Forward Modelling of Carbonate Sedimentology and Diagenesis: Current Status and Issues

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Outline:

Carbonate Sedimentology

- Accomodation and sea level cycles
- Wind waves and facies template models
- Sediment production
- Sediment transport
- Hydrodynamics and timescale issues
- Prediction of porosity

Carbonate Diagenesis

- The hydrozones concept and common links to extrinsic controls
- Prediction of hydrozones (hydraulic conductivity and up-scaling issues)
- Diagenesis by hydrozone template (parameterisation issues)
- Carbonate budgets
- Coupled groundwater flow and geochemical models (RTM)
- Problems of RTM



Focus on Carbonate Developments since 1999

Sedimentological Models

- DIONISOS (Granjeon and Joseph, 1999)
- CSM Carbsim (Taizhong Duan,2000)
- REPRO (Hussner et al, 2001)
- ?? (Burgess et al, 2001)
- SedTec 2000 (Boylan et al, 2002)*
- CARBONATE 3D (Warrlich et al, 2002)*
- SIMSAFADIM (Bitzer and Salas, 2002)
- FUZZYREEF (Parcell, 2003)
- TAWIC+? (Quinquerez et al, 2004)
- CARBONATE GPM (Hill et al in prep)

Diagenetic (Reactive Transport) Models

- PHAST (Parkhurst et al, 2004)
- TOUGHREACT (Xu et al, 2004)
- GEOCHEMISTS WORKBENCH (Bethke, 2007)
- + others in house

Sedimentological and Diagenetic Models

- CARB3D+ (Paterson et al, 2006)*
- FACIES 3D (Matsuda et al, 2004)
- BASIN 2 (Bethke et al, 2007)





Why the move to 3D?



Model Fundamentals : Sea level + Subsidence = Accommodation, Hydrodynamic Environment and Sedimentary Processes > Sediments



CARB3D+ symmetric sea level generator





Symmetric cycles give symmetric sequences



Icehouse (and other?) sea levels are highly asymmetric, so why don't we use them in modelling?





Shallowing Upward Sequences result from asymmetric sea level curves

Facies Template Sedimentology



Wind generated waves and wave refraction: CARB3D⁺



Distribution of wave energy: CARB3D⁺



Wave propagation, long shallow fetch on platform top with wind reinforcement balancing energy loss?



Effect of friction factor on wave energy in platform interior: CARB3D +



Breaking waves should entrain more sediment





Enhanced sediment entrainment: CARB3D+



Facies Template Sedimentology



Facies template models: Need to convert wave energy to actual facies

CSM Carbsim Taizhong Duan (2000)

	1	2	3		4		
water depth <= 200m	1 kenetic energy ≻ 7.3	2 kenetic energy > 3.5	3 keneti energ ≻ 1.5	3 kenetic energy > 1.5		4 kenetic energy ≻ 0.0	
water depth > 200m	5 kenetic energy > 0.8			6 kenetic energy <= 0.8			
		5			6		

E₩-65

Comparison of Wells and Simulated Sections





FACIES 3D: a facies template model based on currents



Calibration issues: Tidal or unidirectional currents?





0

20

40

60

180-

200

Ê 80 coral assemblage C 100 Dept 120 coral assemblage D coral assemblage E 140 bryozoan sand 160 rhodolith 180 Legend of facies 200 5 10 15 20 25 30 35 40 45 50 0 Current velocity (cm/s) Walio Template (Miocene) Current velocity (cm/s) 0 5 10 15 20 25 30 35 40 45 50 reef flat/reef crest 20back-reef slope/patch reef 40interreef agoona 60deep interreef lagoonal reef front (upper) Ê 80reef front (middle) Depth Depth reef front (lower) 120shallow fore reef deep fore reef/basinal 140-160-

Facies selected how?



Miyako Island tidal current calibration (Tsuji et al 1994)

Sediment production and transport models: Carbonate Production



Angle of repose slopes: empirical calibration v fully explicit process specification CARB3D⁺





How many factories? CARB3D⁺ bank margin sediment production by reef and margin (shoal) + interior & pelagic factories



Environmental dependence of production: We know lots.

Eg. Depth (light + suspended sediments etc) reduction of carbonate production with depth: coral *Montrastrea annularis*



Bosscher and Schlager (1992)



We also have good factory production rate data (Although as accommodation is usually limiting this is not so critical)



But are individual species rates and dependencies representative of factories? How do we model changes in community structure in past?



Competition between groups & factories?



SIMSAFADIM

In any case do short term measurements represent long-term rates? And do models account for some of these effects especially nondeposition & platform exposure (oozes v reefs)?



Sadler (1999)



2 key issues affecting sediment availability for transport: cementation





2 key issues affecting sediment availability for transport: cementation and conversely bio-erosion (and geochemical loss of carbonate?)



We need more careful sediment budget studies like this one, and to use the results from them.



We need to be able to incorporate controls on bio-erosion into models: eg nutrients



Carbonate production rates: dependence on carbonate avialability. Residence time & carbonate exhaustion, Great Bahama Bank





Carbonate GPM: Water depth history (central lagoon)



Carbonate GPM: Detail of structure in lagoon sediments











Complex palimpsest of facies or lateral uniformity?


Are models for simulating real examples or for testing ideas or both?



What else does model development do? Formalise existing knowledge and identify areas for further research



Sediment production and transport models: Sediment Transport





From Quinquerez et al, 2004



Dionisos a diffusion-based model: effect of increasing water depth on platform facies



CARB3D⁺ Sedimentology: Advective sediment transport Suspension of sediment by wind generated waves



Wave Amplitude: Windspeed 10 m/s



CARB3D⁺ Sedimentology : Sediment transport by 2D (depth averaged) potential flow currents



Externally specified depth averaged currents: What is the drive and where does the water go to?



What about entrainment by currents? Depth averaged or 2D (3D) currents? Bi-directional wind driven circulation STORMSED 1.0



Coopman & Flemmings (2001): STORMSED 1.0 (2D)

'Large Storm' (20 m/s wind parallel to coast):

based on Mid-Atlantic continental shelf



What about tidal currents (which we can also do well), don't we need them too?



Need to develop criteria for separating different modes of sediment transport + Timescales



Sediment transport timescales: scaling of storm condition advection and magnitude /frequency response



Quinquerez et al, 2004



Sediment Properties



How many grain sizes? CARB3D⁺ Sedimentology : 2 Grain sizes + boundstones



Produced in situ Transported



CARB3D⁺ Sedimentology: The 2 component concept (coarse and fine grains)



Lucia (1995)



CARB3D⁺ sedimentology: The 2 component concept, facies



CARB3D+:Coarse fraction moves as bedload, fine as suspended load



Windward Margin Progrades over Coarse Reworked Slope Debris





Leeward Margin Progrades Over Fines Transported by Current

All Sediment is from reef on windward margin only



Prediction of depositional porosity: CARB3D⁺





Depositional Porosity, an alternative model





CARB3D⁺: Compaction is grain size dependent

0% fines → 100% fines



Cementation and compaction





Budd (2002)

Data handling: digital rocks and facies comparator



Some Conclusions on Modelling of Carbonate Sedimentology:

• Existing models are improving:

- Strong hydrodynamic base (waves and currents)
- Coupling of storm and fair-weather conditions
- More flexible specification of carbonate factories
- Budgeting of carbonate
- Slope transport
- Flexible GUI and output

• Issues for the future:

- Focus on dominant sediment entrainment and transport processes
- More sophisticated 'competition' between carbonate factories
- Development of more sophisticated facies (spatial variability)
- Consideration of role of bio-erosion and cementation on sediment mobility
- Improved prediction of porosity
- Improved simulation of compaction (especially role of cementation)

All are possible, but we must be parsimonious to achieve realistic run times



Why is diagenesis important? Practical as well as intellectual drive



Cemented Grainstone – low porosity

Dissolved Grainstone – high porosity

There is no simple relationship between facies and poro-perm characteristics



The conceptual base:

Common extrinsic controls on sedimentology and diagenesis



CARB3D+ Diagenesis Components:

Hydrozones



CARB3D⁺ Diagenesis : Depositional porosity to permeability based on facies



Empirical poro-perm relationships from published data



CARB3D⁺ Diagenesis : 3D depth-averaged freshwater lens model



- K = hydraulic conduc
- K = hydraulic conductivity,
- α = $\Delta\rho/\!\rho$ density diff sea & freshwater / density of fresh water
- *h* = lens top height above sea level,
- **R** = recharge



Fetter (1972)

CARB3D⁺ Diagenesis: 3D depth-averaged freshwater lens model





Elevation (m)

CARB3D⁺ Diagenesis: Up-scaling of permeability



CARB3D⁺ Diagenesis: Up-scaling of permeability using dissolutional porosity





CARB3D⁺ Diagenesis: Up-scaling of permeability using Kozeny-Carmen model



CARB3D+ Diagenesis: Alternative model non-fabric selective porosity to permeability



Clino & Unda data, Mellim et al (2001)



CARB3D+ Diagenesis:

Alternative model non-fabric selective porosity to permeability

 Use of lattice-Boltzmann model for predicting permeability of vuggy carbonates





(Felce et al., in prep)



CARB3D⁺ Diagenesis: Up-scaling of permeability using dissolutional porosity



Lucayan Limestone, Grand Bahama

(depth/age conversion)



CARB3D+ Diagenesis Components:

Diagenetic Transformations





Hydrozone diagenesis template: Facies-3D

c) Marine 0 %/ka


CARB2D Diagenesis: Diagenetic transformations for each hydrozone



Excluded on thermodynamic grounds



(Whitaker et al, 1997)

CARB3D+ V2.0 Diagenesis:

What determines the extent of diagenetic modification?



Paterson et al (2008) hydrozone residence times



CARB3D+ Diagenesis: Link between hydrozone residence times and sequence types







CARB3D+ V2.0 Diagenetic rates parameterisation eg Using climate parameters such mean annual rainfall



Whitaker & Smart (1997)

But remember as for sediment transport, diagenetic transformations occur as a cumulative result of many individual events in time



CARB3D+ V2.0 Diagenesis rates are uniform with depth (A), have no feedback between zones (B) and are not dependent on grain size (C)



Depth dependence of vadose dissolution, karstified Paleozoic Limestone, UK (Smart & Freiderich 1980)

Dependence of A to C stabilisation on grain size (Whitaker & Smart in prep)

CARB3D+ Diagenesis: uniform hydrozones template (V2.0 top) and (STEP1) sequential carbonate budget approach (V3.0 below)...then

Total Diagenesis = Rate_{Diagenesis} x Time Acting (V2.0)



(Whitaker & Smart, 2006 a and b)

Northern Bahamas field data: Water & Ca budgets

.....distribute reactions along the flow path (Step 2)

Total Diagenesis = Rate_{Diagenesis} x Time Acting

Rate_{Diagenesis} = Flux H₂0 x Reactant Concentration

Reactant Concentration = f (degree of saturation, time, surface area)



Field sampling along the flowpath: We try hard but....



Andros Blue-holes,

exploration, geochemical and hydrological sampling

Shell & Amoco



Reactive Transport Models:

reach the parts that other research techniques don't!



Depth dependence of fresh water lens dissolution, non-karstified Pleistocene Limestone from RTM

(Whitaker and Smart in prep)



Reactive Transport Models: Integrate transport and geochemical reactions including reaction kinetics



Calcite Dissolution: $CaCO_3 + CO_2 + H_2O = Ca^{2+} + 2HCO_3^{-1}$



After Xiao and Jones (2006)

RTM is applicable across a great range of scales



RTM give great results: Reflux dolomitisation



Jones & Xiao (2005)

BUT>>>RTM Issues:

Challenging to parameterise, slow and cumbersome to run



RTM Issues: Need to better model heterogeneous permeability systems



Reflux dolomitisation with spatially random variation in porosity and permeability

(Jones & Xiao, 2005)



RTM Issues: Fractures & high k routes





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South Andros Bank Marginal Fracture
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RTM Issues: Fractures & matrix, conceptual models and numeric formulations (and not just in reservoirs)

Exchange

Dual Permeability



Double Porosity

Multiple Interacting Continua





RTM Issues (geochemistry): Reactive surface area much greater for real carbonate grains than their geometric surface areas



Walter and Morse (1984)



RTM Issues: Reactive surface area changes during dissolution and reaction rates vary between sites





Luttge et al 2005

RTM Issues: Reaction constants from laboratory experiments depend on surface area, and may not be representative of natural conditions



Rate constants for calcite dissolution: Arvidson et al (2003)



RTM Issues: Geochemical reactions are not wholly inorganic but may be driven by organic matter oxidation



RTM Issues: Microbial mediation of reactions is important



RTM Issues: Need to consider changing boundary conditions



Andros

50 km



Eberli et al (2003)

Florida

In the meantime we have CARB3D+ !



- Model complexity and applicability issues:
 - How many processes are explicitly represented?
 - How detailed or realistic are the representations?
 - What are the time and space scales at which the processes can be explicitly represented?
 - Model applicability
 - GUI & run time issues
 - Model purpose (simulator v hypothesis testing)



Model development & parameterisation: the rock record





Model development & parameterisation, a Polemic: More process work, less geological case studies please!



Key: Darker better known





Reactive transport models are great, but

- Slow and complex (precludes use in coupled sedimentological modelling)
- For the future need to:
 - Incorporate heterogeneity in rock properties
 - Model fracture/matrix interaction
 - Improve understanding of reactive surface area and kinetic rates
 - Include biogeochemical reactions
 - Deal with changing sea level and platform geometry





Not for warm water non-coralgal factory, but strong dependence on individual species makeup of factory (larger species ranges)



Enhanced Entrainment Model





Limited field data for parameterisation



Mixing zone thickness, Grand Bahama


The New Mixing Zone Scheme after Bear & Todd, 1960

$$D_{MZ} = a \sqrt{2 D_{\alpha} \overline{u} t}$$

Where D_{MZ} The mixing zone thickness (m)

- a = A constant (normally taken as '5')
- D_{α} = The constant of dispersion (normally taken as 0.01 cm)
- u = The amplitude of the fluctuating velocity (m/day)
- t = The time for the system to reach equilibrium (normally taken as 10,000 d)

$$\boxed{\overline{u} = \frac{2\sqrt{2}}{\pi} \frac{kh_0}{\theta} \sqrt{\frac{\pi S}{t_0 T}} \exp\left(-x \sqrt{\frac{\pi S}{t_0 T}}\right)}$$

- Whereu =The amplitude of the fluctuating velocity (m/d)
 - k = The hydraulic conductivity of the aquifer (m/d)
 - $h_0 =$ The tidal amplitude (m)
 - θ = The porosity of the aquifer (%)
 - S = The storativity of the aquifer (equals the porosity in unconfined aquifer)
 - $t_0 =$ The tidal cycle (normally half a day, in d)
 - T = The transmissivity of the aquifer (m^2/d)
 - x = The distance from the coast (m)

Only Tidal Amplitude is not know (1 parameter)

There are feedbacks to evolving porpo/perm of sediments> dynamic response





CARB3D⁺: externally coupled reactive transport model of mixing zone porosity generation



Sanford and Konikow (1989)



CARB3D⁺ Diagenetic Processes: Aragonite Stabilisation> FW



A complete diagenetic salinity cycle Gldstein slide











Secular variation in seawater chemistry



Fig. 9. Regionalisation of the Australian continental shelf for observed grain size distribution based on ratio of wave and tidal exceedance estimates.





Fig. 1. Division of the Australian shelf (after Harris, 1995) into regions in which sediment transport is caused mainly by tidal currents (17.4% of the shelf area), currents derived from tropical cyclones (53.8%), ocean swell and storm generated currents (28.2%) and intruding ocean currents (0.6%). Contours representing tropical cyclone frequency are from the Burean of Meteorology (http://www.bom.gov.au/climate/averages/ climatology/tropical_cyclones/tropical_cyclones/tropical_cyclones for significant wave height percentage exceedence are from McMillan (1982). Mean spring tidal ranges indicated along the coastline are derived from the Australian National Tide Tables. The location and direction of flow of major ocean currents are indicated.



What do we do at Bristol?





CARB3D⁺ Sedimentology: Comparison with Modern Turks & Caicos Platform



Type of break depends on sea floor gradient + wave energy: CARB3D+



Additional sediment types: Reef derived slope breccias in REPRO



Castell et al, 2007



Angle of repose slopes: empirical calibration CARB3D⁺



