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动网格在非饱和—饱和界面数值模拟中的应用研究进展

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摘　要: 为了探讨结构和非结构动网格技术在地下水非饱和—饱和数值模拟领域未来的发展趋势,总结了非饱和—饱和耦合数值模拟研究现状,介绍了动网格技术原理及运动边界结构和非结构网格的变形方法,综述了动网格技术在非饱和—饱和分界面的应用现状及存在的不足,探讨了相关研究的未来发展趋势。综合分析表明:结构动网格和非结构动网格均存在其固有优缺点,结构、非结构混合网格以及多种动边界处理方法的结合使用在非饱和—饱和耦合数值模拟研究中具有重要的应用价值。在模拟潜水面的变动时,可将多种网格变形方法结合使用,当潜水面位置和形状变动较小时,采用弹簧法更新网格;当潜水面位置变化较大但形状变化较小时,采用重叠结构动网格技术或铺层法更新网格;当潜水面形状变动较大时,则采用网格重构法更新网格,从而更精确地模拟非饱和—饱和分界面的变化和移动。相关研究为场地非饱和带土壤与饱和带地下水协同防治工作提供了科学指导。

关键词: 动网格;非饱和—饱和;土壤;地下水;数值模拟;弹簧法;重叠结构动网格技术;网格重构法
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Research progress on the application of dynamic grids in the numerical simulation of unsaturated-saturated interfaces

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Abstract: In order to discuss the future development trend of structural and unstructured dynamic grid technology in the field of unsaturated-saturated groundwater numerical simulation, this paper summarizes the research status of unsaturated-saturated coupled numerical simulation, introduces the principle of dynamic grid technology and the deformation method of moving boundary structure and unstructured grid, summarizes the application status and shortcomings of dynamic grid technology in the unsaturated-saturated interface, and discusses the future development trend of related research. The review shows that both structural dynamic grids and unstructured dynamic grids have their inherent advantages and disadvantages, and the combination of structural/unstructured hybrid grids and multiple dynamic boundary treatment methods has important application value in the research of unsaturated-saturated coupling numerical simulation. When simulating the change of phreatic surface, a variety of mesh deformation methods can be combined. When the change of the position and shape of the phreatic surface is small, the spring method is

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used to update the mesh; When the position of the water table changes significantly but the shape changes little, the overlapping structure dynamic grid technology or the overlay method is used to update the grid; If the shape of the water table changes greatly, the grid reconstruction method is used to update the grid, so as to more accurately simulate the change and movement of the unsaturated-saturated interface. Relevant research provides scientific guidance for the coordinated prevention and control of unsaturated zone soil and saturated zone groundwater of the site.

Key words: dynamic grid; unsaturated-saturated; soil; groundwater; numerical simulation; spring method; overlapping structure dynamic grid technolog; grid reconstruction method

饱和带地下水及非饱和带土壤中的污染物下渗及其迁移转化问题是地下水污染防治工作和地下水环境研究的重点，已引起国内外学者的广泛关注[1]。通常，非饱和带是水流及地表污染物进入饱和带的必经之路，非饱和带作为饱和带的上边界与饱和带进行水量及溶质交换，形成了统一的非饱和—饱和地下水系统[2]。非饱和带中水流及污染物的运动规律较为复杂[3]。

由于数据采集难度大和模拟计算量受限，大多数研究者在建立非饱和—饱和耦合模型时，抓住非饱和带水流及溶质以垂向运动为主的特点，忽略水流及溶质在非饱和带的水平运动，采用一维垂向运动方程描述非饱和带，仅对饱和带采用三维方程描述，在数值模拟研究中通常对非饱和带进行一维垂向网格剖分，将饱和带剖分成三维网格[4]。用非饱和带模型计算对饱和带地下水的补给流量，将其代入饱和带方程计算新的地下水位，更新非饱和带的下边界[5]，非饱和带的垂向一维网格及饱和带的三维网格也将随之变化。网格剖分是数值模拟前处理过程中尤为重要的一步，在计算成本和精度要求相适应的前提下，网格剖分越精细，所建立的模型越能真实地反映实际模拟场地的地下水流动及溶质运移规律[6]。在非饱和—饱和模拟过程中，随着源汇项和边界条件变化，非饱和带与饱和带分界面的位置和形状也是不断变化的，这导致了描述非饱和带与饱和带的网格发生改变。分界面附近的网格坐标变化，网格单元大小和形状随之改变，进而导致网格质量降低、结果的误差增大[7-8]。为了降低误差出现概率，求解计算时可采用动网格技术对分界面附近的网格进行变形处理[9]，使所建立的模型能够在不同的时间步长内，根据实际分界面的位置与形状，调整网格单元的分布与数量，以适应当前的水流运动及溶质运移规律。

本研究综述了动网格技术在非饱和—饱和耦合水流运动及溶质运移数值模拟研究中的应用现状，并分析了目前该方面研究存在的不足，探讨了该方面研究未来的发展趋势，为非饱和—饱和耦合数值模拟研究提供参考。

1　非饱和—饱和耦合水流运动及溶质运移数值模拟研究现状

目前，描述非饱和—饱和多孔介质水流运动与溶质运移的数学模型主要是 Richards 方程和对流—弥散方程。求解 Richards 方程和对流—弥散方程主要有解析解和数值解 2 种形式。由于 Richards 方程和对流—弥散方程在非饱和带的高度非线性，解析解的推导较为困难，而将非饱和带部分水力参数简化后，可进行解析解的推导。部分研究者基于稳定流和非稳定流的 Richards 方程推导了方程的解析解[10-15]。对流—弥散方程解析解的推导相对较少，Beltman[16]、Domenico[17]针对非饱和—饱和系统中的稳定水流运动，推导出了对流—弥散方程的解析解。但非饱和—饱和系统中的水流及溶质运移大多为非稳定运动，鉴于此，Connell[18]针对非饱和带的非稳定流，采用 Laplace 方法推导出了非饱和—饱和系统的对流弥散方程的解析解。

在推导解析解时，往往需要假设一些比较理想的条件，其实用性较窄，对复杂边界条件下的大多数问题无法推导出其解析解，只能求出数值解。因此，相较于解析解，数值方法求解 Richards 方程和对流—弥散方程的适应性更强。首先，数值模拟可以模拟各种复杂形状的边界条件和不同的初始条件；其次，随着计算机技术的发展，各种数值求解方法和模型不断涌现出来。因此，数值模拟是当前求解多孔介质水流运动及溶质运移方程较为有效的办法。非饱和带与饱和带数值模拟研究已分别形成了成熟的研究方法并开发了相关软件，用于非饱和带数值模拟的软件主要有 HYDRUS、SVAT、SWAT 以及 UZF1 程序包等；用于饱和带的数值模拟软件主要有 MODFLOW、Visual MODFLOW、GMS 等。对于非饱和带—饱和带模拟常用的方法是将非饱和带模拟软件与 MODFLOW 耦合。除此之外，还有一些完全耦合模型也可用于非饱和带—饱和带模拟，包括 COMSOL、FEFLOW、OpenGeoSys、HydroGeoSphere 以及 InHM 等[19-24]。FEFLOW、OpenGeoSys、HydroGeoSphere 以及 InHM 等模型在模

拟过程中网格是不变的[25-29]，而 COMSOL 模型可根据实际情况选择可变动网格或固定网格[30]，基于 MODFLOW 的模型在模拟过程中根据潜水面的变化将非饱和带及饱和带的网格进行重新剖分以适应当前时刻的条件[31-32]。

空间离散是数值模拟的一个重要过程，常用的空间离散方法有有限差分法、有限元法和有限体积法。大多数空间离散方法都需要进行网格剖分，但是由于地下水系统补给和排泄，潜水面的位置和形状在每个时间步长都是不断变化的，这就导致潜水面附近网格发生压缩、拉伸或者扭曲，造成网格质量下降，在很大程度上增大了运动边界处的计算误差，同时会使计算过程中的时间步长减小，延长整体的计算时间。在处理这类问题时，采用动网格生成方法往往能够获得具有较高质量的网格，所求得的解的精度和计算效率都较高。

2 基于动网格更新方法的非饱和一饱和耦合数值模拟研究

2.1 动网格控制方程

动网格方法涉及到计算网格节点的增加、减少和网格单元的变形、移动等过程，一般用于计算流体力学中的自由表面及流体耦合问题等[33]。动网格法是一种基于 ALE(拉格朗日一欧拉)法建立控制方程并按照一定的算法更新网格的方法。兼具 Lagrange 法和 Euler 法的优点：在边界运动的处理上引进了 Lagrange 法的优点，能有效地引入边界的运动；在内部网格的划分上，它吸收了 Euler 法的优点，即使内部网格单元独立于材料而存在，但它又不完全和 Euler 网格相同，其网格可以根据定义的参数在求解过程中适当调整位置，不至于出现负体积[34]。动网格控制方程可表示成如下形式[35]：

$$\frac{\partial}{\partial t}\int_V \boldsymbol{U}\,\mathrm{d}V + \int_{\partial V} \boldsymbol{F}\,\mathrm{d}A = 0 \tag{1}$$

式中：V 为运动的控制体体积；∂V 为其边界；守恒型变量 $\boldsymbol{U}$ 和无黏矢通量 $\boldsymbol{F}$ 定义如下：

$$\boldsymbol{U}=\begin{bmatrix}\rho\\ \rho\boldsymbol{u}\\ \rho\boldsymbol{v}\\ \rho E\end{bmatrix},\ \boldsymbol{F}=\begin{bmatrix}(\boldsymbol{u}_n-\boldsymbol{u}_w)\rho\\ (\boldsymbol{u}_n-\boldsymbol{u}_w)\rho\boldsymbol{u}+pn_x\\ (\boldsymbol{u}_n-\boldsymbol{u}_w)\rho\boldsymbol{v}+pn_y\\ (\boldsymbol{u}_n-\boldsymbol{u}_w)\rho E+pu_w\end{bmatrix} \tag{2}$$

式中：ρ 为流体密度(g/cm^3)；p 为压强(N/m^2)；E 为比总内能(kJ/kg)；$\boldsymbol{u}$，$\boldsymbol{v}$ 分别为速度矢量的 2 个分量(m/s)；$\boldsymbol{u}_n$ 和 $\boldsymbol{u}_w$ 为 $\boldsymbol{u}$ 的 2 个分量；n 为运动边界 ∂V 的单位外法线方向(无量纲)；n_x 和 n_y 是 n 的 2 个分量。

2.2 动网格更新方法

动网格更新方法主要分为两类，分别为基于结构网格的动网格方法和基于非结构网格、混合网格的动网格方法[36]。基于结构网格的动网格方法数据存储形式简单，较易实现区域尺度的边界拟合；但结构网格的结构性、有序性限制了其对复杂几何构型的适应能力，其网格生成较困难，网格生成的人工工作量比非结构网格要多(表 1)。基于非结构网格动网格方法以结构网格的特性为基础，在处理结构网格变形计算中，具备了网格变形速度快、编程易于实现等优点；但非结构网格数据结构的随机性增加了寻址时间，网格的无方向性导致梯度项计算工作量的急剧增大(表 2)；混合网格是将结构网格和非结构网格结合在一起，取其各自的优点，其目的是在提高计算网格质量的同时并降低求解区域网格的离散难度，它能够很好地离散复杂的计算域，节省时间和计算机资源，具有很好的发展前景；但混合网格在结构、非结构网格的交界面处的网格质量较差，需采用一些方式对网格质量进行改善。与结构网格相比，非结构网格、混合网格的动网格方法适用性更广，大多数都可以应用到结构网格中去[59]，各方法主要原理及优缺点如：混合网格的生成方法与非结构网格类似，且目前大多将混合网格数据结构转化为非结构网格的形式进行整体处理，这样使得整个流场的计算方法统一，便于程序设计和调试[60]。

表 1 结构网格动边界处理方法

Table 1 Processing method of moving boundary of structured grid

	原 理	优 点	缺 点
刚性运动网格法[37-38]	网格随物体一起做刚性运动	计算量小	仅适用于单个刚性物体运动
超限插值动网格生成法[39-41]	外边界保持静止，物面边界由物体运动规律或运动方程得到，内场网格由超限插值的方法代数生成	计算量小	网格正交性难以保证
重叠结构动网格技术[42-45]	在计算域的各个子域采用区域共享(重叠部分)的方法来实现信息交换	减轻了子域网格生成的难度且能够保证子域的网格品质	计算量较大
滑移结构动网格技术[46-47]	在物体运动轨迹周围预先划出一个滑移子区域，在子区域和其他区域分别生成多块结构网格；在二者连接处，利用搭接边界与其他区域对接，从而实现整个流场的计算	计算效率高、适用性强	划分子域的多少会影响网格变形质量和计算量

表 2 非结构网格动边界处理方法

Table 2 Processing method of moving boundary of unstructured grid

	原 理	优 点	缺 点
弹簧法[48-51]	将整个网格区域看作一个弹性区域，在边界发生移动且变形较小的情况下，网格发生轻微变形	无需插值，可以保证流场中解的守恒，保证了计算精度	边界位移过大时会使网格严重变形，导致计算出错
扩散法[52-53]	对扩散方程进行求解，基于扩散方程结果更新网格节点位置	网格质量好、计算精度高	不适用时间较长的计算
铺层法[54]	在一个时间步长内，动边界扫过固定的网格，对运动边界周围变形的网格，进行合并或分割	无需对控制方程进行坐标转换，即可实现对复杂动边界的追踪拟合	应用贴体网格及求解 N-S 方程比较困难
网格重构法[55-58]	利用网格变形前后的变形率来判断网格是否符合要求；对于严重变形的网格区域则重新生成网格	对网格拓扑结构没有限制，同时可以保证边界周围网格单元的质量，对于任意的边界变形也可以得到很好的处理	在重新生成以后，空腔内的网格节点的流场参数必须通过插值的方法得到

2.3 动网格更新方法应用

对于地下水系统而言，在进行数值模拟时，对于非饱和带仅作一维垂向网格剖分，而对饱和带则采用三维网格剖分。非饱和带作为饱和带的上边界，与饱和带地下水进行水量及溶质交换，这种交换使得潜水面的位置不断变化，即非饱和带的一维网格和饱和带的三维网格也随之变化，在这个过程中动网格的应用可以大幅提高计算精度[61]。目前，在处理潜水面这种动边界问题时，常用的方法是局部网格重构法，部分研究采用的是弹簧法和重叠结构动网格技术，其他方法应用较少[62]。

2.3.1 网格重构法

该方法是指当边界位移过大时，可能会出现负体积网格，使计算不收敛。针对这种情况，部分模拟软件在计算过程中将变形过大的部分或全部网格重新剖分。大多数非饱和—饱和水流运动及溶质运移数值模型都是基于 MODFLOW 而建立的，因此可以将用于非饱和带的模拟软件与 MODFLOW 耦合(图 1)。根据使用的非饱和带模拟软件的不同，主要分为以下 6 类。

(1)基于网格重构法将 UZF1 程序包与 MODFLOW 软件耦合建立耦合模型[64-71]。模型根据上一时间步长的地下水位计算土壤含水量分布，得到非饱和带对饱和带地下水的补给量，并代入地下水运动方程，进一步计算下一时间步长的水头分布。

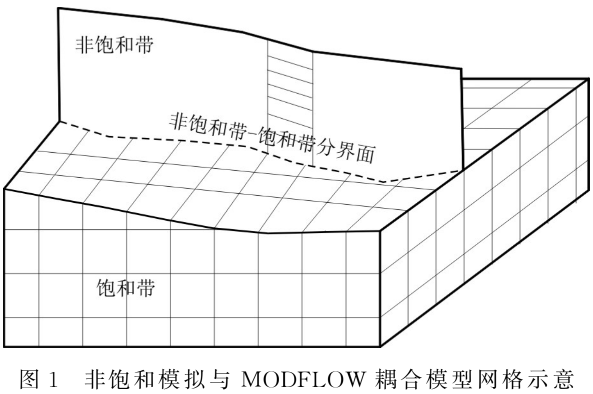


图 1 非饱和模拟与 MODFLOW 耦合模型网格示意图[63]

Fig. 1 Grid diagram of unsaturated-simulation and MODFLOW coupling model

(2)基于网格重构法，采用 HYDRUS-1D 程序包模拟非饱和带水流运动，同时将该非饱和带水流运动与 MODFLOW-2000 进行耦合[72-73]。在模型应用过程中，在水平向进行分区，每个分区采用一个一维运动方程来描述其垂向运动，将计算结果代入地下水模型进行计算。

(3)基于网格重构法将非饱和带垂向 Richards 方程的有限差分解与 MODFLOW 耦合，建立了 LINKFLOW 模型[74]。模型非饱和带以地表作为上边界、潜水面为下边界。一维土壤柱位于三维饱和模型网格的上方，地下水位随时间不断变化。当地下水位变动时，饱和模型网格发生变化的部分将重新剖分以适应新的地下水位。

(4)部分研究者基于网格重构法建立了 SVAT (soil vegetation atmosphere transfer)与 MODFLOW 耦合模型[63,75-76]。SVAT 将土壤由上至下分为 3 层，分别为蒸发层、根系层和渗透层，渗透层从根系层延伸到地下水面；分别建立每层的均衡方程，计算渗透层补给饱和带地下水的量。MODFLOW 计算时，将模拟过程分成不同应力期，每个应力期内，渗透层厚度保持不变，SVAT 每次运行后更新非饱和带厚度，并将潜水面处的网格重新剖分。

(5)在流域尺度上常见的是将水文模型 SWAT (soil and water assessment tool)与 MODFLOW 耦合，建立耦合模型[77-88]。这种基于 MODFLOW 所建立的耦合模型在分界面的位置或形状变动时，将分界面附近的网格重新生成以反映在当前时间步长、非饱和带与饱和带的实际厚度。

(6)朱焱[89]运用网格重构法提出了区域非饱和—饱和水流及溶质运移数值模拟方法。模型将饱和

带地下水与土壤层之间的耦合流量表示为当前时刻饱和带地下水节点水头和土壤层节点水头的梯度，分析饱和带地下水与土壤层相邻节点的水量均衡。在预先剖分网格的基础上，使位于土壤层内紧邻潜水面的节点 N 的压力水头为零(图 2)，位置随时间和迭代不断变化，每次迭代时饱和带地下水网格均需重新剖分。

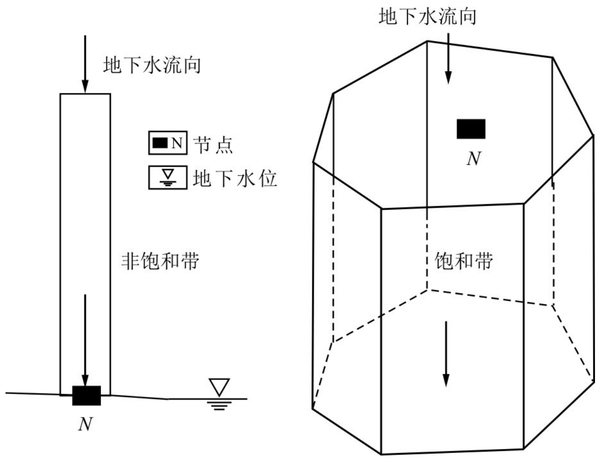


图 2 区域非饱和—饱和带水流运动及溶质运移模型网格示意图[89]

Fig. 2 Grid diagram of regional unsaturated-saturated flow movement and solute transport model

在每次地下水面更新后，基于 MODFLOW 的耦合模型以及区域非饱和—饱和带水流及溶质运移模型仅需对饱和带地下水网格重新剖分，与它们不同的是，COMSOL 软件需将模型网格全部重新剖分(图 3)。焦会青[90]使用 COMSOL 软件构建了区域非饱和—饱和准三维模型，为区域水盐调控和干排盐技术提供了理论依据。根据初始地下水位，模型首先计算土壤层下边界水流和溶质通量，将该通量以源汇项的形式带入饱和地下水计算，再以此调整土壤层的厚度。

2.3.2 弹簧法

弹簧法将网格边界视为节点间相互连接的弹簧，移动前的网格间距相当于边界移动前由弹簧组成的系统处于平衡状态，在网格节点发生位移后，形成的力破坏了弹簧系统原有的平衡，弹簧系统经过调整将达到新的平衡，使网格产生变形，得到新的网格节点的位置。Panday 等[91]基于弹簧法的思路将 Huyakorn 等[92]建立的模型进行了改进，将模型中节点间的直线用曲线代替，形成了六面体正交曲线网格(图 4)，减少了由于网格变形而产生的错误[93]。Jin 等[94]基于弹簧法的思路采用 ALE 法将非承压含水层中的地下水流动问题描述为自由表面问题，模拟中将地下水位设置为允许移动的上边界，通过

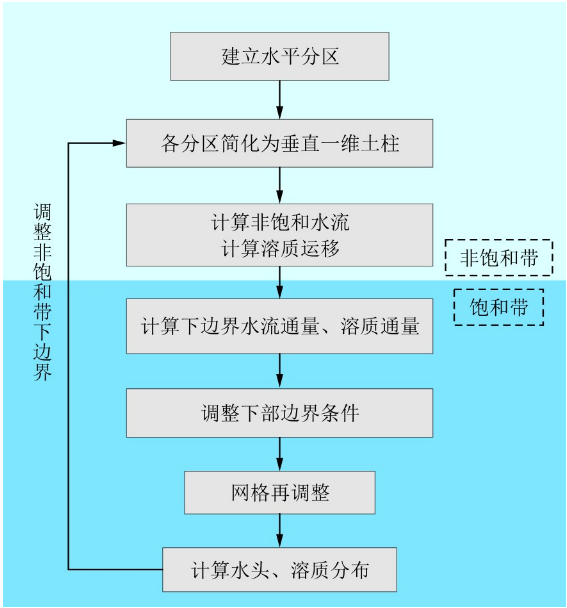
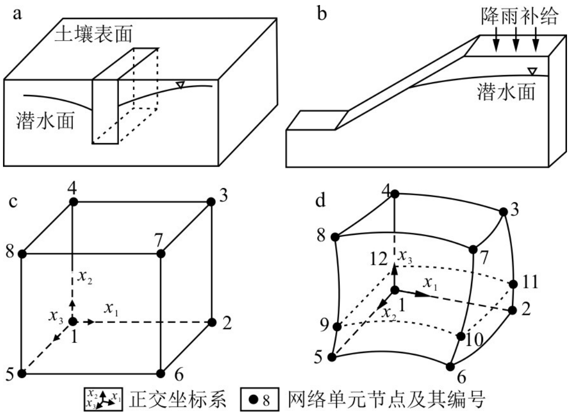


图 3 COMSOL 非饱和—饱和模拟流程图

Fig. 3 Flow chart of soil groundwater coupling simulation based on COMSOL software

网格变形模拟边界的变形和位置的变化，并设置了边界位移距离以防止网格过度变形而使网格质量下降。通过实际案例将数值解与解析解进行对比，确定了新方法的适用性。



a,b 分别为由垂直/倾斜的网格线表示的潜水面；c. 变形前网格形状；d. 变形后网格形状

图 4 弹簧法网格变形示意图(a,b 据文献[91-92]；d 据文献[93])

Fig. 4 Deformation diagram of spring method mesh

2.3.3 重叠结构动网格技术

重叠网格是在计算复杂区域时采用子区域块网格重叠的处理方式，重叠中的子区域网格点的信息共享和交换也要做特殊处理，每个子区域块的动网格计算可以并行计算[95-97]。基于过程的自适应流域模型(以下简称 PAWS 模型)是由 Shen 等[98]开发的分布式水文模型，模型使用重叠结构动网格技术实现了地表水、土壤水和地下水的耦合模拟。

PAWS模型首先将模拟域离散为结构网格，将非饱和带看成一系列土柱，其底部连接潜水面并假设在潜水面以上的水分仅做垂向运动，一维网格贯穿整个含水层，而在饱和带用二维或三维地下水方程进行模拟，此时在饱和带中，一维网格与三维网格产生重叠，这样，非饱和系统与饱和系统形成了无缝连接。以此求出某一时间步长的非饱和带各节点水头以及土壤水补给饱和带的量，并更新下一时间步长的重叠网格以便进行新的时间步长的计算[98-105]。

3　问题分析

动网格技术已经被广泛应用于自由表面及流体耦合等问题，在地下水数值模拟领域应用相对较少。目前，动网格技术在非饱和－饱和界面数值模拟中的应用存在如下问题：

首先，现有的模拟软件在进行非饱和－饱和耦合数值模拟时，大多采用网格重构的方法模拟潜水面的变形及位置的变化，但若每一次迭代都进行网格重构，会耗费大量的计算时间，并且在重新生成网格过程中的插值可能不守恒，采用这种方法增加的计算量及产生的计算误差均较大[106-107]。采用重叠结构动网格法模拟非饱和－饱和系统时，在每个时间步长都需要对重叠区域的网格进行插值和更新，从而导致计算量增大，计算效率低；并且由于插值产生的误差会不断累积，长时间的误差累积将导致误差进一步放大，从而影响计算精度。弹簧法虽然模型较简单，计算效率较高，但是弹簧法一般用于处理边界变形较小的情况，在某些复杂几何变形或者网格大变形的情况下弹簧法失效，容易出现负体积。部分学者为保证网格质量，在模拟时设置了边界位移距离上限[94]。

其次，尽管每一种动网格更新方法在处理运动边界问题时都具有独特的优越性，但不论是基于结构网格、非结构网格还是混合网格的动网格更新方法都存在自身的不足。在模拟过程中最主要的矛盾是：在保证网格质量和计算结果相对准确的前提下，如何尽量减小计算量，提高计算效率。

4　结论与展望

（1）无论结构网格还是非结构网格都存在自身的局限性，混合网格技术是未来的发展方向，并且也逐渐受到更多研究者的关注。对于运动边界的模拟问题，为了保证在运动过程中网格的整体质量，应考虑将多种动边界处理方法结合使用，当潜水面位置和形状变动较小时，采用弹簧法更新网格；当潜水面位置变化较大但形状变化较小时，采用重叠结构动网格技术或铺层法更新网格；若潜水面形状变动较大时，则采用网格重构法更新网格，从而更精确地模拟非饱和－饱和分界面的变化和移动，使整个耦合模型更可靠。

（2）目前，在非饱和－饱和耦合数值模拟中动网格技术的应用主要采用网格重构法、弹簧法和重叠结构动网格技术 3 种方式，其他动网格更新方法的效率、稳健性以及适用性有待研究。对于较大空间尺度的非饱和－饱和耦合水流运动及溶质运移数值模拟研究，由于其水文地质条件的复杂性，计算量较大，因此，需要探寻一种能够精确模拟复杂水文地质条件且具有高计算效率的方法来定量刻画地下水位波动过程，相关研究为场地土壤与地下水协同防治工作提供了科学指导。

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