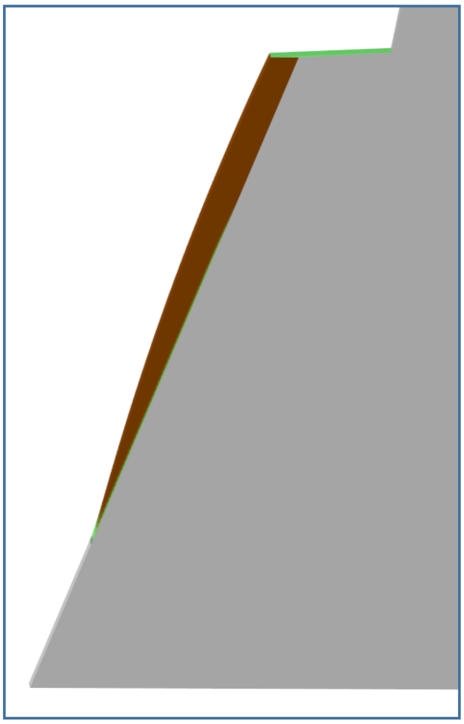

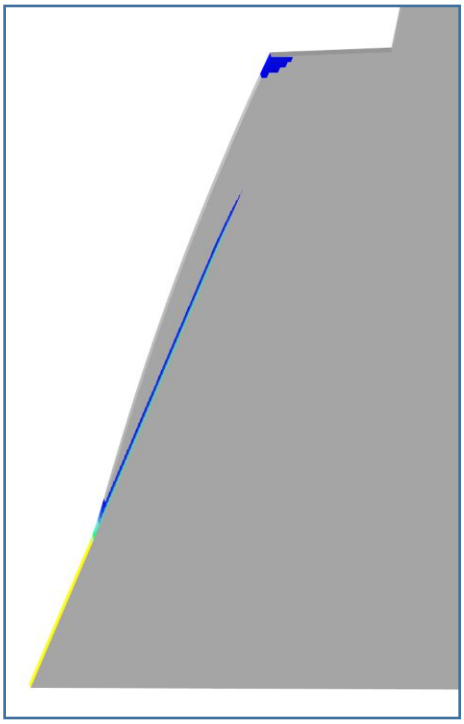

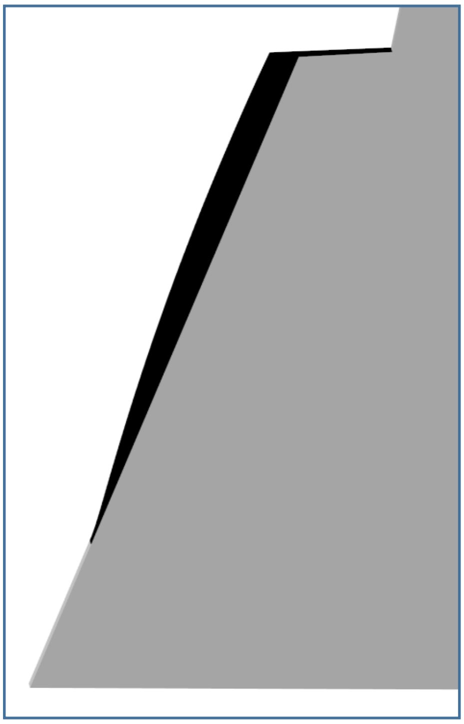

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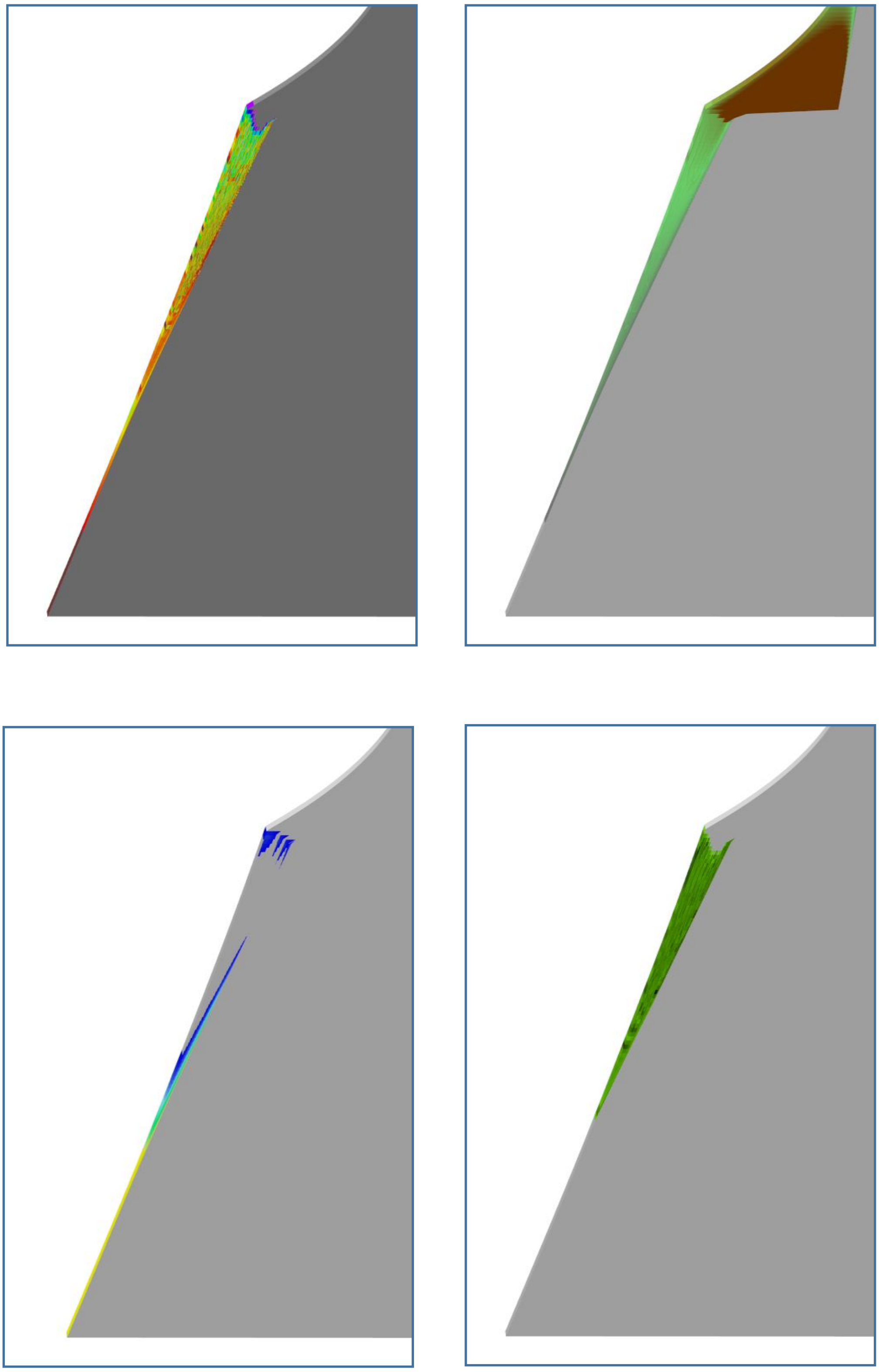

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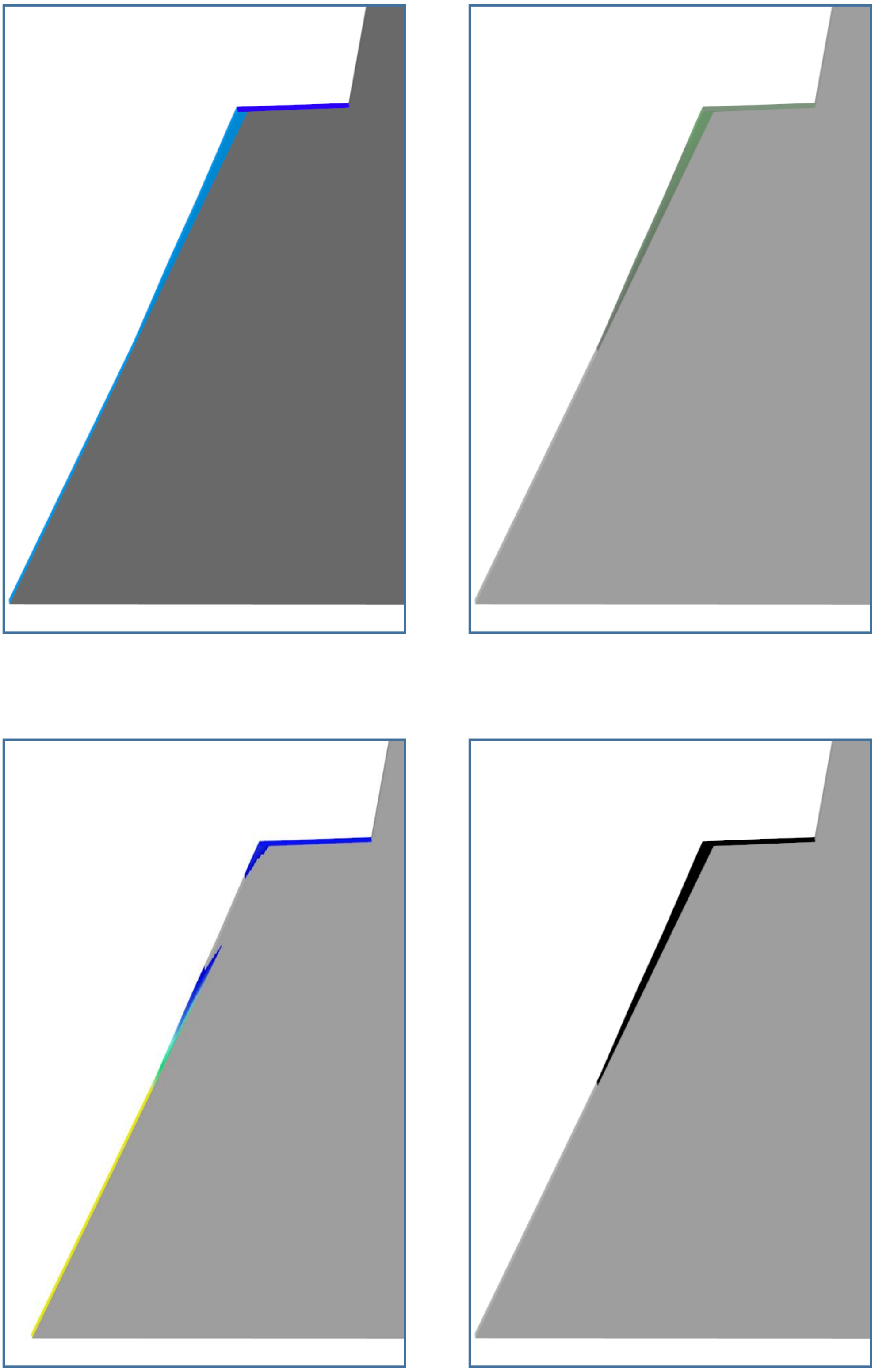

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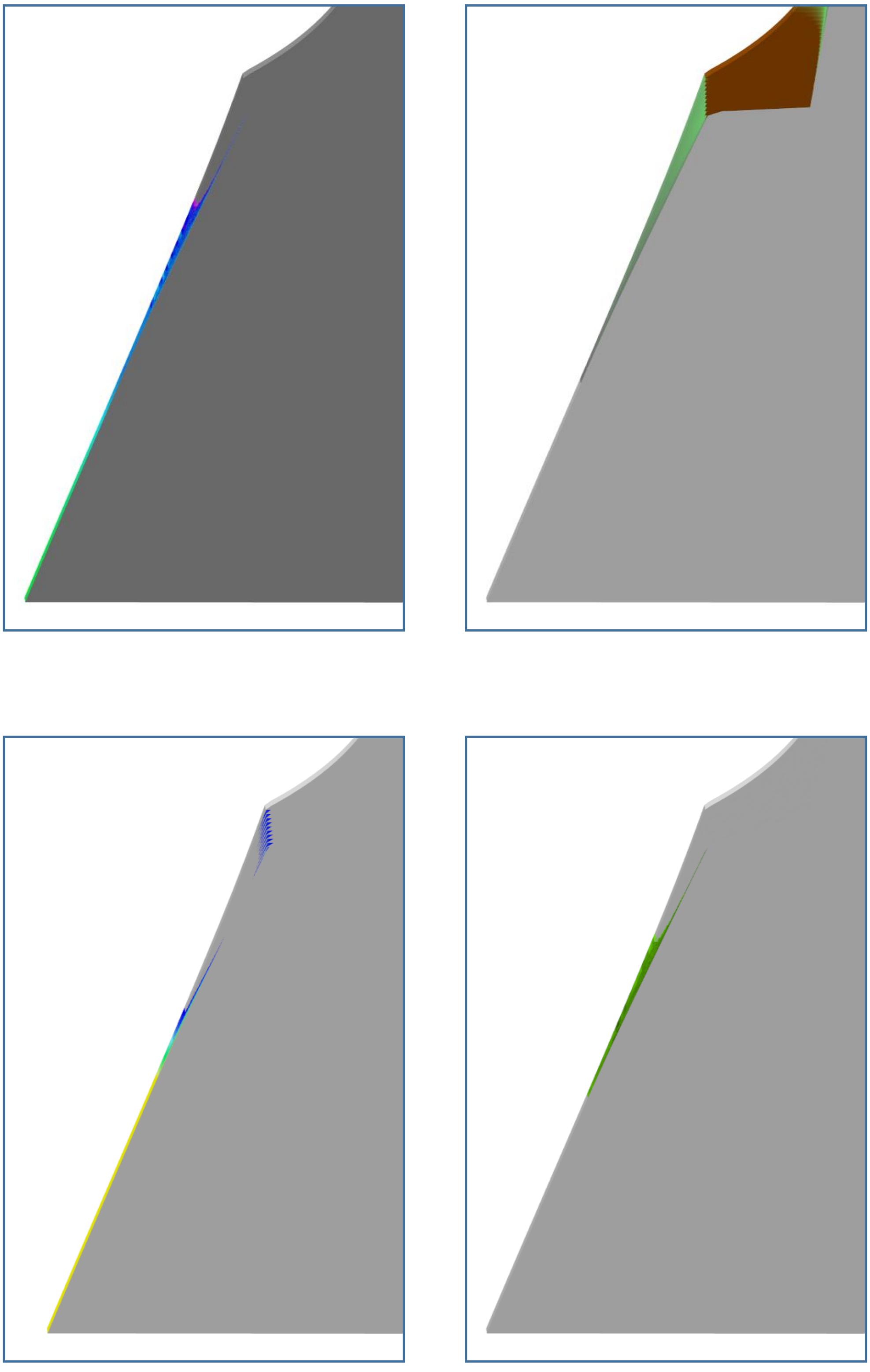

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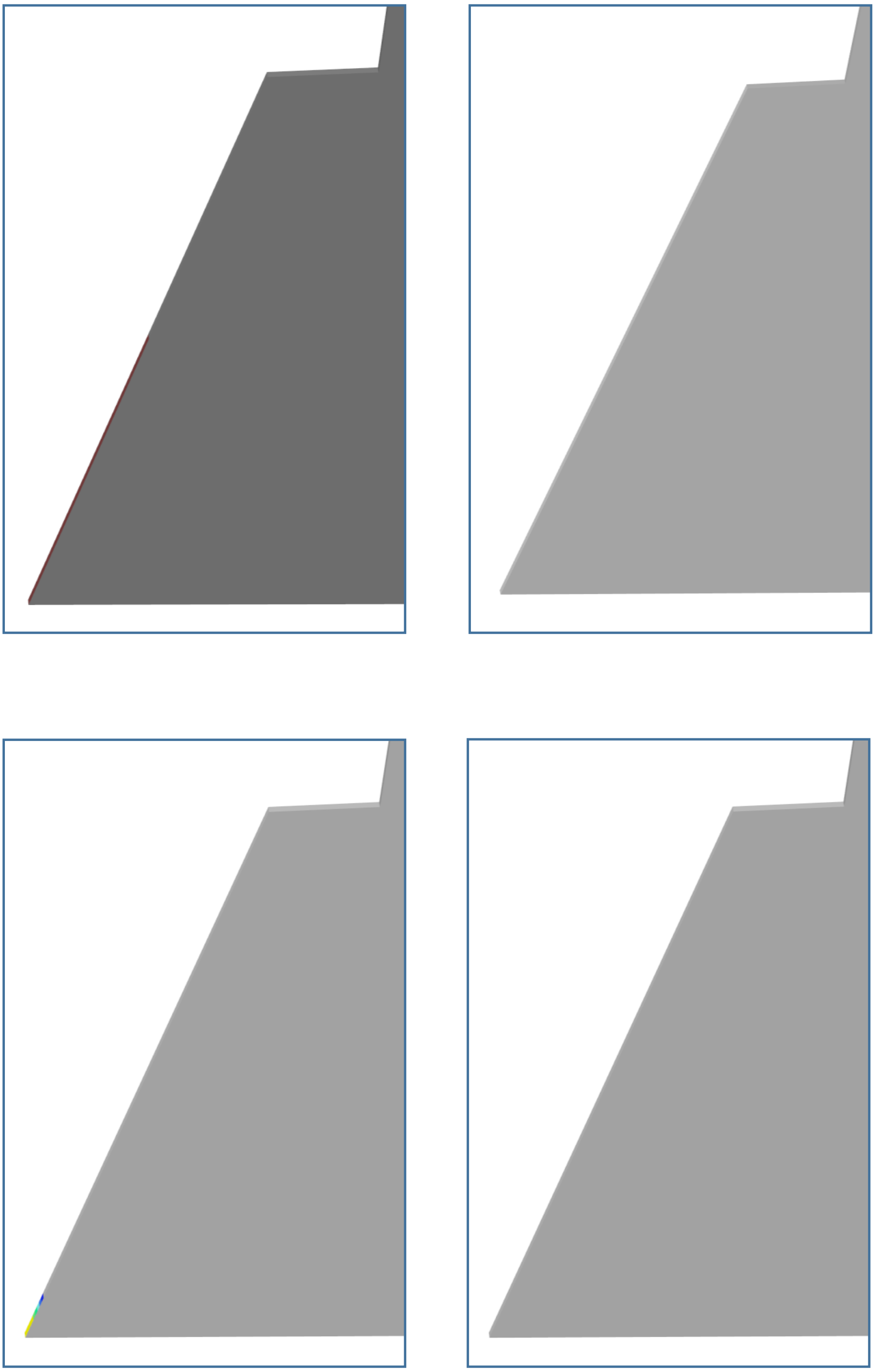

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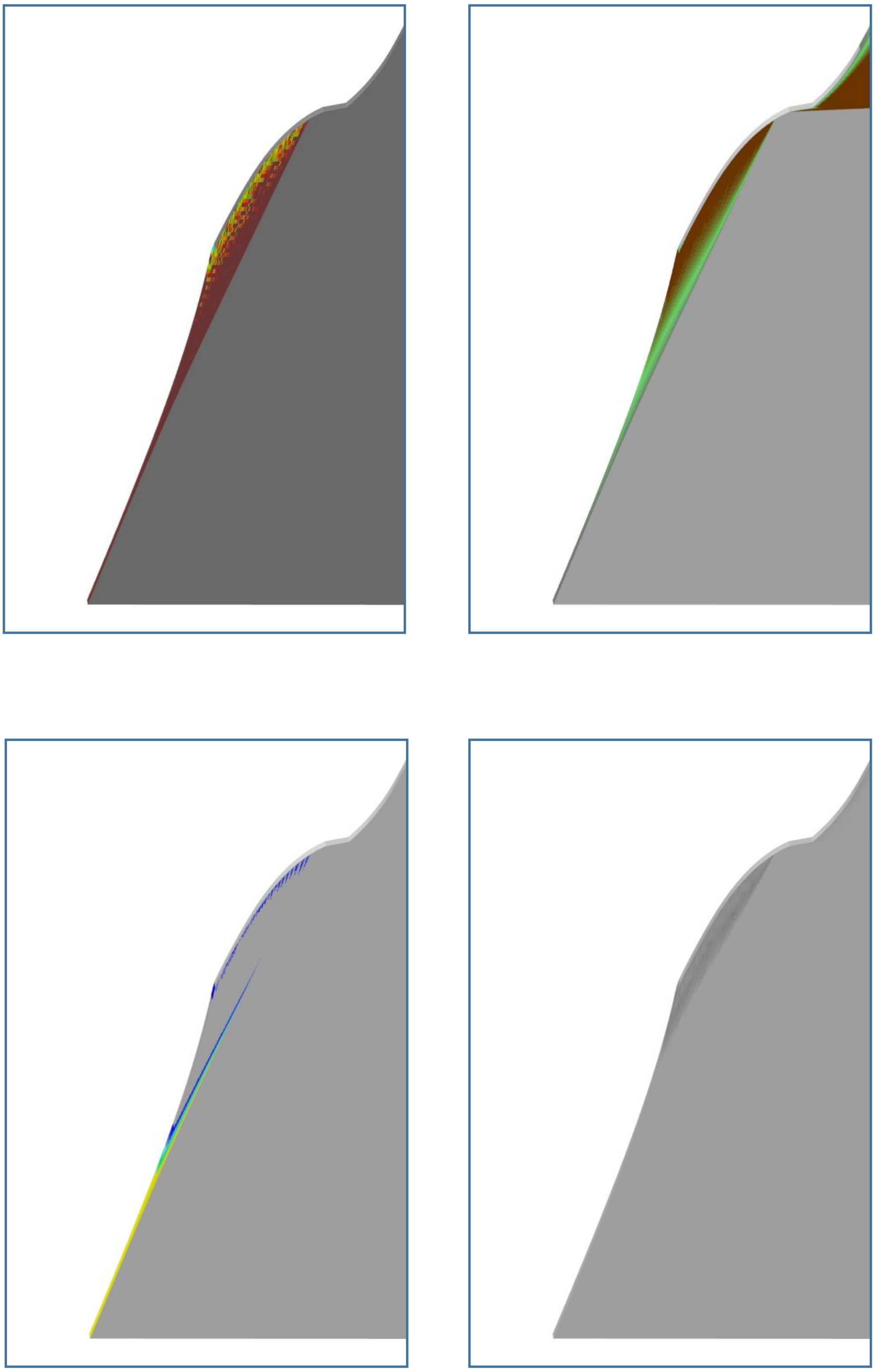

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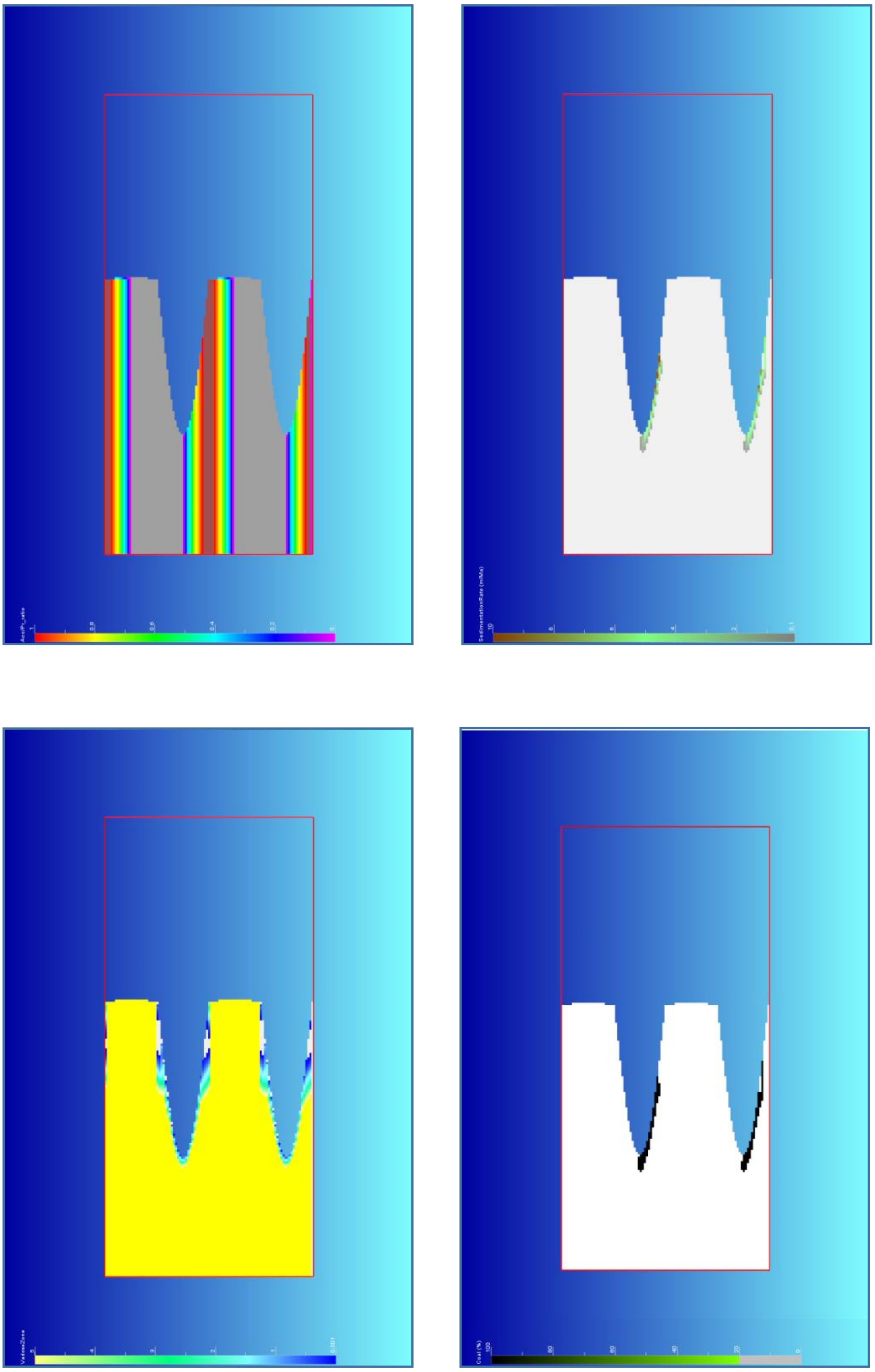

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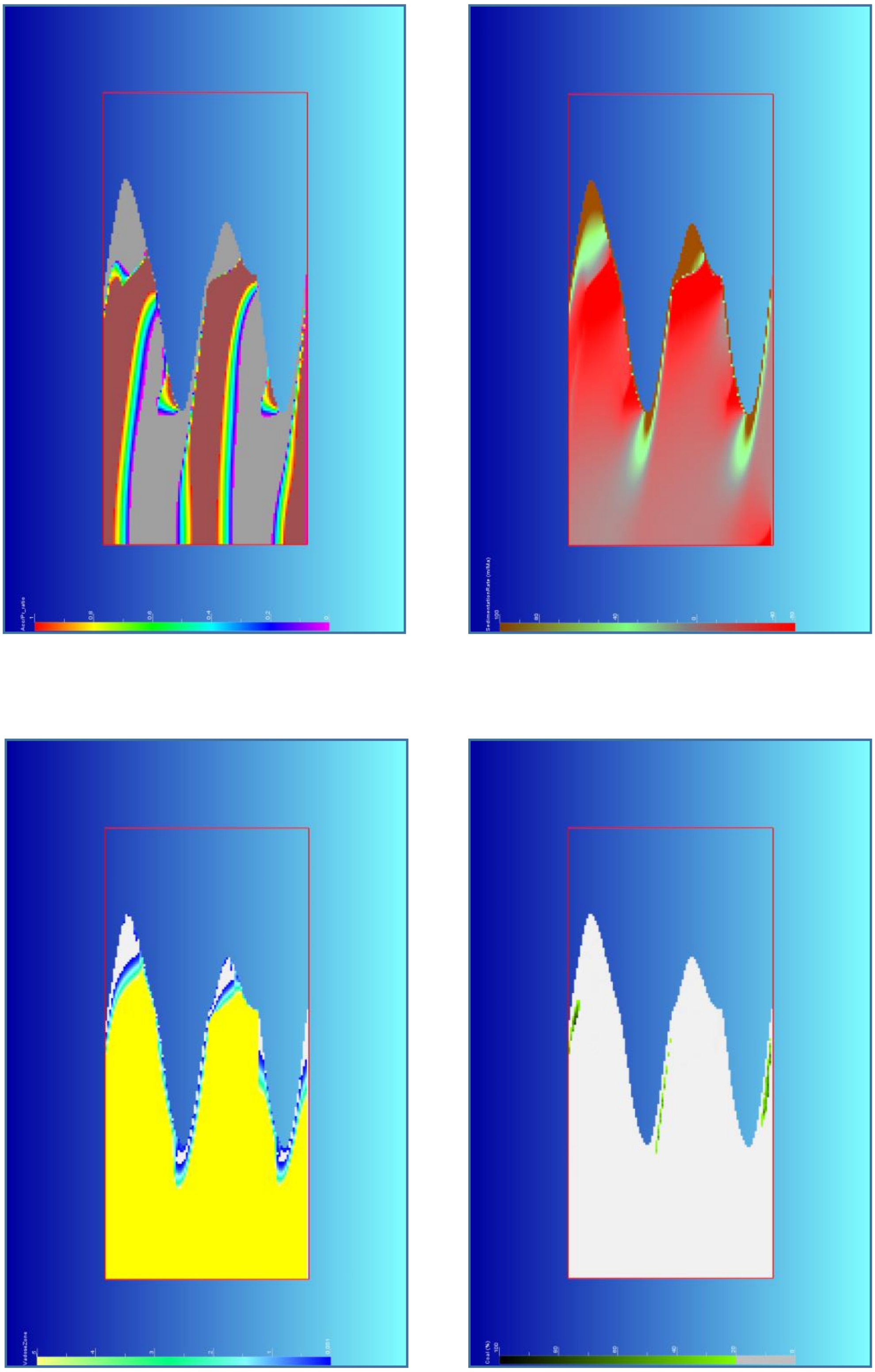

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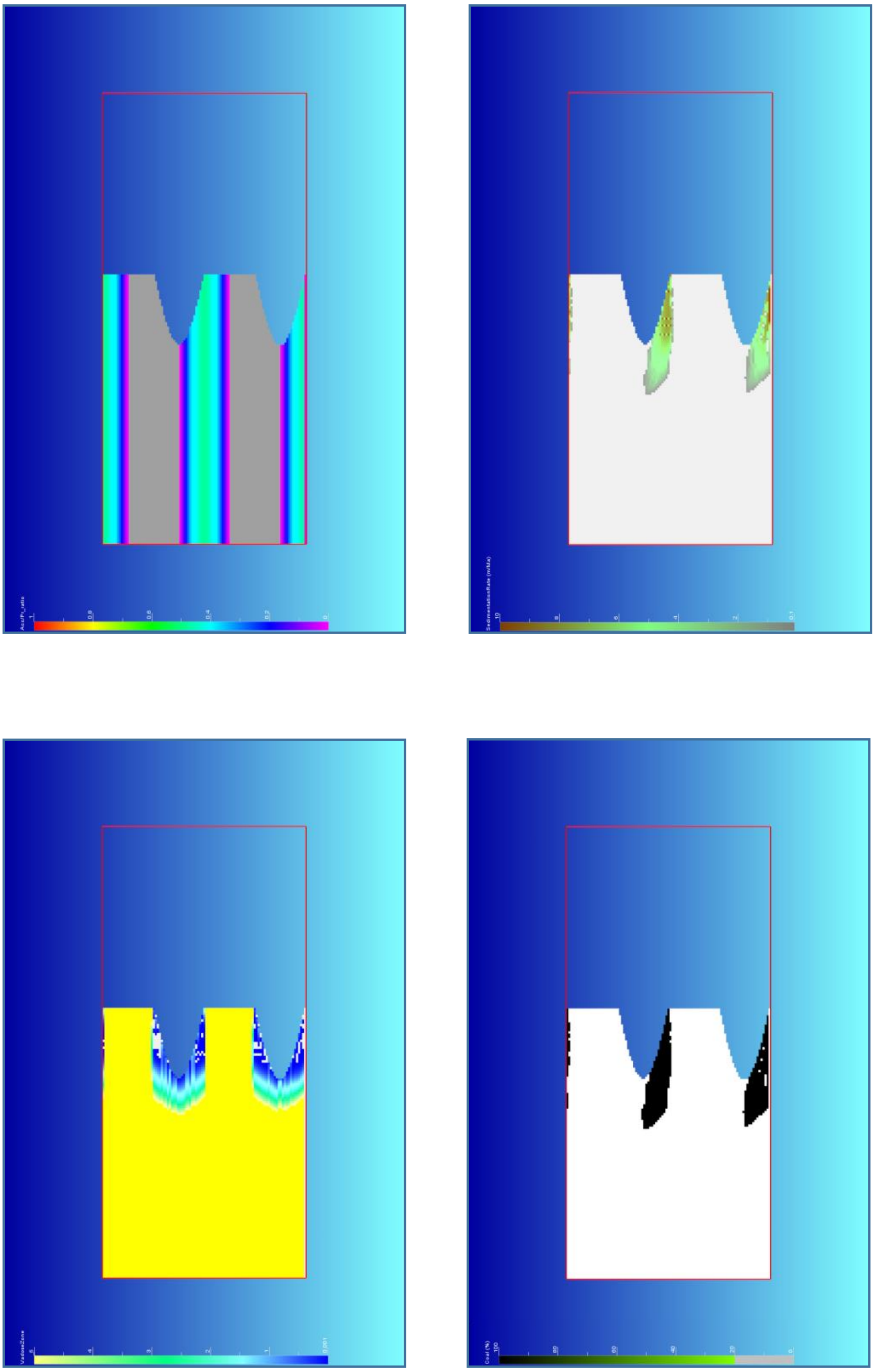

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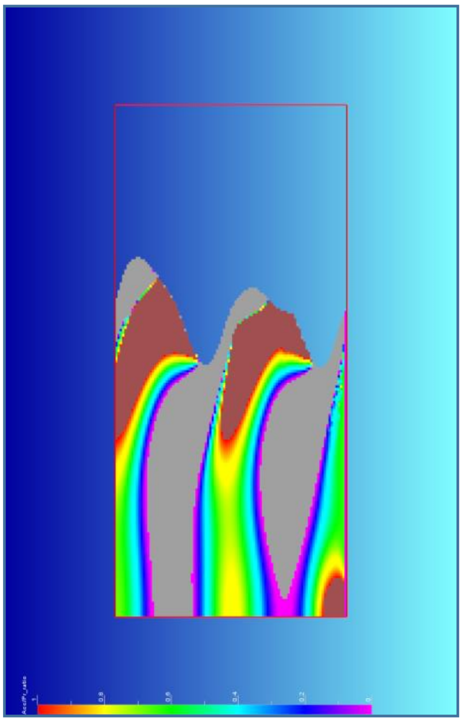

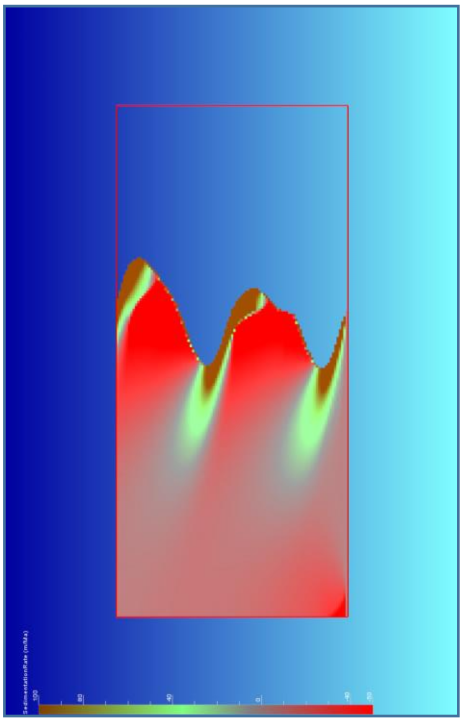

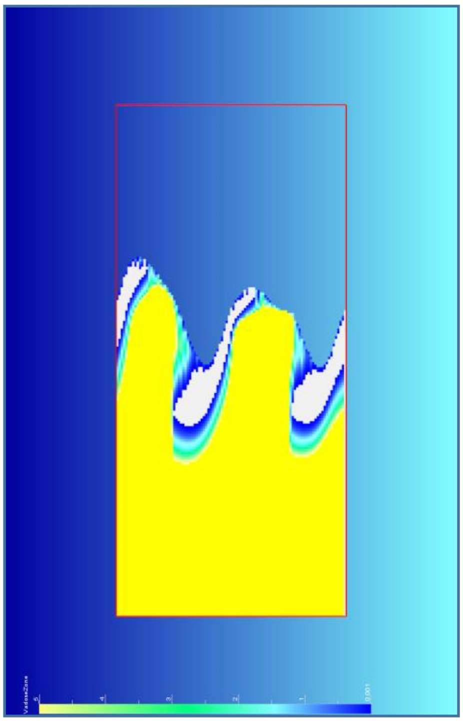

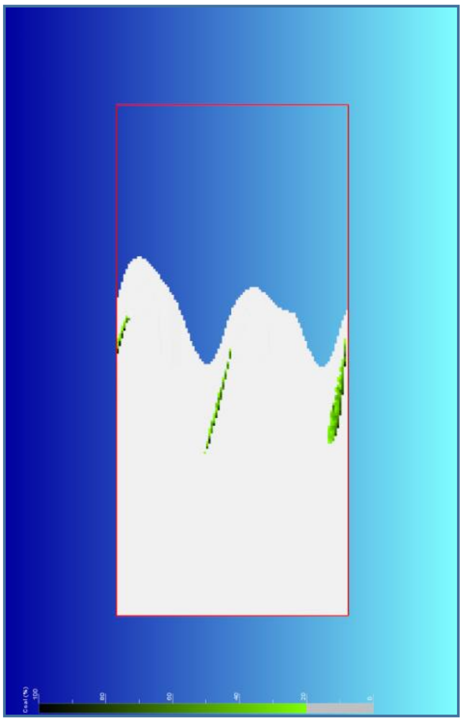

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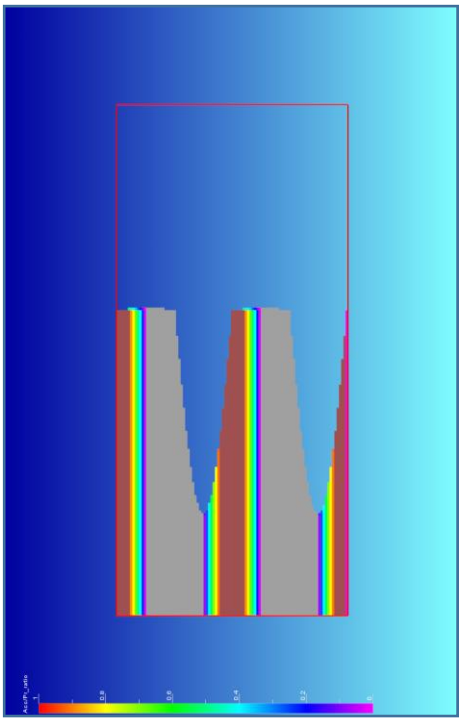

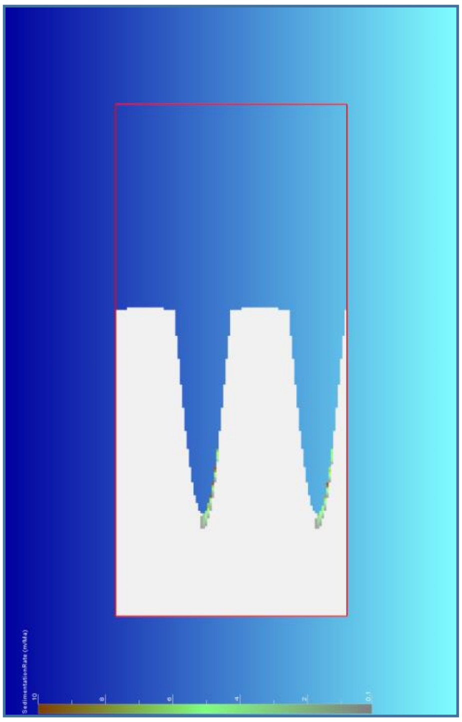

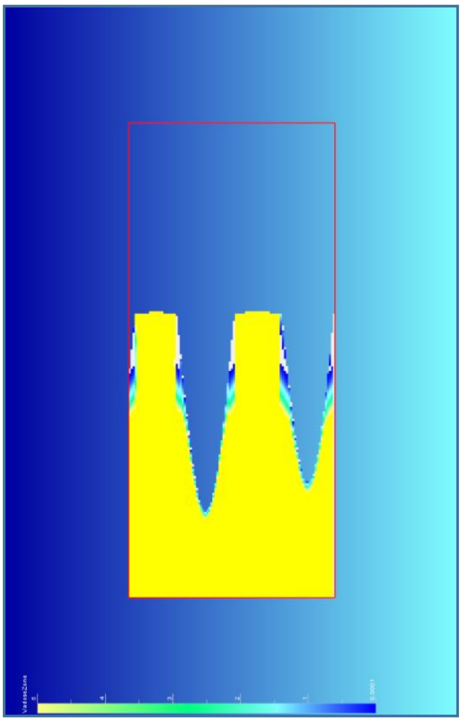

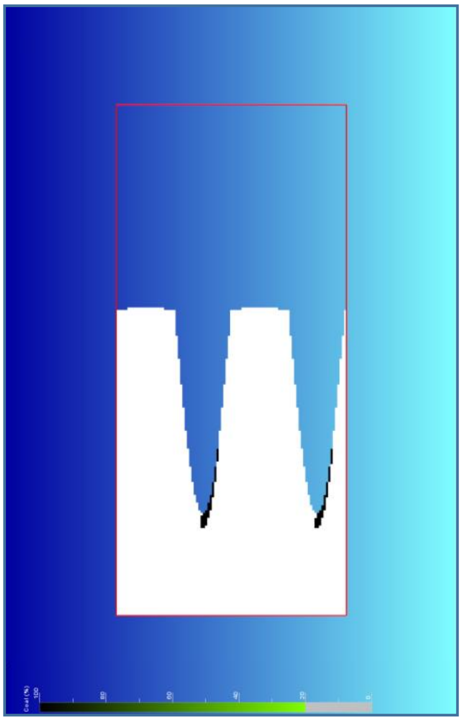

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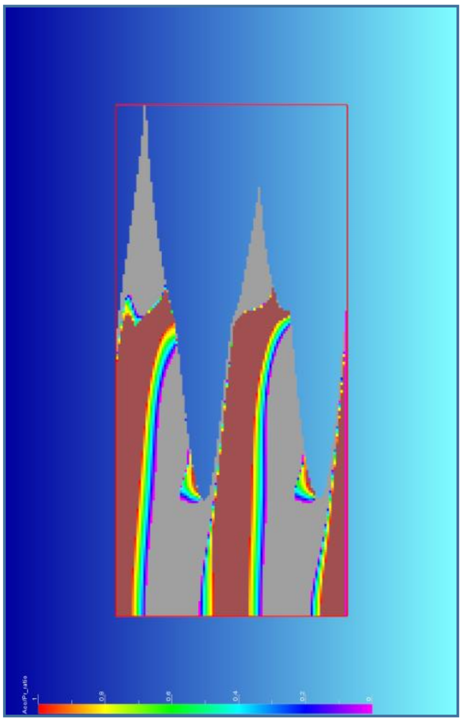

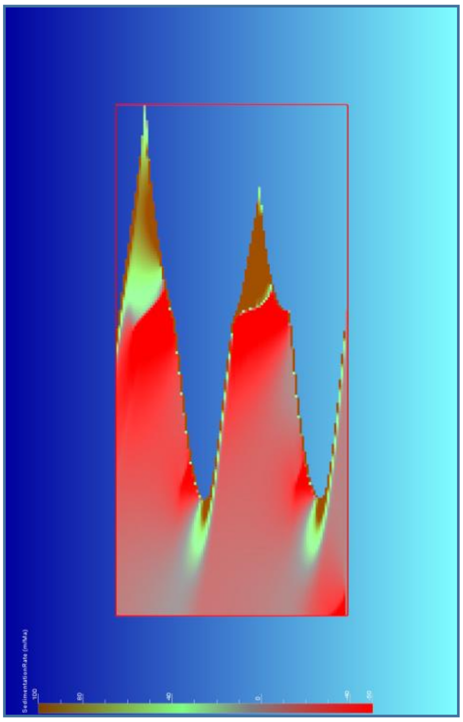

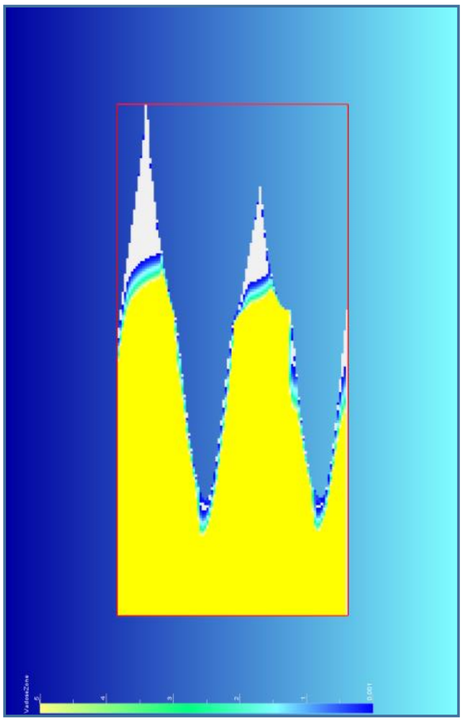

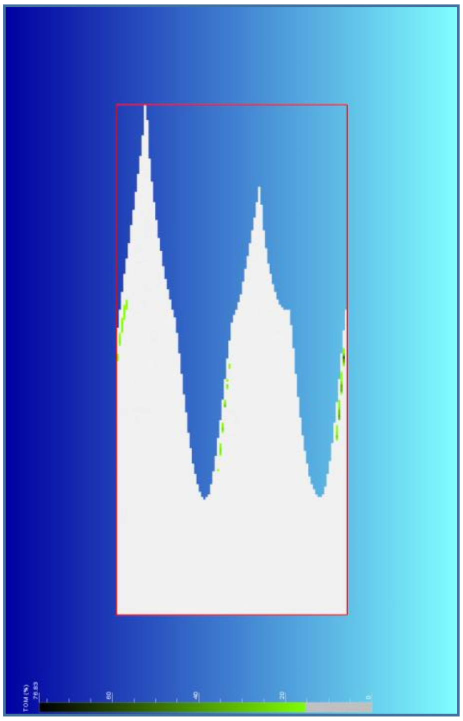

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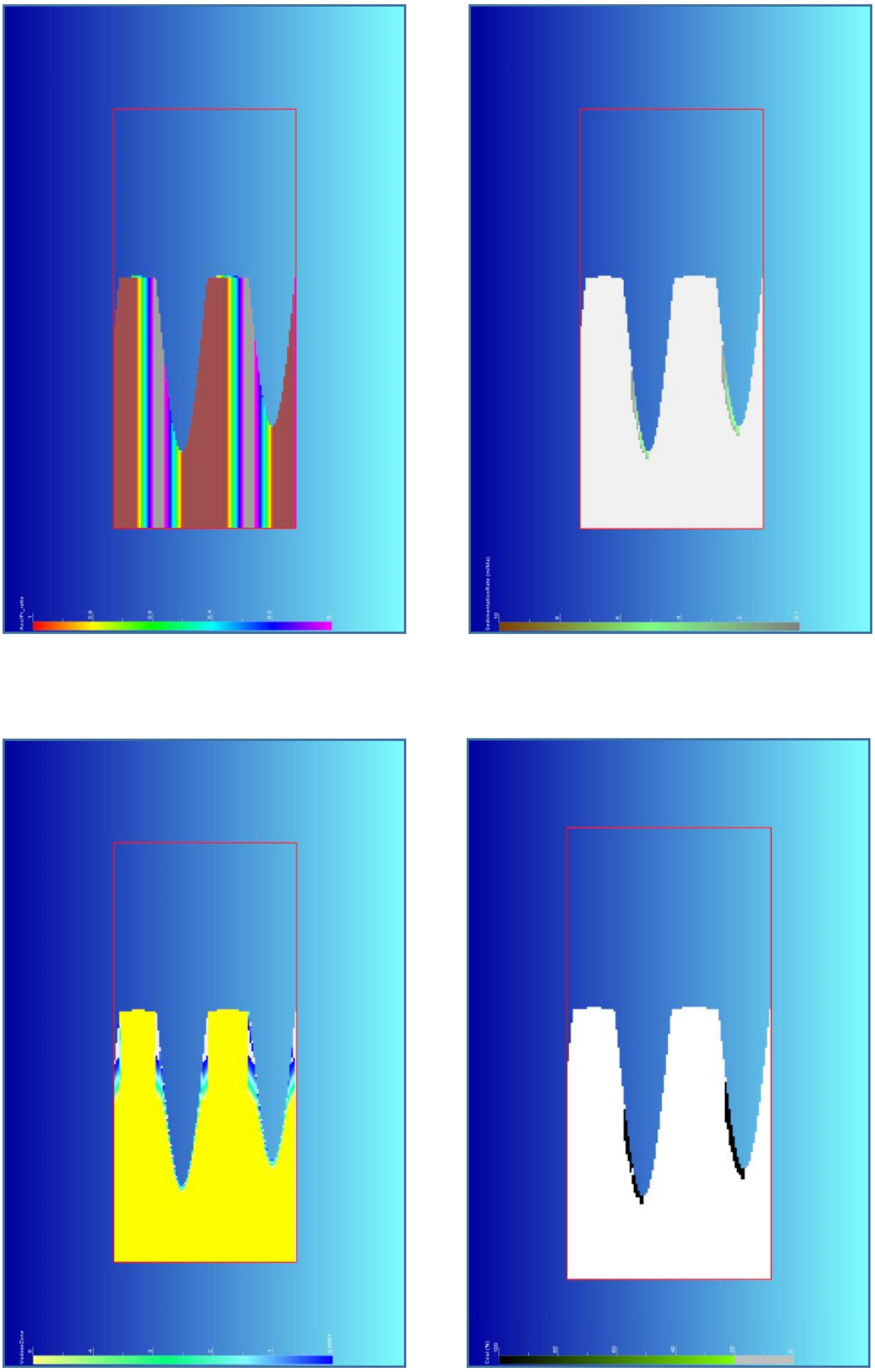

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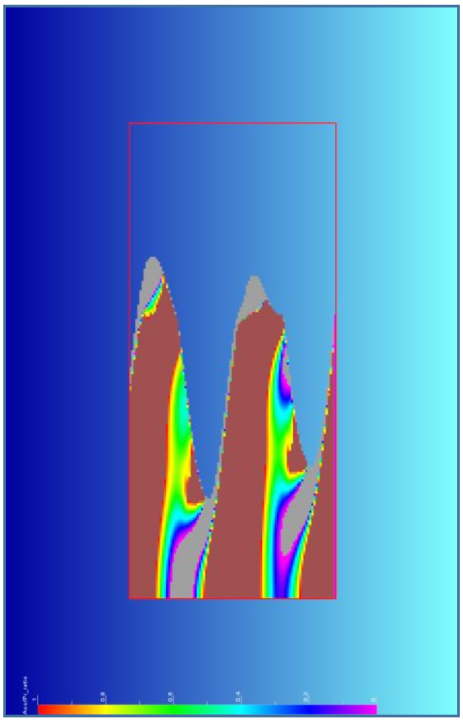

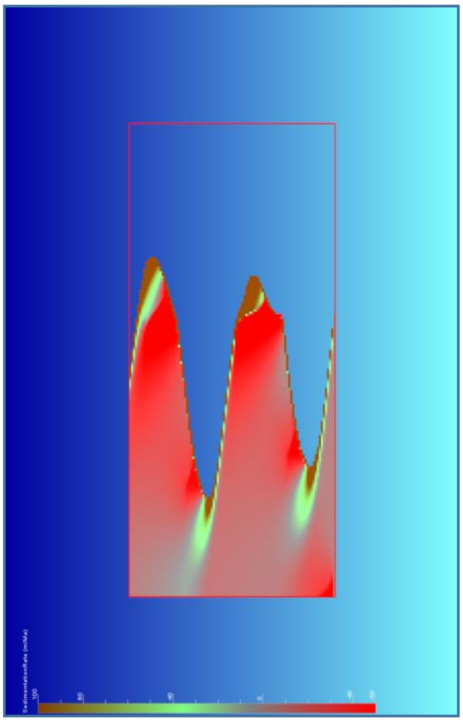

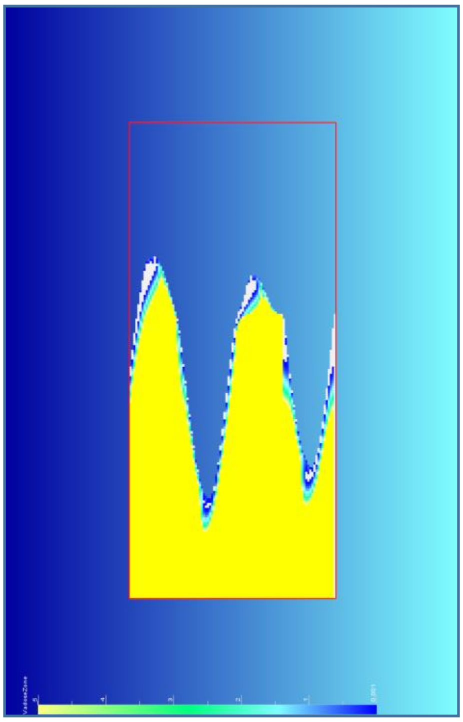

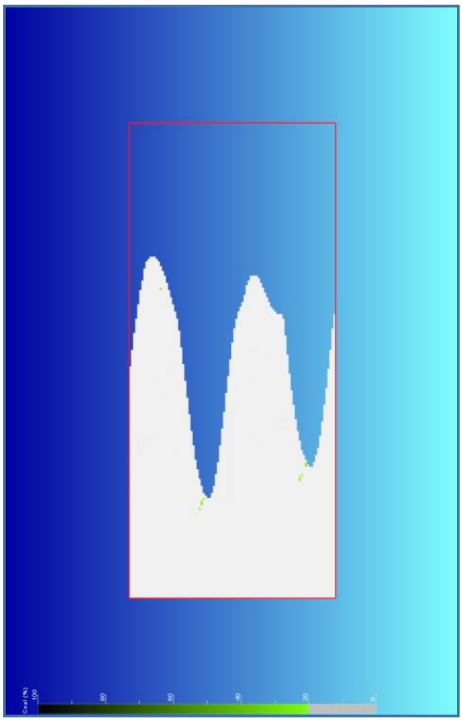

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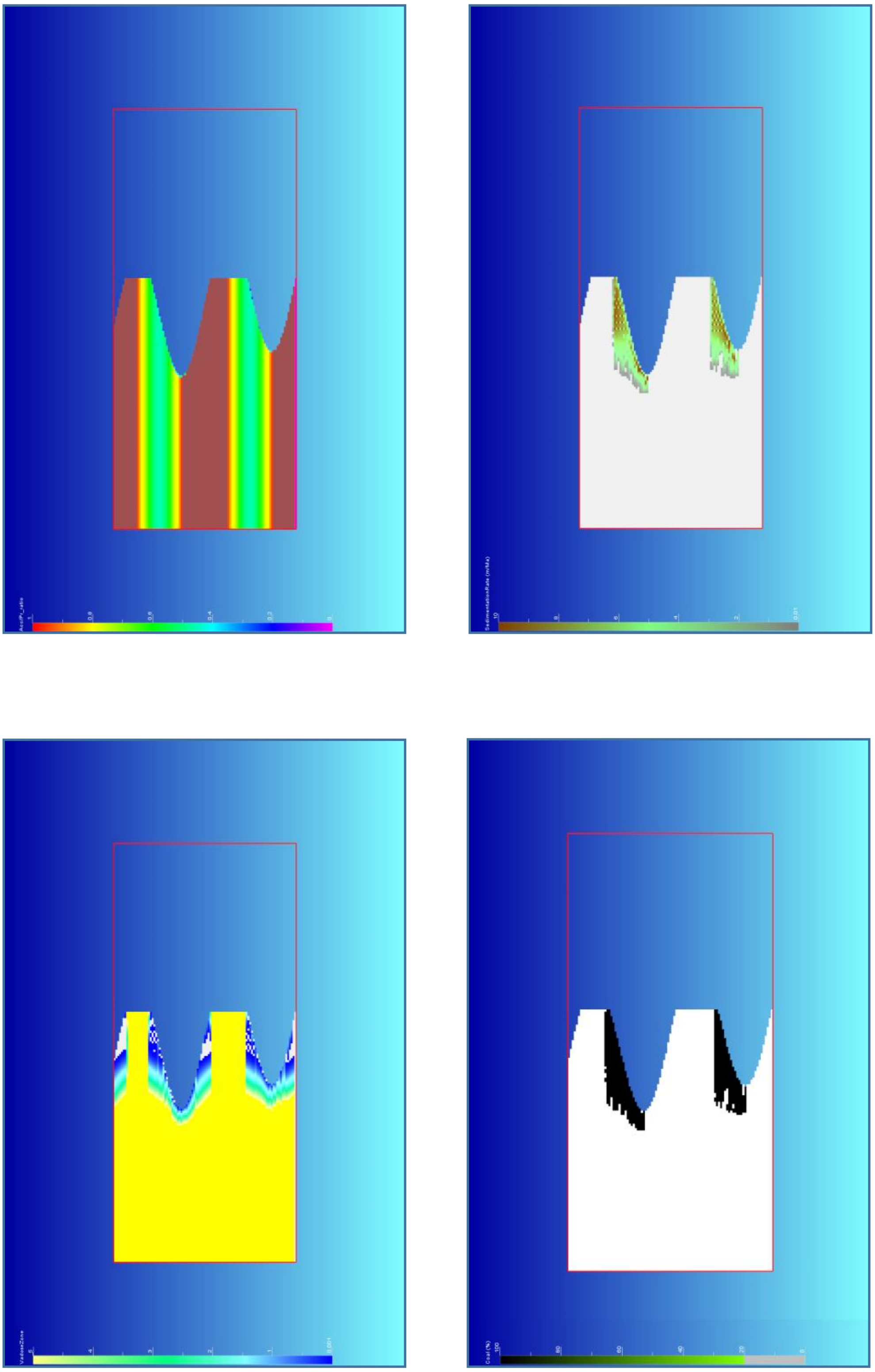

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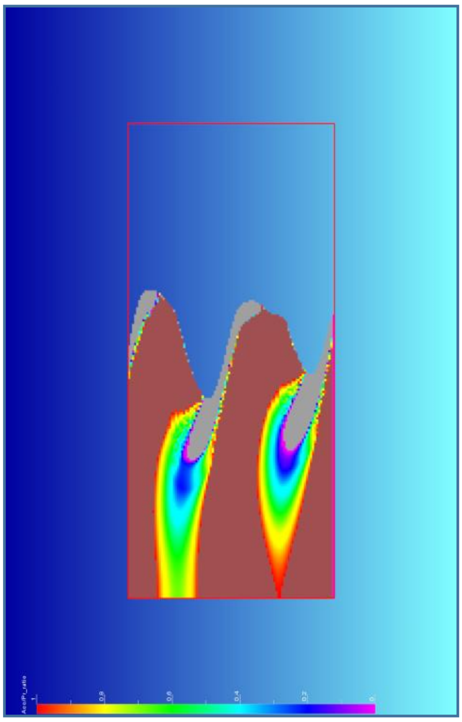

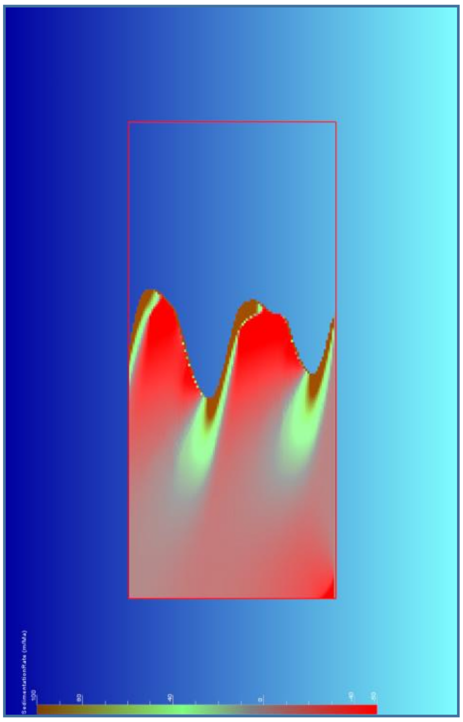

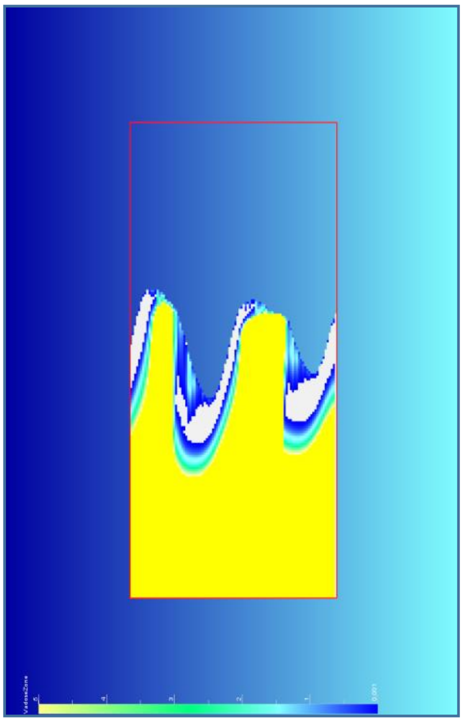

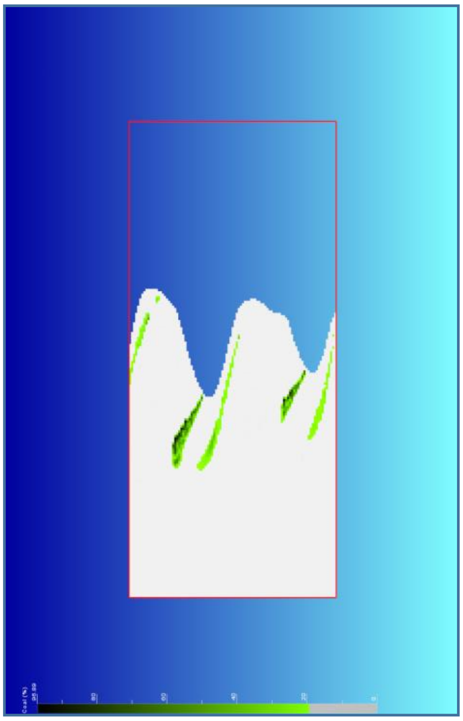

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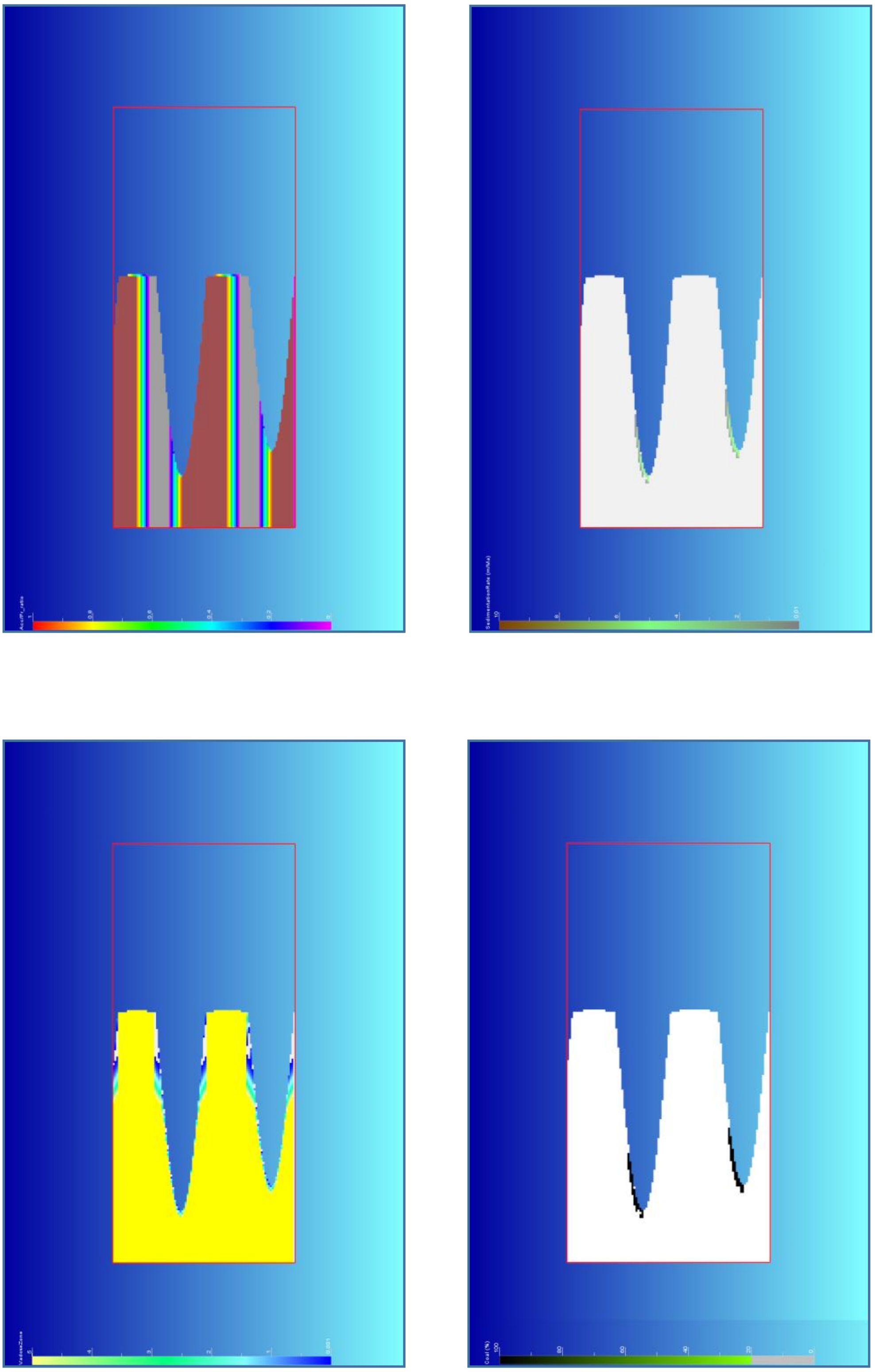

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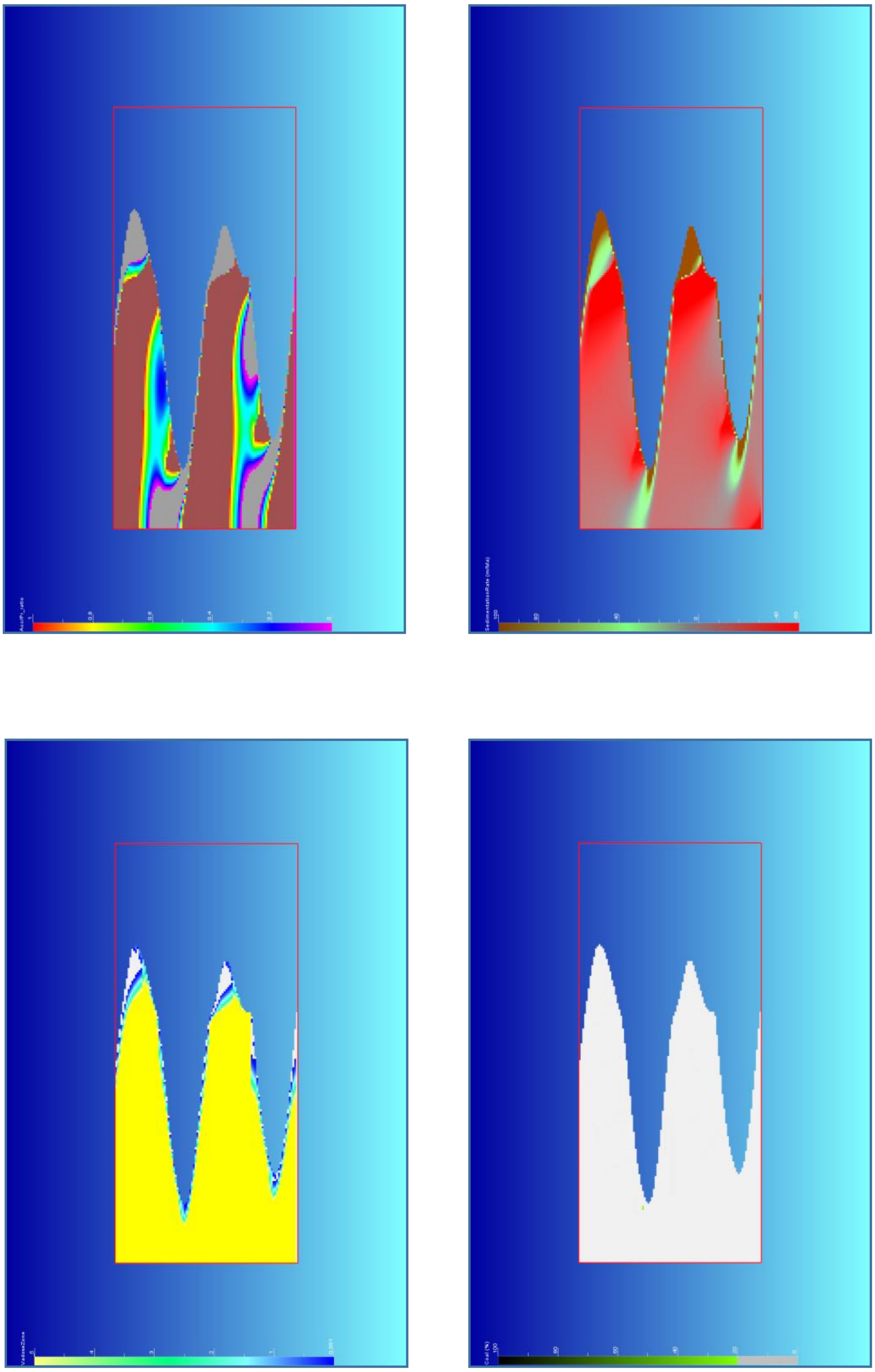

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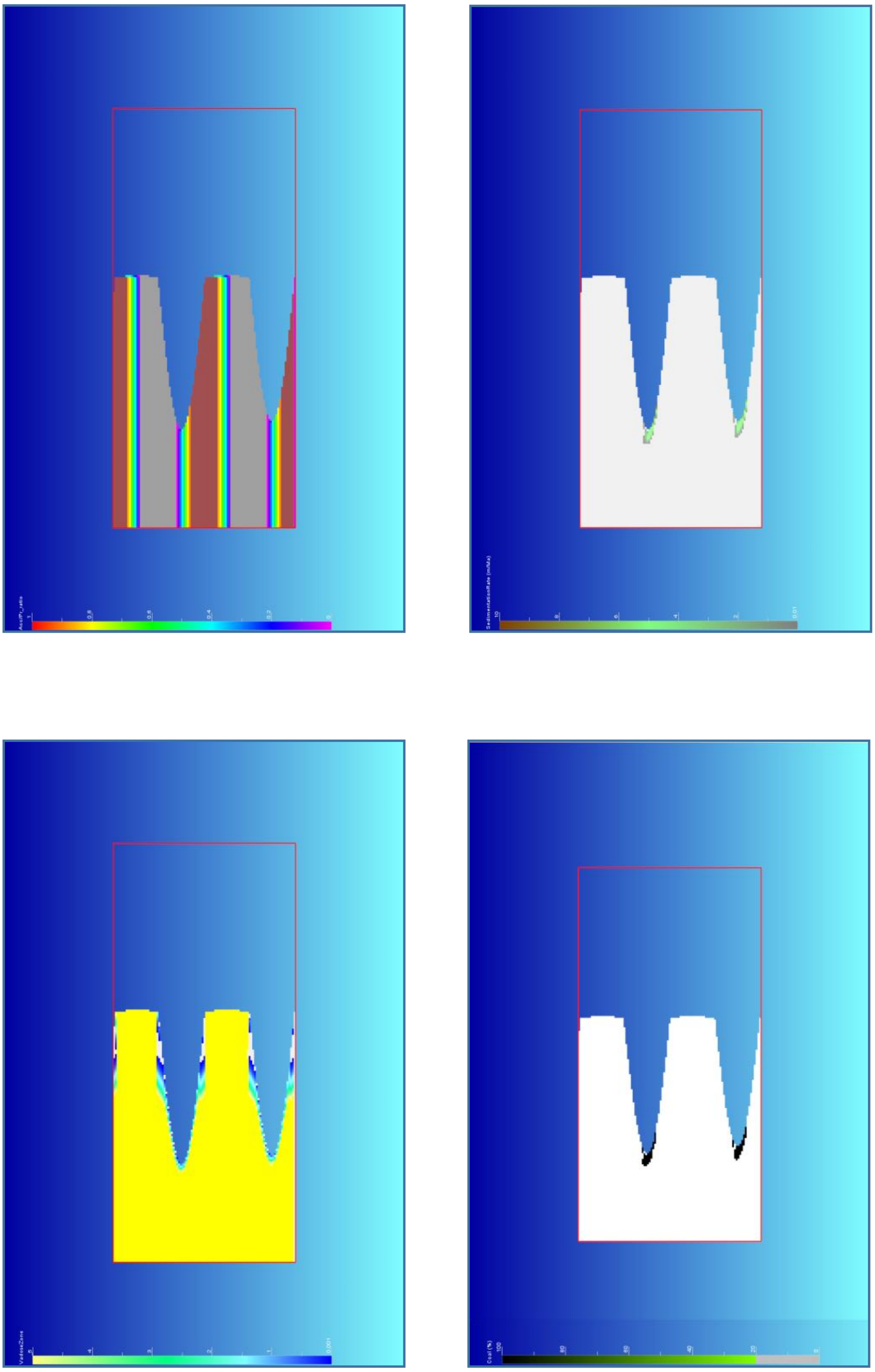

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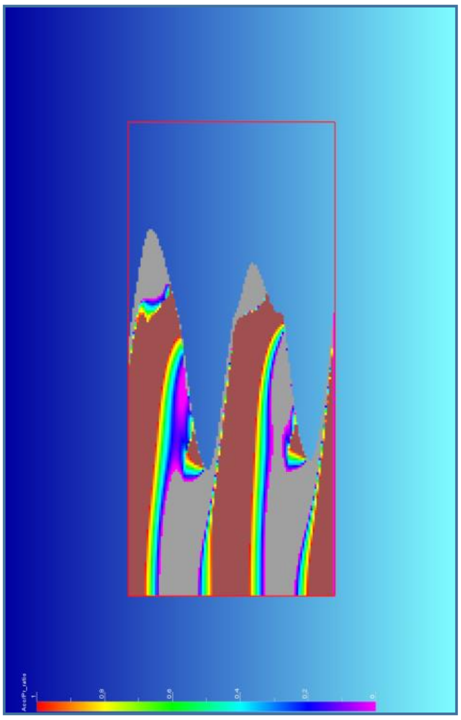

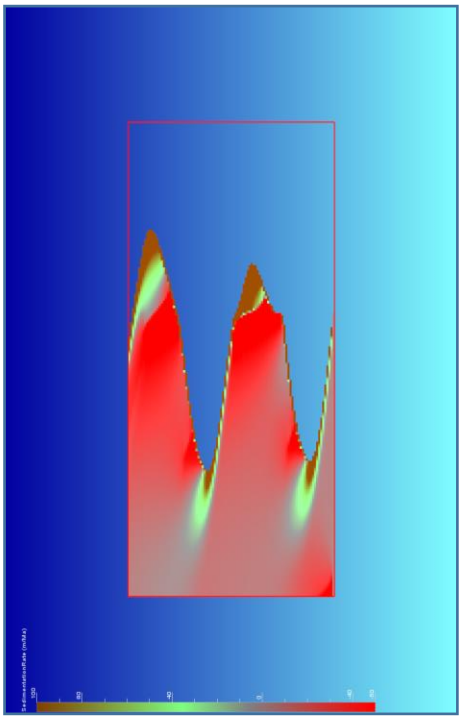

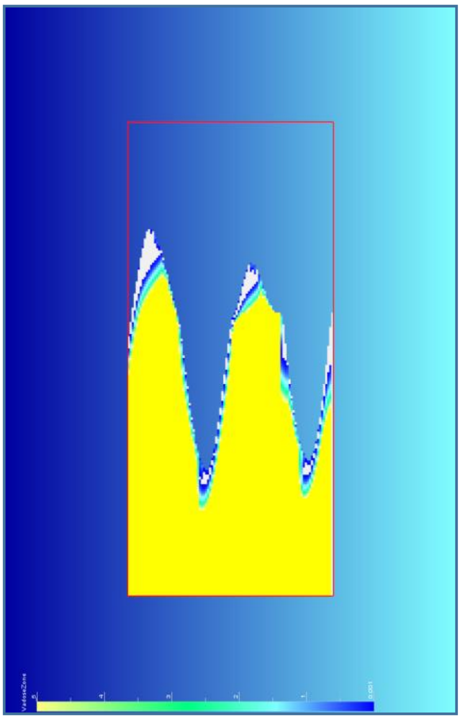

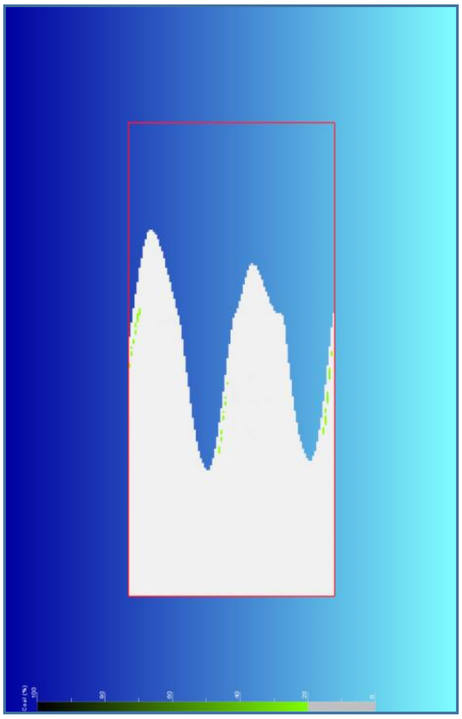

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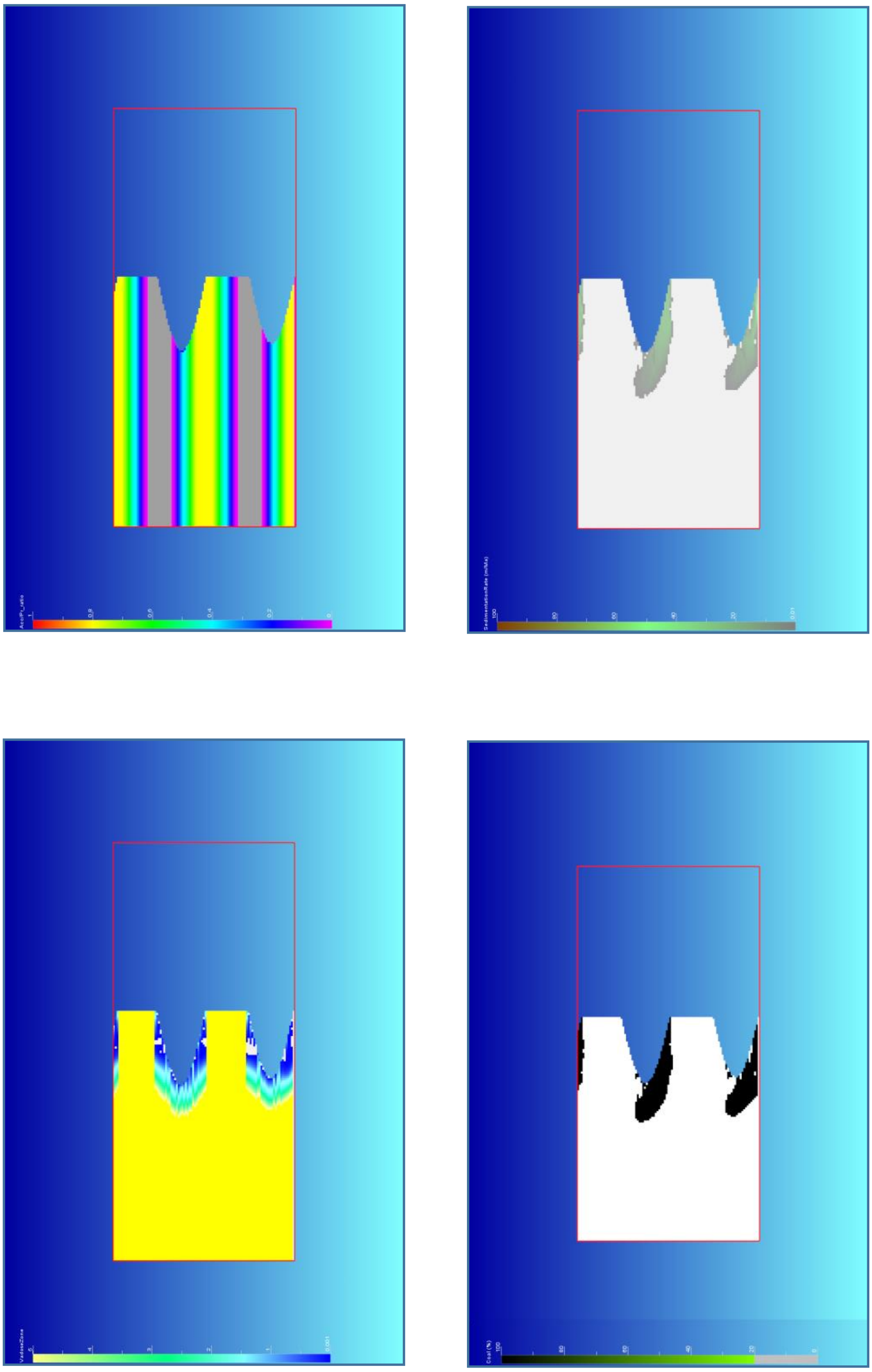

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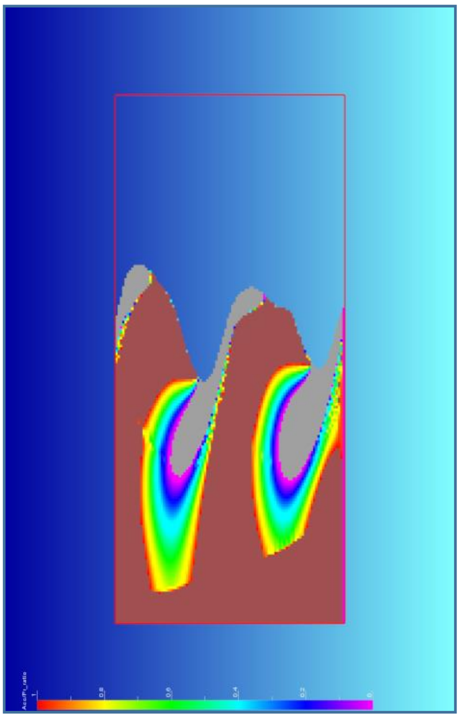

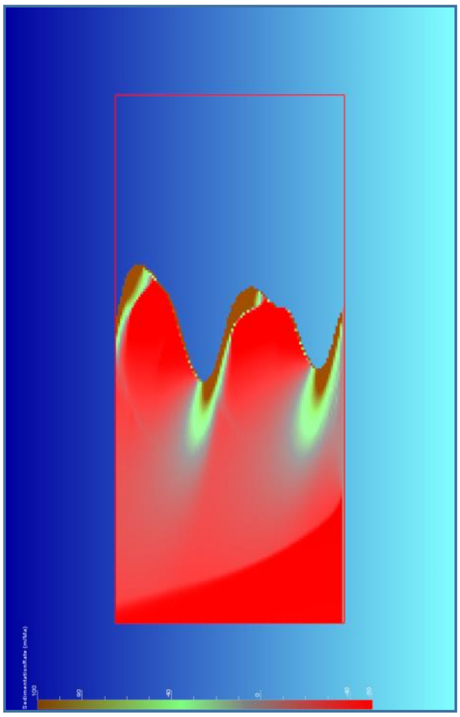

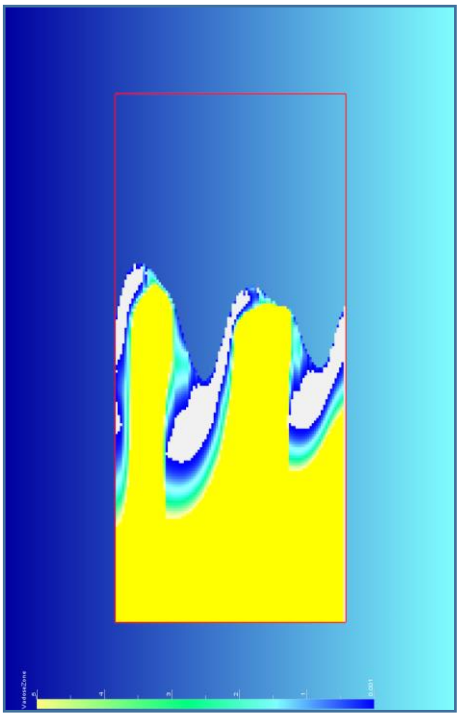

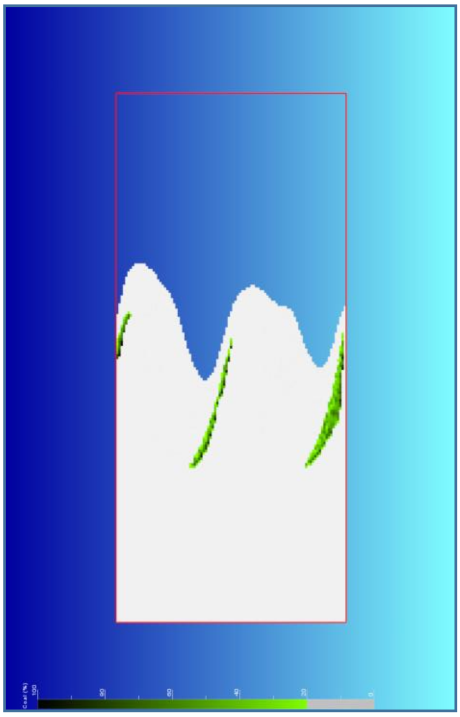

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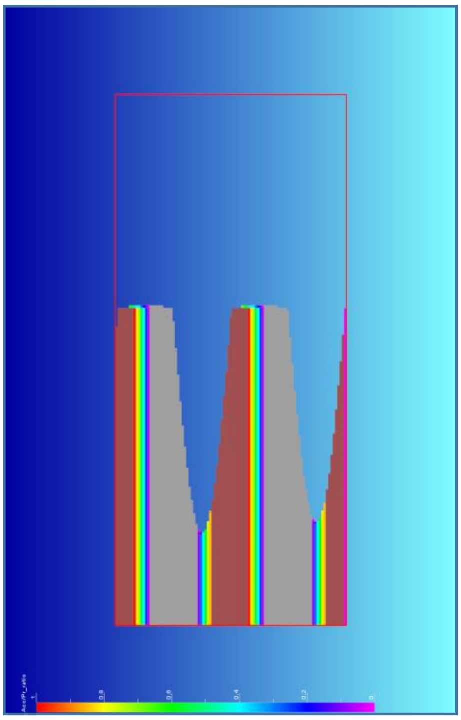

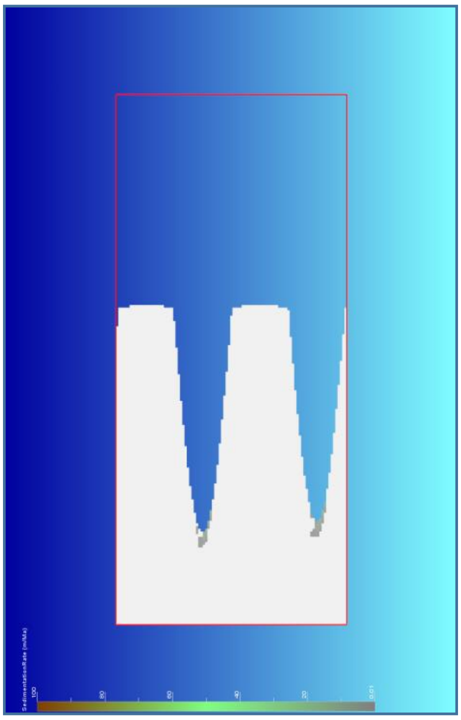

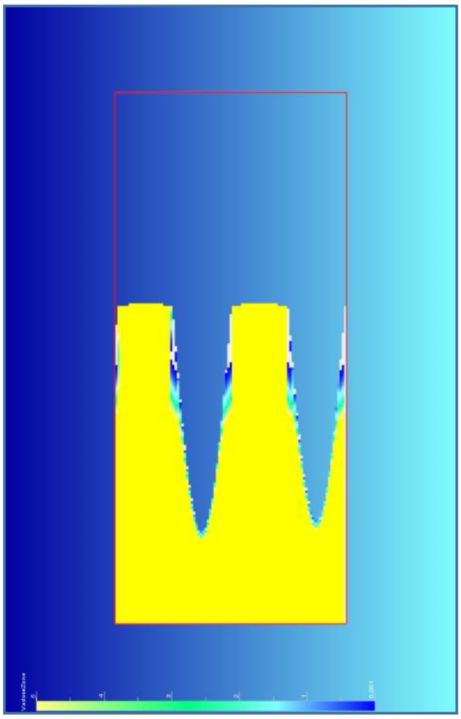

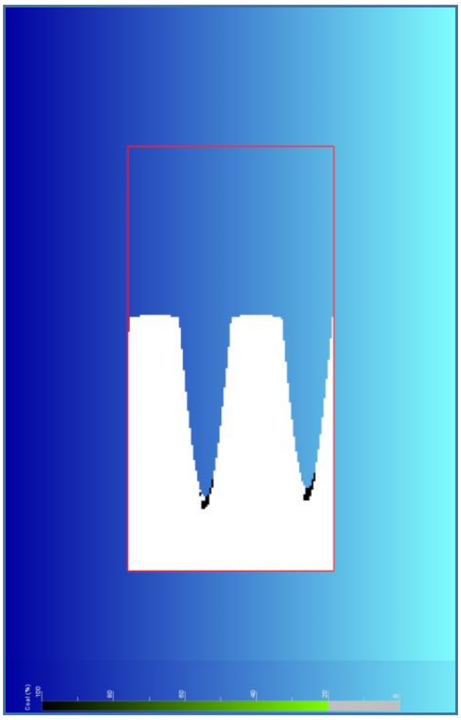

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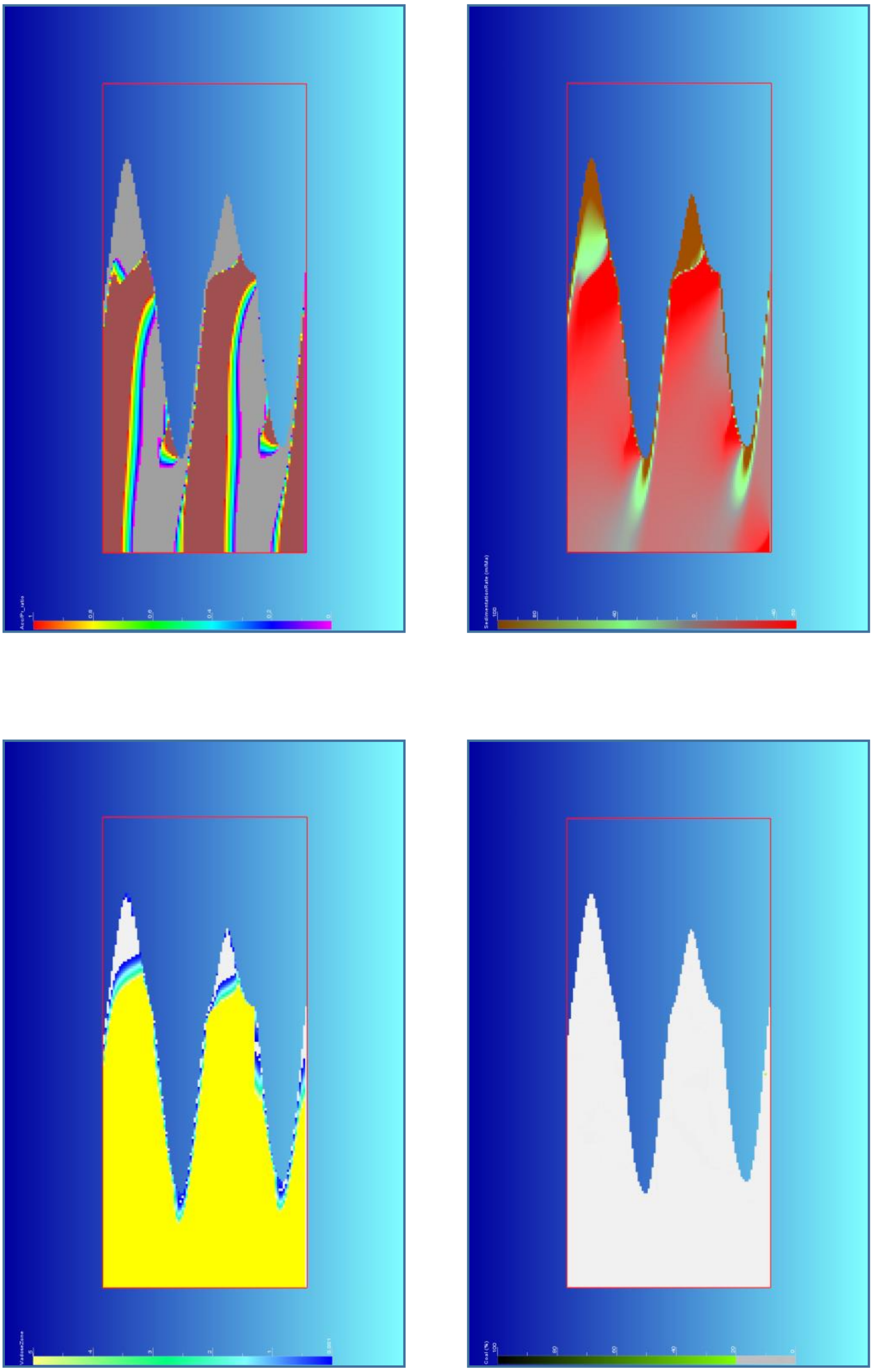

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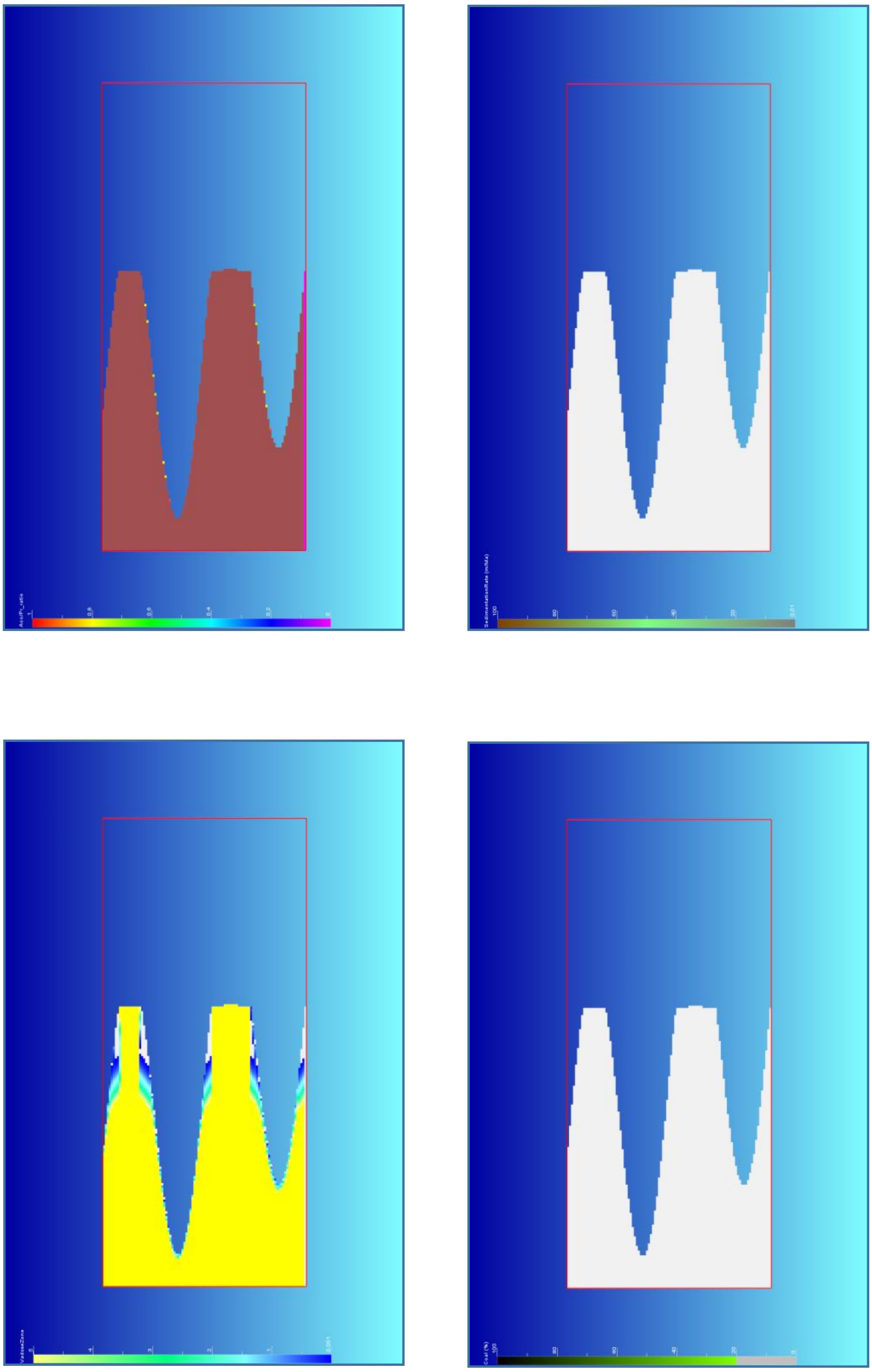

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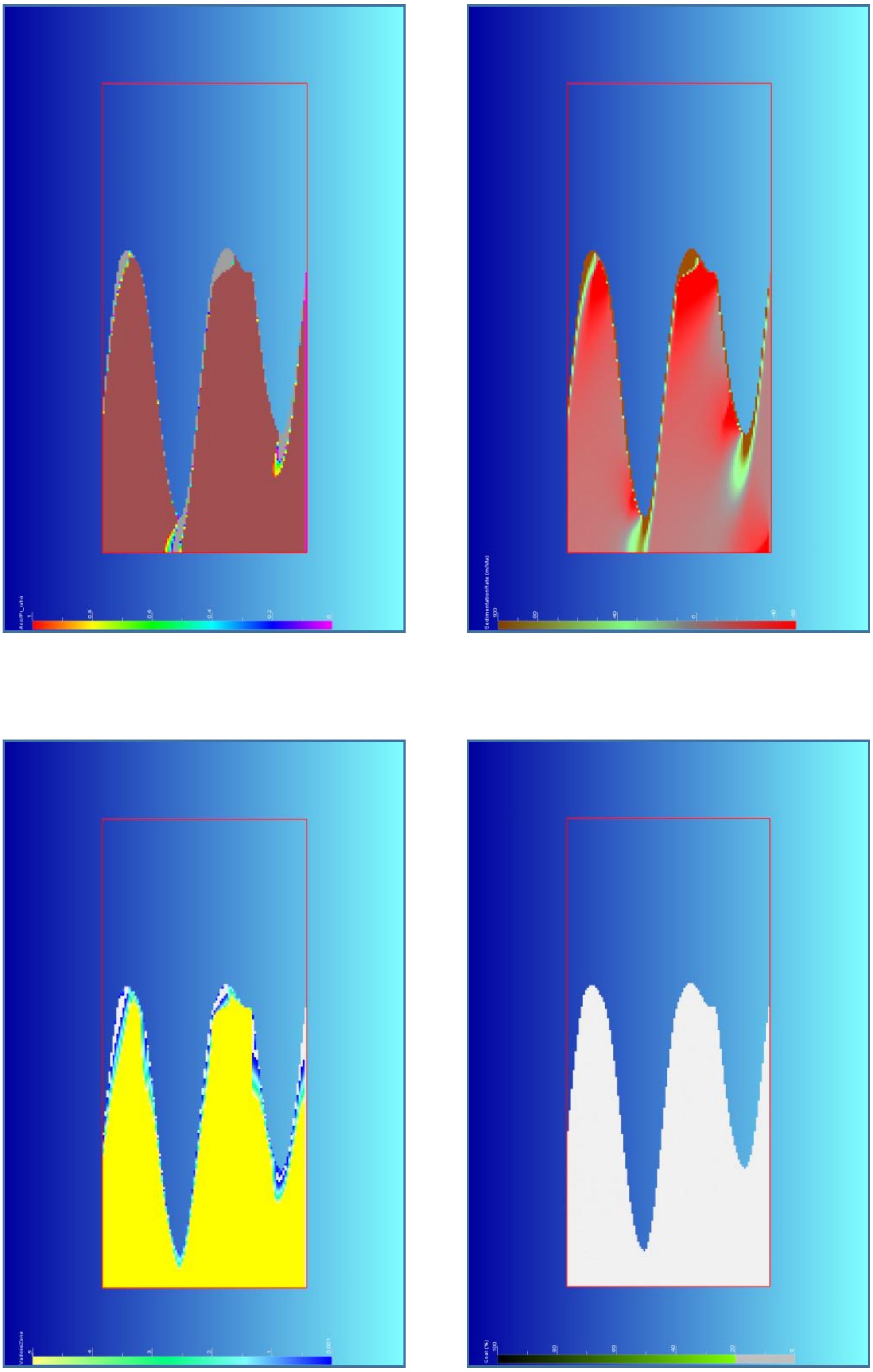

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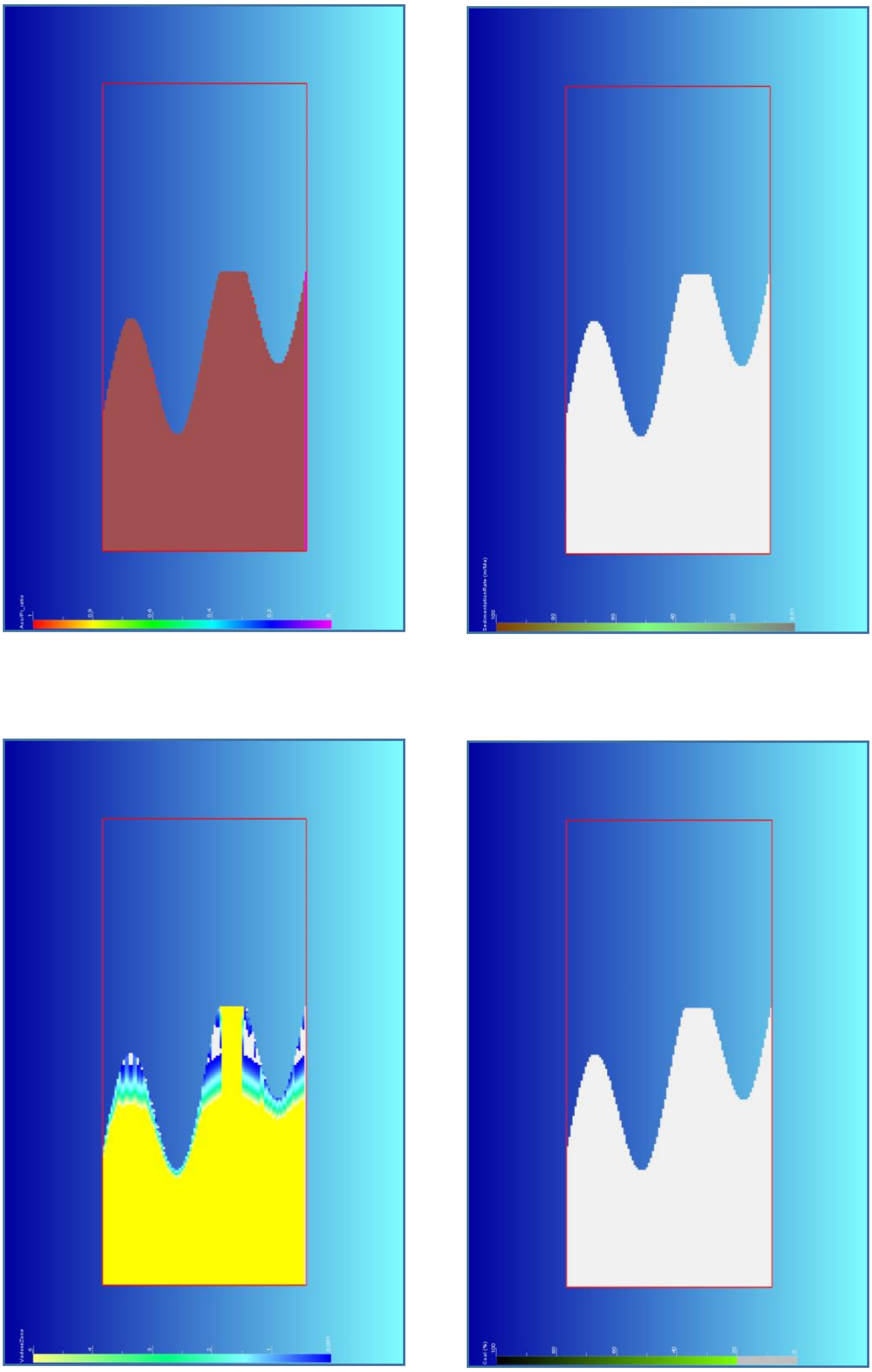

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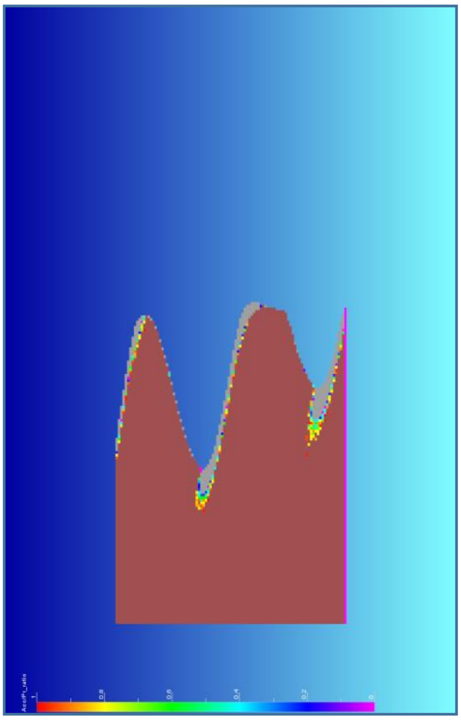
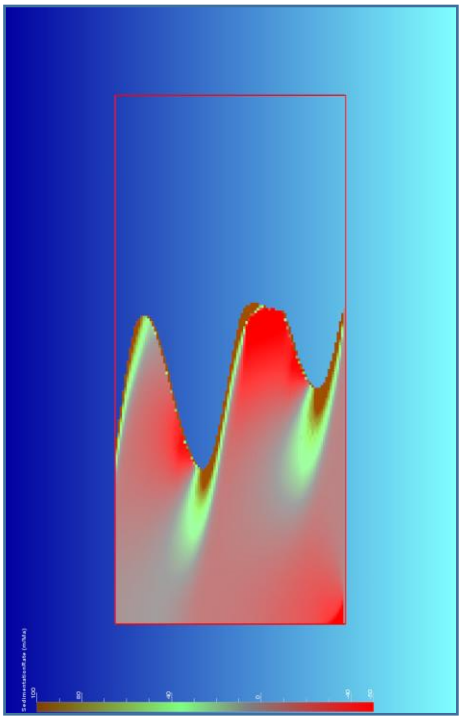
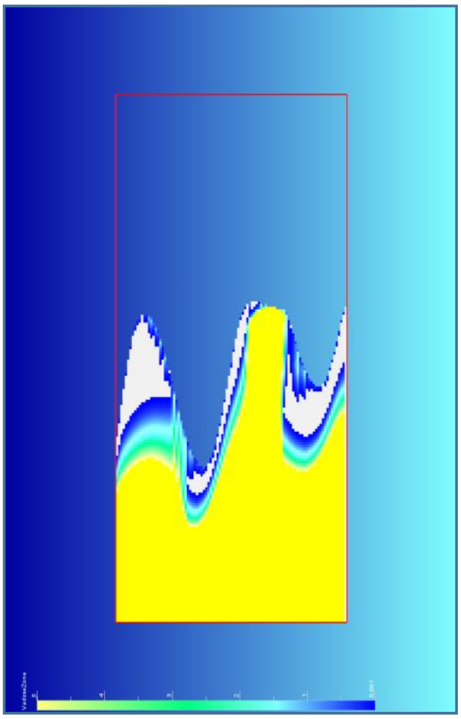
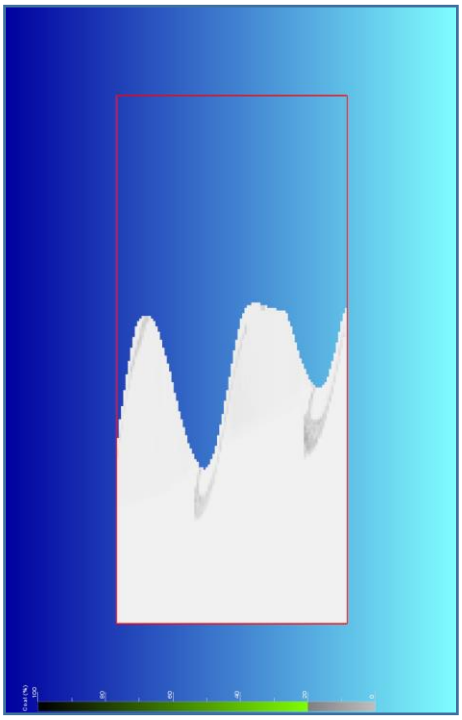
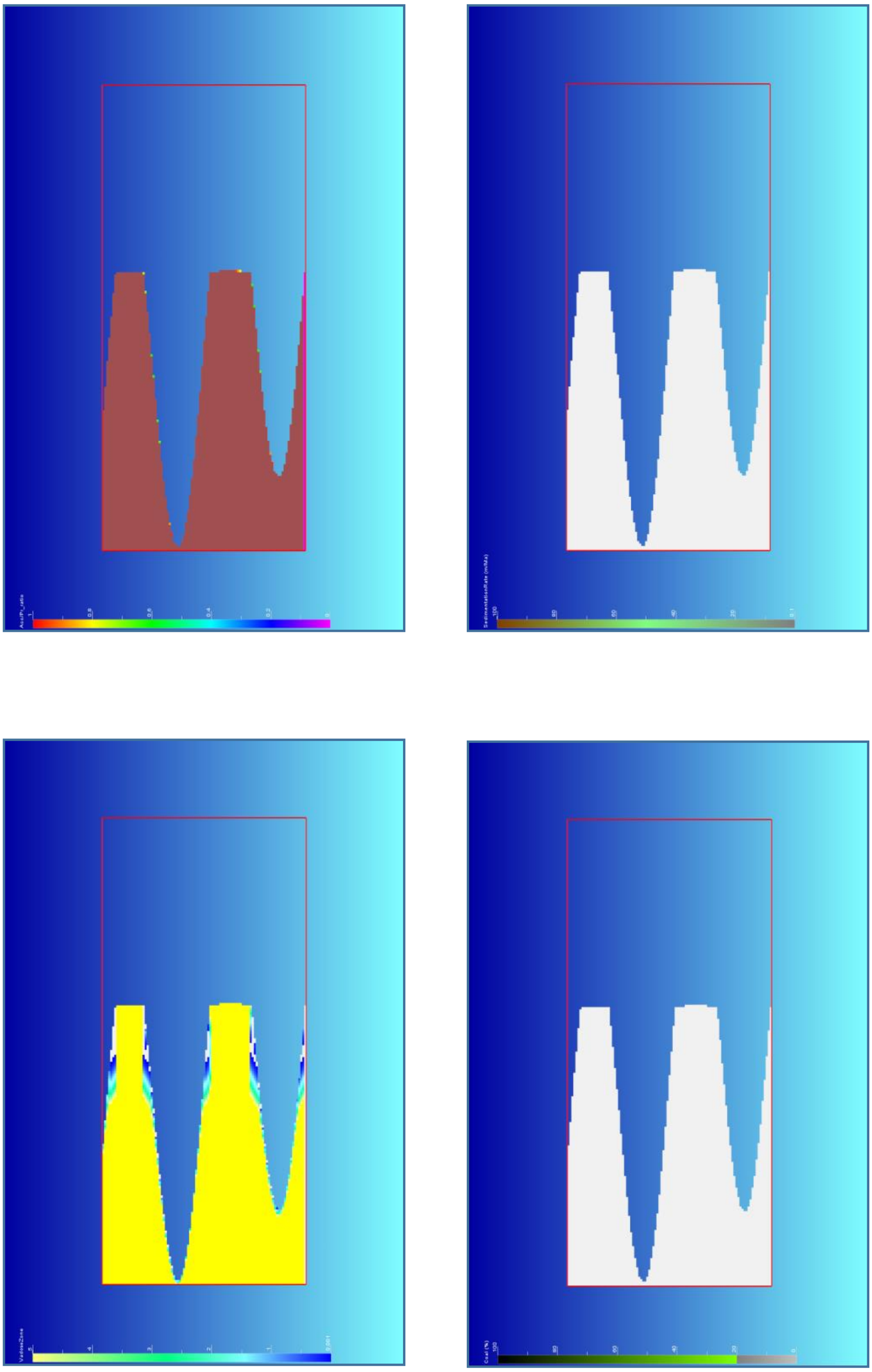








Su_H_Eu_H_nosed



Su_H_Eu_H