

Le développement du modèle intégré des hydrosystèmes Eau-dyssée

Florence. Habets^{1,2*}, Nicolas Flipo², Patrick Goblet², Emmanuel Ledoux², Celine Monteil², Elodie Philippe², Wilfried Queyrel^{1,2}, Firas Saleh^{1,2}, Otmane Souhar¹, Alexandra Stouls^{1,2}, Pascal Viennot², Cédric David³, Alessia Bacchi¹, Hélène. Blanchoud¹, Elodie Moreau-Guigon¹, Marie. Launay⁴, Dominique Ripoché⁴, Bruno Mary⁵, Pierre-Alain Jayet⁶, Eric Martin⁷, Thierry Morel⁸, Julien Tournebize⁹.

¹ UMR Sisyphe, CNRS, EPHE, 4 place Jussieu, 75252 Paris cedex 05 France

² Centre de Géosciences, Mines Paristech, 35 av St Honoré, 77305 Fontainebleau, France

³ Texas University, Austin, TEXAS, USA

⁴ INRA, AgroClim, Domaine St Paul, Site AgroParc, 84914 Avignon Cedex, France

⁵ INRA Agro-Impact, Rue Ferdinand Christ, 02007 Laon cedex, France

⁶ UMR Economie Publique INRA-AgroParisTech, BP01, Centre Inra Versailles-Grignon, 78850 Grignon

⁷ CNRM-GAME, 42 avenue Coriolis, Toulouse, France

⁸ CERFACS, 42 avenue Coriolis, Toulouse, France

⁹ CEMAGREF, Anthony, France

*Auteur correspondant : florence.habets@mines-paristech.fr

1 Objectifs

L'étude des scénarios d'évolution de la ressource en eau (des points de vue qualitatif et quantitatif) selon les différentes contraintes climatiques, économiques ou technologiques passe de plus en plus par la modélisation intégrée des hydrosystèmes.

Le projet Eau-dyssée vise au développement d'un tel outil, en s'appuyant sur des modèles disciplinaires et sur l'utilisation du coupleur externe Palm (Piacentini et al, 2003).

On se base dans un premier temps sur 4 modèles disciplinaires qui sont en cours d'intégration : le modèle hydrologique MODCOU, le modèle agronomique Stics, le modèle d'offre agronomique AROPA-j, et le schéma de surface atmosphérique Surfex (précédemment ISBA).

Ces différents modèles ont déjà fait l'objet de couplages partiels (AROPA-j Stics, ISBA-MODCOU, ISBA-Stics, Stics-MODCOU). Cependant, ces couplages étaient peu interactifs (il s'agissait bien souvent d'un simple forçage, sans rétroaction possible) et souvent peu évolutifs du fait des modifications insérées pour réaliser ces forçages.

Eau-dyssée vise donc au développement d'un couplage interactif, évolutif et modulaire entre modèles experts.

Une première phase dans la construction d'Eau-dyssée a consisté à restructurer MODCOU pour le rendre plus modulaire et lui permettre de gérer de multiples interactions (Habets et al., 2008).

Une deuxième phase qui vient juste de commencer consiste à réaliser le couplage entre MODCOU et les 3 autres modèles experts au sein d'Eau-dyssée. Cela passe d'abord par la prise en main de ces modèles experts, et par des tests de sensibilités avant d'en arriver au couplage.

Ce rapport fait donc le point sur l'état du développement d'Eau-dyssée, avec tout d'abord, les modifications introduites dans le modèle hydrologique MODCOU, puis, le point sur les couplages avec les autres modèles experts.

2 Restructuration du modèle Hydrologique MODCOU

La figure 1 présente une comparaison des structures de MODCOU dans sa version d'origine et dans celle incluse dans Eau-dyssée. La version d'origine était constituée de 4 parties indépendantes (4 exécutables) : Modsur pour l'estimation du bilan hydrique en surface et le routage vers la rivière, Nonsat pour les transferts dans la zone non saturée, MODCOU pour l'estimation des écoulements en nappe et les écoulements en rivière, et enfin NEWSAM pour l'écoulement et le transport convectif en nappe. Chacune de ces quatre parties devait tourner sur la totalité de la période étudiée, et transmettait ensuite les flux aux modules suivants via l'écriture de fichiers de sortie. La nouvelle version conserve les différents éléments constitutifs du modèle hydrologique, mais intègre bien plus d'interaction entre ces éléments. Certaines parties ont évolués. Nous avons : i) introduit un nouveau schéma d'écoulement en rivière (RAPID) ii) introduit un nouveau module permettant d'estimer les hauteurs d'eau en rivière, iii) apporter des modifications au schéma

de transfert dans la zone non saturée, iv) fusionné l'écoulement et le transport en nappe dans un seul et même module dénommé SAM (simulation des aquifères multicouches). Ces modifications ainsi que la gestion des échanges entre les modules sont détaillées dans les sections suivantes.

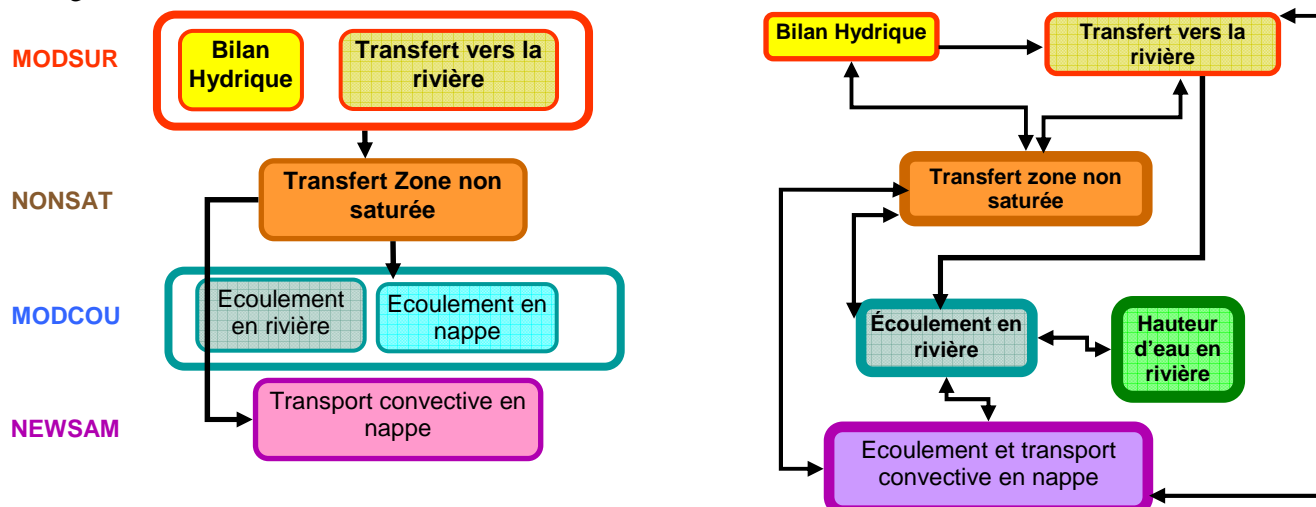


Figure 1 Comparaison entre l'ancienne (à gauche) et la nouvelle (à droite) structure du modèle hydrologique MODCOU.

2.1 Gestion des interactions

Un des objectifs d'Eau-dyssée est de bâtir une modélisation intégrée des hydrosystèmes qui soit modulaire. Cela signifie qu'en fonction des applications, on doit pouvoir remplacer un module par un autre. Ainsi, certains modules sont bien adaptés à des applications à grandes échelles, mais sont moins pertinents à fine échelle. Pour assurer la modularité, chaque élément du modèle est conçu de façon indépendante, et l'interactivité est acquise grâce à un système d'échange de variables. Pour la restructuration de MODCOU, nous avons utilisé le formalisme d'échange défini par le coupleur externe Palm (voir ci-dessous).

2.1.1 Utilisation du coupleur Palm

Palm permet de gérer l'exécution de chaque module en parallèle sur des processeurs différents. Cela signifie que chaque module peut être complètement indépendant (plusieurs exécutables). Dans Palm, pour l'utilisateur, la gestion des interactions repose sur la définition des variables échangées : définition du nom, du type (entier, réel, logique...), de l'espace dimensionnel (0D, 1D, 2D...), et de l'attribut (entrée/sortie). L'échange se fait entre 2 modules si le même nom de variable est appelé. Ce nom peut donc différer du nom de la variable dans le code.

Les échanges entre modules peuvent être visualisés via l'interface PréPalm (Figure 2). En plus des variables physiques, on échange des dimensions, ainsi que des variables dites de synchronisation. Les variables en entrée sont indiquées par PréPalm en haut de chaque module, et les variables de sorties en bas. Une même variable peut être transmise à plusieurs modules.

2.1.2 Développement des échanges hors Palm

L'utilisation de Palm nécessite d'installer le logiciel sur une structure informatique possédant les bibliothèques de calcul parallèle (Message Passing Interface). Cela peut être contraignant, surtout pour les personnes ne désirant utiliser que les fonctions du modèle hydrologique et pas les capacités du modèle intégré Eau-dyssée. Ainsi, afin d'avoir un modèle hydrologique qui puisse être utilisé facilement sur le plus grand nombre de plateformes numériques, nous avons développé une interface transparente pour l'utilisateur permettant de gérer les échanges sans activer Palm. Cette version ne permet évidemment pas le calcul parallèle. Nous avons pour cela conservé le formalisme de déclaration des variables échangées de Palm. Les échanges se font via une sous-routine 'collecteur'. Les versions Palm et Non Palm sont intégrées dans le même code, et sont activées via l'usage d'une option de pré-compilation.

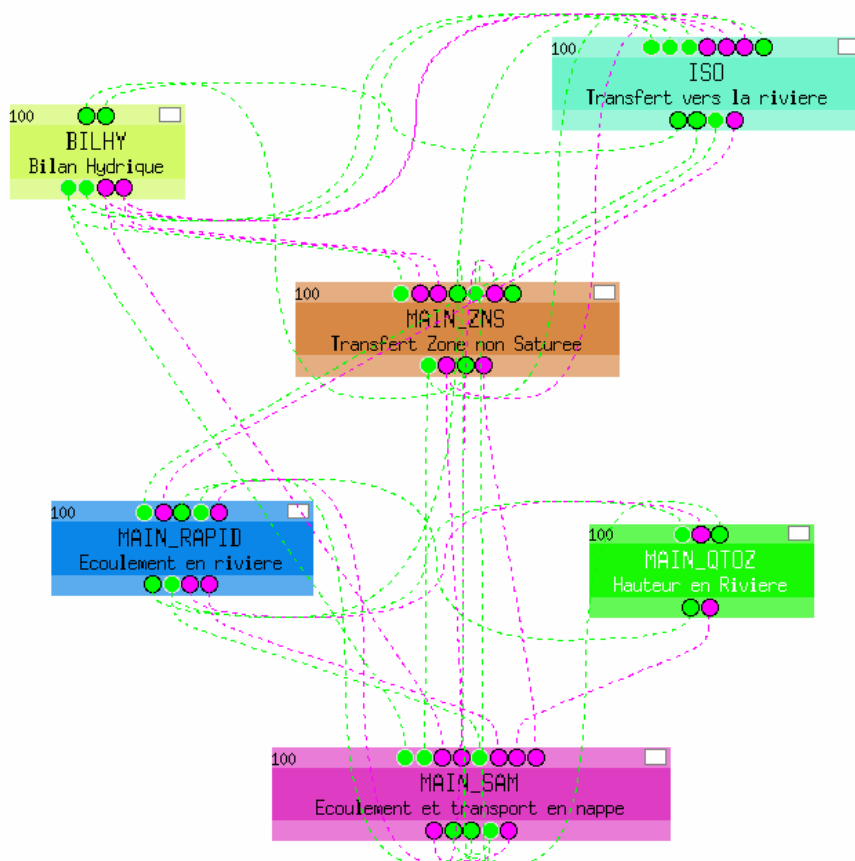


Figure 2 : visualisation des échanges via Prépalm. Les points en haut des modules correspondent à des variables en entrée, et ceux en bas à des variables en sortie. Les connexions entre modules sont indiquées par des courbes

2.2 Implémentation du modèle d'écoulement en rivière RAPID

Dans la nouvelle version de MODCOU, nous n'avons pas pour l'instant repris l'écoulement en rivière de la version d'origine. En effet, le schéma original (un schéma de type Muskingum simplifié) nécessite la gestion d'un zonage isochrone pour chaque station simulée. Cela est assez contraignant (on doit prédéfinir les points où l'on souhaite estimer les débits), et lourd d'un point de vue informatique (nécessité de conserver en mémoire le zonage isochrone pour chaque station). On a donc pour l'instant intégré le schéma de transfert en rivière RAPID (David et al., 2009a,b). Ce modèle est de type Muskingum, et donc conceptuellement proche de ce qui se faisait dans MODCOU à l'origine. Cependant, RAPID permet l'estimation des débits en tout point du réseau de rivière. De plus, RAPID permet le calcul parallèle, ce qui est un avantage lorsqu'on travaille sur des grandes tailles de matrice. Pour son application sur le bassin de la Seine, nous avons tout d'abord utilisé les paramètres définis dans SIM-France (David et al., 2009c). La figure 3 compare les débits simulés par les 2 versions de MODCOU sur la Seine à Poses.

2.3 Implémentation du Module de fluctuation de niveau d'eau en rivière : QtoZ

Le module QtoZ calcule les hauteurs d'eau dans les mailles rivière en fonction du débit routé par le modèle de routage régional. Le module permet trois options afin de faire fluctuer les niveaux d'eau en rivière: a) un niveau d'eau fixe (version initiale d'Eau-dyssée), b) les niveaux d'eau déterminés à partir des courbes de tarage, c) les niveaux d'eau estimés en utilisant l'équation de Manning.

Dans la plateforme de modélisation EAU-Dyssée, le module QtoZ est couplé avec le modèle de routage RAPID et le modèle souterrain SAM (Précédemment MODCOU).

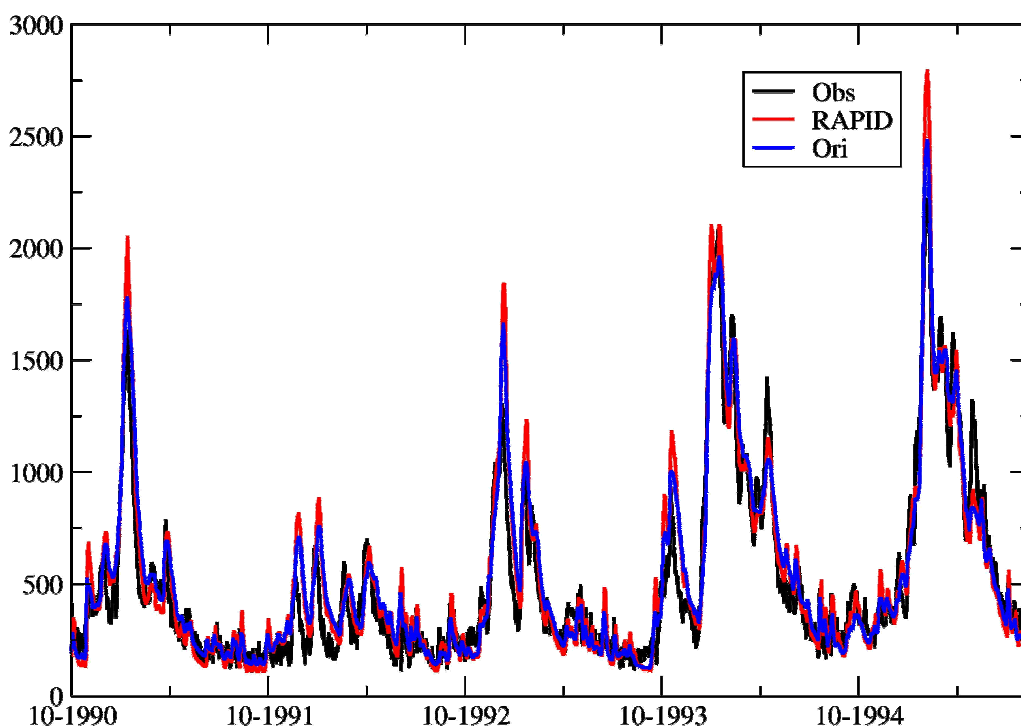


Figure 3 Comparaison des débits observés (noir), et simulés par la version originale de MODCOU (bleu) et la nouvelle version contenant le schéma de transfert en rivière RAPID (en rouge) sur la Seine à Poses.

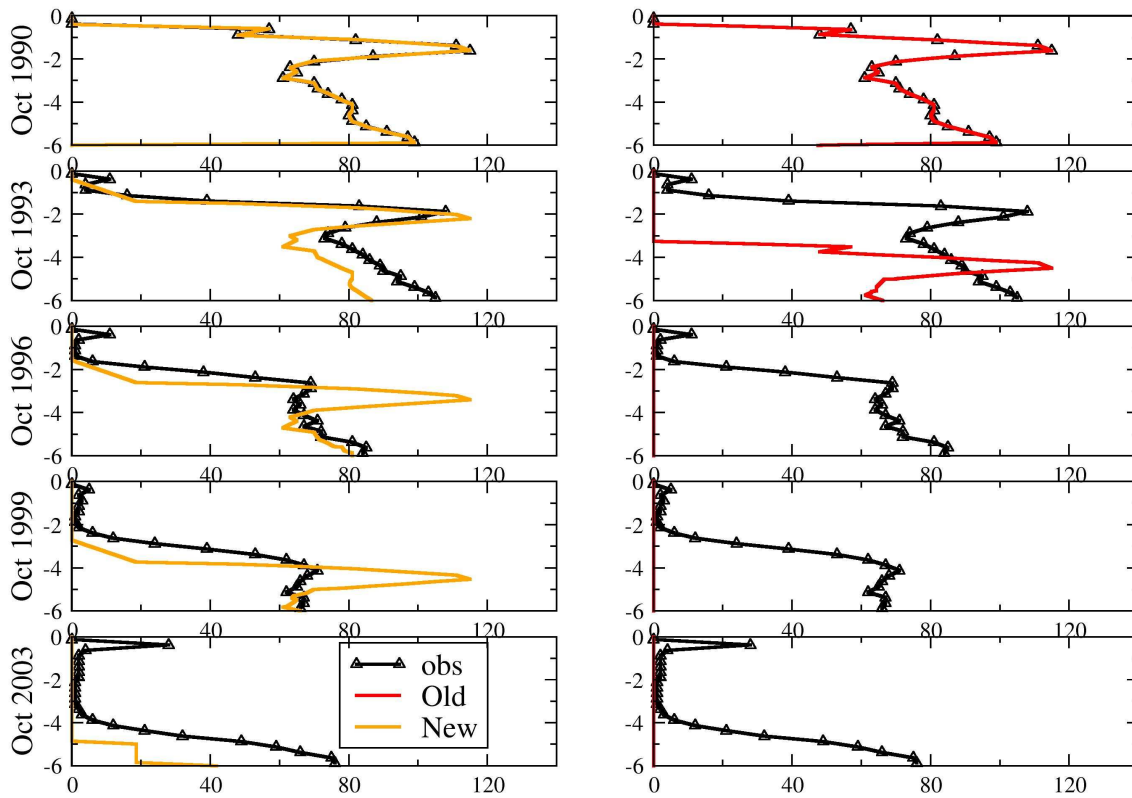
A chaque pas de temps de la simulation, le modèle QtoZ reçoit des débits simulés par RAPID et renvoie des niveaux d'eau au modèle souterrain SAM afin de permettre une meilleure simulation des interactions nappe-rivière. Ce module et son impact sur la modélisation des niveaux piézométriques sont décrits en détails dans Saleh et al., 2010.

2.4 Adaptation du schéma de transfert dans la zone non saturée

Philippe et al., 2009a ont présenté une nouvelle version du schéma de transfert dans la zone non saturée (ZNS). Ce schéma intègre l'équation de Van Genuchten pour estimer le volume d'eau dans la zone non saturée en fonction du type de sol et de la profondeur de la nappe. Nous avons pu valider ce modèle via des comparaisons avec des observations sur deux sites de l'INRA (Philippe et al., 2009b). La figure 4 présente une comparaison entre les concentrations en nitrate observées (noir) et simulées par l'ancienne version (rouge) et la nouvelle version du schéma Nonsat (orange) sur une zone non saturée de 6m de profondeur sur le site de Thibie (craie). Les concentrations observées en octobre 1990 sont utilisées pour initialiser le profil. Les paramètres de Van Genuchten sont définis à partir de la littérature (base de données de Brouyère et al. 2004 pour la craie et Carsel and Parrish 1988 pour les autres types de sol). On constate que la version originale de Nonsat avait tendance à surestimer le temps de transfert des nitrates dans la ZNS (le pic est transmis à la nappe en moins de 6 ans), alors que la nouvelle version estime un temps de transfert plus réaliste (un peu moins de 13 ans pour transférer le pic à la nappe). Au vu de ces validations, nous avons pu estimer les temps de transfert à la nappe d'un polluant passif sur le bassin de la Seine dans des conditions d'infiltration réalistes. Bien sur, il y a de fortes variabilités spatiales, mais il faut en moyenne 17 ans pour qu'un polluant passif atteigne la nappe, alors qu'auparavant, le modèle estimait un temps de transfert moyen de 12 ans (Philippe et al., 2009b, cf annexe).

La validation de la nouvelle version de Nonsat nous a permis de passer à une phase d'exploitation. L'objectif premier de ces développements est de réduire les erreurs entre concentration en nitrate observées et simulées dans les aquifères (Viennot et al., 2006). Nous avons donc refait les simulations Stics-MODCOU de Viennot et al., 2006, en reprenant les quantités d'azote lixiviées estimées sur la période 1970-2005. Pour initialiser les

concentrations en nitrate en nappe et dans la zone non saturée, nous avons comme Viennot et al , 2006 répété le forçage 1970-2005 deux fois. Les résultats obtenus sont présentés figure 5.



Figure

4 : Comparaison des concentrations en nitrate observées et simulées à différentes dates en fonction de la profondeur sur le site de Thibie : observations en noir, ancienne version de Nonsat en rouge (à droite), nouvelle version de Nonsat en orange (à gauche)

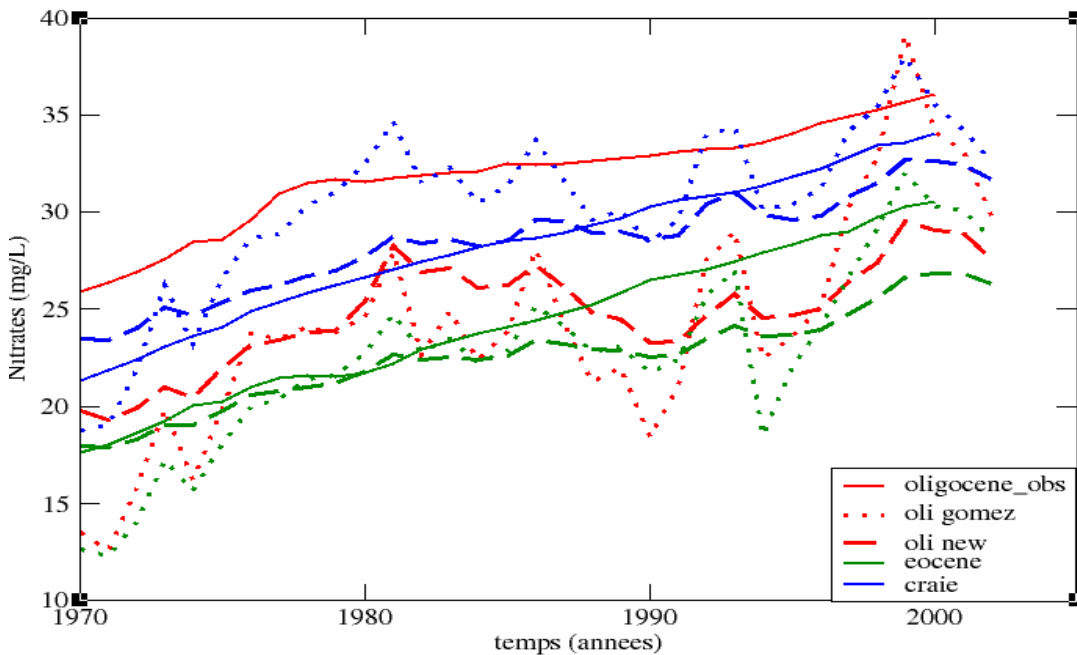


Figure 5 : Concentrations en nitrate simulées en moyenne sur les 3 couches aquifères avec l'ancienne (pointillés) et la nouvelle (tirets) version du schéma de transfert dans la zone non saturée, comparées à la médiane des observations (traits continus). On constate une inconsistance liée aux incertitudes sur l'initialisation. Rouge : Oligocène, Vert : éocène, Bleu : Craie

On constate deux choses : i) les concentrations en nitrate estimées par la nouvelle version de Nonsat en moyenne par aquifère évoluent de façon moins bruitée que celles estimées par la version d'origine de Nonsat et ii) les concentrations estimées en début de période ne correspondent souvent pas à la médiane observée (surtout pour l'Oligocène). Ce dernier point est important, et relève des problèmes d'incertitudes liées à l'initialisation. En effet, les résultats présentés supposent une concentration nulle en nitrate dans la ZNS et la nappe en 1935, puis, une quantité de nitrate lixiviée correspondant à la moyenne 1970-2005 constante sur une période de 70 ans. Cette initialisation est réalisée faute de mieux, mais ne correspond pas à un historique réaliste. En effet, les données anciennes de concentration en nitrate dans les nappes présentent des taux relativement stables de l'ordre de 20mg/l de NO₃ dans les années 1930, puis une augmentation plus ou moins marquée dès les années 1950 (Landreau et Roux, 1984). Cela est cohérent avec l'usage intensif des intrants chimique tel que présenté par l'Ifen et l'Agreste (2001).

Avec des tests de sensibilité, nous avons pu constater qu'il faut des intrants constants sur plusieurs centaines d'années pour équilibrer les concentrations en nitrate de la nappe. Cela est cohérent avec l'usage d'engrais organique avant la révolution agricole.

Nous souhaitons donc nous baser sur l'estimation des quantités lixiviées à partir des intrants organiques (en se basant sur les travaux de Thieu et al., 2010) et sur l'évolution estimée de l'usage d'intrant chimique à partir des années 1930 pour améliorer l'estimation de l'état initiale. Etant donnée la longueur des temps de transfert sur la Seine, cela permettra une meilleure comparaison avec les observations disponibles sur la période 1970 à nos jours.

2.5 Fusion des modules d'écoulement et de transport en nappe

Dans la version originale de MODCOU, le module NEWSAM permettait d'estimer le transport convectif de polluant dans les nappes, mais ne permettait pas l'estimation des débits en rivière (Figure 1). Pour simuler à la fois l'écoulement en nappe, le débit des rivières et le transport convectif en nappe, il fallait faire tourner MODCOU et NEWSAM. La fusion des deux modules d'écoulement en nappe était donc nécessaire. La difficulté résidait dans le fait que le module NEWSAM disposait de fonctionnalités plus évoluées que celles de MODCOU. On ne pouvait donc pas simplement remplacer un module par un autre, mais il était nécessaire de fusionner les deux.

Pour le transport de polluant, nous avons introduit la possibilité de gérer plusieurs types de polluants de façon simultanée, ce qui est nécessaire pour traiter la pollution par les pesticides et leurs métabolites. Des comparaisons entre la nouvelle et l'ancienne version ont été réalisées, et la figure 5 présente un exemple de résultats.

3 Couplage avec le modèle agronomique Stics

Dans Eau-dyssée, nous souhaitons intégrer la dernière version du modèle Stics. La version 7 a été recodée en fortran90 de façon modulaire, et inclut de nouveaux types de culture, en particulier, les prairies permanentes qui sont assez présentes sur le bassin de la Seine. Cette version inclut également le drainage agricole développé par Tournebize et al., 2004. Cependant, cette nouvelle version n'est pas spatialisée, et ne peut tourner que sur une parcelle agricole à la fois. Cela n'est pas très compatible avec la modélisation des hydrosystèmes, qui implique de simuler plusieurs parcelles agricoles de façon simultanée. Ainsi, nous devons essayer de gérer plusieurs appels simultanés à Stics, si possible, de façon parallèle pour ne pas subir des temps de calcul trop long. Cela nécessite de séparer la partie exécutable de la partie gestion de données, et implique une intrusion relativement importante dans le code de Stics, ce qui est contraire aux objectifs d'Eau-dyssée. Cependant, la modularisation de Stics nous permet de conserver toute une partie du code intact, et de ne modifier que la partie amont. Ces travaux de couplage étant menés en collaboration avec l'équipe développant Stics via le projet EC2CO Eau-dyssée, on espère que tous les développements réalisés dans le cadre de ce couplage seront soit réintégrés dans les futures versions de Stics, soit ré exploitables avec ces futures versions.

Pour nous aider dans cette démarche de couplage, le Cerfacs prévoit de réaliser dans le cadre d'un projet ANR un module de Palm dédié au couplage entre modèle 2D et 1D gérant de façon optimale la spatialisation (Figure 6).

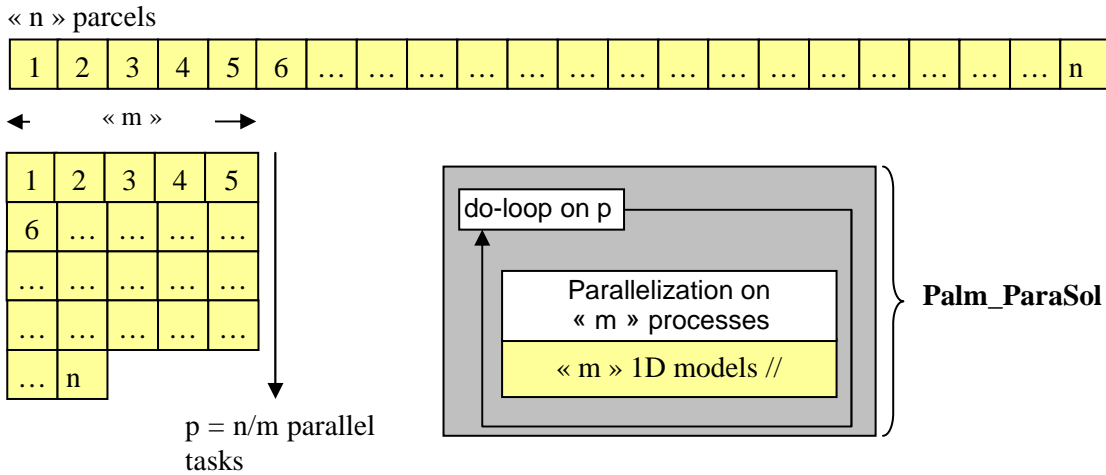


Figure 6: approche par pool de processus : accélération des calculs d'un facteur m, m dépendant du nombre de processeurs disponibles sur la machine (figure préparée par le Cerfacs pour le projet ANR COSINUS Nec-Eau-dyssée)

A ce jour, nous avons pu prendre en main la nouvelle version de Stics, et sommes en train de préparer une filière permettant de la faire fonctionner à partir de la base de données Seine.

L'étape suivante consiste à comparer les résultats obtenus avec la version antérieure de Stics, et d'intégrer cette version dans Palm.

Par ailleurs, des développements sont prévus dans cette version de Stics pour développer une version prenant en compte les produits phytosanitaires.

4 Couplage avec le schéma de surface atmosphérique de Météo-France

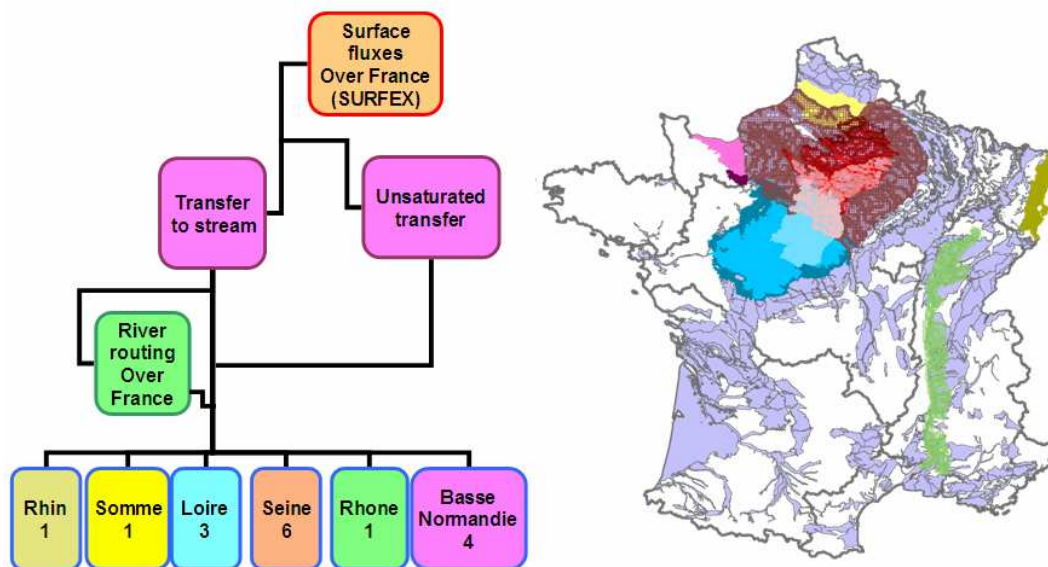


Figure 7 A gauche : principe du couplage hydrométéorologique sur la France : Eau-dyssée doit permettre une gestion simultanée de plusieurs bassins aquifères indépendants (le nombre indiqué sous le nom des bassins correspond au nombre de couches aquifères représentées). A droite : extension spatiale des bassins traités (en couleurs) et en grisé, principaux aquifères selon le BRGM.

Le couplage avec le schéma de surface de Météo-France, développé notamment dans le cadre du projet EC2CO Eau-dyssée et de l'ANR Vulnar n'est pas un objectif purement PIREN-Seine. Cependant, les

développements nécessaires seront sans doute utiles dans le cadre du PIREN-Seine. Ainsi, l'objectif premier de ce couplage est de développer une nouvelle version de l'application SIM-France (Safran-ISBA-MODCOU), capable de gérer de façon simultanée plusieurs nappes indépendantes (Figure 7), connectées à une unique estimation des bilans hydriques et des rivières. Or ce type de schéma est assez proche de ce que l'on souhaite faire dans le cadre d'une simulation avec changement d'échelle. En effet, dans le cadre d'une application grande échelle fournissant des conditions aux limites à une application fine échelle (exemple : bassin de la Seine versus bassin de l'Orgeval), il nous faut gérer simultanément 2 bassins hydrogéologiques, et transmettre des conditions aux limites de l'une à l'autre.

5 Forçage avec le modèle d'offre agricole AROPA-J

La modélisation physique des hydrosystèmes permet d'étudier l'impact de différents scénarios (dans leurs dimensions climatiques et/ou économiques). L'intégration dans Eau-dyssée du modèle d'offre agricole AROPAj vise à faciliter les études économiques portant sur les activités agricoles et leurs relations avec l'environnement (pollutions azotées, gaz à effet de serre). Ainsi, le modèle AROPAj simule le fonctionnement d'un ensemble d'exploitations agricoles représentatives des activités principales de l'agriculture et de l'élevage. Il permet d'évaluer les impacts du changement de l'environnement économique direct (prix, politique agricole, régulation environnementale telle que la « taxe carbone ») ou indirect (lorsque le climat conduit à un changement des rendements par exemple). Ces changements peuvent également être des changements de pratiques agricoles dans la mesure où sont disponibles les références techniques et économiques qui en caractérisent l'impact à l'échelle de la parcelle (rendements et charges variables par exemple). La répartition des terres agricoles disponibles et les productions vendues ou consommées sur la ferme font partie des résultats attendus du modèle qui est structurellement un modèle d'optimisation sous contraintes économiques (PAC,...) et techniques (assolements, alimentation animale, ...). En combinant des informations économiques et physiques, un modèle de distribution spatiale à fin niveau de résolution a été élaboré. Il permet de distribuer dans l'espace géographique les résultats du modèle AROPAj.

En associant les modèles AROPAj et Stics via la sélection et le calibrage de fonctions « dose réponse » (i.e. rendement et perte d'azote fonction de l'apport d'azote), on peut estimer directement l'impact de changements économiques sur les rejets en nitrate. Un premier travail a été mené pour étudier dans quelle mesure les flux estimés par AROPAj Stics pouvaient être directement utilisés dans le modèle hydrologique pour estimer l'évolution de la pollution des nappes par les nitrates. Un des problèmes qui se pose est lié au couplage temporel : en effet, AROPAj Stics fonctionne par pas de temps annuel à partir d'un calibrage effectué sur les années pour lesquelles l'ensemble des données économiques sont disponibles. Ainsi, autant l'espace est finement décrit, autant les variations temporelles infra-annuelles ne sont pas prises en compte. De ce fait, à court terme, on risque d'orienter la modélisation vers un système dans lequel AROPAj Stics estime des assolements que l'on « redistribue » à l'échelle des mailles MODCOU, et ces assolements sont utilisés par Stics-MODCOU dans Eau-dyssée pour simuler des flux de polluant et leurs transferts vers l'hydrosystème.

6 Conclusion

L'année 2009 a été marquée par la fin de la restructuration du modèle hydrologique MODCOU au sein du modèle intégré Eau-dyssée, et par le début des actions de couplage avec les autres modèles disciplinaires. L'année 2010 devrait être consacrée à quelques actions de validation, au développement des couplages, et à leurs applications. L'intégration de Stics est très importante, et devient la pierre angulaire de nos travaux. On bénéficie pour cette action d'une collaboration avec l'équipe développant Stics (INRA Agroclim), de l'investissement du Cerfacs pour la partie couplage, et bien sur, les équipes INRA déjà experte dans l'usage de ce modèle (INRA Laon, EGC, Mirecourt, Cemagref Anthony). En plus du soutien du PIREN-Seine ces collaborations sont soutenues en partie par le CNRS, et l'ANR (www.geosciences.mines-paristech.fr/equipes-de-recherche/systemes-hydrologiques-et-reservoirs/documents/eau-dysee)

Références

Brouyère S, Dassargues A, Hallet V. 2004. Migration of contaminants through the unsaturated zone

overlying the Hesbaye chalky aquifer in Belgium: a field investigation. *Journal of Contaminant Hydrology* 72, 135-164.

Carsel RF, Parrish RS. 1988. Developing Joint Probability Distributions of Soil Water Retention Characteristics. *Water Resources Research* 24: 755-769.

David C., F. Habets, E. Ledoux, 2009, Développement du modèle de routage en rivière RAPID (Routing Application for Parallel computation of Discharge): Principe et intérêt du couplage avec MODCOU pour la gestion des relations nappes-rivières, Rapport 2008 du PIREN-Seine.

David C, Maidment D.R, Niu G-Y, Yang Z-L, F. Habets 2009b River network routing in the Guadalupe and San Antonio River Basins, submitted at WRR 2009WR008688

David C, Habets F., Maidment D. R., 2009c, Rapid applied to the SIM-France model, Submitted to J. Hydrol

Godard C., J. Roger-Estrade, P.A. Jayet, N. Brisson et C. Le Bas, Use of available information at a European level to construct crop nitrogen response curves for the regions of the EU, *Agricultural Systems* Volume 97, Issues 1-2, , April 2008, Pages 68-82

Landreau A. et Roux J.C. 1984, Les nitrates dans les eaux souterraines, exemples de repartition et d'évolution des teneurs dans quelques aquifères français, rapport du BRGM 84SGN 361 ENV

Philippe E., Habets F., Ledoux E, Goblet P. Viennot P., 2009a, Prise en compte du battement de nappe dans la modélisation du transfert de nitrates sur le bassin de la Seine, Rapport 2008 du PIREN-Seine.

Philippe E., Habets F., Ledoux E, Goblet P. Viennot P., Mary B., 2009b, Improvement of the solute transfer in a conceptual unsaturated zone scheme, submitted to *Hydrological Processes*

Saleh F., Flipo N., Habets F., Ducharne A., Oudin L., Poulin M., Viennot P., Ledoux E. , 2010 Contribution de la modélisation hydraulique en rivière pour la quantification des échanges entre la nappe et la rivière dans un modèle hydrologique régional; Rapport du PIREN-Sein

Tournebize J., Kao C., Nikolic N., Zimmer D., 2004, Adaptation of the Stics model to subsurface drained soils, *Agronomie*, 24 (6-7) 305-313.

Viennot P, Ledoux E, Monget JM, Schott C. 2006. Contamination nitrique des aquifères du bassin de la Seine. Document de synth`ese PIREN Seine.

Improvement of the solute transfer in a conceptual unsaturated zone scheme

Elodie Philippe^{*,a,1}, Florence Habets^b, Emmanuel Ledoux^a, Patrick Goblet^a, Pascal Viennot^a, Bruno Mary^c

^a*Mines Paristech, Geosciences Center, 35 rue St Honoré, 77305 Fontainebleau, France*

^b*CNRS/UPMC UMR Sisyphe, Paris, France*

^c*INRA, Agronomical Unit, rue F. Christ, 02007 Laon Cedex, France*

Abstract

For predicting the evolution of solute concentration in groundwater and testing the impact of remediation policies, a coupling between agronomical model Stics and hydrogeological model MODCOU was implemented. Applied on the Seine river basin, this model was shown to represent well the temporal evolution of averaged nitrate concentration in the aquifer, but with some large local errors.

We propose an improvement of the simple unsaturated zone scheme NonsatSW used in Stics MODCOU. Modifications are based on a comparison with a mechanistic model, Metis.

A more realistic saturation profile and a varying percolation rate are integrated in the simple scheme. An assessment of this new model, named NonsatVG, is performed by a comparison with NonsatSW and Metis. In ideal cases, results show that NonsatVG generates a solute transfer and a dispersion more similar to Metis than NonsatSW. In real cases, without additional calibration, NonsatVG and Metis simulate better averaged transfer velocities of observed nitrate profiles.

Furthermore, modifications in NonsatVG allow to integrate a direct link between water table depth and saturation profile. We obtain therefore, as in Metis, an evolution of the solute transfer velocity depending on the piezometric level. Such dynamic is not simulated in NonsatSW.

*Corresponding author

Email address: elodie.philippe@mines-paristech.fr (Elodie Philippe)

¹Tel: +331-64-69-47-47, Fax: +331-64-69-47-03

We show also that, despite a modified water transfer through the unsaturated zone, NonsatVG is as valid as NonsatSW in the modelling of water table fluctuations.

Finally, first results of an application on the Seine basin show that solute transfer velocities are lower with NonsatVG than with NonsatSW, but in better agreement with literature.

Key words: unsaturated zone, hydrogeological modelling, solute transfert, nitrate contamination

1. Introduction

Since the mid 1950's, fertilizers and phytosanitary products are extensively used for agricultural purposes. Such practices have led to an increased diffusion of pollutant in the rivers and aquifers. The Water Framework Directive (#2000/60/CE) adopted by the European Commission requires that each member state's water bodies (rivers, lakes, coastal water and groundwater) reach a good ecological state before 2015. For instance, drinkable water should contain less than 50 mg/L of nitrate. However this threshold is already overpassed in many water bodies in Europe, as noted by Rivett *et al.* (2008). In order to adopt efficient policies regarding agricultural practices and water quality, integrated water models are used to support the decision making (Refsgaard, 2002; Sohler *et al.*, 2009; O'Shea and Wade, 2009; Flipo *et al.*, 2007; Ledoux *et al.*, 2007).

In the Stics-MODCOU model (Gomez *et al.*, 2003; Ledoux *et al.*, 2007), the agronomical model Stics (Brisson *et al.*, 1998) is used together with the hydrological model MODCOU in order to estimate the nitrate contamination of groundwater bodies. The model was first set up over the Seine basin (78650 km²) in northern France, characterized by both an intensive agriculture and an important population and industry, since the basin encompasses the Paris urban area. An important work was done to collect the agricultural data, e.g. crops rotation and agricultural practices (Mignolet *et al.*, 2007). The Stics-MODCOU model was shown to be able to represent the temporal evolution of average nitrate concentration in the aquifer, but some large local errors subsist (Ledoux *et al.*, 2007).

In order to improve this modelling, a special focus is made on the representation of the unsaturated zone in the MODCOU model. The unsaturated zone (UZ) is responsible for the delay for nitrate to reach the water table. This delay can be rather long depending on the UZ thickness and geological nature. Indeed, nitrate transfer velocity varies for example from $2.5m/year$ in eroded granite (Legout *et al.*, 2007) to as low as $0.6m/year$ in chalk (Gutierrez and Baran, 2009; Serhal *et al.*, 2006). Therefore, a good estimation of the transfer through the UZ is required to be able to study the impact of nitrate control policies (O’Shea and Wade, 2009; Sohier *et al.*, 2009).

The UZ is a polyphasic zone (water, air and solid) where phase changes can occur, as well as physico-chemical exchanges between phases due to mechanical and thermal energies variations (Vauclin, 1993). These modifications can influence the dynamics of solutes in the UZ. However, the nitrate transfer phenomenology in the UZ can be simplified assuming that most of the bio-physico-chemical reactions happen in the pedological area (Baran *et al.*, 2007). Thus, although some physically-based models take into account the reaction through the entire hydrosystem, e.g. SHETRAN (Birkinshaw and Ewen, 2000), it is more often considered that no reaction occurs during the transfer of nitrate through the UZ as in EPIC, SWAT and MIKE SHE (Sohier *et al.*, 2009; Neitsch *et al.*, 2005; Refsgaard *et al.*, 1995). We will therefore also assume a passive nitrate transfer through the UZ.

As MODCOU is devoted to be applied on large scale basins, it is not a fully physically-based model. Flow in the UZ is modelled with a simple cascade reservoirs scheme (Besbès and de Marsily, 1984) based on the Nash Cascade Model (Nash, 1960). This model was extended by Gomez *et al.* (2003) to allow the transfer of a passive contaminant. This simple model shares some specific features with recently developed UZ models. For instance, EPIC (Sohier *et al.*, 2009) also uses several reservoirs to reproduce the unsaturated zone. And Jackson *et al.* (2006) developed a model for the Chalk, which uses a piston flow mechanism with a constant velocity for water.

To evaluate the model, a comparison with the physically based model Metis (Goblet, 2007) was done both on ideal and real cases. This comparison showed some discrepancies, leading to a modification of the conceptual model. Both models of the UZ scheme are presented in section 2. Assessment tests results in ideal and real cases are discussed in section 3. And an application over the Seine basin is presented in section 4.

2. UZ model description

Two kinds of models are used for this study: the mechanistic model Metis, based on the resolution of the Richards equation and the convection-dispersion equation, and the conceptual model Nonsat.

2.1. Nonsat model

Nonsat is a conceptual model simulating only the vertical transfers through the UZ. The UZ is assimilated to a series of reservoirs. The original version of Nonsat deals only with water transfer (NonsatW). This version was modified by Gomez *et al.* (2003) to include the transfer of solute (NonsatSW, Gomez *et al.* (2003); Viennot *et al.* (2006)). This model combines piston flow and some interlayer mixing.

2.1.1. Modeling of water transfer with NonsatW

Besbès and de Marsily (1984), by studying the relationship between soil infiltration and groundwater supply at regional scale, showed that the water transfer function in UZ is comparable to a Nash reservoir cascade (Nash, 1960).

Water transfer through the UZ is therefore assimilated to a series of N reservoirs of depth d (in m), flowing in each other. Each reservoir follows an exponential law. Figure 1 presents the principle of the Nash cascade. It shows the effect of the cascade on an impulse input. Continuity of flow between reservoirs i and $i + 1$ writes:

$$Vin_{i+1}(t) = Vout_{i(t)} = Vol_{i(t)} \times \delta \quad (1)$$

with $Vin_{i+1}(t)$ the inflow into reservoir $i + 1$ (m^3), $Vout_{i(t)}$ the outflow of water from the reservoir i (m^3), Vol_i the volume of water in the reservoir i (m^3), δ a drainage coefficient, i the reservoirs index ranging from 1 to N , and t the current time. δ is linked to a percolation time τ in days by the relationship $\delta = 1 - \exp(-\frac{dt}{\tau})$ with dt the computation time step (one day). Water transfer principle is therefore based on the drainage of the water volume in the reservoirs, without any stockage. Thus, it can be considered that NonsatW deals only with gravitational water.

NonsatSW requires only two parameters: τ , that is set according to the soil type, and N . N is set depending on the average thickness of the UZ and the given depth of the reservoir d (Besbès and de Marsily, 1984).

If the number of reservoir increases, the water will take more time to flow

through the UZ. This can be compensated by a decrease of τ . Thus an equivalent velocity transfer can be obtained with different set of parameters, but the dynamic of the flow is different.

2.1.2. Modeling of the water and solute transfer with NonsatSW

NonsatW was modified by Gomez *et al.* (2003) to manage solute transfer. Solute transfer needs to explicitly manage the whole water volume in the UZ, that is to say the gravity water already taken into account in NonsatW, but also the capillary water retained in small pore. Indeed, this immobile phase contributes to solute stockage in the UZ. Therefore, Gomez *et al.* (2003) have introduced a minimal volume V_{min} that represents the water retained in the UZ. V_{min} is set identical in all the reservoirs of a UZ column.

In order to limit mixing within the whole reservoir, Gomez *et al.* (2003) have also introduced a stratification (Figure 2). When an infiltration occurs at a time step, a stratum is introduced at the top of NonsatSW. Strata, defined by a given water volume and a given concentration depending on pedo-climatic and agricultural conditions at the current time step, pile up in the reservoirs and no mixing occurs. Then a piston effect occurs: an inflow at the top of the reservoir leads instantaneously to an outflow at the bottom of the reservoir. Two cases are therefore possible (Figure 2):

- if the outflow from reservoir N_2 is less than or equal to the volume V_1 in the current reservoir, C_r of V_r is equal to the concentration C_1 of V_1 .
- if V_r is greater than V_1 in reservoir N_2 , mixing of two or more strata occurs and C_r is calculated with:

$$C_r = \frac{\sum_{j=1}^{j=nl} C_j V_j}{V_r} \quad (2)$$

with C_r the concentration of drained water ($kg.m^3$), V_r the drained water volume (m^3), nl the number of drained strata and C_j and V_j the concentration ($kg.m^3$) and the volume (m^3) of each stratum j .

Water transfer through the UZ is described by equation 3:

$$Vin_{i+1(t)} = Vout_{i(t)} = (Vol_{i(t)} - V_{min(i)}) \times \delta \quad (3)$$

with $V_{min(i)}$ the minimal water volume in the reservoir i (m^3). For numerical reasons, a maximum number of strata is set. When this maximum is reached,

additional mixing occurs: two strata near the V_{min} are mixed together. In that way, strata mixed due to numerical reasons are located around the top of the reservoir while those mixed during the water transfer are located at the outflow of the reservoir. These mixings lead to a diffusion. However, this diffusion is still limited.

NonsatSW has two additional parameters compared to NonsatW. The maximum number of strata S_{max} is set uniform in the whole domain. The value of the minimal volume V_{min} can vary in space according to the soil type. As initial conditions, water volume in each reservoir of a UZ is equal to the defined V_{min} . These two parameters do not affect the water transfer dynamic, they impact only the solute transfer. A large value of V_{min} generates a longer solute transfer, since the solute has to flow through a larger amount of water. The value of the maximum number of strata affects only the diffusion: a small value leads to a larger diffusion of the solute.

2.2. Improvement of Nonsat

Gomez *et al.* (2003) assessed only partially the solute transfer simulated by NonsatSW through the comparison of passive solute velocity with the literature. The more detailed assessment presented on this study, based on comparisons with physically-based model and in-situ data (cf. section 3) has shown some important bias in the solute transfer. In order to improve the quality of the simulations, we propose two modifications: the integration of a saturation profile and a varying percolation rate depending on the water content.

2.2.1. Introduction of a saturation profile

The UZ is subject to an evolution of the water content through the column, from its base that is almost saturated, to its top that is drier when the equilibrium is reached. Van Genuchten (1980) and Brooks and Corey (1966) have determined the two main equations describing water retention curve in a UZ. Figure 3 presents the evolution of the saturation profile as a function of depth as described by Van Genuchten for a given set of parameters (plain line). In NonsatSW the saturation profile at equilibrium is constant in each reservoir and equal to V_{min} through all the reservoirs of the UZ (dotted line in Figure 3). To improve the realism of the model, a saturation profile is integrated in NonsatSW based on the Van Genuchten (1980) retention curve. This leads to a variation of the minimum volume V_{min} between each reservoir

as presented in Figure 3 (dashed line). For each reservoir, V_{min} is computed as follow:

$$V_{min(i)} = \int_{bottom_i}^{top_i} \frac{1}{[1 + (\alpha \times \phi_x)^n]^m} \times por \times S \times \Delta z \quad (4)$$

with n and α the curve parameters, $m = 1 - \frac{1}{n}$, por the porosity ($m.m^{-1}$), S the surface of the grid cell (m^2), z the depth, and ϕ the capillary pressure head in meters at z that depends on the water table depth. In this study, the discretisation Δz used is $10^{-2}m$.

As the water volume of the UZ reservoirs increases with the depth, the time transfer of the solute increases too, whereas the velocity transfer is constant in the former version of NonsatSW.

2.2.2. Evolution of the percolation rate

τ is related to the time in days required to entirely drain a reservoir. A percolation velocity can therefore be approximated from this data. And as τ is constant in the UZ column, percolation velocity is considered as constant. This transfer is not modified by the introduction of a varying saturated profile (equation 4). However, the velocity should vary according to the saturation. In order to take into consideration this process, we use a generalisation of Darcy's law for the saturated zone by assuming that the water transfer is proportional to the saturation. To take into account such a relationship, a coefficient of percolation *coef* is integrated in the model. *coef* is equal to the saturation fraction of the reservoir:

$$coef = \frac{Vol_{i(t)}}{por \times S \times d} \quad (5)$$

$$Vin_{i+1}(t) = Vout_{i(t)} = (Vol_{i(t)} - Vmin_{i(t)}) \times \delta \times coef \quad (6)$$

Therefore, as the saturation fraction increases in the deeper UZ, the outflow of the reservoir increases too.

The new version of Nonsat (NonsatVG) has therefore 3 additional parameters: the two Van Genuchten parameters α and n , and the porosity. The use of the porosity implies that now NonsatVG takes into account a maximal volume. Indeed, when the volume of water in a reservoir i fills entirely the porosity volume, the excess water is directly added to the V_r (Figure 2) and supplies the reservoir $i + 1$.

The need for three additional parameters may be a problem for regional scale modelling. Indeed, for deep unsaturated zones which are not easily

accessible, observed saturation profiles, allowing to derive n and α as well as porosity data, are rare. Therefore, to specify these three new parameters in regionale scale applications, the Carsel and Parrish (1988) database is used. It gives for each soil type the Van Genuchten parameters and the porosity (table 1). The use of such a database is based on the strong hypothesis that different textural soil types are derived from different UZ types.

2.3. The physically-based model Metis

Metis is a finite element code solving the water and solute transfer equations in the saturated/unsaturated zones (Goblet, 2007). This model was applied in varying studies: estimation of filtration velocity in soils (Goblet, 2008), simulations of heat and helium transfer in groundwater (Castro *et al.*, 2005), calculation of groundwater ages (Castro and Goblet, 2005).

Metis uses Van Genuchten relationships to describe hydrodynamic properties of UZ. The water retention curve is given by:

$$S_e = \frac{1}{[1 + (\alpha\Phi)^n]^m} \quad (7)$$

with S_e the effective saturation, n and α the curve parameters, $m=1-1/n$, and ϕ the capillary pressure head (m).

The hydraulic conductivity curves is described by:

$$K_r = \sqrt{S_e} \left[1 - (1 - S_e^{\frac{1}{m}})^m \right]^2 \quad (8)$$

with K_r the relative permeability.

$$S_e = \frac{S - S_r}{S_m - S_r} \quad (9)$$

S_e is the effective saturation linked to the saturation of the medium S , the maximal saturation S_m and the minimal saturation S_r . S_r is the part of water that can not be displaced by a pressure gradient. S_m is the maximal part of water that can be retained by the medium during a saturation. In this study, S_m is fixed to 1 and S_r to 0. S is therefore equal to S_e .

Richards equation is solved in Metis at each node of a discretized mesh, by the use of finite-element method.

3. Assessment of NonsatVG

To assess the new version of the simple UZ scheme, two kinds of comparison are made. First a comparison with the physically based model Metis is performed in some ideal cases, with various UZ depths in two UZ types. Then two kinds of real cases are studied, and the modelling is compared to observed data. In order to assess in NonsatVG the sole impact of the introduction of a saturation profile and a varying percolation rate, the value of τ is the same as in NonsatSW.

3.1. Ideal cases studies

The first ideal case consists in comparing the dynamic of the transfer simulated by Metis, the former and the new version of Nonsat over a UZ column of 20m depth with constant infiltration flux and an initial impulse flux of solute. In the two versions of Nonsat, the depth of the reservoirs is set to 5 m, the value used for the Seine application (Gomez *et al.*, 2003; Ledoux *et al.*, 2007). In Metis, the column is discretized into 2000 square elements of 10^{-2} m depth.

NonsatSW, NonsatVG and Metis do not use the same physical variables (saturation in % for Metis and volume in m^3 for Nonsat), neither the same kind of parameters, nor the same spatial geometry. Therefore, in order to compare these models we use the following strategy:

- As NonsatSW was already applied over the Seine basin, a set of parameters are available for the 7 dominating soil types of the basin (Gomez *et al.*, 2003). Thus, it was decided to use the results of NonsatSW as a reference. The methodology consists in calibrating Metis in order to have similar solute time transfers at the outflow of the 20 m column as NonsatSW. Default parameters are provided using existing databases. Then, the calibration is made by modifying the saturated hydraulic conductivity and the porosity.
- The Van Genuchten parameters and the porosity used by NonsatVG are set identical to those of Metis.
- The comparison of the solute time transfers is done at each depth corresponding to the output of one Nonsat reservoir (5, 10, 15 and 20m).

The test is done with a constant infiltration (1mm per day) and an input of passive contaminant during the first three days.

Annexe rapport PIREN, soumis à Hydrological Processes

For each UZ types defined by Gomez *et al.* (2003) in the Seine basin, parameters required in Metis are determined from a corresponding textural soil type in the Carsel and Parrish database (Table 1). An exception is made for chalk UZ type, which is characterised by a double porosity of matrix and fractures with a solute transfer occurring mainly in matrix (Lacherez-Bastin, 2005; Normand *et al.*, 2004). Van Genuchten parameters defined by Brouyère *et al.* (2004) for matrix are therefore used for the characterisation of UZ chalk.

In order to avoid generating puddles that cannot be managed by Metis, the value of K_s is adapted to be compatible with the imposed infiltration.

For the calibration, the first strategy is to have a similar water volume in the soil column, and thus, to adjust the porosity in Metis. Then, when solute transfer simulated by Metis is too fast comparing to solute transfer in NonsatSW, K_s is decreased or Por is increased. Reverse modifications are performed when solute transfer velocity in Metis is too slow compared to NonsatSW. This calibration process is performed until a good adequation with the solute transfer at the outflow in NonsatSW is reached.

The first test is performed using the NonsatSW parameters for loam (table 3).

Figure 4 presents the time evolution of the solute transfer simulated by NonsatSW, Metis and NonsatVG at the four depths of a loam UZ. For a given UZ model, the first peak corresponds to the transfer of the solute at 5m, the second at 10m, etc. By construction, the average time period needed by the solute to flow through the entire column are comparable in NonsatSW and Metis.

When looking at the results at 5, 10, 15 and 20 meters depth, the velocity of solute transfer in Metis decreases with depth while it is constant in NonsatSW. Also, the mixing increases in Metis, leading to a diminution of the peak and an increase of the duration of the transfer with depth, while NonsatSW presents almost no mixing. The modifications of NonsatVG yield a dynamic of solute transfer which compares better to Metis. The sole introduction of the saturation profile in Nonsat ('NonsatVG-darcy' in Figure 4) leads to a decrease of the solute transfer velocity with depth, and an increase of the mixing. However, the mixing is not as large as in Metis, and the solute reaches the 20m depth 10% earlier than in Metis. By using the same τ in NonsatVG than in NonsatSW, but considering in addition an evolutive percolation coefficient in the column, results obtained in NonsatVG are more

similar to those of Metis.

To test the robustness of the model, different depths of the UZ are tested. As the saturation profile varies according to the water table depth, the variation of the UZ depth should impact the solute transfer. The tests are done by assuming the same parameters than those calibrated for a UZ of 20 m depth. Results are presented Figure 5 and Table 3 for a loam UZ type.

The time needed by the solute to reach 5m depth is longer for a shallower unsaturated zone as simulated by Metis. This is due to the fact that there is more water contained in the first 5m of the UZ when the water table is closer to the surface. Thus, the solutes need to flow through a more important volume of water to pass the first 5 meters and the percolation velocity decreases. Such dynamic is not represented by NonsatSW which has a constant velocity, but is well captured by NonsatVG.

The same kind of test is also performed on a chalk column. The results presented in Table 3 lead to the same conclusion: the modifications introduced in NonsatVG yield results comparable to those of the physical model Metis, with a decrease of the solute transfer at a given depth when the water table is shallower. However, for this UZ case, the variation of the velocity transfer depending on the water table depth is much less than in the loamy UZ case. Indeed, Van Genuchten parameters used for chalky UZ generate a saturation greater than 90% through the column. Variations of saturation profile with piezometric level are therefore small and generate low variations of solute transfer velocity.

The methodology followed for these comparison tests has led to calibrated parameters that differ significantly from the Carsel and Parrish and Brouyere databases. After calibration, the defined K_s for loam is three orders of magnitude larger than the one from Carsel and Parrish database (respectively $8.15^{-3}m.s^{-1}$ and $2.89^{-6}m.s^{-1}$). For the chalk, the porosity was decreased to an unrealistic value ($por = 0.085m/m$) when compared to the in situ observed water content (Amraoui *et al.*, 2008; Normand *et al.*, 2004). Such parameters are unrealistic, which probably means that the solute transfers simulated by NonsatSW with the parameters defined over the Seine basin are biased. The following section confirms this assumption by using in-situ data.

3.2. Assessment of NonsatVG with observed data

In order to assess more accurately the new model, water and solute transfer dynamics obtained with NonsatVG are compared with in situ data. Two kinds of data are used: some piezometric levels in the Seine basin and monitorings of the nitrate concentration profile in two sites in Northern France located in the Seine basin.

3.2.1. Comparison with the observed piezometric head

The sole introduction of a saturation profile in NonsatVG does not modify the water table fluctuation simulated by Modcou with NonsatSW (equation 3). However the introduction of a relation between the percolation ratio and the saturation ratio modifies the dynamic of the flow. The general tendency is a lower velocity of water transfer through the UZ (equation 6) that generates a modification of the dynamic of the simulated piezometric levels.

In order to evaluate the impact of such a modification in the water transfer, a comparison of the observed and simulated piezometric head is performed over the Seine basin. The simulations are performed using the same module to estimate the surface water budget, and thus, the infiltration in the UZ, and the same aquifer model MODCOU (Ledoux *et al.*, 2007). Thus the differences in the simulation of the piezometric head are only due to the differences in the simulation of the water table recharge.

Figure 6 shows the comparison of the evolution of the piezometric level observed and simulated by Modcou (Ledoux *et al.*, 2007) with NonsatSW and Nonsat VG at the Mainvilliers well (48° 27' 12" North, 1° 27' 43" East) between 1981 and 2004. It can be seen that the fluctuations of the piezometric head are dampened in NonsatVG compared to NonsatSW. However, it is not clear if this dampening leads to an improvement or a degradation of the simulation of the observed piezometric head. Similar results are obtained in the other piezometric wells of the Seine basin. Figure 7 presents the statistical criteria (bias and root mean square error) obtained by NonsatSW and NonsatVG for 32 wells. It appears that the two statistical results are very similar for both models. This result means means that this modification does not make NonsatVG more or less valid than NonsatSW for the simulation of piezometric fluctuations.

3.2.2. Local comparison of the solute transfer

The Agro-Impact group from INRA (Institut National de Recherche Agronomique - National Institute in Agronomical Research) at Laon (North France)

monitors nitrate transfer through two chalky UZ at Haussimont (48° 45' 0" North - 4° 10' 0" East) and at Thibie (48° 55' 49" North - 4° 12' 59" East) in Champagne-Ardenne Region (Normand *et al.*, 2004).

In Haussimont, nitrate concentration profiles from 1 to 20 meters depth are available on a long run, from 1982 to 2004. At Thibie, nitrate concentration profiles from 0.13 to 6 meters depth were monitored from 1990 to 2008. For both sites, propagation of a nitrate peak through time can be observed. This type of long term experiment is not very common and provides very useful data to both understand the transfer of nitrate through the UZ, and to assess its modelling.

We use therefore this data set to test the three UZ schemes.

All the data needed to perform a simulation of the experimental site are not available. For instance, the time evolution of the infiltration and its nitrate concentration are unknown. Therefore to simulate this real case, some approximations are done. First, the first nitrate concentration profile (1982 for Haussimont and 1990 for Thibie) is imposed as an initial condition, and no more additional nitrate input is supposed. Then the water percolation flux is determined with the water balance module of the MODCOU model (Ledoux *et al.*, 2007) that was already applied over the Seine basin. Thus, it does not take into account the real land use, and while the site has experienced annual rotation of winter wheat, sugar beet, lucerne and winter barley, we will consider only a generic crops type. Daily precipitation and Potential Evaporation data for both sites are provided by the SAFRAN analysis of Meteo-France (Quintana Seguí *et al.*, 2008). A constant depth of the water table is assumed, and is set equal to 25 meters depth at Haussimont and 15 meters depth at Thibie according to neighbouring piezometric wells. An initial profile along the nodes in Metis and the strata in NonsatSW and NonsatVG was extrapolated from the observed data (triangular lines in Figures 8 and 9).

Three simulations are performed: the first one is done with NonsatSW with the parameter calibrated by Gomez *et al.* (2003) for a chalk UZ. The two other ones are done with Metis and NonsatVG.

Required Van Genuchten parameters and porosity in Metis and NonsatVG are determined from Brouyère *et al.* (2004). In order to avoid generating puddles in the physically-based model, the defined K_s in Metis is fixed at $9.0^{-7}m.s^{-1}$. In NonsatVG, value of τ defined by Gomez *et al.* (2003) is used. In Metis, the dispersivity is set according to the simulation of the LIXIM model (Mary *et al.*, 1999) on the Haussimont site (dispersivity=12.5cm).

Annexe rapport PIREN, soumis à Hydrological Processes

Haussimont site. From 1982 to 1999, total amount of nitrate in the UZ at Haussimont increased due to successive supplies from the agricultural activities. Then from March 2001, a significant decrease of the total amount of nitrate in the UZ was observed. At the same time, the nitrate peak is not in evidence anymore. We consider therefore that the main peak was transferred through the UZ. Thus, the comparison between observed and simulated profiles only focuses on the evolution of the nitrate peak observed in 1982 through 18 years.

The nitrate peak is at 5m depth in may 1982, 7m in march 1986, and at 14m depth in March 2000. The average transfer velocity (ATV) of this peak in this UZ is therefore 0.5m/year which is comparable to results of other studies (Serhal *et al.*, 2006). The results of comparison are presented Figure 8.

Metis simulates an evolution of the concentration profiles that is closed to the observed one. The depth of the peak for each given date and the diffusion are however slightly underestimated (AVT=0.4 m/year).

NonsatSW is not able to reproduced the observed profiles: the modelled solute peak is transferred too quickly (almost 10m in only 4 years, AVT=2.5 m/year).

Compared to NonsatSW, profiles simulated by NonsatVG are improved, with a longer solute time transfer. However, the transfer velocity is too slow, since the peak reaches in 18 years only 13 meters instead of the observed 14 meters (AVT=0.44 m/year). During all the simulation, the peak simulated by Metis is shallower than the observed one. It is not the case in NonsatVG. In April 1991, the solute peak simulated by NonsatVG has an average depth closed to the observations. But from March 97, the peak simulated by NonsatVG is still shallower than the observed one. Then it seems that the solute transfer simulated in NonsatVG is faster at the top of the UZ and is slowing closer to the aquifer. Such behavior could be seen also in the ideal case (Figure 4). It can be also noticed that the dispersion simulated by NonsatVG does not compare well to the observed one. At Haussimont, the peak intensity decreases by 30% in 18 years. In Metis, this peak decreases by more than 20% whereas in NonsatVG, the peak is almost identical at the beginning and at the end of the simulation.

Thibie site. The main peak observed in the first available profile in October 1990 is almost totally transferred through the UZ in october 2008. Thus, the comparison between observed and simulated profiles is focused on the evo-

lution of the nitrate peak from 1990 to 2003. The nitrate peak is at 1.65m depth in October 1990, 1.88m in October 1993, 4.13m in October 1999 and at 5.88m in October 2003. ATV of this peak is therefore 0.32m/year. The results of comparison are presented Figure 9. Contrary to Haussimont, the depths of the peak are surestimated in NonsatVG and Metis. The AVT is respectively 0.38 m/year and 0.47 m/year for the new version of Nonsat and the physically-based model. The closest simulated evolution of concentration profiles is therefore performed by NonsatVG. However, almost no dispersivity is simulated in this latest. In Metis, the nitrate peak intensity decreased by 35% through the simulated period which is in good agreement with the observed peak decreased of 40%.

None of the three models is able to accurately reproduce the observed profiles. Part of the error is due to the physic of the model, but also to error on the estimation of the infiltration or the estimation of the parameters. It is assumed that with an improved physics, realistic parameters as those derived from available databases should lead to realistic results. Thus, several additional tests are performed by varying the infiltration and the parameters.

A first test is done with an annual average infiltration value set according to the simulation of the LIXIM model (Mary *et al.*, 1999). The infiltration flux is 25% larger for Haussimont and 33% lower for Thibie. These modifications seems to improve the solute time transfer simulated by Metis and NonsatVG.

Then, instead of using parameters defined for the chalk, we used Van Genuchten parameters from the Carsel Parrish database for the closest soil type, ie, clay. For NonsatSW, several tests are done by increasing the minimal water volume V_{min} to get closer to realistic value, or by increasing the τ (which is equivalent to decrease the hydraulic conductivity).

For each test, an error is computed as

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (Dpeak_i^{obs} - Dpeak_i^{simu})^2} \quad (10)$$

with n the number of compared profiles, and $Dpeak_i^{obs}$ and $Dpeak_i^{simu}$ the depth of respectively the observed and simulated nitrate peak at the profile i .

Figure 10 presents mean values of this RMSE for the three models at Haussimont.

The three models are able to obtain good results (RMSE close to zero). However, it can be seen that the parameters from NonsatSW need to be adjusted (V_{min} multiplied by a factor of 5). With the default parameters, the RMSE was large (around 1m). As the parameters from NonsatSW do not rely on classical physical parameters, they could not be set according to the available database. On the contrary, both Metis and NonsatVG obtained reduced RMSE (lower than 4m) for the four tests (varying infiltration and varying soil types). Similar results were also observable at Thibie site.

From these results, it is clear that without additional calibration, the new version of Nonsat is in better agreement than the former version with the physically-based model and with the observed data. Good adequation between the former version of Nonsat and observed data is obtained only after an appropriate calibration of the V_{min} .

Furthermore, Nonsat VG model is still far less time expensive than the physically-based model Metis and is expected to be less sensitive to the exact value of the parameters.

4. Impact on the estimation of the solute transfer time in the Seine basin

The comparisons with local observations have shown that NonsatVG seems to simulate the solute transfer than NonsatSW. It is interesting to see how these differences impact the solute time transfer to the aquifers of the Seine basin. In order to estimate this time, a 35-years simulation is done, with an intransient solute imposed at the beginning of the simulation, and the real atmospheric forcing imposed from 1971 to 2006. The estimation of the infiltration in the UZ is computed by the MODCOU model (Ledoux et al. 2007). The Seine basin is characterised by a weak infiltration in the center of the basin (lower than 100mm/year), where the aquifers lie (Figure 11). Figure 12 presents the solute transfer velocity for the cells located on chalky, clay and sandy soil types as a function of the accumulated annual infiltration simulated both by NonsatVG and NonsatSW. As expected, the velocity increases with the accumulated infiltration, and can vary by a factor of 3. On average, it seems that the solute velocity for chalk, sand and clay is around 2m/year for NonsatSW. In NonsatVG, the solute velocity is around 1m/year

in chalky and clay UZ and around 3 m/year in sand.

Solute time transfer in sandy column seems to be more scattered than in the chalk for a given mean infiltration rate. This is due to the fact that the water volume in a sandy UZ is varying according to the unsaturated depth. In the chalk, such variation is attenuated because the column is almost saturated along the whole column. The velocity value obtained with NonsatVG in chalky UZ is closer to the observed data for similar soil type (0.8 to 0.9 m/year (Jackson *et al.*, 2006), 0.6 to 1.25 m/year (Serhal *et al.*, 2006)). It is also the case for clay UZ type (0.27 to 0.42 m/year (Johnson *et al.*, 1989)). Concerning sandyUZ, solute transfer velocity obtained with NonsatVG seems also in better agreement with literature (2 m/year (Legout *et al.*, 2007))

Figure 13 shows the distribution of the solute time transfer in the basin as simulated by NonsatSW and NonsatVG. There is a shift between the two simulations: in NonsatVG, a significant part of the UZ in the Seine basin transfers pollutant in about 10-15 years whereas, while in NonsatSW, the most important transfer of pollutant to the saturated zone occurred before 10 years of simulation. In NonsatVG 17 years are needed for a solute to reach the water table on 50% of the basin, while it was only 12 years with NonsatSW.

Figure 14 presents the map of the solute time transfer in the Seine basin. It easily reaches 30 years and even more than 50 years where the aquifer is deep.

This solute time transfer seems to be longer than the one obtained by Sohier *et al.* (2009) in a chalk basin in Belgium, where most of the solute reached the watertable in 15 years. This might be due to a deeper unsaturated zone depth in the Seine basin.

5. Conclusion

An improvement of a simple scheme that simulates the transfers of solute and water in the unsaturated zone using a cascade of reservoirs is proposed. Two modifications are made: a) an introduction of a saturation profile with depth, according to the Van Genuchten equations and b) an evolution of the drain velocity of the reservoir according to the saturation of the reservoir. In order to assess such modifications, comparisons with the physically based model Metis are presented in both ideal and real cases. These comparisons

show that the original version of the simple model NonsatSW was not able to represent the evolution of the solute transfer for different water table depths. The new version, NonsatVG, is better able to reproduce this dynamic. As this model is dedicated for regional scale application, one critical aspect is the determination of the three additional parameters. To define these latter, we use the Carsel and Parrish (1988) database that links these parameters to 12 FAO soil types.

An exception is made for chalky UZ type. Indeed, this medium is characterised by a double porosity of matrix and fractures with a dominant matrix water transfer (Normand *et al.*, 2004; Brouyère *et al.*, 2004). The matrix is almost saturated and generates a water transfer through the UZ by piston effect (Headworth, 1972). To take into account this particular unsaturated dynamic, Van Genuchten parameters defined by Brouyère *et al.* (2004) for UZ chalk matrix are therefore used. Sensitivity tests presented in this study show the relevance of using such parameters for this type of UZ.

As tests in ideal and real cases demonstrate that NonsatVG allows to obtain a better solute transfer through the UZ than NonsatSW, a comparison test was performed on the whole Seine basin from 1971 to 2006. Results show that, without significant modifications of water table fluctuations, solute transfer through the UZ is globally slower with NonsatVG than with NonsatSW and in better agreement with literature. NonsatVG modifies therefore significantly nitrate transfer dynamic at the Seine basin scale.

Legout *et al.* (2007) and Brouyère *et al.* (2004) have shown that fluctuations of piezometric level also modify greatly contamination dynamic in the groundwater. Indeed, when this latter rises, solute in the UZ is washed and when it drops, contamination from the UZ to the saturated zone decreases. In order to improve the dynamic of solute transfer at the interface unsaturated-saturated zones, fluctuations of water table should therefore be taken into account. Modifications provided in NonsatVG allow to integrate a direct link between water table depth and saturation profile in the UZ. We can therefore take into account explicitly water table fluctuations in the UZ. Details are presented by Philippe *et al.* (2009) and work is underway to simulate this phenomenon on the Seine basin. By the fact that it will have a direct impact on the groundwater nitrate concentration modelling, we expect to improve simulation quality of Stics-MODCOU in the Seine basin by reducing the large local errors that subsist locally in the simulation of the groundwater contamination (Ledoux *et al.*, 2007).

6. Acknowledgments

The authors would like to thank R2DS Ile-de-France for the funding of this research project, and the PIREN-Seine research program.

References

- Amraoui N, Machard de Gramont H, Robelin C, Wuilleumier A, Noyer ML, Feret MJ. 2008. Flow processes in the unsaturated Chalk of the Hallue Basin (France). In *Unsaturated Soils: Advances in Geo-Engineering*, Toll et al. (eds).
- Baran N, Richert J, Mouvet C. 2007. Field data and modelling of water and nitrate movement through deep unsaturated loess. *Journal of Hydrology* **345**: 27-37.
- Besbès M, De Marsily G. 1984. From infiltration to recharge: use of parametric transfer function. *Journal of Hydrology* **74**: 271-293.
- Birkinshaw SJ, Ewen J. 2000. Nitrogen transformation component for SHETRAN catchment nitrate transport modelling, *Journal of Hydrology* **230**: 1-17.
- Brisson, N, Mary B, Ripoche D, Jeuffroy MH, Ruget F, Nicoullaud B, Gate P, Devienne-Barret F, Antonioletti R, Durr C, Richard G, Beaudoin N, Recous S, Tayot X, Plenet D, Cellier P, Machet JM, Meynard JM, Delecalle R. 1998. STICS: a generic model for the simulation of crops and their water and nitrogen balances. I. Theory and parameterization applied to wheat and corn. *Agronomie* **18**: 311-346.
- Brooks RH, Corey AT. 1966. Properties of porous media affecting fluid flow. *Journal of the Irrigation and Drainage Division, Proceedings of the American Society of Civil Engineers* **92**: 61-88.
- Brouyère S, Dassargues A, Hallet V. 2004. Migration of contaminants through the unsaturated zone overlying the Hesbaye chalky aquifer in Belgium: a field investigation. *Journal of Contaminant Hydrology* **72**, 135-164.
- Carsel RF, Parrish RS. 1988. Developing Joint Probability Distributions of Soil Water Retention Characteristics. *Water Resources Research* **24**: 755-769.

-
- Castro MC, Goblet P. 2005. Calculation of Ground Water Ages - A comparative Analysis. *Ground Water* **43**: 368-380.
- Castro MC, Patriarche D, Goblet P. 2005. 2-D numerical simulations of groundwater flow, heat transfer and He transport - implications for the He terrestrial budget and the mantle helium-heat imbalance. *Earth and Planetary Science Letters* **237**: 893-910.
- Flipo N, Even S, Poulin M, Théry S, Ledoux E. 2007. Modeling nitrate fluxes at the catchment scale using the integrated tool CAWAQS *Science of the Total Environment* **375**: 69-79.
- Goblet P. 2007. Spécifications pour la simulation de l'écoulement en zone non saturée. Rapport final. IRSN/DSU/SSIAD.
- Goblet P. 2008. Estimation des vitesses de filtration de l'eau dans les sols de CNPE - Identification de régime-types d'écoulement. Rapport technique No R080318PGOB, Centre de Geosciences, Ecole des Mines de Paris, Fontainebleau, France.
- Gomez E, Ledoux E, Viennot P, Mignolet C, Benoit M, Bornerand C, Schott C, Mary B, Billen G, Ducharne A, Brunstein D. 2003. Un outil de modélisation intégrée du transfert des nitrates sur un système hydrologique: application au bassin de la Seine. *La Houille Blanche* **3**.
- Gutierrez A, Baran N. 2009. Long-term transfer of diffuse pollution at catchment scale: Respective roles of soil, and the unsaturated and saturated zones (Brévilles, France). *Journal of Hydrology* **369**: 381-391.
- Headworth HG, BSC, DIC, FGS (Professional Associate), Hydrologist Hampshire River Authority 1972. The analysis of natural groundwater level fluctuations in the chalk of Hampshire. *Journal of the Institute of Water Engineering* **26**: 107-124.
- Jackson BM, Wheeler H, Mathias SA, McIntyre N, Butler AP. 2006. A simple model of variable residence time flow and nutrient transport in the chalk. *Journal of Hydrology* **330**: 221-234.
- Johnson RL, Cherry JA, Pankow JF. 1989. Diffusive Contaminant Transport in Natural Clay: A Field Example and Implications for Clay-Lined Waste Disposal Sites. *Environmental Science & Technology* **23**: 340-349.

Annexe rapport PIREN, soumis à Hydrological Processes

-
- Lacherez-Bastin S. 2005. Contribution à l'étude de la migration des nitrates dans le sol et la zone non saturée de la nappe de la Craie dans le Nord de la France. Thèse de Doctorat, Ecole Polytechnique Universitaire de Lille.
- Ledoux E, Gomez E, Monget JM, Viavattene C, Viennot P, Benoit M, Mignolet C, Schott C, Mary B. 2007. Agriculture and Groundwater Nitrate Contamination in the Seine Basin. The STICS-MODCOU modelling chain. *Science of the Total Environment* **375**: 33-47.
- Legout C, Molenat J, Aquilina L, Gascuel-Oudou C, Faucheux M, Fauvel Y, Bariac T. 2007. Solute transfer in the unsaturated zone-groundwater continuum of a headwater catchment. *Journal of Hydrology* **332**: 427-441.
- Mary B, Beaudoin N, Justes E, Machet JM. 1999. Calculation of nitrogen mineralization and leaching in fallow soil using a simple dynamic model. *European Journal of Soil Science* **50**: 549-566.
- Mignolet C, Schott C, Benoît M. 2007. Spatial dynamics of farming practices in the Seine basin: Methods for agronomic approaches on a regional scale. *Science for the Total Environment* **375**: 13-32.
- Nash JE, ME, AMICEI. 1960. A unit hydrograph study, with particular reference to british catchments.
- Neitsch SL, Arnold JG, Kiniry JR, Williams JR. 2005. Soil and Water Assessment Tool Theoretical Documentation.
- Normand B, Mary B, Czernichowski I, Beaudoin N, Mouvet C, Bazerque MF, Groell F. 2004. Programme expérimental de suivi de la qualité de l'eau sur trois bassins versants de Picardie faisant l'objet de mesures agri-environnementales. Rapport de synthèse.
- O'Shea L, Wade A. 2009. Controlling nitrate pollution: an integrated approach. *Land Use Policy* **26**: 199-808.
- Philippe E, Habets F, Ledoux E, Goblet P, Viennot P. 2009. Improvement of nitrate transfer modelling in a drainage basin: consideration of water table fluctuations in the unsaturated zone. *Proceedings of the 16th Nitrogen Workshop, Turin*.

-
- Quintana Segui P, Le Moigne P, Durand Y, Martin E, Habets F, Baillon M, Canellas C, Franchisteguy L, Morel S. 2008. Analysis of Near Surface Atmospheric Variables: validation of the SAFRAN analysis over France. *Journal of Applied Meteorology and Climatology* **47**: 92-107.
- Refsgaard JC, Storim B. 1995. MIKE SHE. Computer Models of Watershed Hydrology. *Water Resources Publication*, 809-846.
- Refsgaard JC. 2002. Harmonising Quality Assurance in model based catchment and river basin management. State-of-the-Art Report on Quality Assurance in modelling related to river basin management. Contract EVK2-CT2001-00097. HarmoniQua project.
- Rivett OM, Buss SR, Morgan P, Smith JWN, Bemment CD. 2008. Nitrate attenuation in groundwater: a review of biogeochemical controlling processes. *Water Research* **42**: 4215-4232.
- Serhal H, Bastin-Lacherez S, Bernard D, El Khattabi J. 2006. Etude de la migration des nitrates dans la nappe à travers la zone non saturée: enjeux et impact sur la qualité de l'eau exploitée. Darcy 67. Colloque international - Gestion des grands aquifères - 30 mai-1er juin 2006. Dijon, France.
- Sohier C, Degré A, Dautrebande S. 2009. From root zone modelling to regional forecasting of nitrate concentration in recharge flows - The case of the Walloon Region (Belgium). *Journal of Hydrology* **369**: 350-359.
- Van Genuchten MTh. 1980. A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. *Soil Science Society of American Journal* **44**: 892-898.
- Vauclin M. 1993. Modélisation du transport de solutés dans la zone non saturée du sol. *Revue des Sciences de l'Eau* **7**: 81-102.
- Viennot P, Ledoux E, Monget JM, Schott C. 2006. Contamination nitrique des aquifères du bassin de la Seine. Document de synthèse PIREN Seine 2006.

Table 1: Averaged values for selected soil water retention and hydraulic conductivity parameters for 12 major soil textural groups according to Carsel and Parrish (1988). θ_r and θ_s are the minimal and the maximal saturation of the medium ($m.m^{-1}$), α and n are Van Genuchten parameters and K_s is the saturation permeability ($m.s^{-1}$). In the last column, corresponding soil type defined by (Gomez *et al.*, 2003) on the Seine basin.

<i>Carsel and Parrish</i>						<i>Nonsat</i>	
<i>Texture</i>	θ_r	θ_s	$\alpha(1/m)$	n	K_s		
<i>sand</i>	0.045	0.430	14.500	2.680	$8.250.10^{-5}$	<i>urban crystallin</i>	
<i>loamy sand</i>	0.057	0.410	12.400	2.280	$4.050.10^{-5}$		
<i>sandy loam</i>	0.065	0.410	7.500	1.890	$1.220.10^{-5}$		
<i>loam</i>	0.078	0.430	3.600	1.560	$2.890.10^{-6}$		
<i>silt</i>	0.034	0.460	1.600	1.370	$6.940.10^{-7}$		<i>alluvium</i>
<i>silt loam</i>	0.067	0.450	2.000	1.410	$1.250.10^{-6}$		<i>loam</i>
<i>sandy clayloam</i>	0.100	0.390	5.900	1.480	$3.640.10^{-6}$		<i>sand</i>
<i>clay loam</i>	0.000	0.410	1.900	1.310	$7.220.10^{-7}$		<i>chalk</i>
<i>silty clayloam</i>	0.089	0.430	1.000	1.230	$1.940.10^{-7}$		
<i>sandy clay</i>	0.100	0.380	2.700	1.230	$3.330.10^{-7}$		
<i>silty clay</i>	0.070	0.360	0.500	1.090	$5.550.10^{-8}$		
<i>clay</i>	0.068	0.380	0.800	1.090	$5.550.10^{-7}$		<i>clay</i>

Table 2: Set of parameters used in NonsatSW, NonsatVG and Metis for ideal cases. N is the number of reservoirs, *thick* is the thickness of the UZ (m), nqu is the number of nodes, τ is the time percolation (m/s), V_{min} is the minimal water volume in each reservoir ($m.m^{-1}$), *por* is the porosity ($m.m^{-1}$), n and α are Van Genuchten parameters, K_s is the saturation permeability ($m.s^{-1}$), dispersivity is the solute dispersion ($10^{-2} m$).

<i>Loam UZ</i>			<i>Chalky UZ</i>		
<i>NonsatSW</i>	<i>NonsatVG</i>	<i>Metis</i>	<i>NonsatSW</i>	<i>NonsatVG</i>	<i>Metis</i>
$N = 4$	$N = 4$	$nqu = 2000$	$N = 4$	$N = 4$	$nqu = 2000$
$\tau = 1, 15.10^{-5}$	$\tau = 1, 15.10^{-5}$	$K_s = 8, 15.10^{-3}$	$\tau = 1.15.10^{-5}$	$\tau = 1.15.10^{-5}$	$K_s = 9, 00.10^{-7}$
<i>thick</i> = 20	<i>thick</i> = 20	<i>thick</i> = 20	<i>thick</i> = 20	<i>thick</i> = 20	<i>thick</i> = 20
$V_{min} = 0.07$	<i>por</i> = 0.33	<i>por</i> = 0.33	$V_{min} = 0.08$	<i>por</i> = 0.085	<i>por</i> = 0.085
	$n = 1.56$	$n = 1.56$		$n = 1.1$	$n = 1.1$
	$\alpha = 3.6$	$\alpha = 3.6$		$\alpha = 0.1$	$\alpha = 0.1$
		<i>dispersivity</i> = 1			<i>dispersivity</i> = 1

Table 3: Mean solute velocity transfer (m/year) obtained with NonsatSW, NonsatVG and Metis to reach a given depth D (m) considering a given water table depth (WT in m) for ideal cases.

		<i>Loam UZ</i>			<i>Chalk UZ</i>		
<i>WT</i>	<i>D</i>	<i>NonsatSW</i>	<i>NonsatVG</i>	<i>Metis</i>	<i>NonsatSW</i>	<i>NonsatVG</i>	<i>Metis</i>
20	5	8.7	11.4	13.0	7.6	7.9	7.9
	10	8.7	11.4	12.2	7.6	7.8	7.9
	15	8.7	11.06	11.4	7.6	7.7	7.9
	20	8.7	8.8	8.8	7.6	7.7	7.8
15	5	8.7	11.4	14.8	7.6	7.8	7.9
	10	8.7	10.9	13.0	7.6	7.7	7.8
	15	8.7	8.1	8.7	7.6	7.6	7.6
10	5	8.7	11.1	11.4	7.6	7.6	7.7
	10	8.7	7.0	7.2	7.6	6.5	7.6

Table 4: Set of parameters used in NonsatSW, NonsatVG and Metis for comparison with observed data. N is the number of reservoirs, *thick* is the thickness of the UZ (m), nqu is the number of nodes, τ is the time percolation ($m.s^{-1}$), V_{min} is the minimal water volume in each reservoir ($m.m^{-1}$), *por* is the porosity ($m.m^{-1}$), n and α are Van Genuchten parameters, K_s is the saturation permeability ($m.s^{-1}$), dispersivity is the solute dispersion ($10^{-2} m$).

<i>NonsatSW</i>	<i>NonsatVG</i>	<i>Metis</i>
$N = 5$	$N = 5$	$nqu = 5000$
<i>thick</i> = 25	<i>thick</i> = 25	<i>thick</i> = 25
$\tau = 1.15^{-5}$	$\tau = 1.15^{-5}$	$K_s = 9.00.10^{-7}$
$V_{min} = 0.08$	<i>por</i> = 0.41	<i>por</i> = 0.41
	$n = 1.1$	$n = 1.1$
	$\alpha = 0.1$	$\alpha = 0.1$
		<i>dispersivity</i> = 12.5

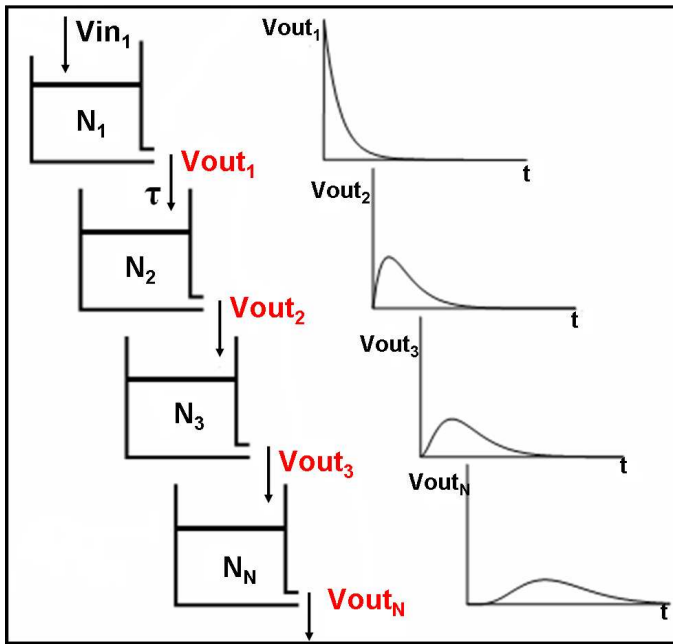


Figure 1: Representation of the Nash cascade. N is the reservoir, varying from N_1 to N_N , Vin_1 is the infiltration at the surface of the UZ, $Vout_i$, i varying from 1 to N is the outflow from each reservoir N_i . The amplitude of the given infiltration is modified by the transfer through the cascade.

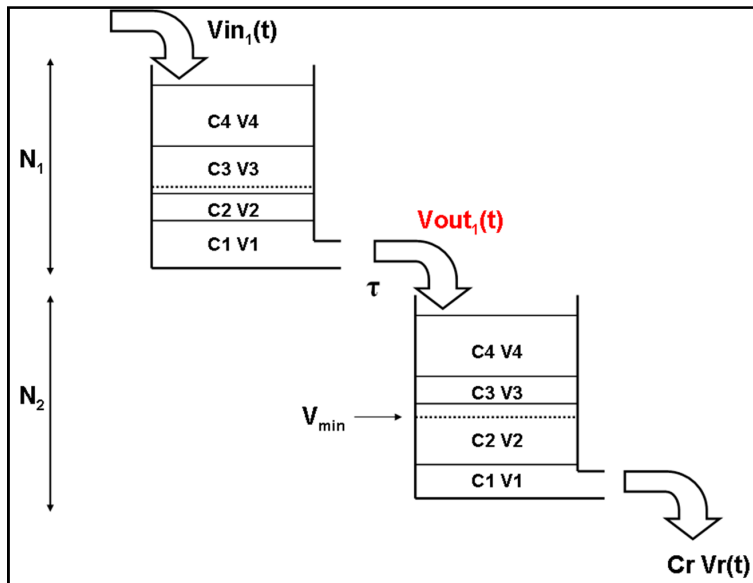


Figure 2: Representation of the passive solute transfer through the UZ in NonsatSW with 2 reservoirs N . V_{min} is the minimal water volume in each reservoir, τ is the percolation time and C and V the concentration and the volume of each stratum. An infiltration at the surface of the unsaturated zone at the time step t generates an immediate outflow of water with a volume V_r and a concentration C_r by piston effect.

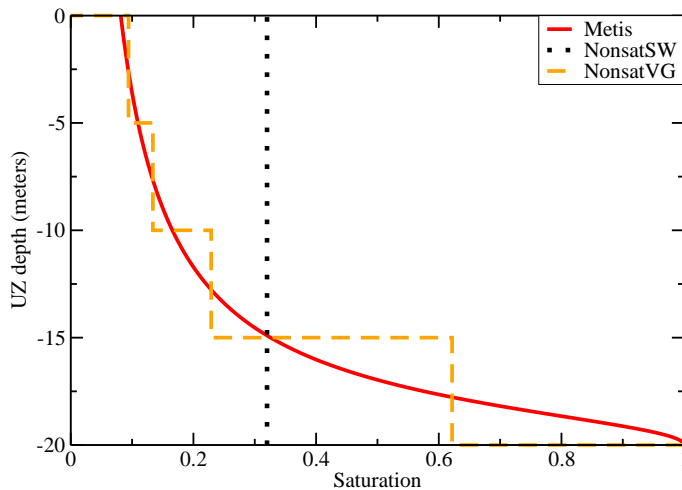


Figure 3: Evolution of the saturation with depth in Metis, NonsatVG and NonsatSW.

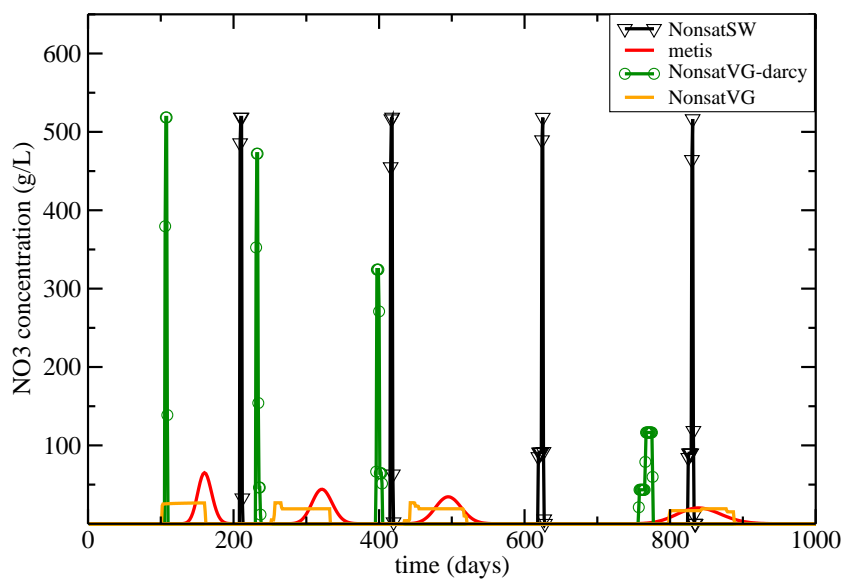


Figure 4: Transfer of passive solute in ideal cases at 4 depths (5, 10, 15 and 20 meters depth) through a loam UZ column in Metis, NonsatSW, NonsatVG with only a Van Genuchten saturation profile (NonsatVG-Darcy) and NonsatVG.

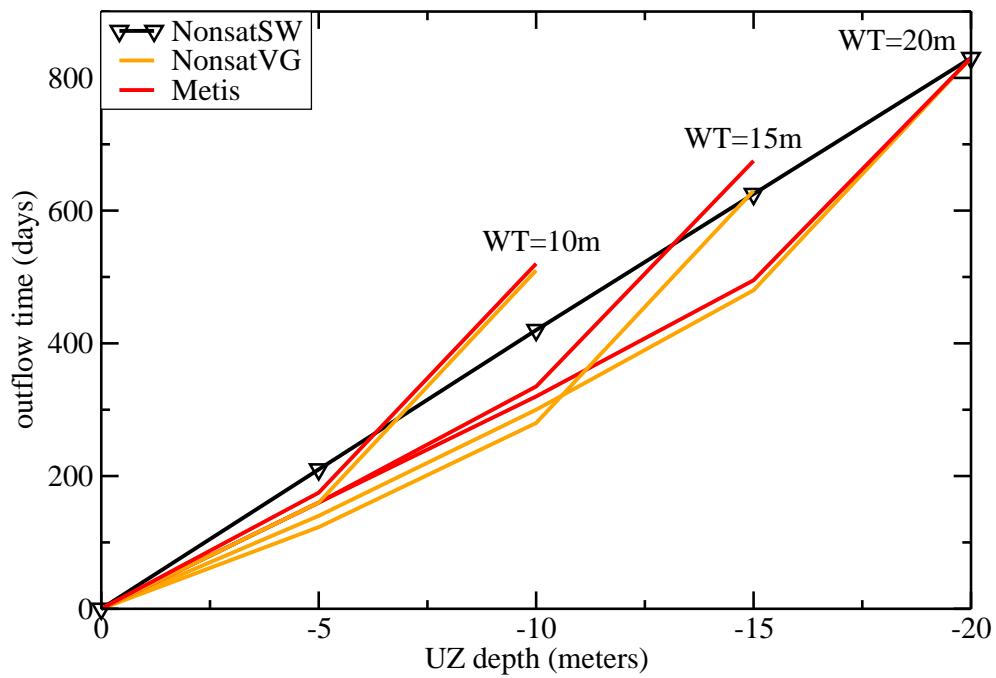


Figure 5: Time in days required for a passive solute to reach 5, 10, 15 and 20 meters depth in a loam UZ for three different water table depths (WT in meters) in NonsatSW, NonsatVG and Metis.

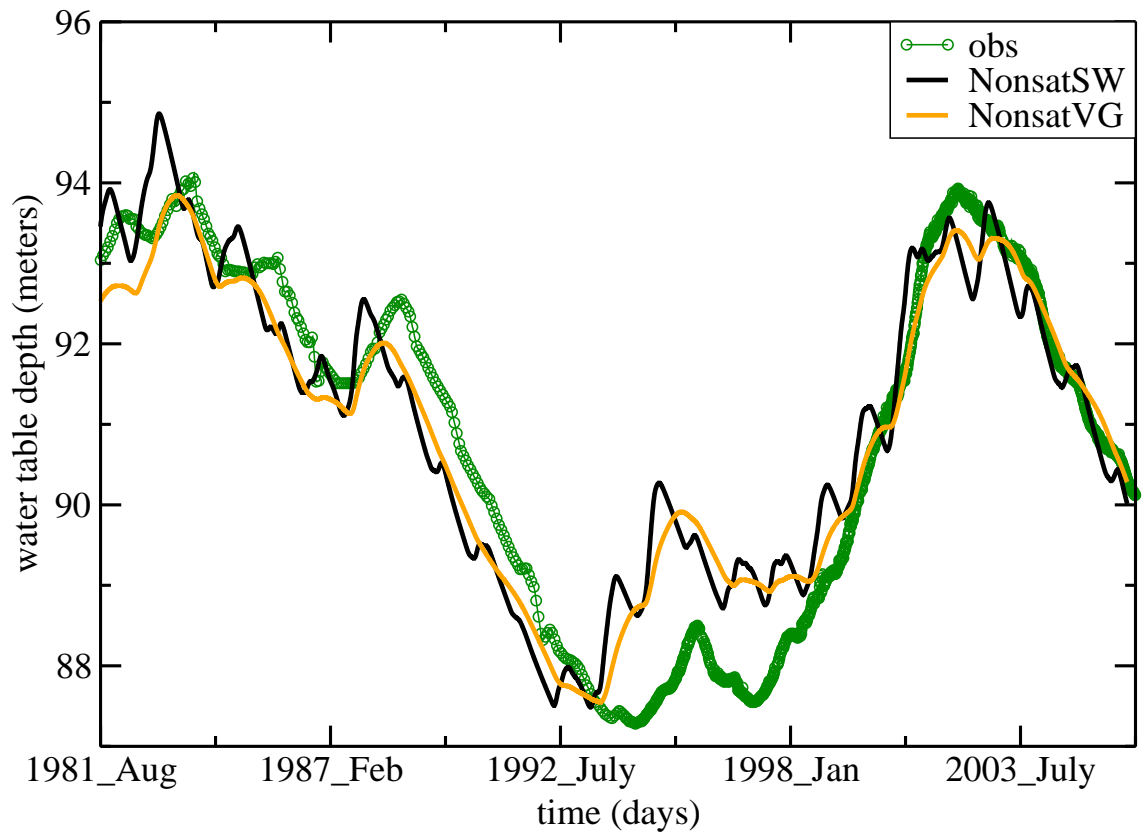


Figure 6: Comparison of the piezometric head observed at the Mainvilliers well and simulated by NonsatSW and NonsatVG, from 1981 to 2004.

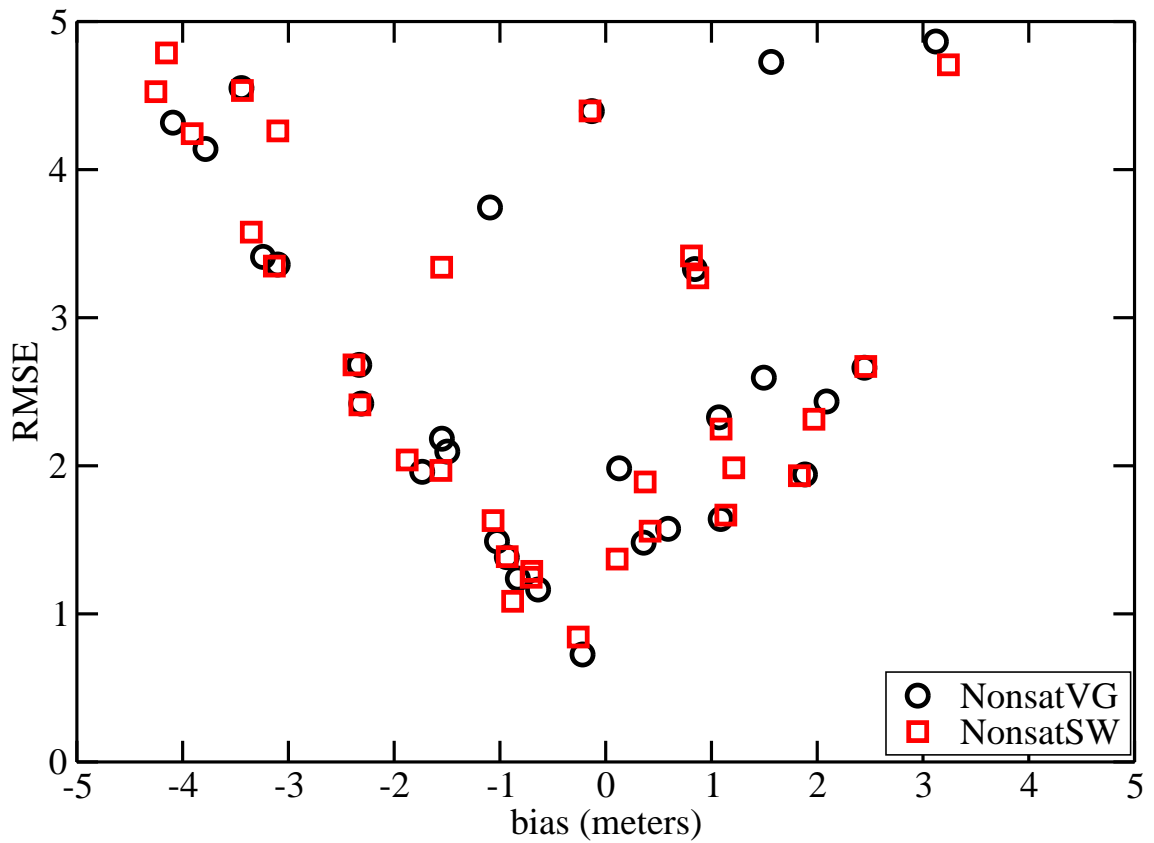


Figure 7: Root mean square error and bias in the modelling of water table fluctuation by NonsatSW and NonsatVG on 32 wells over the Seine basin, from 1981 to 2004.

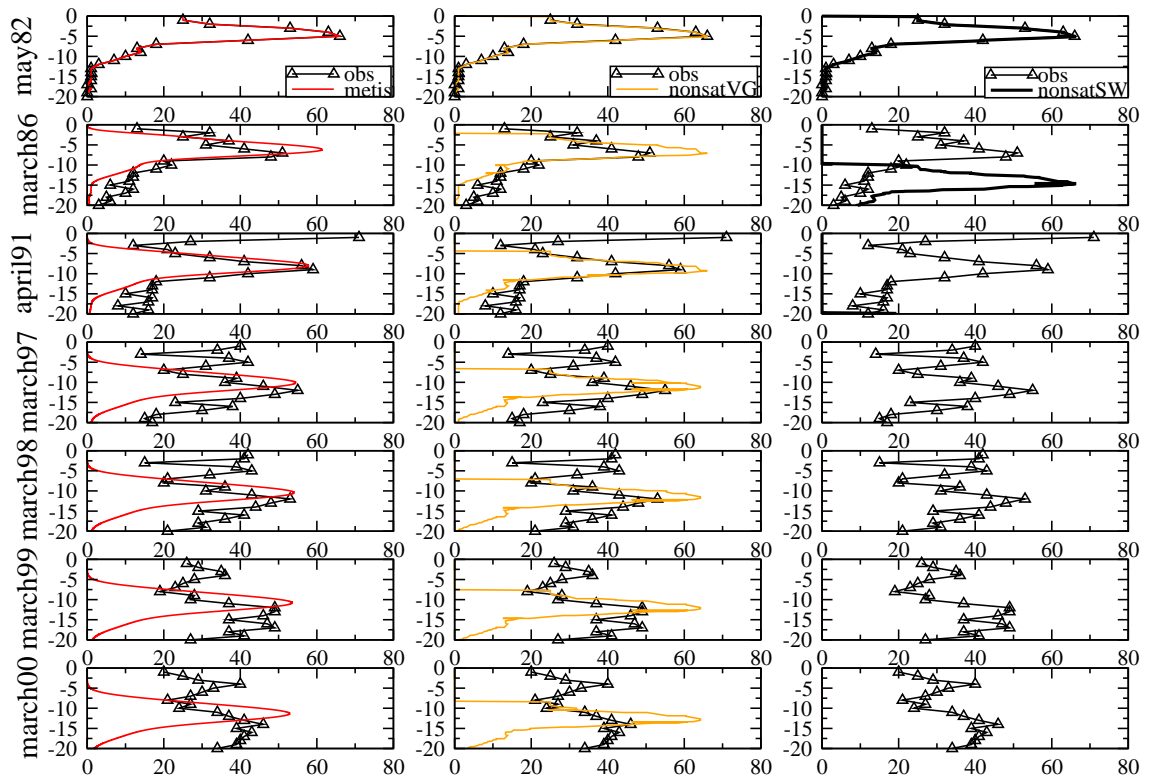


Figure 8: Nitrate concentration profile (x axis) in g/L observed at Haussimont from 1982 to 2000 in a UZ of 25 meters depth (y axis) and simulated by Metis (left), NonsatVG (center) and NonsatSW (right). Modelling is performed by considering as initial conditions the nitrate profile observed in may 82, with no additional solute input during the simulation. Water percolation flux is determined with the water balance module of the MODCOU model (Ledoux *et al.*, 2007).

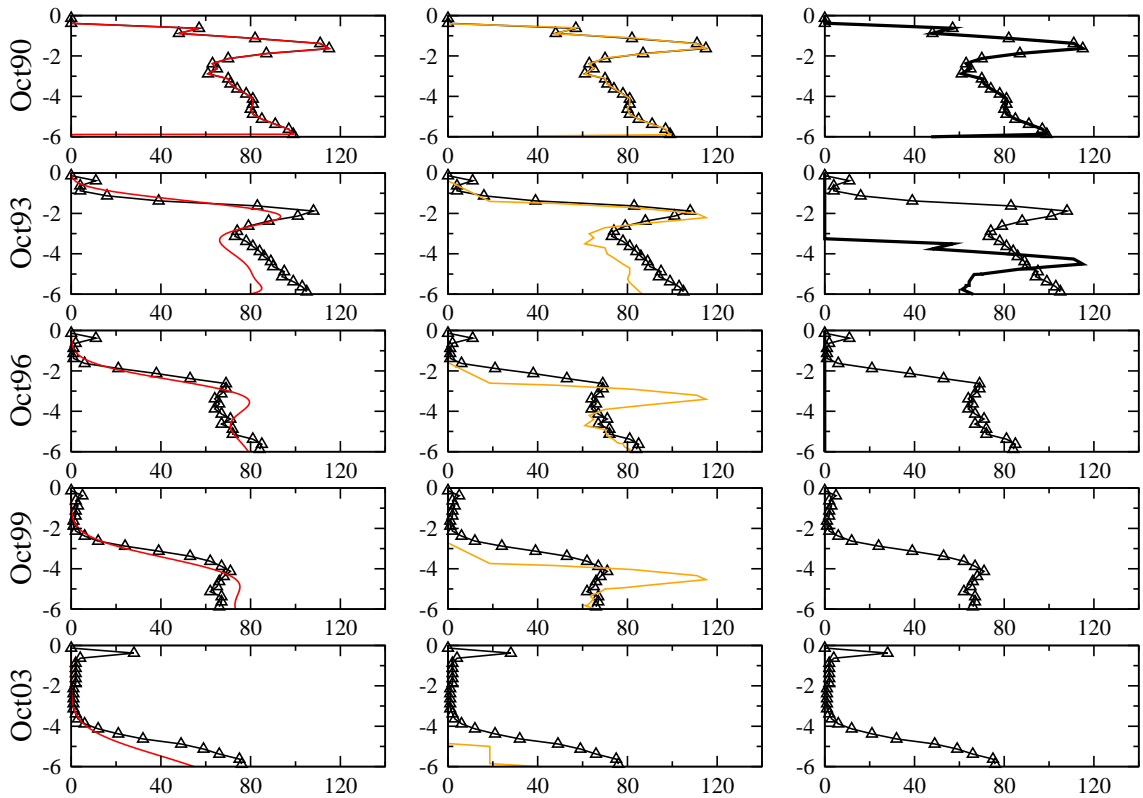


Figure 9: Nitrate concentration profile (x axis) in g/L observed at Thibie from 1990 to 2003 in a UZ of 15 meters depth (y axis) and simulated by Metis (left), NonsatVG (center) and NonsatSW (right). Modelling is performed by considering as initial conditions the nitrate profile observed in octobe 1990, with no additional solute input during the simulation. Water percolation flux is determined with the water balance module of the MODCOU model (Ledoux *et al.*, 2007).

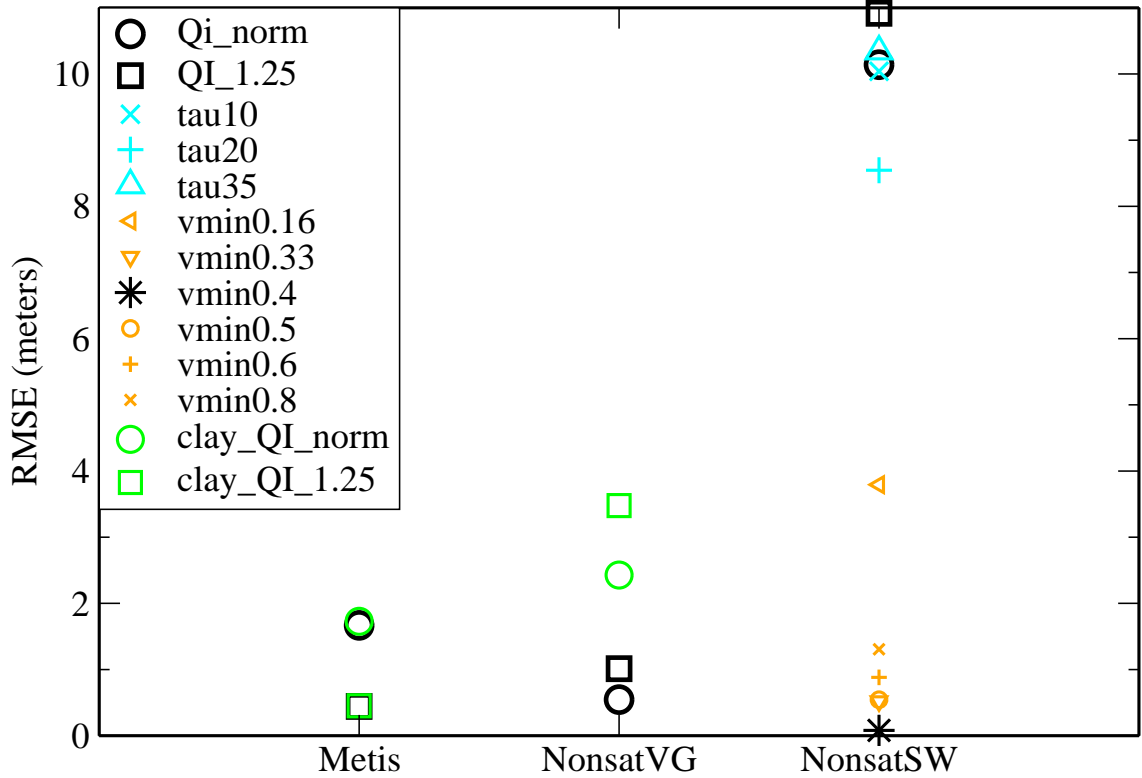


Figure 10: Root Mean Square Error (RMSE) of the nitrate peak depth simulated by NonsatVG, NonsatSW and Metis, from 1982 to 2000 at Haussimont. Results are obtained with parameters defined in table 4. QI_{norm} are obtained with infiltration determined from the water balance module of the MODCOU model (Ledoux *et al.*, 2007). $QI_{1.25}$ are obtained with an infiltration flux 25% larger. *Clay* are performed with clay class parameters (table 1) with MODCOU infiltration ($ClayQI_{norm}$) and infiltration 25% larger ($ClayQI_{1.25}$). With MODCOU infiltration, points $V_{min}x$ are obtained with a minimal water volume value in each reservoir equal to xm/m and points τx are obtained with a $\tau=x$ days.

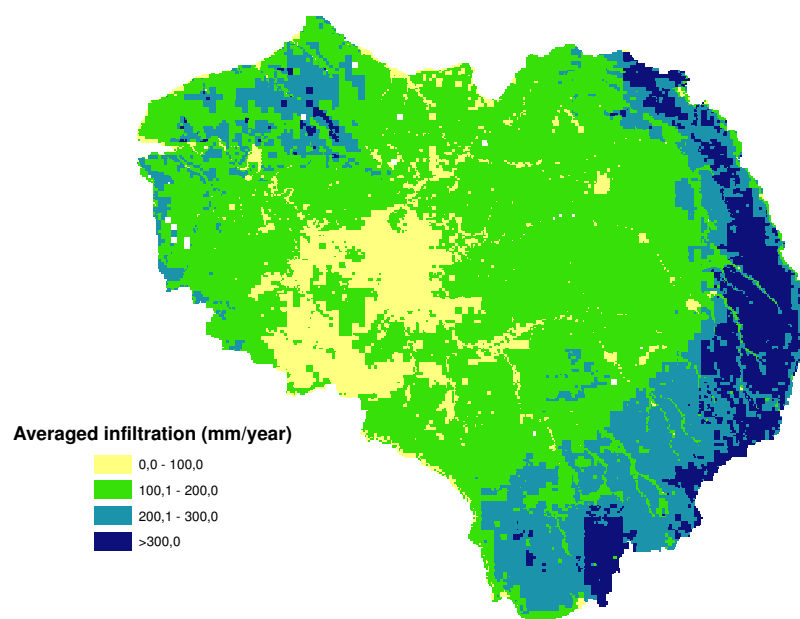


Figure 11: Average annual infiltration estimated from 1971 to 2006 over the Seine basin with the water balance module of the MODCOU model (Ledoux *et al.*, 2007).

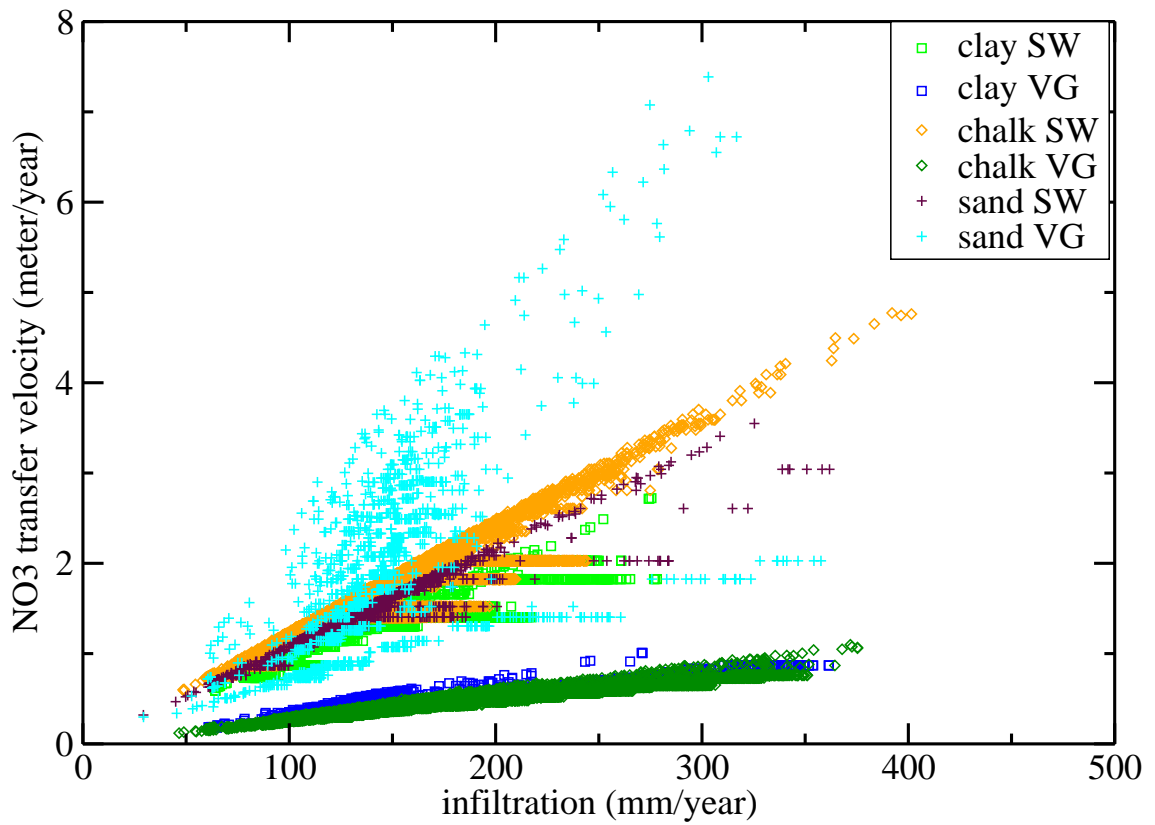


Figure 12: Comparison of the solute transfer velocity simulated by NonsatSW (SW) and NonsatVG (VG) for each cell located on chalk, clay and sandy soil types in the Seine basin, as a function of the average annual infiltration.

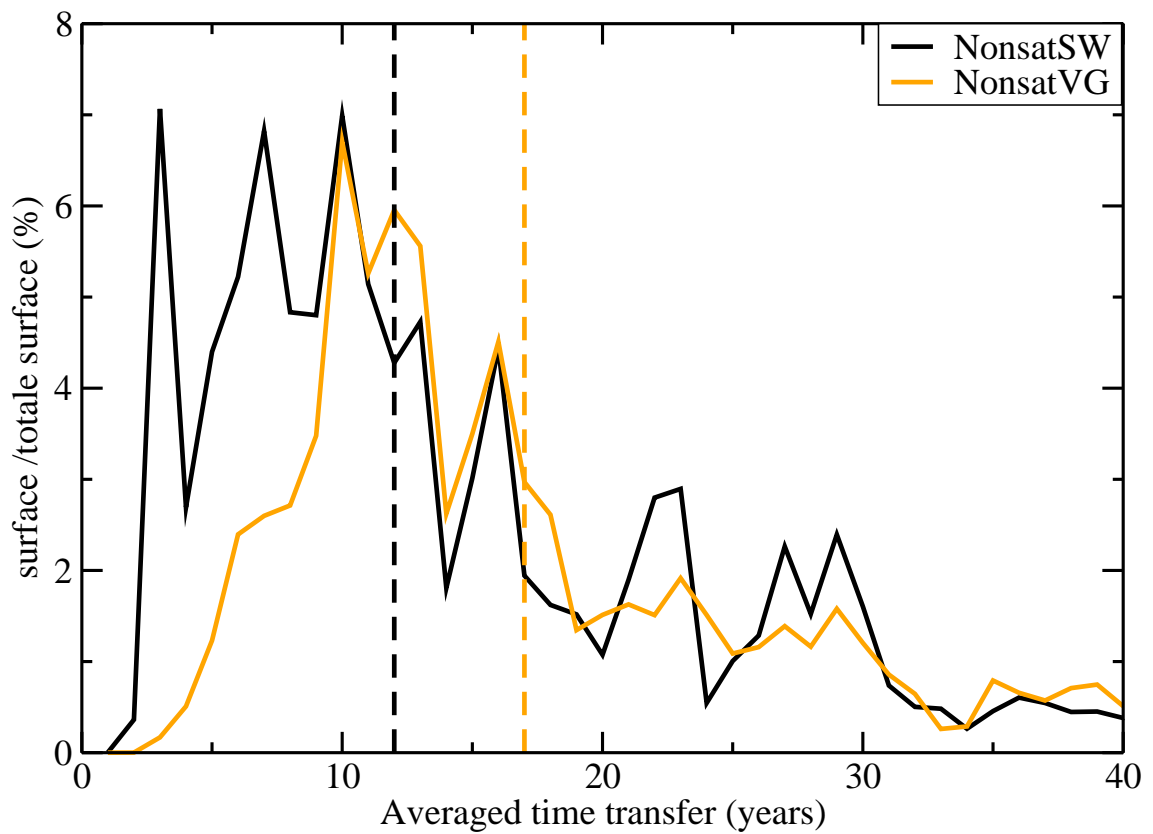


Figure 13: Surface repartition of the Seine basin depending on the averaged time required in years for an outflow of nitrate from the unsaturated zone to the saturated zone. Infiltration is determined with the water balance module of the MODCOU model (Ledoux *et al.*, 2007) from August 1971 to August 2006 and a nitrate input occurs from the 181th to the 196th days of the simulation. At the dashed line, 50% of the unsaturated zone in the Seine basin have transferred nitrates to saturated zone.

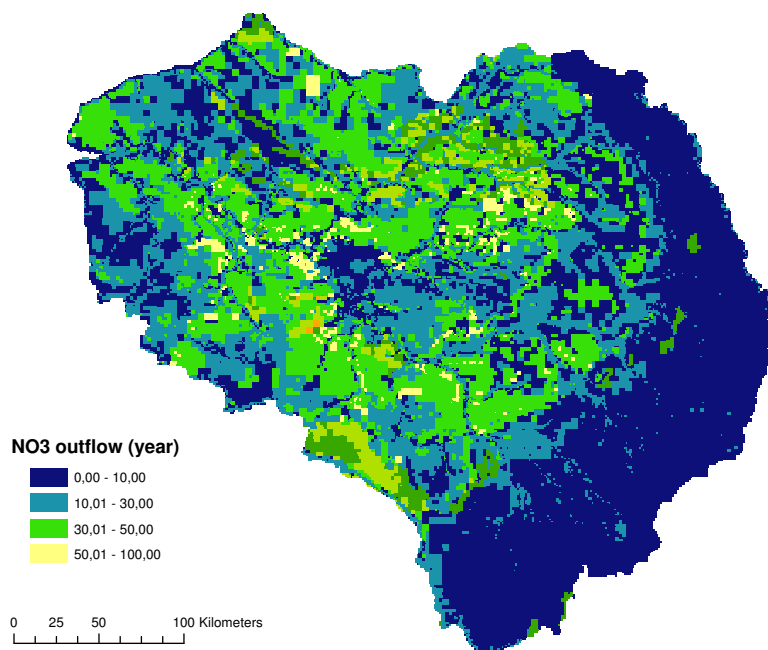


Figure 14: Averaged time required in years for a nitrate transfer through the unsaturated zone in the Seine basin with NonsatVG. Infiltration is determined with the water balance module of the MODCOU model (Ledoux *et al.*, 2007) from August 1971 to August 2006 and a nitrate input occurs from the 181th to the 196th days of the simulation.