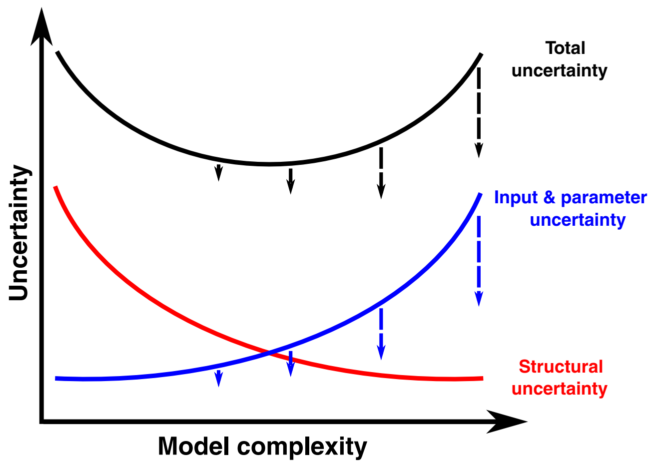

Fig. 18. Idealised dependency of various sources of uncertainty on model complexity (i.e. components, resolution and represented processes). Blue arrows depict an improvement of input or parameter uncertainty using SA and empirical methods (see text) which results in a decrease in total model uncertainty (black arrows).
Source: Adapted from Solomatine and Wagener (2011).

biogeochemical reaction rates and their combined influence on the ambient pH. The conservative boundary approach does not capture this biogeochemical complexity and thus does not appropriately represent the sedimentary response.

In order to illustrate how different sediment boundary conditions affect biogeochemistry in the ocean we compare a GENIE set-up using the reflective boundary with the conservative boundary for two climate scenarios (see Box 2 for more information). The impact of including organic carbon burial on global mean water-column O_2 and PO_4 concentration during the Eocene is shown in Fig. 16 (A + B). Global deep water O_2 concentration increases as POC reaching the seafloor is buried and not remineralised. In contrast, nutrient concentration in the deep ocean is decreasing as less PO_4 is released to the ocean. But not just the global O_2 concentration changes, also the spatial difference of bottom water oxygenation for the two sediment schemes varies significantly for the modern and the Eocene (Fig. 16C + D). Ocean redox differences are even more pronounced when applying the two sediment representations for the Late Cretaceous. Fig. 17 (A) highlights the problem of the reflective lower boundary by showing an unrealistically high concentration of H_2S at the seafloor. This result is an artifact of the lower boundary condition as all POC gets instantaneously remineralised at the seafloor. On the other hand, the conservative boundary (Fig. 17B) shows very little H_2S in the deeper ocean as it neglects completely the degradation of POC at the seafloor. However, the employed lower boundary condition does not only have implications on redox conditions at the bottom of the ocean but can also be seen in the photic zone (Fig. 17C).

3.3.2.3. Vertically-integrated dynamic model. In the vertically-integrated approach, the sediment is represented as a single box (Fig. 14C). The average concentration of the represented species in this box is calculated as the balance between the deposition and burial flux, as well as the sum of consumption processes. The diffusive flux of dissolved species through the sediment-water interface in turn equals the sum of consumption/production processes that are usually tightly linked to the transformation of particulate material (e.g. Maier-Reimer, 1993). The model thus neglects temporary storage of dissolved species and fluxes in porewaters. However, this approach is clearly superior to the two simpler approaches. It has the merit of simplicity and is computationally efficient. In addition, it also reproduces some of the complexity associated with the short- and long-term evolution of benthic recycling fluxes. Such an approach also allows differentiating between various fractions of organic matter (if POC is represented) and therefore is able to resolve some of the biogeochemical complexity associated with the decrease of organic matter reactivity with sediment depth. Most paleo-EMICs incorporate a vertically-integrated sediment model for PIC only, sometimes considering oxic-only sediment respiration of organic carbon (compare Table 1). Bern 3D being a notable exception, as it includes a vertically-integrated dynamic model also considering oxic degradation and denitrification of organic carbon (Tschumi et al., 2011),

3.3.2.4. Vertically resolved diagenetic model. So-called diagenetic models provide the most robust description of the benthic-pelagic coupling (Fig. 14D). Those models solve the one-dimensional, fully coupled reaction-transport equation for solid and dissolved species (e.g. Berner, 1980b; Boudreau, 1997). This approach thus accounts for all important transport processes, such as burial, compaction, bioturbation, molecular diffusion and bioirrigation. In addition it resolves the fully coupled biogeochemical dynamics of the carbon, oxygen and nutrient cycles and the resulting characteristic redox-zonation of marine sediments (also compare Fig. 12). However, controversy still revolves around the formulations of organic matter degradation (e.g. Arndt et al., 2013) and calcite dissolution (e.g. Jourabchi et al., 2005). In addition, the parameterisation of diagenetic models requires a good understanding of diagenetic dynamics and careful consideration of the environmental conditions. For instance, rate constants that are typically used in state-of-the art diagenetic models may predict the benthic response in the modern-day, well ventilated ocean, but might not be applicable under extreme environmental conditions such as OAEs and the PETM. The major drawback of those models is the computational cost associated with the computation of vertically-resolved reaction-transport equations for a number of interacting species. Therefore, paleoclimate models that include a diagenetic model generally reveal a very low spatial resolution of the benthic environment (e.g. GEOCLIM *reloaded* only resolves three sediment columns; Arndt et al., 2011) or use other methods to reduce computational demands: DCESS for instance uses a semi-analytical, iterative approach considering $CaCO_3$ dissolution and (oxic and anoxic) organic matter remineralisation (Shaffer et al., 2008). One exception here is the early diagenesis model MEDUSA which is coupled to the multi-box model MBM (Munhoven, 2007). MEDUSA operates in a fully transient way at 100 m depth intervals over the whole model sea-floor, in five regions, totalling 304 columns.

3.3.3. Conclusion

Marine sediments represent the largest reservoir of carbon among the exogenic reservoirs (Mackenzie et al., 2004). The assessment of the response of the ocean to variabilities in atmospheric CO_2 concentrations requires a robust quantification of the benthic-pelagic coupling and the sedimentary carbon sink (Archer and Maier-Reimer, 1994; Archer et al., 1998; Sigman et al., 1998; Heinze et al., 1999). However, it appears that convenience rather than a careful mechanistic representation and the ability of the approach to provide an answer to the problem guides the choice of the lower boundary condition for the ocean model. Paleoclimate modelling has developed to a stage where increasingly complex and multi-dimensional ocean, atmosphere and continental vegetation models are coupled (e.g. McGuffie and Henderson-Sellers, 2005; Randall et al., 2007). Yet, compared to these developments, considerably less effort has been devoted to the coupling between ocean and sediment models. However, sophisticated, comprehensive and carefully calibrated and tested diagenetic models (e.g. Aguilera et al., 2005; Archer et al., 1998; Cappellen and Wang, 1996; Soetaert et al., 1996), as well as computationally efficient pseudo dynamic approaches (e.g. Ruardij and Van Raaphorst, 1995; Arndt and Regnier, 2007) are now available and could be incorporated into paleoclimate models in numerically efficient ways, such as for instance look-up tables (see e.g. Ridgwell and Hargreaves, 2007) and neural networks (see Section 4.3). Ultimately, our ability to understand past climate change critically