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Review of groundwater flow and contaminant transport modelling approaches for the Sherwood Sandstone Aquifer, UK; insights from analogous successions worldwide

Medici G. [1]*, West LJ[2]

[1] Morwick G360 Groundwater Research Institute, College of Engineering and Physical Science, University of Guelph, Guelph, Ontario, N1G2W1

[2] School of Earth and Environment, University of Leeds, Woodhouse Lane, Leeds, W Yorkshire LS2 9JT, UK

* Correspondence: giacomo.medici@g360group.org

Abstract

Sandstones are characterized by different hydraulic behaviours and need to be modelled in various ways to represent groundwater flow and contaminant transport. This review shows how sandstone aquifers within the UK Triassic Sherwood Sandstone Group, can be represented using three modelling approaches; the Conduit Network, Discrete Fracture Network and Equivalent Porous Medium.

The Sherwood Sandstone Aquifer is dominated by matrix flow in the Eastern England Shelf, Worcester, Needwood and Staffordshire basins. Here, the aquifers are modelled as Equivalent Porous Media at a range of scales. Fractures represent the principal flow pathways in the Cheshire Basin. Here, Discrete Fracture Network models that account for diffusivity in the matrix can be used where the scale of the model domain is small. The Sherwood Sandstone aquifer across north-western England shows evidence of intense

groundwater alteration and high flow velocities in conduits. Turbulent flowing pipe-elements can be inserted in the modelling domain represented by Equivalent Porous Medium at specific sites. The review shows how the Sherwood Sandstone Aquifer as well as other siliciclastic deposits across the world need to be represented using a range of modelling approaches, as they behave as matrix or fracture flow aquifers, or in specific cases show a karst-like behaviour.

Keywords: Flow modelling, Sherwood Sandstone Aquifer, Scale, Fracture, Porosity, Conduit

Introduction

Contaminants are transported at different rates in sandstone aquifers at relatively shallow depths depending on the proportion of intergranular to fracture permeability (Gogu et al. 2003; Powell et al. 2003). Indeed, hard sandstones tend to be heavy fractured and characterized by low values of effective porosity and hence relatively high groundwater flow velocities occur and large well-head protection areas are designed around abstraction wells (Freeze and Cherry 1976; Cook 2003; Ofterdinger et al. 2019; Troeger and Chambel 2021). Such sandstone-types can also be characterized by karst-like conduits, due to dissolution of primary and secondary calcite, dolomite and aragonite. These carbonate minerals precipitated and sealed fractures and adjacent pores before subsequent dissolution as a consequence of lithospheric uplifts and exposures to freshwater circulation (Burley 1984; Barker et al. 1998; Kůrková et al. 2019; Meus and Willems 2021). This telogenetic process coupled with elevated flow velocities allows for genesis of cavities by also dissolving felspathic grains, and occurrence of turbulent flow in sandstones of fluvio-aeolian origin (Burley 1984; Kůrková et al. 2019). Conversely, porous and poorly fractured sandstones are characterized by laminar flow and slow dispersal of pollutant species in groundwater at relatively slow rates (Worthington 1977; Tellam and Barker 2006).

To face this hydraulic complexity, hydrogeologists need to consider that to model groundwater flow in a porous and fractured sandstone, three alternative modelling approaches might be necessary as function of modelling objective, observation scale and proportions between intergranular and fracture permeabilities: Equivalent Porous Medium (EPM), Discrete Fracture (DFN) and Conduit (CN) network approaches (Barker et al. 1998; Selroos et al. 2002). From a computational standpoint, the simplest flow modelling approach is EPM where the flow velocities exclusively depend on the hydraulic gradient, the bulk hydraulic conductivity and the effective porosity. This method treats a sandstone using bulk properties rather than the physical characteristics of the intergranular pores, platy fractures and conduits of approximately pipe-shape (Selroos et al. 2002). By contrast, DFN and CN approaches represent groundwater flow in individual fractures and channels, respectively (Shoemaker et al. 2008; Hill et al. 2010; Gallegos et al. 2013; Parker et al. 2019: Medici et al. 2021). These approaches to modelling groundwater flow and contaminant transport were recently reviewed by Medici et al. (2021) with respect to the carbonate aquifers of Great Britain and North America. In contrast, in this review, we focus our attention on modelling groundwater flow in a sandstone aquifer of fluvio-aeolian origin, the Triassic Sherwood Sandstone Aquifer of Great Britain, which shows a spectrum of hydraulic behaviours across the country (Allen et al. 1997; Tellam and Barker 2006; Medici et al. 2019a, b).

The Sherwood Sandstone Aquifer (Figs. 1, 2) is particularly suitable for studying the different approaches to groundwater flow modelling in siliciclastic aquifers for two reasons. Firstly, calcite, aragonite and dolomite represent the principal minerals that fill bedding discontinuities and fractures in this sandstone of Triassic age (Burley 1984; Strong et al. 1994; Medici et al. 2018). These minerals are highly soluble in groundwater and can dissolve, resulting in the formation of karst-like conduits. Together with pores and fractures, such conduits represent further hydraulic elements to be inserted in a model domain. Secondly, a diverse suite of background hydrogeological materials (e.g., core plug porosity and permeability tests, fluid logging, tracer tests and groundwater flow models) is available on the Sherwood Sandstone Aquifer since it represents the second most important UK aquifer in terms of volume of abstraction (Harris and Lowe 1984; Allen et al. 1997; Smedley and Edmunds 2002; Gooddy et al. 2005; Streetly et al. 2000, 2006; Rivett et al. 2007; Abesser and Lewis 2015), and it serves as the bedrock lithology of large industrial cities such as Birmingham, Liverpool, Nottingham and Manchester (Waltham 1993; Ford and Tellam 1994; Tellam 1995; Allen et al. 1997, 1998; Bottrell et al. 2008; Banks et al. 2013; Colyer et al. 2021). Hence, establishing a link between the hydraulic behaviour of the Sherwood Sandstone Aquifer and appropriate modelling techniques is achievable.

Large availability of background data on the hydrogeology of the Sherwood Sandstone Aquifer has prompted other review papers in the last thirty years. A collection of permeability tests on core plugs, pumping tests and tracer tests on the Sherwood Sandstone Aquifer can be found in Allen et al. (1997). Further hydraulic data were acquired on the Sherwood Sandstone Aquifer to characterize the aquifer properties at a variety of scales (e.g., Rivers et al. 1996; Hitchmough et al. 2007; Bashar and Tellam 2011; Medici et al. 2016, 2018). New advances were made by numerous authors in understanding the three dimensional fracturing pattern that controls groundwater flow in the Sherwood Sandstone Aquifer of Great Britain (e.g., Allen et al. 1998; Gutmanis et al. 1998; Wealthall et al. 2001).

Tellam and Barker (2006) reviewed the physical and chemical properties of the Sherwood Sandstone Aquifer in detail, but without incorporating groundwater flow models. A recent review analysed the existing background information to extract useful hydraulic information for the analogue Triassic successions that host hydrocarbon resources off-shore (Medici et al. 2019a). However, Medici et al. (2019b) studied the ratio between the hydraulic conductivity at the scale of the pumping test ($K_{well\text{-}test}$) and the core plug ($K_{core\text{-}plug}$) that regionally varies across the Sherwood Sandstone Aquifer in Great Britain. This ratio ($K_{well\text{-}test}/K_{core\text{-}plug}$) appears sensitive to the sedimentary basin in the country (see locations of grabens in Figures 1a, b) and is diagnostic to define the hydraulic behaviour of the aquifer and variation in permeability with scale (Allen et al. 1997; Medici et al. 2019a, b). Hence, the above mentioned ratio represents a starting point for this review. Details on the influence of mechanical strength and style of deformation on permeability type (i.e,. fracture versus matrix flow) of the Sherwood Sandstone Group across the UK basins were also recently reviewed (Medici et al. 2019b). In contrast with previous reviews on the hydrogeology of Sherwood Sandstone Aquifer, the physical properties of the aquifer are here reviewed focussing on groundwater flow modelling. The review aims to relate the different hydraulic behaviours of the Sherwood Sandstone Aquifer to the three different approaches to difference and finite element modelling (see Fig. 3) used to model groundwater flow in porous and fractured rocks. The review focuses on the initial choice of the modelling approach to groundwater and contaminant transport representation based on the purpose and scale of the project, and the hydraulic properties of the sandstone. In terms of modelling purpose, we distinguish between simulations that only need to predict bulk water movement (e.g., for water resource assessment), and those that require groundwater velocity simulation (e.g., for reactive transport modelling of pollutant migration). Note that parameters required for reactive contaminant transport modelling of specific pollutants were not considered in this review.

Specific objectives are as follows: (i) identify the principal hydro-mechanical features of the aquifer across the country, (ii) review previous groundwater flow and contaminant transport modelling studies, and (iii) address future modelling research needs in the Sherwood Sandstone Aquifer through comparisons with similar aquifers overseas.

Geological background

Basin evolution and stratigraphy

The Triassic Sherwood Sandstone Group comprises a continental sedimentary succession of fluvial and aeolian deposits accumulated in a series of sedimentary basins. Such geological basins developed as a consequence of the break-up of the Pangaea supercontinent during the Permo-Triassic and host the sedimentary succession studied in this research (Mountney and Thompson 2002; Brookfield 2008; McKie and Williams 2009; Medici et al. 2015; Newell 2018). Fluvial deposits were related to the major braided fluvial system that filled the rift basins of Great Britain under semi-arid to arid climate conditions (Thompson 1970; Schmid et al. 2006).

Extensional tectonics characterized NW Europe after the Permo-Triassic time throughout the Jurassic and Cretaceous (Chadwick and Evans 1995). After this time, NW Europe was uplifted during the Cenozoic Era (Carminati et al. 2009; Kortas and Younger 2013). This lithospheric uplift is considered responsible for the development of high-angle (70° – 90°) inclined stratabound joints (*sensu* Odling et al. 1999) which terminate in correspondence of fractures at very low angle (0° – 15°) relative to bedding (Gutmanis et al. 1997; Odling et al. 1999). The Sherwood Sandstone Group has also been affected by deep mining of underlying Carboniferous Coal Measures in the coalfields on Nottinghamshire, Staffordshire and Yorkshire that has resulted in coal working collapse and fracturing in the lower parts of the overlying strata (Allen et al. 1998; Barker and Tellam 2006). The sediments that formed the Sherwood Sandstone Aquifer filled a series of sedimentary basins in Great Britain which are illustrated in Figure 1b. The Wessex, Worcester, Staffordshire, Needwood, Cheshire, Eastern Irish Sea and Vale of Eden basins are all at least partially bounded by palaeo-rift faults. However, the Eastern England Shelf is a shelf-edge type basin not-bounded by faults and therefore it represents an exception in the Triassic realm of Great Britain.

In all the above mentioned Triassic basins, the basal part of the Sherwood Sandstone Group is dominated by fluvial deposits, which are primarily characterized by channel-fill architectural elements (Fig. 2, Ambrose et al. 2014). The fluvial palaeocurrent direction is towards the north due to the principal sediment source which is represented by the Armorican Massif in northern France (Newell 2018; Figs. 1a, 2). Northward decrease in mean grain-size and maximum clast-size characterizes the fluvial deposits of the Sherwood Sandstone Group as a consequence of the increasing distance from the fluvial sediment source (Fig. 2; Smith 1990; McKie and Williams 2009). Fluvial deposits of Lower Triassic age range from conglomerates (LA1 Lithofacies Association 1, Fig. 4a, b) in the Wessex, Worcester, Staffordshire, Needwood, Cheshire and southern parts of the Eastern England Shelf basins, to fine-grained sandstone in the northern part of the Eastern England Shelf, Eastern Irish Sea Basin, Vale of Eden and Carlisle basins (Fig. 4 c, d; Mickie and Williams 2009; Ambrose et al. 2014; Medici et al. 2019b). The Sherwood Sandstone Group shows an upward trend from conglomerates (LA1) via feldspatic sandstone of fluvial origin (LA2), into sand-prone and quartz-rich deposits which are characterized by facies of exclusively aeolian origin (LA3 Lithofacies Association 3, Figs. 2, 4c, 5a, b).

Fluvial lithofacies associations are characterized by conglomerate and pebbly sandstone lithofacies (LA1), and sandstone channels interbedded with floodplain mudstone (LA2). However, lithofacies associations of aeolian origin (LA3) are dominated by cross-bedded dune deposits. Fine grained sandstones related to damp interdune and mudstone of wet interdune and mudstone wet interdune origin also characterize the aeolian deposits (LA 3) of the Sherwood Sandstone Group. Note that, reference to these three facies associations (LA 1-3) is crucial in this manuscript to establish a link between lithology, mechanical behaviour and flow modelling approach.

Structural style and mechanical behaviour of the stratigraphic units

Development of stratabound and non-stratabound joints and bedding plane fractures is highly determined by lithology and mechanical properties in the Sherwood Sandstone Aquifer. The bedding plane fractures in the Eastern Irish Sea Basin (Figure 4c) are characterized by lateral continuities up to 300 m (Medici et al. 2015). Stratabound and bedding plane discontinuities reactivated by tectonic stresses are particularly well developed in the relatively brittle, highly mechanically resistant (17-36 MPa of uniaxial compressive strength under natural saturation conditions, UCS_{nat}) Sherwood Sandstone Aquifer of the Eastern Irish Sea and Cheshire basins (Fig. 4c, 5a, 6a-c; Allen et al. 1998; Hitchmough et al. 2007). Here, high angle joints have been found partially filled by clays in the vadose zone in the Runcorn Peninsula (Wealthall et al. 2001). By contrast, sub-vertical joints are more widely spaced and non-stratabound in the Eastern England Shelf. This structural pattern arises from the relatively ductile, low mechanical resistance (UCS_{nat} <20 MPa; Yates 1992) of the Sherwood Sandstone Group in the shelf-edge basin of England as illustrated in the conceptual scheme in Figure 7. Stratabound joints are exclusively present in the 1-2 m thick sandstone layers interbedded with conglomerates (LA1 lithofacies association) in the Kidderminster Sandstone Formation (Figure 7 upper panel) of the Worcester, Needwood and Staffordshire basins. Notably, the low-mechanical resistance (UCS_{nat} < 16 MPa; Whitaker and Turner 1989) of the conglomerates also in the latter case impedes development of stratabound fractures. Scanline surveys of rock discontinuities undertaken at road cuts in the Helsby and Wildemoor Sandstone formations show higher fracturing density in the fluvial deposits (which are less porous and more mechanically resistant) than in the aeolian deposits (Fig. 7 middle and lower panels; Allen at al. 1997, 1998). The fluvial channels (LA2 Lithofacies Association) and aeolian dunes (LA3 Lithofacies Association) are characterized by an average lateral spacing of sub-vertical joints of 2.0 and 3.1 meters, respectively (Allen et al. 1998; Wealthall et al. 2001; Hitchmough et al. 2007).

Fault zones in aeolian dunes are also characterized by development of low permeability deformation bands rather than open fractures, as seen in fluvial sequences worldwide (Aydin 2000; Bense et al. 2013). Extensional faults are highly permeable in the fluvial St Bees Sandstone of west Cumbria and dilatational jogs enlarged by groundwater flow and cavities are recognized in outcrop (Fig. 5c). Boreholes collapse in correspondence of such tectonic structures, cavities with apertures in the range 0.05 - 0.6 m large are recognized by optical televiewer logs in correspondence of bedding plane fractures (Fig. 6a, b), and calcite dissolves in sub-vertical joints (Fig. 6c) in the Sherwood Sandstone Aquifer of west Cumbria (Medici et al. 2016). Further details on the hydro-structural pattern of fault zones and development of extensional features in fluvial and aeolian deposits can be found in Medici et al. (2019b).

Physical Hydrogeology

Core plug and well-test scale properties

Intergranular hydraulic conductivities measured using the Darcy's law on core plugs vary within eight orders of magnitude from 1.2×10^{-11} to 1.0×10^{-4} m/s in the Sherwood Sandstone Aquifer (Allen et al. 1997). This high variability is related to heterogeneities (e.g., mudstone) that characterize the three distinct lithofacies associations (LA1-3), as illustrated in Figures 4, 5 and 7.

Intergranular hydraulic conductivities are only slightly reduced (by 6-20 %) in response to an increase in lithostatic pressure of 7 MPa (overburden pressure of 300 m below the subsurface) as tested at the core-plug scale by Daw et al. (1974). In contrast, fracture flow is strongly reduced (by 65-80%) in experiments that applied the same amount of overburden pressure (7 MPa) to plugs with a single discontinuity (Daw et al. 1974). The aquifer is highly anisotropic and the ratio between horizontal (K_h) and vertical hydraulic conductivity (K_v) ranges from 1.5 to 100 and 2 to 34 at the core plug and well test scale, respectively (Allen et al. 1997; Streetly et al. 2000; Pokar et al. 2006; Medici et al. 2018).

Transmissivities in the Sherwood Sandstone Aquifer show similar values across the regions of Great Britain, i.e. median values range from 1.6×10^{-3} m^2/s to 3.5×10^{-5} m^2/s in the various Permo-Triassic basins (Brassington and Walthall 1985; Allen et al. 1997, 1998; Tellam and Barker 2006; Medici et al. 2019a). Such transmissivity values show a positive correlation with the well-screen length (Allen et al. 1997).

In contrast to transmissivity values, the ratio ($K_{well\text{-}test}/K_{core\text{-}plug}$) between hydraulic conductivity values from pumping tests and core plugs shows a regional distribution across the Triassic basins of Great Britain. Notably, the hydraulic conductivity from pumping tests is ~10^2 times higher than that derived testing core-plugs collected from the Eastern Irish Sea Basin of west Cumbria at shallow depths (<~150 mBGL; Allen et al. 1997; Streetly et al. 2000). Here, pumping tests show the highest transmissivity value, 1.0×10^{-2} m/s, in a valley. This is a hydraulic scenario common to moderately karstfied aquifers such as the Magnesian Limestone and the Chalk in England (Allen et al. 1997; Worthington and Ford 2009), suggesting that the sandstone here is locally characterized by a karst-like behaviour. The ratio between well-test derived hydraulic conductivity and those from core plugs measured by mini-permeameters is ~5 in the Sherwood Sandstone Aquifer in the

Cheshire Basin. This value is the result of a pervasive fracture network due to the high mechanical resistance (UCS_{nat} = 30 MPa) combined with a relatively low hydraulic conductivity matrix (Brassington and Walthall 1985; Hitchmough et al. 2007). The area of the Sherwood Sandstone Aquifer that shows the lowest difference between well-test and core-plug hydraulic conductivities (< 2.0) is the Eastern England Shelf and Worcester Basin (Allen et al. 1997; Ramingwong 1974). This hydraulic scenario arises from low values of mechanical resistance (UCS_{nat}< 20 MPa) that impedes development of a pervasive fracturing network in the latter two Triassic basins (Whitworth and Turner 1989; Yates 1992); the aquifers developed in these basins are thus mainly dominated by intergranular flow.

Fluid logging

Bedding plane discontinuities, sub-vertical joints and extensional faults are all capable of facilitating flow in the Triassic Sherwood Sandstone Aquifer (Tellam and Barker 2006; Medici et al. 2016). In fact, bedding plane fractures were detected as pathways at shallow depths (< 150 mBGL) by borehole fluid electrical conductivity and temperature logging under natural conditions in the Eastern Irish Sea Basin (Medici et al. 2016, 2018), Cheshire (Hitchmough et al. 2007), Worcester (Allen et al. 1998) basins and the Eastern England Shelf (Rivers et al. 1996). In the Eastern Irish Sea Basin, high angle (70° – 90°) inclined stratabound joints also provide occasional support to flow at their intersection with bedding plane fractures in the shallow (<100 mBGL) Sherwood Sandstone Aquifer (Medici et al. 2016, 2018).

This hydraulic scenario was characterised by borehole flow logging under natural condition in the highly mechanically resistant (UCSnat = 17-36 MPa) St Bees Sandstone aquifer of the Eastern Irish Sea and Cheshire basins (Medici et al. 2016; Hitchmough et al. 2007). Fluid temperature and electrical conductivity logs were also undertaken in the Sherwood

Sandstone Aquifer in the Vale of York (Allen et al. 1998) and Nottinghamshire (Rivers et al. 1996). Here, inflows from fissures were detected only in the first 10 meters below the water table due to greater dissolution in the shallow part of the aquifer zone. Below this threshold, the aquifer behaved as a matrix flow aquifer and variation in fluid temperature and electrical conductivity were absent in the Vale of York and Nottinghamshire.

Quantitative flow logging analysis was performed using the Flow Log Analysis Single Hole (FLASH, Day-Lewis et al. 2011) program in the St Bees Sandstone of west Cumbria. Here, the latter methodology developed by the United States Geological Survey (USGS) to compute profiles of hydraulic conductivity has been applied due to the availability of both fluid velocity logs and pumping tests (Medici et al. 2016). Notably, the use of the USGS FLASH program failed on three boreholes matching experimental and modelled fluid flow velocities in wells characterized by sharp variation of velocities in correspondence of conduits 5-10 cm in diameter (Medici et al. 2016). This scenario can arise from turbulent flow occurring in correspondence of such conduits enlarged by dissolution of the high-solubility cement (Day-Lewis et al. 2011; Medici et al. 2016).

Tracer testing

Very few successful field-scale point-to-point tracer tests have been carried out in the Sherwood Sandstone Aquifer due to the simplistic assumption that the sandstone is primarily a matrix flow aquifer across all the Great Britain (Allen et al. 1997, 1998; Barker et al. 1998; Streetly et al. 2002; Tellam and Barker 2006; Riley et al. 2011). Tracer movement was considered slow by hydrogeologists and high dilution a problem that might prevent detection at field-site scale (Allen et al. 1998).

However, results from a few point-to-point tracer tests are available in the Sherwood Sandstone Aquifer of the Yorkshire, West Midlands and Cheshire regions. Low travel times of 1.7×10^{-5} and 3.5×10^{-5} m/s, perhaps indicating matrix flow, characterize this sandstone aquifer at Carlton in the Eastern England Shelf and Hodnet in the Worcester Basin, respectively (Allen et al. 1997, 1998). Hydrogeologists injected fluorescent dye into an observation borehole and recorded the breakthrough at inflows along a tunnel in Liverpool in the Cheshire Basin (Barker et al. 1998; Streetly et al. 2002). Here, the average linear flow velocity was 1.6×10^{-3} m/s which more typically can be found in karst aquifers of carbonate origin instead of porous sandstone (Hartmann et al. 2014; Worthington 2015).

In summary, the physical hydrogeology of Sherwood Sandstone Aquifer shows a range of scale effects depending on the important of matrix versus fracture or conduit flow. In Sherwood Sandstone Aquifer where matrix flow dominates, it is likely that a Representative Elementary Volume (REV, *sensu* Schulze-Makuch et al. 1999; Schulze-Makuch 2005) can be defined at the approximately 10m scale. In these cases, the hydraulic conductivity above that scale becomes constant and tracer testing is not necessary. Where fracture flow dominates, it may also be the case that REV can be defined at such a scale, taking into account that the spacing of bedding plane fractures and joints is smaller than 10m, provided that the effect of large faults is taken into account separately, where these occur on the 100m – 1km scale (Medici et al. 206; Bense et al. 2013). However, where karst-like conduits are present, no REV can be defined (Schulze-Makuch et al. 1999; Hartman et al. 2014; Medici and West 2021). In such cases, the hydraulic conductivity will continue to increase with scale, up to the characteristic length of the connected conduits that can be detected by tracer testing.

Groundwater Flow Modelling

Previous models

Groundwater flow models in the shallow (< 120 mBGL) Sherwood Sandstone Aquifer were developed in most cases using the EPM as the modelling approach and MODFLOW as the numerical code, respectively (see type of approach, location and numerical code used for flow models in Table 1). MODFLOW groundwater flow models at a relatively large (~ 200 km^2) scale were developed in the Eastern England Shelf to constrain aquifer recharge and designate capture zones around areas of abstraction in both the Vale of York (Bottrell et al. 2006) and Nottinghamshire using MODFLOW/MODPATH to trace unreactive particles (Tab.1; Bishop and Ruston 1993; Allen et al. 1997; Zhang and Hiscock 2010). However, exclusively in Nottinghamshire, MODFLOW-MT3DMS large-scale contaminant transport models are publicly available that represent plume development in the subsurface and predict nitrate concentrations in supply wells (Davison and Lerner 2000; Zhang and Hiscock 2011, 2016). All the above mentioned groundwater flow models were calibrated using horizontal hydraulic conductivity (1.2×10^{-6} - 6.9×10^{-5} m/s) values that are within the range of the values derived from core plugs and pumping tests in the Sherwood Sandstone Aquifer of the Eastern England Shelf (Bishop and Ruston 1993; Davison and Lerner 2000; Neumann and Hughes 2003; Bottrell et al. 2006; Pokar et al. 2006; Zhang and Hiscock 2010, 2011). Note that matching the hydraulic conductivity values of the core-plug with those of the regional scale is common for aquifers largely dominated by intergranular flow and characterized by a small REV (*sensu* Schulze-Makuch et al. 1999; Schulze-Makuch 2005).

The Sherwood Sandstone Aquifer was treated as a single hydraulic unit in groundwater flow models developed for the Eastern England Shelf (Bishop and Ruston 1993; Davison and Lerner 2000; Neumann and Hughes 2003; Bottrell et al. 2006; Zhang and Hiscock 2010, 2011). In this sedimentary basin, the latter choice is reasonable given the relative homogeneity of the sandstone and the fact that the British Geological Survey could not recognize stratigraphic members in quarries and core logs (Ambrose et al. 2014; Wakefield et al. 2015). The Sherwood Sandstone Aquifer was also modelled as a single-layer in the MODFLOW-EPM model developed in the Birmingham area of the Worcester Basin (Knipe et al. 1993; Rivett et al. 2012). Here, the Bromsgrove, Wildmore and

Kidderminster Sandstone formations were treated as a single unit with a hydraulic conductivity of 1.7×10^{-5} m/s and an effective porosity of 0.25. This assumption overlooks the fact that the aeolian facies of the Bromsgrove Sandstone Formation is more porous and has fewer connective fractures than the fluvial units of the Wildmore and Kidderminster Sandstone formations (see contrast of fracture density in fluvial vs. aeolian lithofacies associations in Figure 7). Thus, the Bromsgrove Formation is likely characterized by higher values of effective porosity (typically set up to around 0.15-0.25 in particle tracking modelling) and therefore ideally should be represented as different unit for particle tracking and solute transport modelling (Allen et al. 1997, 1998; Tellam and Barker 2006; Medici et al. 2019a).

The Sherwood Sandstone Aquifer in the Merseyside area of the Cheshire Basin was also modelled in MODFLOW as a single unit in an EPM. Here, a 2.3×10^{-5} m/s background horizontal hydraulic conductivity was assigned to the entire aquifer. A reduction of three orders of magnitude was applied in correspondence of faults to simulate the sharp changes in hydraulic head moving from the footwall to the hanging wall (Tab. 1; Seymour et al. 2006). The Sherwood Sandstone Aquifer is anisotropic and the ratio between horizontal and vertical hydraulic conductivity was defined through calibration in MODFLOW-EPM models. In such models, the ratio K_h/K_v is typically tenth-one fitting values (2-34) from pumping tests in the studied aquifer (Streetly et al. 2000; Zhang and Hiscock 2010).

In contrast to the models described above (see Tab. 1), Hitchmough et al. (2007) developed a DFN flow model using NAPSAC (by AMEC, Harwell, Oxfordshire; Wilcock 1996) as the numerical code for the Sherwood Sandstone Aquifer in the Cheshire Basin of the Merseyside area. This research used DFN modelling to assess fracture network connectivity in its minimum REV of 35 x 35 x 35 m (Tab. 1). In the latter basin, fractures are highly conductive ($K_{well\text{-}test}/K_{core\text{-}plug}$=5; Medici et al. 2019b) and a DFN approach at the scale of the industrial field site (~ 10^1 km^2) can be used based on a robust characterization of the fracture network. DFN modelling generates distributions of fractures and bedding planes and compares these values with observed data from outcrop scanlines and/or borehole acoustic televiewer logging to represent positions, sizes and mechanical apertures of those features. To develop the DFN model generated by Hitchmough et al. (2007), 979 rock discontinuities were characterized performing outcrop scanlines, and measurements of fracture orientation, aperture, spacing and tortuosities were recorded. In terms of flow modelling, the latter DFN model of the Sherwood Sandstone Aquifer of the Merseyside assumes a non-conductive matrix; hydraulic conductivity of bedding plane discontinuities was extrapolated from packer testing (Hitchmough et al. 2007). Note that groundwater flow models that incorporate discrete karstic conduits have not been built for the British Sherwood Sandstone to the authors' knowledge. This scenario might be either related to absence of a robust characterization that supports the latter modelling solution, apart from tracer testing in Liverpool (Barker et al. 1998), or an assumption that this approach is not necessary for the purposes to which their models were developed.

Comparisons with other sandstone aquifers

The EPM modelling approach is commonly used in sandstone aquifers for the management of aquifer water resources across the world (Freeze and Cherry 1976; Hill and Tiedeman 2006). In this case, EPM modelling is suitable at a variety of scales from that one of industrial sites (<~10 km^1) up to the one of a sedimentary basin (~10^4 km^2) for sandstone aquifers as depicted on the left side of Figure 8. For example, the EPM using MIKE-SHE (by DHI Water & Environment, Cambridge, Ontario; Jaber and Shukla, 2012) as numerical code was used in the Californian Cretaceous Sandstone at the watershed (~15^2 km^2) scale in a model that include the vadose zone and the shallowest and highly permeable saturated zone (Manna et al. 2019). A similar approach to groundwater flow modelling has been used in the Sherwood Sandstone Aquifer to constrain aquifer resource by model calibration in the shallowest and highly permeable 150 m below the ground surface (Bottrell et al. 2006). Moving at a smaller (1-5 km^2) scale to model contaminant transport the DFN approach was chosen in the Cretaceous sandstones of California and Colorado and the Cambrian Sandstone of Wisconsin (McKoy and Sams 1997; Pierce et al. 2018; Morgan 2019; Pilato 2021). In the above mentioned case studies, the use of FRACTRAN and MAFIC (both by Golder Associates, Toronto, Ontario; Miller 1995) as numerical codes allowed representation of solute advective transport and diffusivity in the rock discontinuities and matrix (Figure 8 central-right portion of the panel describing fractured sandstones), respectively. This approach named DFN-M combines EPM and DFN and can be exported in the Sherwood Sandstone Aquifer where both fractures and matrix are hydraulically conductive, and diffusivity cannot be neglected (Figure 8 central portion; Bloomfield and Williams 1995; Bloomfield et al. 2006; Bouch et al. 2006; Tellam and Barker 2006; Hitchmough et al. 2007).

The DFN approach in sandstone aquifers has also been used in the Carboniferous Sandstone of NE England. This Carboniferous sandstone is highly mechanically resistant (UCS > 20 MPa) and hydraulic aperture and hence flow velocities are highly sensitive to stress release in proximity to mineral-pit excavations, i.e. within the so-called excavation disturbed zone (Foster et al. 2018). This finding was demonstrated via applying a DFN approach using the ELFEN code (by Rockfield Global, Cardiff, Wales; Rockfield 2001) to geomechanical modelling by investigating fracture aperture response to stress relaxation in the Carboniferous Sandstone of Northumberland for a range of excavation profiles. The mechanical resistance of the Sherwood Sandstone Aquifer is very high (up to 30 MPa) in north-west England and here similar scenarios can occur with mechanical aperture increased by stress release within excavations disturbed zones. Indeed, the fracture hydraulic conductivity changes by 65-80% from a 7 MPa normal stress change (Daw et al. 1974).

Groundwater flow can enlarge rock discontinuities via dissolution processes in a variety of rock-types including sandstones. Also, after dissolution of the carbonate cement, silicate mineral grains can be washed out from fractures in areas characterized by elevated groundwater flow velocities (Worthington et al. 2016). Note that, the Sherwood Sandstone Aquifer in west Cumbria where cavities were detected by optical and acoustic televiewer logs is located in the proximity of the Lake District mountains and hence elevated hydraulic gradients (0.15-0.35) and intense groundwater flow occur (Black and Brightman 1996; Medici et al. 2016, 2018, 2019b). Karst-like cavities and caves have been reported in some other sandstones with calcite cement in five continents; the Devonian in Australia (Young 1986, 1988), the Carboniferous in Scotland (Balin 2000), the Permian in China (Yang et al. 2011), the Jurassic in Luxembourg (Meus and Willems 2021), the Cretaceous in Czech Republic (Kůrková et al. 2019), and the Miocene in Nigeria (Wray 1997). Karst-like groundwater flow velocities have been found in the Sherwood Sandstone Aquifer in England (1.6×10^{-3} m/s average peak flow velocity), the Jurassic Sandstone of Luxembourg (4.4×10^{-3} m/s and 9.7×10^{-2} m/s as average pick and maximum flow velocities, respectively), and the Cretaceous in Czech Republic (maximum flow velocities reported 2.2×10^{-2} – 2.02×10^{-1}m/s) by using tracer testing (Barker et al. 1998; Kůrková et al. 2019; Meus and Willems 2021). Occurrence of high flow velocities and turbulent flow should not be discounted in some sandstone aquifers to designate well-head protection areas. For example, high turbidity was found in the groundwater of the Sherwood Sandstone Aquifer in the Worcester basin by South Staffs Water (Hudson 2008). Solute transport occurs through matrix, a network of discrete fractures and a small number of karst-like conduits. In the latter case, the EPM, DFN and CN needs to be combined to represent this complexity as shown in the right-lower portion of the panel in Figure 8.

Modelling strategy and future research

The shallow (<150 mBGL) Sherwood Sandstone Aquifer is characterized by different hydraulic behaviours across Great Britain. Hence, the strategy to model groundwater flow can vary and different approaches may be combined depending on modelling objectives, observation scale, degree of heterogeneities and nature of permeability as illustrated in Figure 8. Where modelling is at a relatively large scale (more than 10 km^2 plan area) representation of individual features such as fractures and conduits may be too computationally demanding to be feasible. Furthermore, fractures and conduits can lose connectivity at the basin scale (plan areas ~ 10^2-10^4 km^2). In such circumstances, representation using the EPM approach is likely to represent the only practicable solution, whatever the modelling objective. This option requires to estimate the equivalent bulk properties of the modelled layers, for example the EPM hydraulic conductivity, and where transport is modelled, the effective porosity (Worthington et al. 2012, 2019; Medici and West 2021; Medici et al. 2021). The EPM methodology has commonly been applied to trace particles to abstraction wells for the purpose of wellhead protection due to uncertainties related to constraining the fracture network even in heavily fractured sandstones (e.g., Freeze and Cherry 1979). The use of the EPM is reasonable for particle tracking and contaminant transport purposes at a variety of scales where the Sherwood Sandstone Aquifer is porous and dominated by matrix flow (the case of the upper-right portion of the panel). Here, the REV is small, and values of core plugs can be used to calibrate groundwater flow models. Notably, the Sherwood Sandstone Aquifer has been modelled across the Great Britain using the EPM approach as a single hydraulic unit for contaminant transport purposes (Knipe et al. 1993; Allen et al. 1998; Seymour et al. 2006; Bottrell et al. 2006). This assumption (Figure 8, right-upper portion of the panel) is certainly reasonable in the case of the Eastern England Shelf where the sandstone is highly porous, relatively homogeneous, no individual stratigraphic members are identifiable and aeolian lithofacies are absent (Ambrose et al. 2014; Wakefield et al. 2015; Medici et al. 2019a). However, where present we recommend the use of contrasting values of EPM effective porosity to characterize aeolian and fluvial units separately, with aeolian-dominated deposits such as the Helsby Sandstone and the Ormskirk Sandstone formations of the Cheshire and Eastern Irish Sea basins characterized by higher values of effective porosity. Such formations of primary aeolian origin are more porous and permeable at the core-plug scale and less heavily fractured compared to fluvial-dominated formations (Fig. 7; Allen et al. 1997; Tellam and Barker 2006; Medici et al. 2018). This difference arises because the aeolian dune sandstones are petro-physically different from fluvial channel sandstones as shown by wireline logging in the Sellafield. Here, the Triassic aeolianites are characterized by a dominant component of matrix flow (Jones and Ambrose 1994; Sutton 1996).

In contrast, fluvial units may be fracture-flow dominated where the Sherwood Sandstone Aquifer has relatively high mechanical resistance. The fracturing network can be spatially constrained and modelled using a DFN-M approach at scales of less than $\sim$ 10 km^2 in systems where fracture flow is important (see right-central portion of the panel in Figure 8). This approach may provide model simulation benefits to be used in the Sherwood Sandstone in the Cheshire Basin, allowing representation of both chemical advection and diffusivity in the fractures and matrix blocks, respectively to model contaminant transport. To allow representation of this complexity, a network of discrete flowing fractures need to be inserted in an EPM in sandstone aquifers as proposed by Pierce et al. (2018) and illustrated in the right-central portion of the panel in Figure 8.

DFN solutions should also be considered where geomechanical effects, e.g. stress changes within the disturbed zones around tunnels and excavations could potentially influence hydraulic conductivity via increasing fracture apertures. A geomechanical approach to DFN modelling can be used in the future in the high-mechanically resistant areas of the Sherwood Sandstone Aquifer. This rock-type is subject to large excavations in west Cumbria, Lancashire and Merseyside to meet the demands of the UK national market for building stones (Yates 1992).

A one end of the spectrum of hydraulic behaviours that the Sherwood Sandstone Aquifer shows across the Great Britain, this aquifer locally behaves as moderately (pseudo-) karstified with occurrence of conduits 0.05-0.6 m large. This sandstone is characterized by a transmissive zone in the first 100-150 m below the ground in west Cumbria (Streetly et al. 2000). Here, the transmissivity (1.0×10^{-1} m^2/s) is much higher in valleys with axis of 2 km and at this scale conduits should be inserted in groundwater flow models (Figure 8 lower-right portion of the panel). Additionally, high ($\sim 10^{-3}$ m/s) flow velocities characteristic of karstic carbonate systems where identified in the Sherwood Sandstone of the Liverpool area (Barker et al. 1998). The use of the Darcy-Weisbach equations (mathematical details in Valiantzas 2008) that describe laminar and turbulent flow in discrete pipe-conduit elements may be appropriate here. More research is needed to verify the widespread presence of karst-like conduits in the Sherwood Sandstone Aquifer in NW England. New tracer tests in the highly transmissive valleys in west Cumbria might reveal higher flow velocities than 1.6×10^{-3}m/s found in Liverpool by Barker et al. (1998). More tracer testing would also determine the effective porosity which is inadequately characterised in the Sherwood Sandstone Aquifer and is necessary to run contaminant transport models (Allen et al. 1997; Tellam and Barker 2006; Medici and West 2021). Note that, values of effective porosity used to run contaminant transport models in the range 0.1 - 0.35 and are not experimentally supported (Bottrell et al. 2006; Rivett et al. 2012; Zhang et al. 2010, 2011, 2016). Much lower values are expected in the Sherwood Sandstone Aquifer of north-west England. In this area, groundwater flow is largely dominated by bedding plane fractures. Fracture flow aquifers are characterized by effective porosities in the range $\sim 10^{-3}$ $\sim 10^{-5}$ (Ren et al. 2018; Medici and West 2021; Moore and Walsh 2021).

To treat fractured aquifers with occurrence of some conduits, the hydrogeologists of the USGS have applied the Darcy-Weisbach solution to MODFLOW-2005, and they found the models are highly sensitive to the diameter of conduits (Valiantzas 2008; Shoemaker et al. 2008; Hill et al. 2010; Gallegos et al. 2013; Saller et al. 2013; Medici et al. 2019b). According to the methodology of the USGS, the Darcy-Weisbach equations need to be embedded and either DFN or EPM codes are used to model groundwater flow away from such conduits in sandstones (right-lower portion of the panel in Figure 8). This methodology can be used in the Sherwood Sandstone Aquifer of north-western England at the sites where conduits are identified by tracer testing, pumping tests, optical and acoustic televiewer logs or inferred from geomorphological surveys.

Conclusions

The fluvio-aeolian deposits of the Sherwood Sandstone Aquifers across Great Britain are complex from a hydrogeological point of view as demonstrated by core plug tests, field pumping tests, borehole fluid logging analysis and tracer testing. Consequently, three different approaches to groundwater flow modelling: EPM, DFN and CN modelling need to be considered for these and other sandstone aquifer-types, depending on modelling objectives, observation scale, degree of heterogeneities and nature of permeability. The findings of the review can be summarized as follows.

1. The Sherwood Sandstone Aquifer of Great Britain behaves as a matrix flow aquifer in the Eastern England Shelf, as well as the Wessex, Worcester, Needwood and Staffordshire basins, i.e. $K_{well\text{-}test}/K_{core\text{-}plug} < 2$. Here, the EPM approach can be used to model both groundwater flow and contaminant transport at a range of scales. The Sherwood Sandstone Aquifer is particularly homogeneous in the Eastern England

Shelf and characterized by exclusively fluvial deposits. Thus, use of a single layer with EPM properties can characterize the grid.

2. Multiple hydraulic-units should be modelled for contaminant transport purposes where both fluvial and aeolian deposits form part of the groundwater system. Aeolian lithofacies are more porous and less densely fractured than fluvial units, and likely are dominated by matrix flow. Hence, such deposits need to be characterized by higher effective porosities in EPM models, which implies that contaminant dispersal is likely to be slower than in deposits of fluvial origin.
3. Fractures represent the principal flow pathways in the Sherwood Sandstone Aquifer of the Cheshire and Eastern Irish Sea Basin. Here, either EPM or DFN models may be appropriate, depending on the modelling scale and the extent of available information on the conductive fracture network. For large scale (defined here as > 10 km^2) modelling areas, a EPM approach, with and appropriate number of layers to correctly represent both fracture and matrix flow units, may the only practicable approach. For smaller scale models (plan area < 10 km^2, but including much smaller domains), a DFN approach may be considered, which accounts for both chemical advection and diffusion in fractures and matrix, respectively. Similar approaches have been applied to siliciclastic rocks in California, Colorado and Wisconsin.
4. Tracer tests indicate karst-like velocities in the Sherwood Sandstone Aquifer in the north-west of England. Cavities with apertures 0.05 - 0.60 m have been detected, where calcite cements have been dissolved in correspondence of fractures, similar to limestone or dolostone aquifers. In such scenarios, the Sherwood Sandstone Aquifer can be modelled by embedding discrete conduits elements in a DFN-M with flowing pores and fractures, to appropriately simulate the karst-like flow velocities detected by tracer testing.

Overall, the review has shown that aquifers developed in the Triassic Sherwood Sandstone Aquifer exhibits a spectrum of hydraulic behaviours from matrix, to fracture flow with secondary intergranular porosity, up to moderately karst-like behaviour. Consequently, various flow modelling approaches may be appropriate. Further field studies to determine effective porosity and assess characteristics of fractures and scale of conduit networks are recommended to support contaminant transport models in these aquifers, and similarly for analogous sandstones worldwide.

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Figures

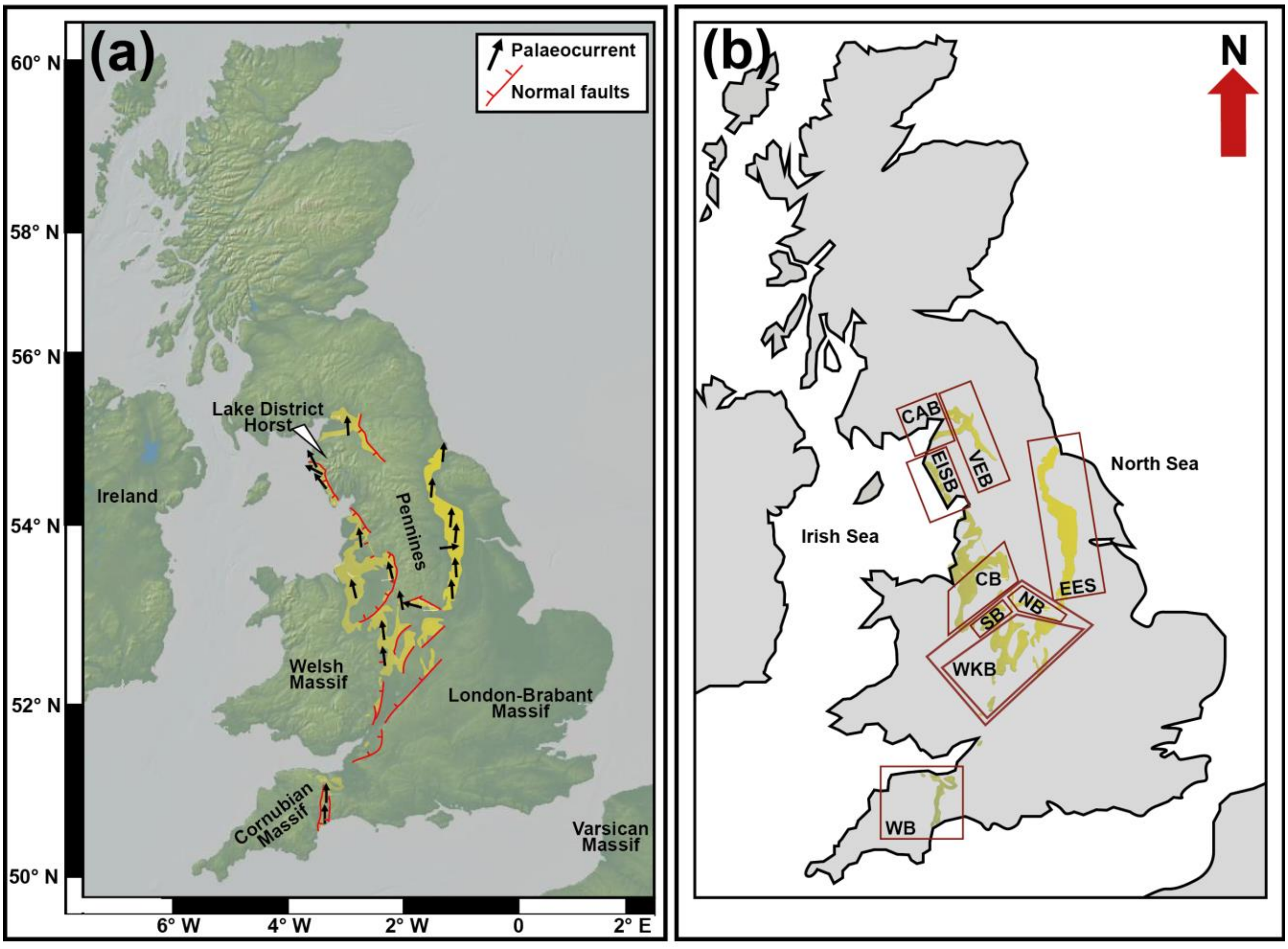

Fig. 1 Siliciclastic deposits of the Sherwood Sandstone Group in England and Wales. (a) Triassic fluvio-aeolian deposits, direction of palaeocurrents shown by arrows (basemap from GeoMappApp 2021), (b) Triassic basins in the Great Britain: Worcester (WKB), Staffordshire (SB), Needwood (NB), Eastern England Shelf (EES), Cheshire (CB), Eastern Irish Sea (EISB), Vale of Eden (VEB), Wessex (WB) and Carlisle (CAB) basins (adapted from Wakefield 2015)

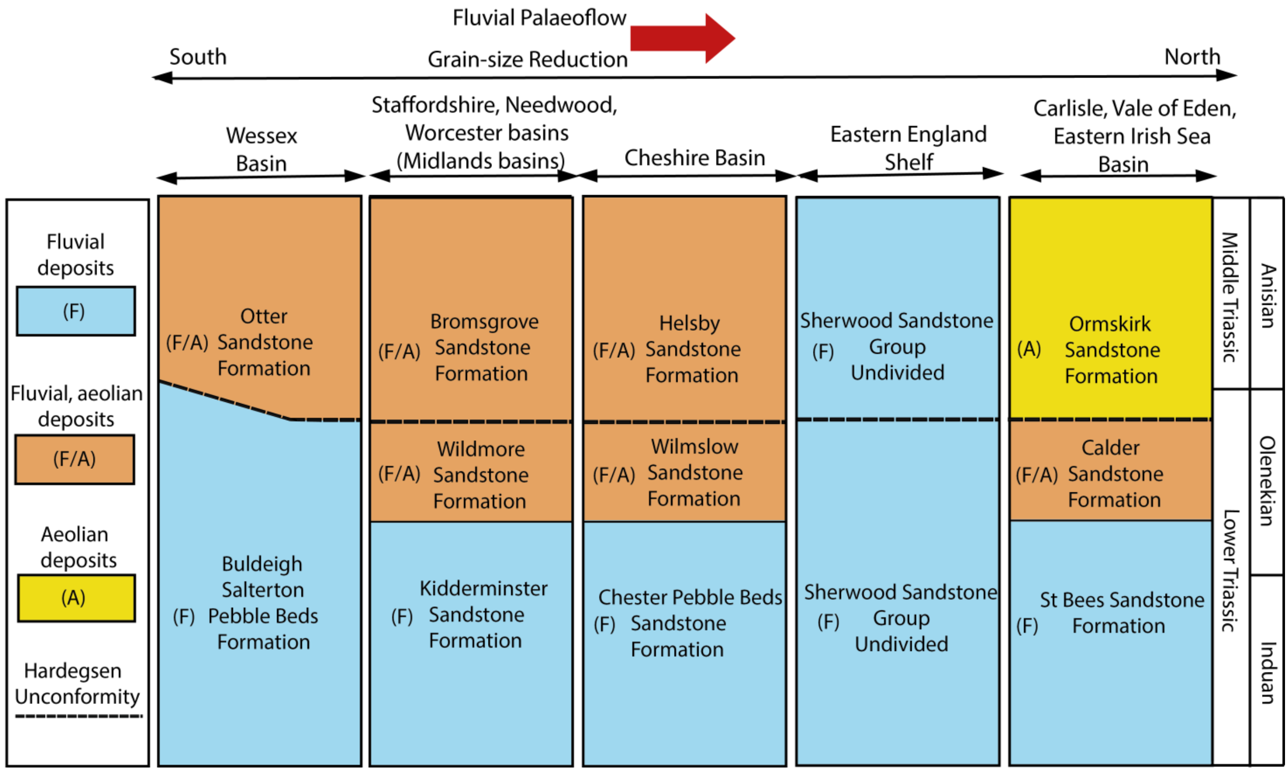

Fig. 2 Litho-stratigraphic scheme and nomenclature of the Triassic Sherwood Sandstone Group in the Triassic Basins of Great Britain (adapted from Ambrose et al. 2014 and Medici et al. 2019b).

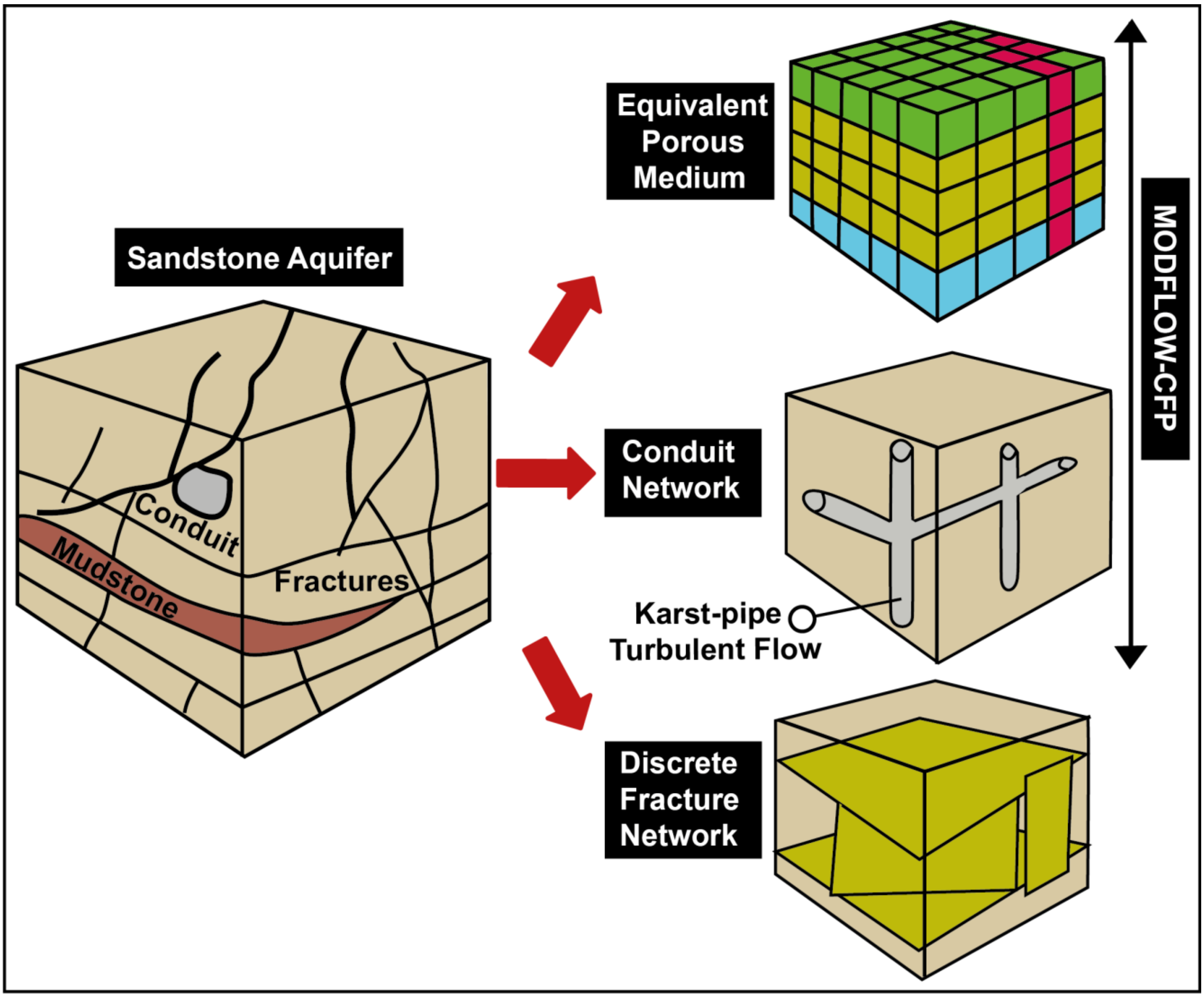

Fig. 3 Conceptual model of a sandstone aquifer and the EPM, CN and DFN approaches to numerical flow modelling (adapted from Selroos et al. 2002 and Medici et al. 2021).

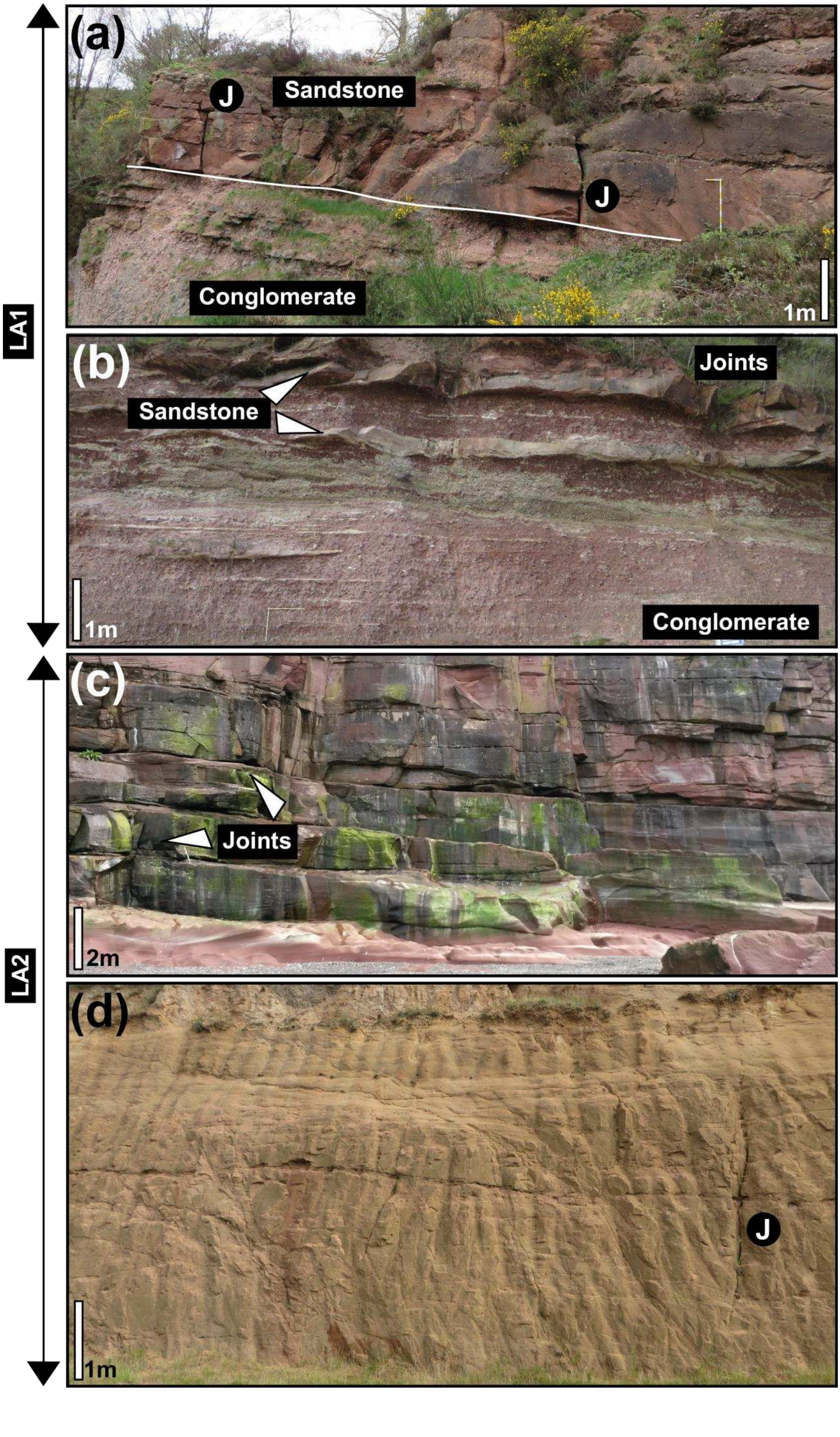
LA1
LA2
(a)
J
Sandstone
J
Conglomerate
1m
(b)
Joints
Sandstone
1m
Conglomerate
(c)
Joints
2m
(d)
J
1m

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Fig. 4 Outcropping lithofacies associations (LA1, 2) in the fluvial deposits of the Sherwood Sandstone aquifer in England. (a) Kidderminster Sandstone Formation in the Needwood Basin, Hulme Quarry, Stoke on Trent, (b) Kidderminster Sandstone Formation in the Staffordshire Basin, Croxden Quarry, Staffordshire, (c) St Bees Sandstone Formation, Fleswick Bay, west Cumbria, (d) Undivided Sherwood Sandstone Group, Dunsville Quarry, Doncaster, South Yorkshire.

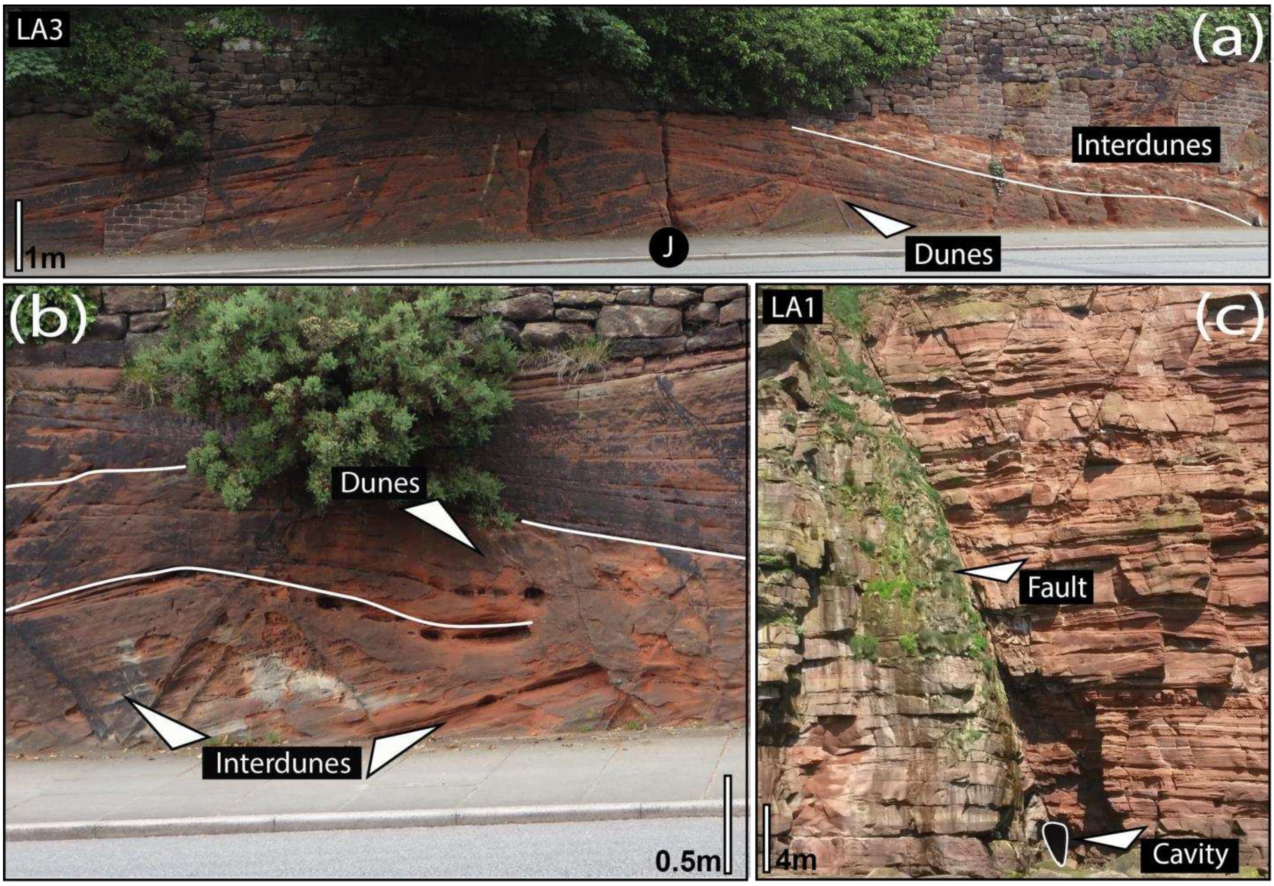

Fig. 5 Outcropping fluvial (LA1) and aeolian (LA2) lithofacies association in the Sherwood Sandstone Group. (a) Aeolian deposits Helsby Sandstone Formation, South Thurstaston, Wirral Peninsula, (b) Aeolian deposits Helsby Sandstone Formation, North Thurstaston, Wirral Peninsula, (c) Large cavity in fault zone, fluvial deposits of the St Bees Sandstone Formation at St Bees, west Cumbria.

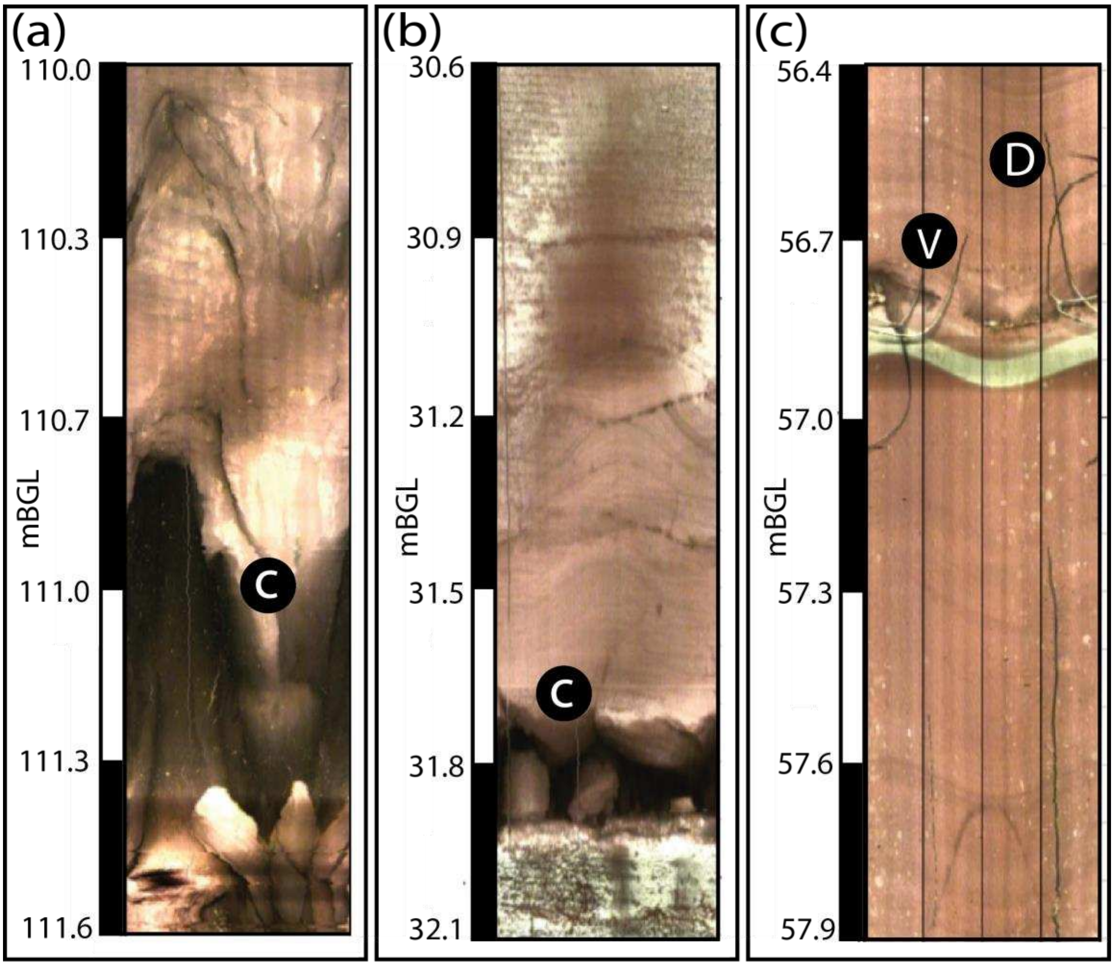

Fig. 6 Fluvial deposits of the St Bees Sandstone Formation, optical logs in the St Bees-Egremont area (west Cumbria, UK) from Medici et al. (2016). (a) Large cavity (C) in fault zone, (b) cavity (C) in correspondence of a bedding plane discontinuity, (c) Dissolution (D) of calcite veins (V).

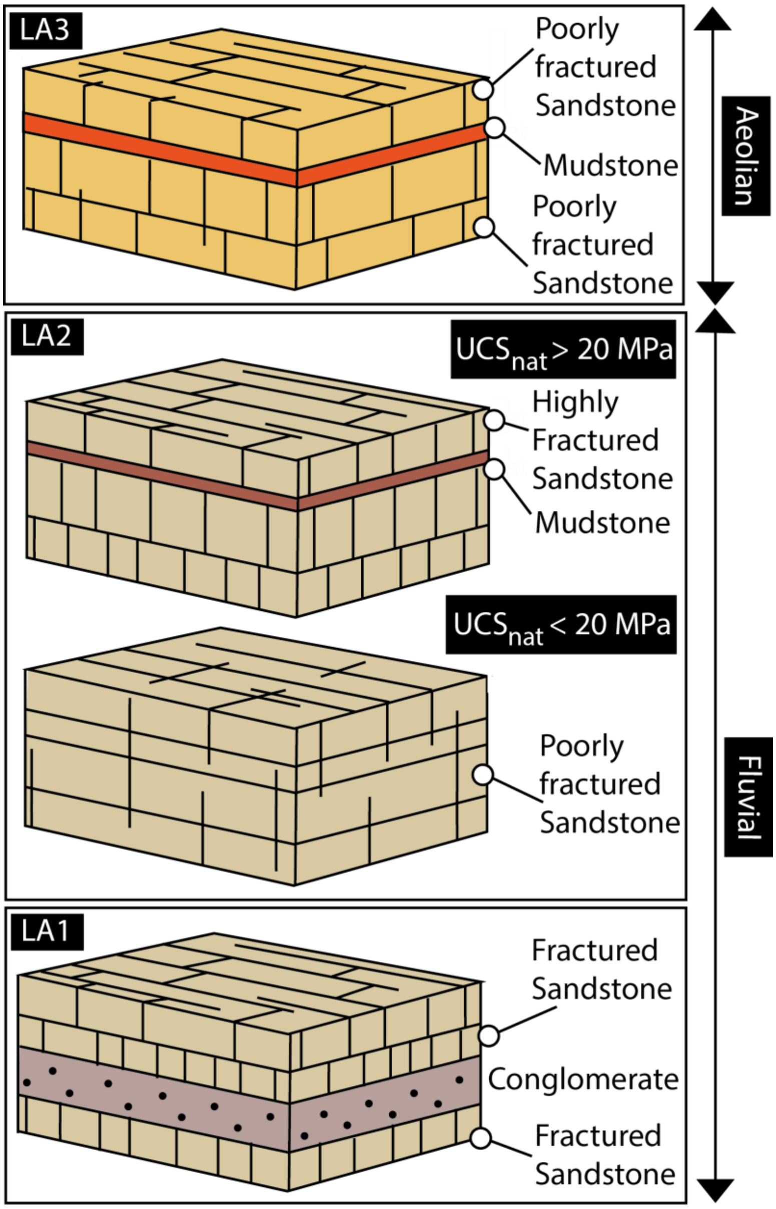

Fig.7 Conceptual model of the fracturing network in the three lithofacies associations (LA1-3) of the Sherwood Sandstone Aquifer (LA1 is fluvial conglomerate and pebbly sandstone, LS2 sandstone channels interbedded with floodplain mudstone, LA3 cross-bedded dune deposits of aeolian origin).

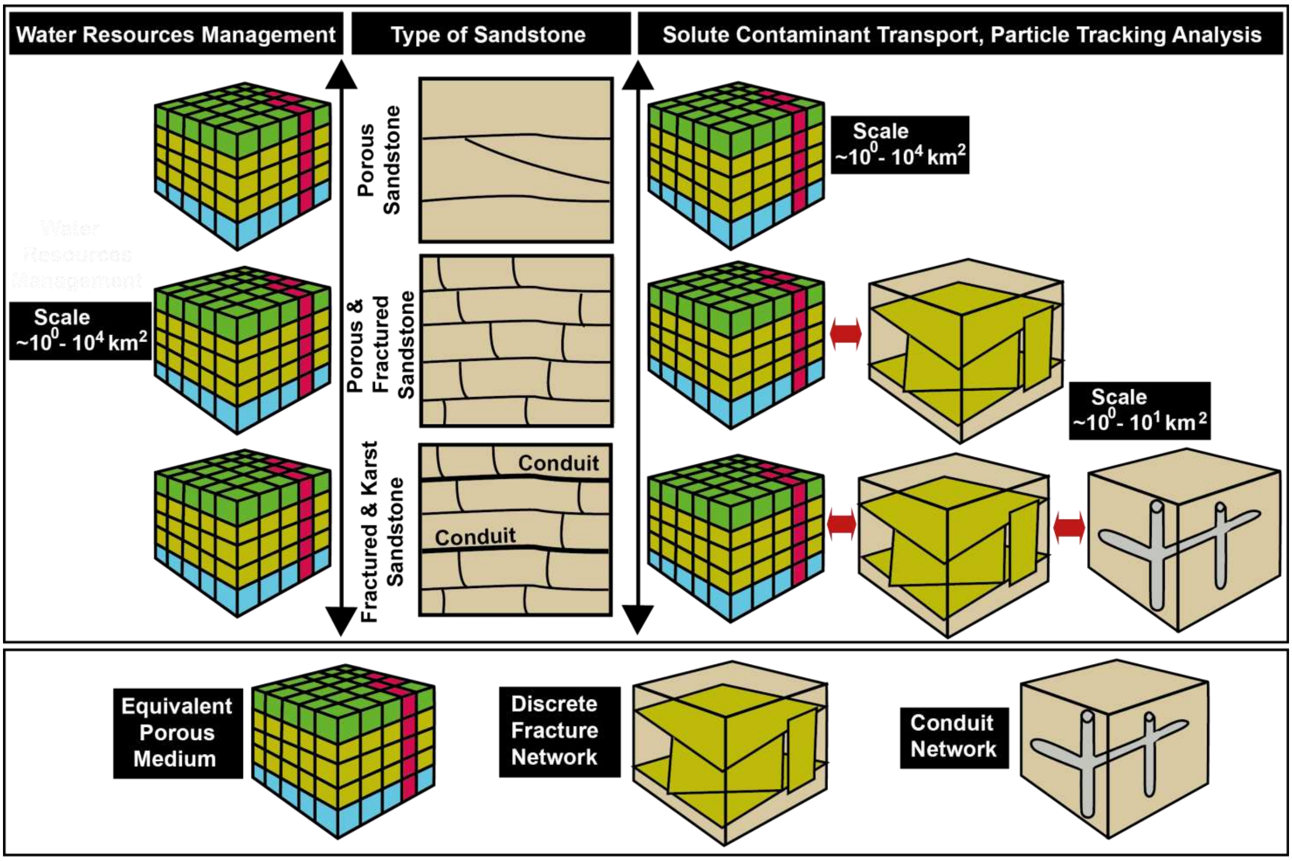

Fig. 8 Selection of difference and finite elements modelling approaches (EPM, DFN and CN) in sandstone aquifers as function of the permeability-type, observation scale and modelling purpose.

Numerical code	Sedimentary basin	Modelling objective	Reference
Equivalent Porous Medium			
MODLOW, MODPATH	Eastern England Shelf	Water balance, capture zone definition	Bottrell et al. 2006
			Zheng and Hiscock 2010
MODFLOW		Water balance	Bishop and Ruston 1993
			Neumann and Hughes 2003
MODLOW, MT3DMS		Water balance, solute contaminant transport	Davison and Lerner 2010
			Zheng and Hiscock 2011
			Zheng and Hiscock 2016
MODFLOW	Worcester Basin	Water balance	Knipe et al. 1993
MODFLOW, MODPATH		Capture zone definition	Rivett et al. 2012
MODFLOW	Cheshire Basin	Fault compartmentalization assessment	Seymour et al. 2006
Discrete Fracture Network Models			
NAPSAC	Cheshire Basin	REV definition	Hitchmough et al. 2007

Tab. 1. Type of approach, sedimentary basins and numerical code used for used for the groundwater flow, particle tacking models and solute contaminant transport models used in the Sherwood Sandstone Aquifer.