# Chapitre 2

## 2 Description des modèles

Nous avons argumenté dans l'introduction l'intérêt de développer des chaînes pertinentes de modèles pour étudier les phénomènes influençant les pollutions de l'air et de l'eau induites par le trafic routier. Plusieurs outils ont été utilisés pour ces quatre phénomènes : trafic, émission, qualité de l'air et de l'eau.

Le choix du modèle dépendra de l'échelle spatio-temporelle à modéliser mais aussi de la résolution des données d'entrées et de sorties des modèles ou encore de la compatibilité des modèles disponibles pour le mettre en œuvre. Par exemple pour modéliser la qualité de l'eau, nous ne pouvons pas utiliser une chaîne de modèles dynamique à petite échelle temporelle car les modèles d'émissions instantanés actuels n'estiment pas encore les émissions non-échappement et les particules ayant un diamètre supérieur à 10 µm ; or, ces particules peuvent être la source principale de certains polluants dans les eaux de ruissellement (diamètre médian 30 µm). Il convient aussi de choisir des modèles en fonction des cas d'étude et de la précision attendue. Ces questions sont traitées dans le chapitre 3 qui présente un état de l'art des modèles disponibles pour simuler le trafic, les émissions de polluants, la qualité de l'air et la qualité des eaux de ruissellement.

Ce chapitre est consacré à la description des modèles utilisés dans les chaînes de modélisation construites dans cette thèse, particulièrement les chapitres 3, 4, et 5. Ils incluent le modèle dynamique de trafic (Symuvia), le modèle d'émissions pour vitesse moyennées (CopCETE), le modèle d'émissions instantanées (PHEM), le modèle de dispersion atmosphérique (Polyphemus), et le modèle de quantité et qualité de l'eau (SWMM).

### 2.1 Modèle de trafic (Symuvia)

Le modèle de trafic Symuvia de l'IFSTTAR est un modèle microscopique à loi macroscopique du 1er ordre de type LWR (Leclercq et al., 2007). Le modèle LWR de Lighthill et Whitham (1955) et Richards (1956) calcule trois variables macroscopiques du trafic (le débit $Q$, la concentration $K$ et la vitesse $V$) par deux lois de la mécanique des fluides et la relation du diagramme fondamentale qui décrit le comportement des véhicules.

$$\frac{\partial K}{\partial t} + \frac{\partial Q}{\partial x} = 0 \quad (2.1)$$

$$Q = KV \quad (2.2)$$

Les modèles du 1er ordre de type LWR supposent que le système est en permanence à l'équilibre et que la vitesse n'est fonction que de la concentration : $Q = KV_{eq}(k(x,t))$, donc le système se réduit à une seule équation hyperbolique scalaire de la variable K (Godlewski et Raviart, 1991).

$$\frac{\partial K}{\partial t} + \frac{\partial Q_{eq}(K)}{\partial x} = 0 \qquad 2.3$$

Cette équation est généralement calculée au moyen du schéma numérique de Godunov (Godunov, 1959) en tenant compte de la condition CFL ($V_{max}\, \Delta t \leq \Delta x$).

Le modèle Symuvia a été enrichi avec diverses extensions de manière à décrire plus finement les diverses situations de trafic en milieu urbain et notamment l'accélération bornée pour améliorer la reproduction de la cinématique des véhicules, les différentes classes de véhicules, la gestion particulière des transports collectifs et les conflits aux carrefours urbains (giratoire, feux, les interactions entre les piétons et les véhicules, etc.) (Leclercq et Laval, 2007 ; Laval et Leclercq, 2008 ; Chevallier et Leclercq, 2008 ; Chevallier et Leclercq, 2008b).

Les données d'entrée du modèle incluent : la matrice origine-destination (O/D), les niveaux de demandes aux entrées (veh/h), les réglages des cycles de feux aux carrefours ainsi que les types de véhicules (véhicules légers, bus, trolleys bus, tramways, etc.). Ce modèle est susceptible de calculer à chaque instant la position, la vitesse et l'accélération de chaque véhicule présent sur le réseau.

## 2.2 Modèle d'émission basé sur la vitesse moyenne (CopCETE)

CopCETE a été développé pour des cas d'études français par le Ministère de l'Écologie (MEDDE) et coordonné par le CETE (Centre d'études techniques de l'équipement ; actuellement CEREMA) Normandie-Centre. CopCETE est un outil basé sur les méthodologies et équations de COPERT (Ntziachristos et al., 2009), avec en plus certains facteurs d'émissions spécifiques dérivés de travaux français. Le logiciel COPERT est orienté sur le calcul d'inventaire macroscopique (inventaires nationaux d'émissions) alors que CopCETE permet de travailler à partir d'une grande série de tronçons ou segments routiers, plutôt que les 3 seuls cas urbain / rural / autoroutier envisagés par l'outil COPERT.

Les méthodologies de COPERT4 sont présentées brièvement à l'Annexe A et de manière détaillée à http://www.emisia.com/copert/Documentation.html.

CopCETE offre la plupart des possibilités de calcul abordées dans la méthodologie COPERT : (source, Notice CopCETE, 2010)

- les émissions à chaud pour les véhicules légers et lourds ;
- les surémissions à froid pour les véhicules légers ;
- les surémissions liées à la pente pour les poids lourds ;

- les surémissions liées à la charge des poids lourds ;
- les corrections liées aux améliorations des carburants ;
- les corrections liées au vieillissement des catalyseurs et leur maintenance ;
- les émissions par évaporation pour les véhicules légers ;
- les émissions hors échappement ;

Il faut noter que le logiciel CopCETEv3 a été utilisé pour calculer les émissions échappement et évaporation en utilisant des données COPERT, or l'approche des émissions de démarrage à froid et par évaporation n'est pas toujours appropriée au niveau du tronçon. Par ailleurs, pour les émissions non échappement, le document « Sélection des agents dangereux à prendre en compte dans l'évaluation des risques sanitaires liés aux infrastructures routières et ferroviaires » a été utilisé (http://www.sante.gouv.fr).

Pour appliquer le modèle, if faut connaître les paramètres suivants : (1) pas de temps (horaire, journalier, mensuel, annuel), (2) la période (mois) renvoyant aux conditions de température, (3) le chargement des véhicules lourds (0, 50% ou 100%), (4) la longueur des trajets (ou un facteur de démarrage à froid) et leur nombre journalier pour la détermination des surémissions de démarrage à froid et par évaporation de carburant, (5) la longueur du tronçon et sa pente moyenne (par classe de 2% jusqu'à ±6), (6) le milieu (urbain diffus, urbain dense, campagne, autoroute), (7) les nombres de véhicules légers et lourds ayant circulé pendant la période sur ce tronçon, un pourcentage du VUL dans le flux VL, le nombre de bus et de camions, (8) la vitesse de circulation des VL, PL et bus, (9) des données liées au démarrage à froid et aux évaporations (taux de froid, nombre d'arrêt au cours de la période) et (10) le parc automobile français élaboré par l'Ifsttar-LTE (version 2011) qui a été intégré dans CopCETE (cependant, le modèle peut utiliser des parcs différents selon le cas d'étude). Le calcul d'émissions sur un réseau routier peut être effectué pour chaque tronçon et pas de temps, on ne définit qu'une vitesse moyenne par groupe de véhicules ; en conséquence, tous les véhicules circulent à la même vitesse sur le tronçon, stable au cours de la période, et on ne capte pas plus finement qu'à ce niveau la dynamique du trafic.

Le modèle fournit des émissions échappement et non échappement par tronçon et par catégorie détaillée de véhicules pour un pas de temps choisi par l'utilisateur (horaire, journalier, mensuel, annuel). COPCETE peut également agréger les résultats par grandes catégories (VP, VUL, PL, etc.), par tronçon, et pour l'ensemble des tronçons. Les données fournis par CopCETE comprennent la consommation de carburant et les émissions de 26 polluants qui incluent $CO_2$, CO, $NO_x$, COV, benzène, PM, $SO_2$, Pb, Cd, $CH_4$, COVNM, $N_2O$, $NH_3$, HAP, Cu, Cr, Ni, Se, Zn, Ba, As, acroléine, formaldéhyde, 1,3-butadiène, acétaldéhyde et benzo(a)pyrène. La liste des types d'émissions pris en compte pour chaque polluant est présentée en Annexe B.

Il faut noter que les facteurs d'émission non-échappement de COPERT 4 ont été utilisés ici pour les polluants qui ne sont pas inclus dans modèle CopCETE.

## 2.3 Modèle d'émissions instantanées (PHEM)

Le modèle PHEM (Passenger Car and Heavy Duty Emission Model) est développé par Graz University of Technology, Autriche (Zallinger et al., 2008). Ce modèle calcule la consommation de carburant et l'émission instantanée des véhicules sur la base de cycles de conduite donnés et de cartes du moteur du véhicule. Ces cartes du moteur sont produites par la puissance et la vitesse de moteur (1 Hz) pour chaque norme Euro. Les données d'entrées (cycle de conduite et caractéristiques du véhicule) calculent à la fois la puissance du moteur liée à la résistance du véhicule et la perte de transmission, et aussi la vitesse du moteur basée sur le taux de transmission, le diamètre de roue et le modèle de changement de vitesse. En effet, les différents paramètres tels que les charges des véhicules, la pente de la route en combinaison avec les variations de la vitesse et de l'accélération peuvent être illustrés dans le modèle par différents effets de changement de vitesse. La Figure 2.1 montre différents paramètres mis en jeu avec le modèle PHEM.

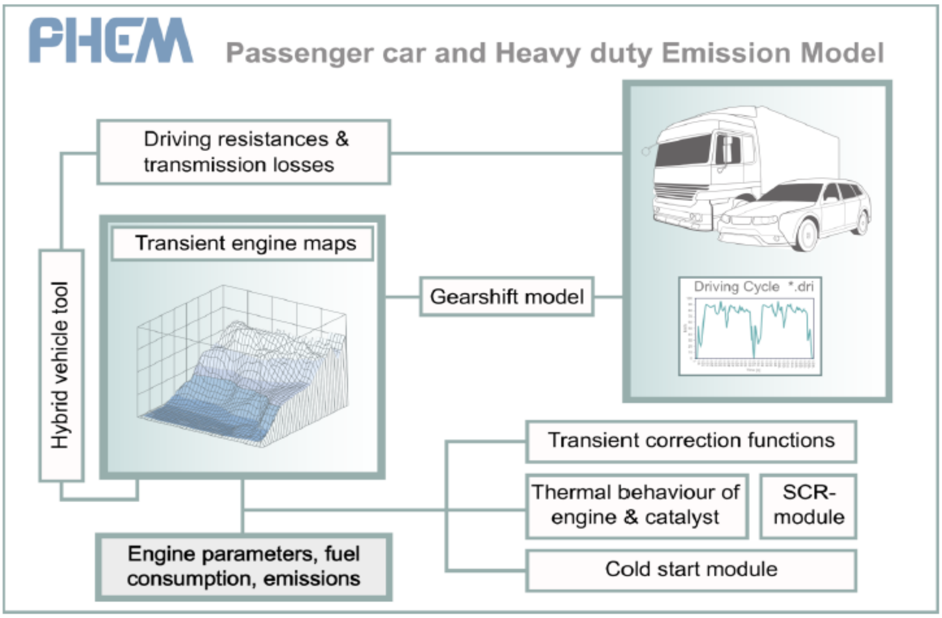


Figure 2.1. Schéma du modèle PHEM.

Il existe trois versions de ce modèle : (1) PHEM Standard simule l'émission d'un véhicule individuel à l'aide de ses caractéristiques et de son cycle de conduite, (2) PHEM Batch peut être utilisé pour un groupe des véhicules ; cette version utilise aussi les caractéristiques du véhicule et le cycle de conduite, (3) PHEM Advance calcule les émissions d'un parc automobile dans les réseaux routiers. Pour PHEM Advance, l'utilisateur n'a besoin d'entrer que les positions et les vitesses des véhicules en chaque instant (e.g., GPS) ou les laisser être calculées par le modèle de trafic.

Nous sommes intéressés ici par la version PHEM Advance qui est capable de calculer les émissions à petites échelles spatio-temporelles et peut aussi être couplé grâce à une interface avec le modèle de trafic. Ce modèle nécessite 4 fichiers entrés pour la mise en œuvre opérationnelle : (1) données de trafic (FZP) qui incluent le temps, la position, la vitesse, la catégorie de véhicule, et le numéro de tronçon et sa pente. Ces données peuvent être fournies par le modèle de trafic (e.g., VISSIM), (2) la composition du parc automobile (FLT), (3) les données de température (TEM) et (4) la segmentation de réseaux (STR). Une compatibilité de la segmentation avec celle d'un modèle de qualité de l'air facilite le transfert des résultats. Les résultats de PHEM se présentent sous trois formes : (1) résultats seconde par seconde d'information sur les véhicules: les coordonnées, les identifications de véhicules, la puissance, la vitesse, l'accélération, les émissions de plusieurs polluants (NO, $NO_x$, CO, HC, PM, PN (nombre de particule)) et la consommation du carburant, (2) les valeurs moyennes d'émissions de chaque véhicule en fonction du temps de conduite, (3) des résultats qui peuvent être importés dans le modèle de qualité de l'air (e.g., MISKAM) et qui incluent $NO_x$, CO, HC, $CO_2$, $PM_{10}$, benzène, carbone suie (soot) et $SO_2$.

## 2.4 Dispersion atmosphérique (Polyphemus-Gaussien)

La plateforme de modélisation Polyphemus (Mallet et al., 2007) est développée par le CEREA. Cette plateforme propose différents modèles de simulation de qualité de l'air tels que des modèles Eulérien, Lagrangien, Plume-in-Grid et Gaussien. Ce dernier a été largement utilisé pour modéliser la dispersion atmosphérique à l'échelle locale grâce à ses formulations simples qui offrent l'avantage d'être une bonne approximation pour un grand nombre de cas proches des sources avec des temps de calcul convenables. La formulation gaussienne peut s'appliquer à des rejets instantanés (modèle à bouffées) et à des rejets continus (modèle de panache) ; par ailleurs, un rejet continu peut être discrétisé dans le temps pour être représenté par une série de bouffées. Un modèle à bouffées permet d'avoir une meilleurs représentation de la trajectoire d'un panache sur de longues distances où la direction du vent peut varier. Le modèle Gaussien de panache est utilisé pour les émissions du trafic routier car un modèle à bouffées est coûteux en temps de calcul du fait de la longueur des sources (routes) et un modèle de panache est approprié car les impacts ont lieu à seulement quelques centaines de mètres de la source. Les modèles gaussiens supposent que les conditions météorologiques sont uniformes et stationnaires ce qui est acceptable à l'échelle locale. La formule analytique de dispersion gaussienne est valable pour une source ponctuelle si l'on tient compte des hypothèses sur la stationnarité et l'homogénéité. Elle est aussi valable pour une source linéique dans le cas où vent est perpendiculaire à la route. Une autre formulation a été ajoutée au modèle gaussien de Polyphemus par Briant et al. (2011, 2013) ; elle est basée sur la formulation de Venkatram et Horst (2006) qui consiste à évaluer l'intégrale en approximant l'intégrande et en excluant du calcul certaines portions de la source. Cette formulation induit des erreurs sous le vent par rapport à la source linéique et aussi par rapport aux deux extrémités de la source. Les erreurs induites par cette approche ont été minimisées en ajoutant deux sources ponctuelles à chaque extrémité de la source linéique pour l'erreur sous le vent par rapport aux deux extrémités. L'erreur sous le vent par rapport à la source linéique est minimisée selon trois régime définis en fonction de l'angle du vent par rapport à la route. Pour des angles de 0° à 40°, (0° représente un vent perpendiculaire à la route), l'erreur est négligeable, pour des angles de 40° à 75° l'erreur peut être minimisée avec des fonctions gaussiennes, et pour des angles de 75° à 90° l'erreur est minimisée en utilisant une fonction exponentielle. Par ailleurs, l'équation gaussienne diverge lorsque la direction du vent est parallèle à la source ; par conséquent, pour les cas où l'angle est supérieur à 80°, une combinaison de concentrations calculées par la formulation pour une source linéique et de concentrations calculées par la discrétisation de la source en sources ponctuelles est utilisée. Un coefficient qui dépend de l'angle du vent définit les fractions relatives de ces deux concentrations. Par ailleurs, le modèle a été amélioré pour modéliser la largeur de la route au moyen d'une intégration de Romberg. La formulation a été développée à l'origine pour des polluants gazeux. Dans le cadre de cette thèse, le modèle a été modifié pour traiter les particules.

Ce modèle donne de bons résultats pour les cas où la vitesse du vent est importante (>1 m/s), mais a des mauvaises performances pour les cas où la vitesse du vent est faible, car la direction du vent est alors mal définie. Une solution a été proposée par Venkatram et al. (2013) qui suppose que les polluants peuvent être dispersés sur 360° lorsque la météorologie est calme. Cette approche est développée et évaluée au chapitre 4.

Les données d'entrées nécessaires pour la simulation des concentrations des polluants et les dépôts atmosphériques comprennent les éléments suivants: (1) les coordonnées et longueurs des sources (tronçons de route), (2) les taux d'émissions horaires associées au trafic, (3) les positions des points récepteurs où sont calculées (et parfois mesurées) les concentrations, (4) les données météorologiques qui comprennent la vitesse et la direction du vent, la température et la nébulosité (la stabilité atmosphérique est estimé à partir de la période (jour ou nuit), vitesse du vent et nébulosité). Par ailleurs, les précipitations sont nécessaires pour le calcul des dépôts humides et des hypothèses doivent être faites sur la granulométrie des particules pour estimer les vitesses de dépôts secs et les coefficients de lessivage par la pluie.

## 2.5 Hydrologie (SWMM)

Le modèle SWMM 5 (Rossmann, 2004) simule à la fois la quantité (débit à l'exutoire d'un bassin versant) et aussi la qualité des eaux de ruissellement. Il s'agit d'un modèle assez répandu pour les études d'hydrologie urbaine pour des périodes continues et longues ou à l'échelle d'évènements de pluie. Ce modèle représente le bassin versant sous la forme de trois objets principaux : les sous-bassins versants en surface, les nœuds et les conduits du réseau d'assainissement. Dans ce modèle, le bassin versant est divisé en plusieurs sous-bassins pour mieux estimer la quantité et la qualité des eaux de ruissellement en fonction de la variabilité spatiale de la topographie, des ouvrages de drainage, de l'occupation de sol, etc.

La transformation pluie-débit est modélisée par un réservoir non-linéaire qui comprend l'infiltration, le stockage sous forme de pertes initiales et l'évaporation. Le transfert sur la surface est modélisé en suivant l'approche de l'écoulement d'une onde cinématique sur un plan (Singh, 1988). Les équations correspondantes sont:

$$\frac{dV}{dt} = A(p - perm * i - e) - Q(V) \tag{2.4}$$

$$Q(V) = kWn^{-1}\left(d - d_p\right)^{5/3} s^{-1/2} \qquad 2.5$$

où, V ($m^3$) est le volume stocké dans un sous-bassin versant, Q ($m^3$) est le volume d'eau sortant du sous-bassin versant, A ($m^2$) est la surface du sous-bassin versant, W (m) est la largeur moyenne du sous-bassin versant, p (m) est la hauteur de pluie, d (m) est la hauteur d'eau (*V/A*), perm est la pourcentage de surface perméable, $d_p$ (m) est la hauteur des pertes initiales, i (m) est l'infiltration, n est la constante de Manning qui dépend de la typologie de la surface, e (m) est l'évaporation et s est la pente moyenne du sous-bassin versant.

L'écoulement est transporté dans les conduits représentant le réseau sur la base des équations de Saint-Venant.

La modélisation de la qualité des eaux nécessite la modélisation de l'accumulation de la pollution sur le sol durant le temps sec, du lessivage des polluants durant les pluies et du transport des polluants dans le réseau. Pour cela, le modèle a besoin que soient définies des informations telles que le type de polluant, les catégories d'occupation de sols qui produisent ces polluants et les concentrations des polluants dans les précipitations et dans les eaux souterraines. Les méthodes de calcul de ces paramètres seront expliquées au chapitre 5.

Ce modèle nécessite de fournir les discrétisations et de définir les caractéristiques des sous-bassins versants (surface, largeur, pente, surface imperméable, coefficient de rugosité), l'occupation des sols, les réseaux de conduits, les données de précipitation, le modèle d'infiltration, ainsi que l'accumulation de polluant et le lessivage. En sortie, l'utilisateur peut récupérer les résultats de débit, de hauteur d'eau, et la concentration des polluants en chaque nœud du réseau.

# Chapitre 3

## 3 Chaînes de modélisation

La nécessité de développer une chaîne de modélisation pour simuler la pollution de l'air et des eaux pluviales due au trafic routier a été expliquée au chapitre 1. Ce chapitre présente un état de l’art des outils de modélisation des différents phénomènes (trafic, émissions, pollution atmosphérique, qualité des eaux de ruissellement), mettant en exergue les enjeux liés à l’intégration des différents modèles et le choix de modèles pour constituer une chaîne cohérente en termes de polluants et d’échelles spatio-temporelles.

Les modèles de trafic sont classés en 3 grandes catégories : statique, dynamique agrégée, et dynamique. Les méthodes et outils sont présentés pour différentes échelles, données d’entrée et résultats. Par exemple, un modèle statique tel que VISUM estime le débit et la vitesse moyenne sur un tronçon, alors qu’un modèle dynamique microscopique tel que Symuvia est capable de déterminer la position des véhicules, leurs vitesse et accélération sur l’ensemble du réseau de routes considéré. Les modèles d’émissions relèvent de 7 catégories en fonction des données nécessaires pour calculer les taux d’émissions ainsi que les différents types de polluants émis par les véhicules. Par exemple, le modèle CopCETE peut utiliser les résultats d’un modèle de trafic statique (donnant des flux de véhicules horaires et des vitesses moyennes) pour simuler les taux d’émissions de nombreux polluants issus de diverses sources d’émissions (échappement, non-échappement et évaporation). Si l’on souhaite connaître les émissions avec plus de précision, le modèle PHEM peut estimer l’émission à l’échappement à chaque instant et sur chaque segment de route. De nombreux types de modèles de dispersion atmosphérique faisant appel à diverses techniques de modélisation et couvrant différents échelles spatiales sont présentés. Le choix du modèle dépendra du cas d’étude local, régional ou continental. Les modèles de chimie-transport basés sur une approche Eulérienne ou Lagrangienne peuvent être utilisés aux échelles régionales et continentales (voire globales). À l’échelle locale sans obstacle et avec des données d’entrée uniformes spatialement (e.g., météorologie), les modèles Gaussiens sont appropriés. Les modèles de type « street-canyon » ont été développés pour tenir compte de l’effet des bâtiments sur la dispersion en milieu urbain. Pour les cas avec des géométries complexes, les modèles CFD peuvent être choisis, cependant, leurs besoins en temps de calcul limitent leurs applications à des domaines limités (quartier) et des courtes périodes (journée). Les modèles hydrologiques sont classées en 4 catégories selon le degré d’homogénéisation des données d’entrée spatiales qui peuvent caractériser un bassin versant (localisé), un sous-bassin versant (partiellement distribué), une surface avec des données d’entrée hydrologiques similaires (HRU) ou une région avec un maillage spatial (distribué). La disponibilité de données telles que celles d’occupation des sols et d’intensité de la pluie et la résolution désirée des données d’entrée déterminent le choix du modèle. Les limitations et les incertitudes associées à ces modèles sont aussi brièvement présentées dans ce chapitre.

Le lien entre les émissions du la circulation, les dépôts atmosphériques et la contamination des eaux de ruissellement n'a pas encore été traité d'une manière globale. C'est pourquoi différents couplages entre modèles sont étudiés dans ce chapitre séparément à travers trois cas d'étude.

Le premier cas d'étude considère le couplage entre un modèle de trafic (Symuvia) et deux modèles d'émissions distincts : l'un utilisant des vitesses moyennées et l'autre des vitesses instantanées (PHEM). La comparaison des résultats de ces deux couplages montrent des émissions plus importantes pour la plupart des polluants avec le modèle d'émissions utilisant les vitesses instantanées pour une voie urbaine lorsque les vitesses de circulation sont faibles.

Le deuxième cas d'étude considère le couplage des modèles d'émissions et de qualité de l'air. Une application de ce couplage a été réalisée pour un segment de l'autoroute A31 près de Metz avec une comparaison des résultats de la simulation avec des mesures de dépôts de cadmium obtenues à différentes distances des deux côtés de l'autoroute pendant février 1997. Les émissions ont été calculées avec le modèle CopCETE. Le modèle Gaussien de Polyphemus, alimenté par ces émissions, a alors été utilisé pour calculer la dispersion et les dépôts secs et humides de cadmium. Les résultats des simulations sont satisfaisants sauf pour les zones proches de la bordure de l'autoroute où des particules grossières non-prises en compte dans les émissions pourraient contribuer significativement aux dépôts.

Le troisième cas d'étude considère le couplage entre les modèles de qualité de l'air et des eaux de ruissellement. En particulier, la cohérence et les interfaces des modèles sont discutées. Le cas d'étude réalisé traite le calcul du dépôt avec des données expérimentales de dépôt, de trafic et de conditions météorologiques. Une comparaison entre deux scénarios, l'un qui inclut les émissions du trafic local et les concentrations de fond et l'autre qui traite seulement les concentrations de fond, montre que les concentrations de métaux dans les eaux de ruissellement sont jusqu'à six fois plus élevées en considérant explicitement le trafic local pour les sous-bassins versants situés au voisinage des routes très fréquentées.

Cette étude a permis de proposer deux configurations de chaînes de modélisation, l'une statique avec des pas de temps horaires, la seconde envisageant une approche dynamique. La première chaîne peut estimer à la fois les concentrations de polluants dans l'air et aussi dans les eaux de ruissellement, grâce à son modèle d'émission (CopCETE) qui détermine une large variétés des polluants émis par les véhicules. Des facteurs d'émission de COPERT peuvent en particulier être utilisés pour les particules de diamètre supérieures à 10 µm, car celles-ci sont des polluants potentiellement importants dans les eaux de ruissellement. Une application de cette chaîne de modélisation sera présentée en détail au chapitre 5.

La seconde chaîne considère les émissions et la dispersion des polluants de manière plus détaillée, en analysant le comportement individuel des véhicules, l'effet du régime moteur sur les émissions du véhicule, ainsi que la turbulence créée par les obstacles et les véhicules. Cette seconde approche conviendrait pour une simulation précise de la qualité de l'air mais pas pour la qualité de l’eau car les modèles d'émissions instantanés ne traitent pas encore les polluants d'intérêt pour l'eau tels que les HAP, métaux lourds, et la fraction grossière des PM produites par les émissions non-échappement (usure des freins et des pneus).

Ce chapitre est constitué de Fallah Shorshani et al., (2014) :

Fallah Shorshani M., André M., Bonhomme C., Seigneur C. (2014). Modelling chain for the effect of road traffic on air and water quality: Techniques, current status and future prospects. Submited to Environmental Modelling & Software.

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**Abstract**

Modelling approaches for simulating air and stormwater pollution due to on-road vehicles in an urban environment are reviewed and discussed. Models for traffic, emissions, atmospheric dispersion and stormwater contamination are studied with particular emphasis on their couplings to create a modelling chain. The models must be carefully selected according to the requirements and level of necessary details required for the integrated modelling chain. Although a fair amount of research has been conducted to link air pollution and road traffic, many questions related to spatio-temporal scales, domains of validity, consistency among models, uncertainties of model simulation results and interfaces between models remain open. Furthermore, the link between traffic emissions, atmospheric deposition and the contamination of stormwater runoff in urban areas has not yet been treated in a comprehensive manner. The aim of this work is to review the current status of the relationships between traffic, emissions, and air and water quality models, to recommend modelling approaches and to propose some directions for improving the state of the art. The difficulties and challenges associated with model coupling are illustrated with specific examples.

## 3.1 Introduction

It is expected that in 2050 more than 70 percent of the world’s population will live in urban areas. The growing amount of vehicles in densely populated areas increases traffic congestion and contributes to the deterioration of air (e.g., Zmirou et al., 2004) and stormwater quality (e.g., Obropta and Kardos, 2007). Thus, traffic is a major source of pollution in cities. Currently, traffic models can predict the position and kinematic parameters of the vehicles and emission models can estimate the amount of different types of pollutants emitted by vehicles, albeit with some uncertainty. Then, the dispersion and transformation of pollutants in the atmosphere can be modelled using atmospheric dispersion models and/or chemical-transport models. A fraction of the air pollutants deposits to surfaces by dry and wet processes. These pollutants may be entrained by the water runoff during rainfall events, which can be simulated by stormwater models. They may also be resuspended in the atmosphere due to mechanical disturbance (e.g., traffic, wind). Various models have been designed to simulate each of these phenomena; however, little work has been done to develop integrated modelling systems that can simulate the impact of traffic on both the air and water environments in urban areas. It is essential that such capabilities be developed and evaluated as their needs are primordial for the planning of the sustainable cities of the future. Thus, there is a need for a global and systemic approach of pollutant mitigation policies in urban areas in order to decrease globally their pressure on the environment and human health.

Traffic pollutants are emitted by the internal combustion engine of the vehicles, tyre, clutch and brake wear, fuel evaporation, and road wear. Exhaust emissions consist mostly of carbon dioxide ($CO_2$), carbon monoxide (CO), nitrogen oxides ($NO_x$: NO and $NO_2$), volatile organic compounds (VOC), particulate matter (PM), nitrous oxide ($N_2O$), ammonia ($NH_3$), persistent organic pollutants (POP) including polycyclic aromatic hydrocarbons (PAH), and metals. VOC are also emitted by evaporation. Non-exhaust emissions such as brake and tyre wear are also sources of PM. PM includes inorganic species, trace metals, and carbonaceous compounds. Emission factors are available only for the major air pollutants and large uncertainties exist for many air pollutant emissions.

First, we present and classify the models for each phenomenon (traffic, emissions, air quality, and water quality) according to their input data and scales of application. Next, we discuss the strengths and weaknesses of these models. Then, we address the development of modelling chains and various approaches to link these models. Finally, we present recommendations for further model development and suggest alternative models that could be considered as integrated modelling systems. Specific issues such as differences in PM size ranges relevant to air and water quality are identified and actions to resolve those issues are proposed. This work provides the basis to improve the integrated modelling approach to relate traffic to air and water pollution, which today is typically limited to spatially or temporally averaged conditions (average fleet composition, average traffic speed, stationary atmospheric conditions) and separate media (i.e., either air or water).

## *3.2* Model description

### 3.2.1 Traffic models

Three major classes of models can represent the behaviour of vehicles for various applications to an urban network:

i) Static models rely on the spatial distribution of population and calculate average traffic volumes in different areas of a network. Such models (e.g., VISUM, Fellendorf et al., 2000) are typically divided into four steps: trip generation, trip distribution, modal split and assignment. The numbers of trips in each area of the network are estimated based on housing, office density, and their locations. These trips are used to construct an origin-destination (OD) matrix. The OD matrix, in combination with information such as the different modes of transport and speed flow curves, is used to calculate the travel times on the road network. Thus, they provide the vehicle flux for each link of the road network. These models are highly simplified, but they are useful to provide a static description of the road traffic in terms of flow and speed over large spatial scales (e.g., city scales).

ii) Dynamic models describe the temporal variations of traffic conditions and how they affect vehicle movement. These models use an explicit representation of congestion and operate at a smaller spatio-temporal scale than the static models. They calculate the location and kinematic parameters of vehicles, which can subsequently be used to predict pollutant emissions and traffic noise as a function of space and time. They are discussed in grater detail below.

iii) Aggregated dynamic models (e.g., Daganzo, 2007) keep an explicit representation of congestion by describing the temporal evolution of traffic states of a simplified road network (spatial aggregation). These models divide the city into neighbourhood-sized reservoirs (commensurate with a trip length) and shift the modelling emphasis from microscopic predictions to macroscopic monitoring. Upon the assumption of a homogeneous distribution of the traffic, it is possible to estimate the average speed and the congestion level as a function of time. These models are based on relationships between the amount of displacement per unit of time (generation) and the number of vehicles on the network (accumulation), which are denoted MFD (Macroscopic Fundamental Diagram), and traffic demand (OD-matrix) among different neighbourhoods. The typical application of such models is the evaluation of the level of congestion to reduce traffic.

We are interested here in dynamic models that provide appropriate traffic conditions for a more accurate estimation of air pollution. Dynamic models can be classified into three categories according to different aspects of traffic flow operations:

(1) The macroscopic models (e.g., METACOR, Diakaki and Papageorgiou, 1996) use an aggregate representation of vehicles and the assumption of continuous traffic flow. They are, therefore, characterized by variables such as traffic flow and vehicles density.

(2) The microscopic models take into account the time-space behaviour of individual vehicles under the influence of other vehicles in their proximity. These models determine vehicle location, speed, and acceleration.

(3) Mesoscopic models represent the behaviour of vehicles without explicitly distinguishing their time-space behaviour, but instead taking into account the behaviour of groups of several vehicles.

Macroscopic dynamic modelling is based on the collective behaviour of vehicles; therefore, vehicles are not followed individually. The point of view is rather that of a continuum. The Euler and Navier-Stokes equation of fluid dynamics describing the flow of fluids may also describe the motion of cars along a road. The three main variables of traffic (flow, vehicle density, and average speed) are connected by two fluid laws proposed by Lighthill and Whitham (1955) and Richards (1956) (LWR). This model can be adapted to represent the diversity of urban traffic situations (e.g., Leclerq and Bécarie, 2012). This system must be supplemented by an independent third equation (fundamental diagram of traffic flow) which describes a relationship between traffic flow and traffic density. Two classes of macroscopic models can be identified. The first class uses the sole mass conservation equation supplemented by suitable closure relations that represent equilibrium states (first-order models). The second class uses a coupled system of mass conservation and momentum balance equations that represent equilibrium states or the behaviour of the flow acceleration (relaxation flow velocity) (second-order models). The main parameters for the implementation of macroscopic models include the fundamental diagram of traffic flow, OD-matrices, and the traffic control devices (e.g., traffic lights). The simulation outputs are traffic density in each cell as a function of time as well as the traffic flows simulated across the model cells.

Dynamic microscopic traffic models (e.g., VISSIM, Fellendorf and Vortisch, 2010) consider individual vehicle interactions with other vehicles and the road network. There are two main classes of microscopic models: (1) microscopic models with macroscopic law, which in fact correspond to a Lagrangian representation of macroscopic models, (2) microscopic models that are built up using submodels that control specific tasks in the simulation process. The car-following model is one of the most important submodels. A car-following model controls the driver's behaviour with respect to the interactions between two successive vehicles. These models can be completed by other submodels. In such models, typical submodels include the effect of overtaking as a function of vehicle categories and incoming traffic. For example, another submodel will allow one to simulate the response of vehicles to the control systems such as traffic lights, and an intersection submodel will manage the conflicts and the priorities at crossroad intersections and the arrival of new vehicles on the road network. These microscopic models calculate instantaneously the location, speed, and acceleration of the vehicles on the road network.

The mesoscopic models are intermediate between the macroscopic and the microscopic approaches. The objective is to describe the traffic given by aggregate laws. For example, vehicles may be grouped in packs, which then move on the road network (e.g., CONTRAM, Leonard et al., 1989). Table 3.1summarizes the classification of traffic models and provides an example for each category. An exhaustive list of available models cannot be provided here. Various traffic models, including their strengths and weaknesses, have been reviewed by Boxill and Yu (2000).

Table 3.1. Summary of traffic model categories.

| Models | | Solving method | Application domain | Results | Example |
|---|---|---|---|---|---|
| Static | | O/D matrix | Urban area | Average quantity of vehicles | VISUM<br>(Fellendorf et al., 2000) |
| Aggregated dynamic | | Relation<br>flow-density | Several neighbourhoods | Average speed, congestion | Daganzo, 2007 |
| Dynamic | Macroscopic | First order (LWR) | Neighbourhood | Density & speed of vehicles | METACOR<br>(Diakaki & Papageorgiou, 1996) |
| | | Second order (AZR) | Highway | | |
| | Mesoscopic | Aggregate flows<br>Traffic details | Neighbourhood | Vehicle trajectory | CONTRAM<br>(Leonard et al., 1989) |
| | Microscopic | Macroscopic Lagrangian | Urban network | Location, speed, acceleration per second | VISSIM<br>(Fellendorf et al., 2010) |
| | | Car following | | | |

**Uncertainties of traffic models**

The different types of errors that may cause incorrect estimations of traffic have been studied by Ortuzar and Willumsen (2011). These errors are summarized below

1) Measurement errors: Those are network measurement errors or errors due to information incorrectly registered by the interviewer.

2) Sampling errors: These errors depend on the number of observations. Optimal sampling strategies are defined by Daganzo (1980).

3) Computational errors: These errors are based on the iterative procedures of most models; they are typically small in comparison with other errors.

4) Specification errors: These errors are due to simplifications of processes in the models or the omission or misrepresentation of a phenomenon that is not well understood (e.g., using linear function to represent non-linear effects)

5) Transfer errors: They refer to cases when a model developed in one context (time and/or place) is applied in a different one.

6) Aggregation errors: They result from data aggregation that overlooks the individual behaviour.

A remaining question is whether complex models produce better results than simpler ones. Ortuzar and Wilumsen (2011) argued that if the complexity of a model with more variables reduces specification error ($e_s$), data measurement error ($e_m$) will probably increase with model complexity. As shown in Figure 3.1, the more realistic results that include a minimum of total modelling error ($E=\sqrt{(e_s^2+e_m^2)}$) are generally obtained for an optimal level of model complexity.

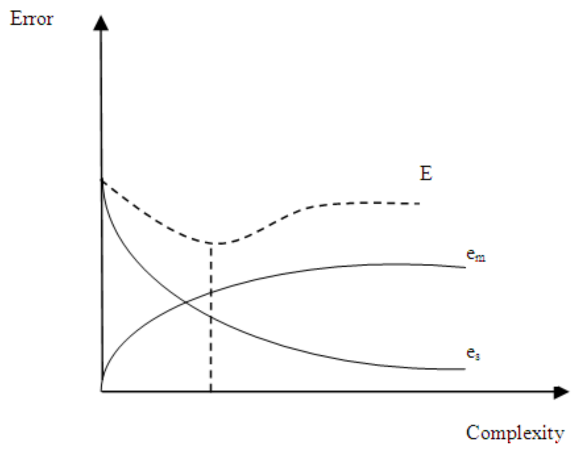


Figure 3.1. Variation of error with complexity, source: after Ortuzar and Wilumsen, 2011.

### 3.2.2 Emission models

There is a large variety of tools to calculate emissions and to develop on-road transportation emission inventories. Emissions from traffic are estimated by multiplying emission factors with appropriate activity data for different vehicle classes. The emission factors are measured in a laboratory using a chassis or engine dynamometer according to several specific driving cycles. A driving cycle is representative of driving behaviour for specific categories of vehicles, roads and speeds experienced.

Traffic emissions can be divided into four types: exhaust emissions, evaporative emissions, non-exhaust vehicle-wear emissions (mostly vehicle tyre and brake wear), and road wear and dust resuspension caused by vehicle traffic. Different categories of emission models are presented below. They can be classified according to the input data, the spatio-temporal scale of the study and the type of pollutants being considered.

1. Models based on fuel quantities

Models such as IPCC (Houghton et al., 1996) use fuel consumption as input data (i.e., fuel sale data) and the categories of vehicles. Such models can only be used for large-scale (e.g., national) emission inventories.

2. Models based on average traffic volumes per categories of vehicles

These models, such as NAEI (Choudrie et al., 2008) and IVE (Davis et al., 2005), use a single emission factor to represent a particular type of vehicle and driving cycle. The emission factors are calculated as mean values of measurements on a number of vehicles over given driving cycles and are usually stated in terms of the mass of pollutant emitted per vehicle distance or fuel consumption. The user only needs to provide the number of vehicles and the annual mileage per category. These models are mostly used in national and regional emission inventories.

3. Models based on average traffic speed

These models (e.g., COPERT; Ntziachristos et al., 2009, MOBILE, U.S. EPA; 1994) predict average emission factors for a vehicle class that is driven over a number of different driving patterns, which are a function of the mean travelling speed. The total emissions can be calculated as the sum of the exhaust emissions (hot and cold), evaporative emissions and for some models (e.g., COPERT) emissions due to vehicle tyre and brake wear as well as road wear resulting from the traffic. These models are based on time-averaged inputs (traffic mean speed) that may not be representative of actual traffic conditions because a given mean speed may correspond to different conditions. Nevertheless, they cover the major emission processes and most pollutants of interest and, accordingly, they are widely used in air quality modeling studies.

4. Models requiring detailed descriptions of traffic situations

These models (e.g., HBEFA, 2010) use distinct emission factors for predefined traffic situations (e.g. stop-and-go, saturated, heavy, free flow) and road configurations. Corresponding emission factors are available for pollutants emitted by the hot and cold exhaust emissions as well as by fuel evaporation. The methodologies were also developed for small scales such as for a single street (André et al., 2006). Traffic situation models require vehicle-kilometer-travelled (VKT) data per traffic-situation as input, which can be acquired from traffic models. It is important to note that there is no universal definition of traffic situation, which is to some extent a subjective concept. These models provide emissions for a large number of different regulated and non-regulated pollutants.

5. Models based on traffic-related variables

Emission factors obtained from traffic-variable models (e.g., Matzoros, 1990) are estimated from traffic flow variables such as average speed, traffic density, queue length and signal settings. In fact, they use a correction of the average speed to assume the effects of the traffic onto pollutant emissions, Previous work (Smit, 2006) suggests that this approach is approximate and that the consideration of the impact of the congestion on emissions is not entirely correct.

6. Models representing a detailed description of the speeds experienced

These emission models (e.g., VERSIT+, Smit et al., 2007) are based on tests conducted on a large number of vehicles according to various driving cycles to calculate exhaust emission inventories. Within the model, each driving cycle used is characterized by a large number of descriptive parameters (e.g., average speed, number of stops per km, kinematics of vehicles such as acceleration, cruising, etc.). For each pollutant and vehicle category, a regression model is fitted to the average emission values over the different driving cycles. These models require detailed information on the movement of the vehicles (instantaneous speed, acceleration), which can be obtained from microscopic traffic models or from traffic measurements.

7. Model based on chronological speeds (instantaneous models)

These models (e.g., PHEM, Zallinger et al., 2008; CMEM, Barth et al., 2000) represent explicitly the vehicle emission behaviour by relating emission rates to vehicle operation during a series of short time steps. In some models, vehicle operation is defined in terms of a relatively small number of modes (idle, acceleration, deceleration, and cruise). For each of the modes, the emission rate for a given vehicle category and pollutant is fixed and the total emission rate is calculated by weighting each emission rate by the time spent in each mode. Several instantaneous models relate vehicle engine power, speed and acceleration to each point of a driving cycle. These models estimate exhaust emissions only. This type of model can be coupled with a dynamic traffic model, which estimates the kinematics of vehicles (using typically 1 second time steps).

Models of categories 1 and 2 are not appropriate for considering traffic variation since they are based on average traffic volumes and do not account for vehicle speed. Models of categories 3 and 4 account for traffic condition (but only via average values) and cover the major emission processes and most pollutants from a single road up to a city. Models of category 5 require traffic flow variables for each road and category 6 is defined by individual vehicle movement data. However, both types of models use databases, which are limited to specific conditions and pollutants. Models of category 7 represent explicitly the vehicle emission behaviour by relating emission rates to vehicle operation (engine power, speed, and acceleration) during a series of short time steps. They require detailed information on vehicle movements, which can only be acquired from on-board measurements, or derived from microscopic traffic models. However, they use databases of emission factors, which are limited to specific emission processes and pollutants.

Table 3.2. Summary of emission model categories.

| Categories of Models | Application domain | Input | Example |
|---|---|---|---|
| Models based on fuel quantities | Country | Fuel consumption | IPCC<br>Houghton et al. 1996 |
| Models based on average traffic volumes per categories of vehicles | Country<br>Region | Number of vehicles<br>Average kilometer travel | NAEI<br>Choudrie et al., 2008 |
| Models based on average traffic speed | City<br>Neighbourhood | Average speed | COPERT<br>Ntziachristos et al., 2009 |
| Models requiring detailed descriptions of traffic situations | Neighbourhood | Average speed<br>Traffic condition | HBEFA, 2010 |
| Models based on traffic-related variables | Intersection area | Driving cycles | Matzoros, 1990 |
| Models based on a detailed description of the speeds experienced | | Driving cycles | VERSIT+<br>Smit et al., 2007 |
| Models based on chronological speed (instantaneous models) | | Driving cycles<br>Vehicle characteristics | PHEM<br>Zallinger et al., 2008 |

**Limitations and uncertainties of emission models**

The model output uncertainty depends on the uncertainties in the model internal parameters (emission factors) and input data. The most typical sources of uncertainty in emission models include: (1) ambient conditions, (2) parameters with temporal variation (e.g., temperature) , (3) vehicle fleet composition, (4) vehicle mileage, (5) traffic data, (6) estimation methods of emissions based on steady-state emissions that ignore transient vehicle operation (for some emission models), and (7) emission factors.

The uncertainty of the emission factors can be divided into random sampling error (statistical error), measurement errors (imperfections in sampling and analytical methods), different conditions between the case study and the source test (e.g., vehicle aging or modification of car equipment by users), averaging time for measured or reference data, omissions (missing data), surrogate data (estimated data when data are not available), and in the absence of relevant data or surrogate data, other approaches (e.g., conversion of a trace species in a fuel to an air pollutant, Frey, 2007).

Most European countries (22 out of 27) use the COPERT model for emission inventory estimation. Uncertainties associated with this model have been studied by Kouridis et al. (2010). They calculated the contribution of four sources of errors for two case studies (Italy and Poland) by considering fifty-one uncertainty inputs. The most important inputs were (1)

meteorological and temporal parameters (e.g., temperature, time series, vapour pressure), (2) the activity data (e.g. vehicle fleet composition and mileage), (3) traffic and model parameters (e.g., vehicle velocity, driving shares among cycles, load factor for heavy-duty vehicles, average trip length and fuel properties), and (4) cold-start emissions and emission factors, which were all identified as influential parameters. A limitation of this study is that the parameters have been considered separately. For example, the emission factors cannot be considered as true input data as they may change depending on other parameters.
The limited number of measurements made for various emission processes and pollutants are insufficient to provide all the necessary data needed for most advanced emission models, for example, instantaneous emission models are limited to a few pollutants from exhaust emissions. In addition, emission models are not able to consider completely the processes associated with mechanical abrasion and corrosion (tyre, brake, clutch, and road surface wear, corrosion of chassis and body work). Particles greater than 10 µm in diameter are not considered in those emission models because current air quality regulations apply only to particles with an aerodynamic diameter below 10 µm. However, tracking PM above 10 µm is essential when modelling water contamination.

### 3.2.3 Air quality models

Air quality models calculate pollutant concentrations and deposition fluxes at various locations and times using mathematical equations describing the atmospheric transport processes and chemical and physical transformation processes between the point(s) of emissions and the receptor location(s). The different approaches available differ in terms of inputs and levels of spatial and temporal resolution of the results.

1. Box models

Box models consider that the concentrations are homogeneous within the modelling domain (i.e., the box). Pollutants are emitted, undergo chemical and physical processes, and are advected in and out of the box. These models are not used operationally, but they are useful to investigate specific processes under simple configurations (e.g., single airshed, Pun and seigneur, 2001) under controlled conditions (e.g., smog chamber experiments, Goliff at al., 2013) or to obtain annual average deposition fluxes, which can be used to estimate water contamination due to air pollutants (e.g., Petrucci et al., 2014).

2. Near-source dispersion models

Near-source dispersion models use parameterizations to represent the transport and dispersion of pollutants from one or a selected number of sources. In the absence of obstacles to atmospheric transport and under stationary atmospheric conditions, the atmospheric dispersion process can be approximated by a Gaussian distribution of the time-averaged pollutant concentrations. Therefore, Gaussian dispersion models, which are based on the assumption that atmospheric dispersion leads to a Gaussian distribution of the concentrations of the emitted pollutant in the vertical and horizontal directions are widely used (Csanady, 1973). In the case of steady-state atmospheric conditions, the impact of a source is represented by a Gaussian plume model. In the case where atmospheric conditions are variable, one may represent the atmospheric dispersion process by releasing distinct puffs from the source at successive intervals of time; Gaussian puff models present the advantage over Gaussian plume models that they are not limited to steady-state conditions (e.g., constant wind speed and direction); however, the computational requirements are greater for puff models than for plume models. Gaussian plume models are not designed to model atmospheric dispersion under low wind-speed conditions and the wind is assumed to be constant in time and space. Hybrid models, which use a combination of the Gaussian plume and puff models, can provide better estimates of concentrations under low wind-speed conditions (Sharan et al., 1996; Thomson and Manning, 2001). Gaussian plume models treat deposition processes and can treat simple chemical reaction systems (i.e., first-order kinetics and steady-state systems). Gaussian puff models can treat complex chemically reacting systems (Karamchandani et al., 2000). Algorithms have been developed for some Gaussian models to treat atmospheric dispersion around buildings; the effect of wakes from buildings can be achieved by modifying the dispersion coefficients. However, the Gaussian equation is not able to calculate recirculation effects caused by multiple buildings or atmospheric flow at street intersections (Holmes and Morawska, 2006) and other formulations must then be used (e.g., Soulhac et al., 2011). Gaussian plume models may be used to estimate concentrations up to 50 km from the source and are typically applied with averaging times of one hour (or less) so that the assumptions of constant and uniform meteorology hold. Gaussian puff models have been used for long-range impacts, when coupled with an appropriate meteorological model; they are however limited to the impacts of a few specific sources.

For situations where the atmospheric dispersion of pollutants is constrained by obstacles such as buildings, noise-barriers or vegetation, other parameterizations must be used. For street-canyon situations, parameterizations based on the assumption of a well-mixed zone within the canyon can be used. One widely-used approach is the Operational Street Pollution Model (OSPM) (Hertel et Berkowicz, 1989 a, b, c).
Another method proposed for road pollution is SIRANE (Soulhac et al., 2011, 2012), which simulates each street with a box model and calculates the corresponding advective fluxes balance at intersections. This model accounts for three important transport mechanisms within the urban canopy to better estimate the effect of the complex street configuration in urban area: 1) advective mass transfer along the street due to the mean wind along their axis, 2) turbulent mass transfer across the interface between the street and the overlying atmospheric boundary layer, and 3) advective transport at street intersections (this last term is not treated by OSPM). The simulation at street level is completed by a standard Gaussian plume model for atmospheric transport and dispersion above roof level.

### 3. Lagrangian trajectory models

Lagrangian trajectory models (which include Gaussian dispersion models) consist in following the trajectory of an air mass along the mean wind flow. In addition to Gaussian models, we can mention the numerical particle models and the grid-based Lagrangian models (e.g., AUSTAL2000, Graff, 2002; Hysplit, Draxler and Hess, 1998; FLEXPART, Stohl et al., 1998). In a particle-trajectory model, the model particles are advected and dispersed as the air mass moves along the trajectory by advection and pollutants are dispersed by turbulent diffusion. Thus, particle models work well for both stationary conditions over flat terrain and variable conditions over complex terrain (e.g., Holmes and Morawska, 2006). Grid-based trajectory models consist of a column (1D) or a wall (2D) of cells that is advected by the mean wind; turbulent dispersion spreads the air pollutants among those cells as the air mass moves downwind from the source along the trajectory (e.g., Seigneur et al., 1997). Because of the gridded nature of the model, it is possible to model non-linear chemistry, as discussed below for Eulerian models. However, complex meteorological conditions such as wind shear, land-sea breezes and mountain-valley winds are poorly represented by grid-based Lagrangian models.

4. Eulerian models

An Eulerian model considers an element of volume of homogeneous properties (air pollutant concentrations, meteorological variables) and studies the flow of those variables through a 3-D gridded mesh of such volumes, i.e., grid cells. The atmosphere is discretized into cells and the equations of mass conservation are solved iteratively for each grid cell. Such models take as input the meteorological variables that have been calculated previously using a meteorological model; they are typically referred to as chemical-transport models (CTM) (e.g., Polair3D, Sartelet et al., 2007; CHIMERE, Bessagnet et al., 2009; CMAQ, Byun and Ching, 1999; CAMx, ENVIRON., 2011. Alternatively, the Reynolds-Averaged Navier-Stokes (RANS) equations of the meteorology may be solved jointly with the chemical-transport equations; such a modelling approach is referred to as integrated on-line meteorology air quality modelling (WRF-Chem, Grell et al., 2005; Zhang, 2008; Zhang et al., 2012; Baklanov et al., 2014). The on-line approach is well suited to the study of feedbacks between air quality and meteorology (e.g., the effect of PM on clouds) and air quality forecasting. Eulerian models can handle a large number of sources, complex chemistry and, given the appropriate meteorological fields, complex atmospheric transport phenomena. They are used to simulate air quality from the urban scale to regional, continental, hemispheric and global scales. One class of Eulerian models combines the advantages of Eulerian models (large domain and multiple sources) and Lagrangian models (fine resolution near sources); these models, which are referred to as plume-in-grid models (PinG), simulate selected sources using a Lagrangian model (such as a puff model) imbedded within the 3D Eulerian model, which simulates the fate and transport of all other emissions (Karamchandani et al., 2011; Briant and Seigneur, 2013; Kim et al., 2014).

5. CFD models

The most common CFD (Computational Fluid Dynamics) techniques are direct numerical simulation (DNS), large-eddy simulation (LES), and Reynolds-averaged Navier-Stokes (RANS) equations with turbulence closure models. Each technique handles turbulence in a different manner. DNS solves the Navier-Stokes equation without approximations. It requires a very fine grid resolution to catch the smallest eddies in the flow. This makes the calculations extremely time consuming. DNS for either indoor or outdoor environment simulations is not realistic in the near future. LES separates turbulent motions into large and small eddies. The small eddies are modeled independently from the flow geometry with parameterizations and large eddies are simulated explicitly for time-dependent flow. LES is a more practical technique than DNS; nevertheless, it is still time consuming and its application has been mostly limited to meteorology with no operational applications to air pollution yet to date. RANS is the fastest approach since the computational burden is significantly less than those of LES and DNS. It solves the time-averaged Navier-Stokes equations by using approximations to simplify the calculation of turbulent flow. RANS is useful for applications in air quality (e.g., Code_Saturne, Milliez and Carissimo, 2007; MISKAM, Eichhorn and Kniffka, 2010), which are limited to local applications, such as the impact of a single pollution source in complex terrain or in a built environment, where the flow characteristics are complex (e.g., Milliez and Carissimo, 2007; Yuan et al., 2014). Chemical transformations have recently been incorporated into RANS models. A comparison of two different modeling approaches (RANS and LES) has been presented by Gousseau et al., (2011) for an actual urban area.

Table 3.3. Summary of air quality model categories

| Models | Application domain | Solution method | Examples |
|---|---|---|---|
| Chemical Transport Models (CTM) | Urban to global (from 1 km to several 100 km resolution) | Some Lagrangian models | Flexpart, Hysplit AUSTAL2000 |
| | | Eulerian models | Polair3D, CMAQ, WRF-Chem, CAMx CHIMERE |
| | | Plume-in-Grid models | PinG , CMAQ-Urban |
| Near source dispersion models | Local impact (up to 1 km) | Gaussian models & some Lagrangian | Polyphemus, ADMS, SIRANE, AERMOD |
| | | Street-canyon models | SIRANE, OSPM |
| Computational Fluid Dynamics models (CFD) | Complex environment Local scale (up to 10 km) | RANS | Code_Saturne, MISKAM |
| | Research (turbulence) | LES | FAST3D-CT (Patnaik and Boris, 2010) |

### Limitation and uncertainties of air quality models

The limitations of most models are as follows: (1) dispersion in urban areas is complicated by the aerodynamic effects of street/building geometry and traffic-induced turbulence., (2) air quality impacts of traffic include a local component as well as an urban background component, which differ in terms of pollutants, temporal and spatial scales, (3) the estimation of wet and dry atmospheric deposition fluxes strongly depends on the particle size distribution; wet scavenging and dry deposition velocities still remain difficult to estimate as a function of particle size, atmospheric conditions and, for dry deposition, surface configuration and types (e.g., Sportisse, 2007, Duhanian and Roustan, 2011).

The major source of uncertainties is typically due to model inputs (e.g., emissions, meteorology and boundary conditions). The sensitivity and uncertainty analysis of model applications have been reviewed by Russel and Dennis (2000). Some studies found that the uncertainty of all input data can reach 50%, but can be greater for emission data (Hanna et al., 1998, Hanna et al., 2001). The second source of uncertainties is the mathematical representation of the physico-chemical processes simulated by the model; for example, chemical mechanisms include many simplifying assumptions and atmospheric turbulences is highly parameterized. Another significant source of uncertainty lies in the necessary numerical approximations including numerical schemes, time steps, and the horizontal and vertical resolutions.

### 3.2.4 Stormwater models

Several hydrological models are commonly used to model pollutant transport in waters. First of all, the models must simulate the water flow (quantity) in order to model water quality (i.e., pollutant concentrations and loads). These models may be classified in terms of their functionality, accessibility, water quantity and quality components included in the model, and their temporal and spatial scales. State-of-the-art reviews of stormwater models, including discussions of their capability, strengths and weaknesses have been conducted by Elliott et al., (2007), Zoppou (2001), Cheah (2009), and Jacobson (2011). Hydrological models may be classified according to their spatial distribution:

1. Lumped models (e.g., SLAMM, Pitt and Voorhees, 2002): A lumped model is based on spatial averaging of the input parameters over the catchment. Therefore, these models provide outputs only at the outlet of the catchment without an explicit consideration of spatial variability.
2. Semi-distributed models (e.g., SWMM, Rossman, 2010): Semi-distributed models take into account the variability inside the catchment by dividing a catchment into several subcatchments. Therefore, spatial resolution is related to the size and number of subcatchments.
3. Hydrological Response Unit models (e.g., URBS, Rodriguez et al., 2008): An HRU represents an area of similar runoff generation. The hydrological processes, which can be determined by different factors depending on the catchment and scale, should be similar in one HRU and must characterize the greatest variation in the dominant hydrologic process.
4. Fully-distributed models (e.g., MIKE-SHE, Refshaard et al, 1995; El-Tabach, 2010): They represent surface flow by using physical laws on a grid mesh. They often include spatial and temporal variability (such as soil properties, land use, etc.) depending on the grid size.

These models were listed above from the lowest to the highest spatial resolution. A lumped model often needs to be calibrated. On the contrary, a fully-distributed model is supposed to be based on more physical concepts and may not need to be calibrated. These different models have different aims in terms of temporal and spatial scales and model outputs. Fully-distributed models are mostly used to model individual storm events at the intra-event scale, whereas lumped models are used to simulate water and/or pollutant fluxes over long periods (annual scale). Many of these water quality models have been reviewed by Obropta and Kardos (2007), Vassilios et al. (1997), Elliot and Trowsdale (2007), and Cheah (2009).

Depending on the model type, processes related to pollutant behaviour may be described by deterministic or stochastic laws. Deterministic, stochastic, and hybrid (combination of deterministic and stochastic approaches) stormwater quality models have been presented by Obropta and Kardos (2007). In deterministic models, the transport and transformation of pollutants are mostly modeled by using an advection-diffusion equation and/or the conservation of mass coupled to different reaction rates involving the pollutants in different forms (particles, colloids, dissolved matter). In urban areas, these models couple hydrologic (for surface water) and hydraulic (for water flow through channels) modules. Surface flow is modeled with the shallow water wave equation or its simplified version (kinematic, diffusion wave equation). In lumped models, water contaminants are simply transferred from one compartment to another depending on rainfall intensity and flow rates among the modeled compartments. Another classification of models distinguishes conceptual and empirical models (Zoppou, 2001).

There is added complexity when modelling water quality in addition to water quantity because pollutant forms are highly diverse and variable: some pollutants may be transferred from the dissolved phase to suspended solids during their transport (thereby having a different dynamics of transport) and/or they may be degraded during their transport. Moreover, the phenomena involved in their build-up on urban surfaces and their wash-off are still poorly understood. Therefore, several processes in water quality models must often be simplified using empirical parameterizations. For example, four types of build-up models are generally used: linear, power, exponential, and Michaelis-Menten. Wash-off is usually modeled as a first-order decay function of runoff or with simpler methods such as a constant concentration and rating curves (graph of discharge versus stage for a given point on a stream). The prediction of pollutant transport and transformation in water is very complex and its simulation by current models includes large uncertainties (Kanso et al., 2004).
Atmospheric pollutants are introduced into the stormwater runoff by two processes: dry deposition under the effect of turbulence and, for particles only, gravity, and wet deposition via the scavenging of particles and gaseous pollutants by water droplets. These processes can be modelled by several parameterizations (Sportisse, 2007, Duhanian and Roustan, 2011). Other processes such as road surface abrasion and tyre wear also bring pollutants onto the road surface (Boulter, 2007).
Although these atmospheric processes are well-known, their impact on water quality is rarely treated in current water quality models.

Table 3.4. Summary of urban water quality model categories

| Models | Scales | example |
|---|---|---|
| Lumped | Spatial average of the input for catchment | SLAMM<br>Pitt and Voorhees, 2002 |
| Semi-distributed | Spatial average for each sub-catchment | SWMM<br>Rossman, 2010 |
| Hydrological Response Units | Spatial average at HRU scale ( be create by combined different factors) | URBs<br>Rodriguez et al. 2008 |
| Fully-distributed | Explicity spatial variability (mesh) | MIKE-SHE<br>Refshaard et al. 1995 |

Water pollutants associated with on-road traffic include mainly polycyclic aromatic hydrocarbons (PAHs) and heavy metals such as Pb, Zn, Cd, Sb, Pt and Cu. Some of these pollutants may exist in a dissolved form. They may be complexed with organic matter or attached to suspended solids (SS), which can then be considered as pollution vectors.

**Limitations and uncertainties of stormwater models**

It is challenging to implement all these processes in a model and simplifications are needed, which may induce errors. The uncertainty of water quality model outputs is typically greater than that of water quantity because of the additional treatment of pollutants in an urban catchment. Moreover, there is a lack of knowledge on most pollutant emissions relevant to water quality impacts of traffic, which include a component caused by direct deposition on the roadway (road abrasion and tyre wear) and a component resulting from atmospheric processes, followed by water runoff. These processes are particularly difficult to model in water quality models.

Three major uncertainty sources are model parameter values, model formulation, and data (which are used for input, calibration and validation). The uncertainty of a flow measurement in a pipe is estimated to be about 20% and that of a suspended solid concentration is around 30 to 40%. Several studies have discussed the issue of uncertainties in urban hydrology, (e.g., Lindblom et al., 2007; Willems, 2008; Kanso et al., 2003; Dotto et al., 2010). The discussion of uncertainty and validation with special reference to the development and use of models was reviewed by Beck et al. (1987) and Mannina et al., (2006). Other studies (Kanso et al., 2004; Freni et al., 2011) investigated parameter uncertainties in urban runoff quality models. Uncertainty of the model inputs and calibration data have been presented by Freni et al. (2009), Park et al. (2012), and Sun et al. (2013). Finally, different uncertainty techniques in urban stormwater modelling have been compared by Dotto et al. (2012).

## 3.3 Modelling chain

The main building blocks of such a simulation framework are (1) the structure of the modelling chain which contains traffic, emission, air quality and water quality models (Figure 2) and (2) the interfaces between the output from a model and the input to the next model. Examples of modelling systems to link traffic flow, emission and air quality modelling tools have been described by Lim et al. (2005), Schmidt and Schäfer (1998) and Hatzopoulou (2010). Modelling the effects of atmospheric pollutant dispersion on water quality has been studied mostly at regional scales to address the impact of air pollutants on ecosystems (e.g., Burian et al., 2002, Vijayaraghavan et al., 2010, Gunawardena, 2012). However, there have been few studies of atmospheric deposition on urban watersheds (e.g., Sabin et al., 2005; Fallah Shorshani et al., 2014). We focus below on the interfaces between the various models.

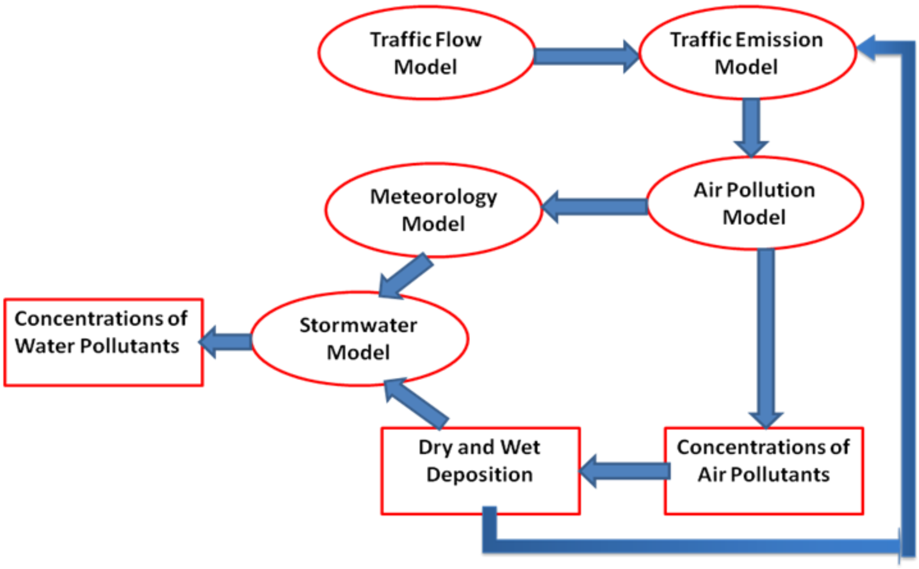


Figure 3.2. Schematic representation of the modelling chain (components are represented with ellipses) with expected input and output data (represented with boxes).

### 3.3.1 Coupling of traffic and emissions models

The factors relevant to the estimation of vehicle emissions are the vehicle operation (e.g. speed, acceleration, and engine load), the traffic flow conditions and the road and vehicle characteristics. These parameters can be determined by traffic models, so an appropriate coupling is examined here to link the input requirements of emission models with the outputs of traffic models. A traffic model must be chosen according to its capacity to produce the inputs of the emission model: road type and gradient, vehicle category, kinematic parameters (speed, acceleration, idling). Vehicle category information required by emission models is based in Europe on the Euro standard (Kousoulidou et al., 2008) and the capacity of the engine. The traffic models do not provide these data because they only require vehicle types (passenger cars, heavy-duty vehicles, motorcycles, etc.). Therefore, the fractions of different vehicles must be defined by a vehicle fleet composition estimated separately from the traffic model. The variety of traffic/emission models can be presented according to four major types:

- **Macroscopic (static traffic models and aggregated emission models)**

Macroscopic emission models (models based on average vehicle speeds) are combined with a static traffic model or an aggregated dynamic traffic model. Vehicle fleet composition must be provided. Macroscopic traffic flow and emission models are used for large road networks. Static models simply calculate the traffic volume that provides the number of vehicles and average speed on each link needed by average-speed emission models. Such coupling can induce a high level of uncertainty due to several parameters: (1) the OD matrix, which is a central element of the traffic, (2) the parameters and mathematical formulation of the traffic model such as speed-flow curves (which determine the free-flow and congested branches), and (3) the vehicle fleet composition, which has a significant impact on pollutant emissions. In general, both static traffic and average speed emission models use aggregate methods that include significant uncertainty due to the averaging process.

Situation-traffic emission models, such as HBEFA and MOBILE, can also be coupled with aggregated dynamic models of traffic, which can provide the average speed and degree of congestion. It is possible to use average-speed emission models with aggregated dynamic models but one needs to provide a sub-model that defines the level of congestion based on vehicle speed and speed limit. There has been a large number of studies that have integrated macroscopic traffic flow and exhaust emissions (Schmidt and Schafer, 1998; TEMMS project, Namdeo et al., 2002; TEIS, Xia and Shao, 2005). These couplings provide long-run estimates of vehicle emissions for large-scale applications, which would be challenging to calculate with more detailed models.

- **Mesoscopic (macroscopic traffic model and microscopic emission model)**

Emissions can be modeled more accurately with both vehicle speed and acceleration as inputs. Macroscopic traffic models do not provide the acceleration, unlike microscopic models. However, microscopic traffic models need large inputs and computational times when applied to a large road network. We are interested in finding a way to integrate macroscopic traffic models with instantaneous emission models so that the macroscopic variables can be used to produce estimates of the instantaneous emissions on large scales. Cappiello et al. (2002) proposed a combination of a probabilistic acceleration approach and a dynamic emission model (EMIT). The proposed model uses random variables distributed according to some known distribution, for a given speed range and other parameters. In spite of the use of an instantaneous emission model, the emissions calculated with this approach cannot represent accurately second-by-second emissions. The combined model must be used for cases where vehicles have homogenous characteristics within a given speed range.

Another study by Zegeye et al., (2010) proposed integrating the macroscopic traffic flow model METANET and the microscopic emission model VT-micro. METANET is a macroscopic traffic model that describes the average behaviour of vehicles into a number of segments by a system of discrete-time dynamic equations (average traffic density, flow and speed for each segment). VT-micro is a microscopic dynamic emission model that yields emissions of individual vehicles using second-by-second speed and acceleration. Since

METANET is discrete in both space and time, there are two possible accelerations: “temporal” (acceleration of the vehicle flow within a given segment) and “spatial” (acceleration of the vehicles flowing from one segment to another in one simulation time step). The temporal and spatial accelerations of vehicles in a segment are obtained from speed variation. The number of vehicles corresponding to each acceleration can be obtained according to density, flow, length of the segment, and time step. These spatial and temporal speed-acceleration pairs determine the spatial and temporal emissions using VT-micro. The combination of emissions and number of vehicles gives the total traffic emissions.
Information on vehicle category, which is needed by emission models, is not available in macroscopic traffic models. Therefore, the applicability of this approach is limited to cases where vehicles have homogenous characteristics within a given speed range.
These approaches may include important uncertainties associated with the coupling of the traffic and pollutant emission models.

- **Mesoscopic (microscopic traffic model and macroscopic emission model)**

The parameters of macroscopic emissions (average speed and traffic situation) can be precisely estimated by microscopic traffic models but may require large computation times for a large-scale network. To get a balanced trade-off between computational burden and accuracy, one may want to combine a microscopic traffic model with a macroscopic emission model. The main advantage of this coupling is the ability to simulate a large number of pollutants, because macroscopic emission models have a more complete pollutant database compared to instantaneous models. A study by Chanut and Chevallier (2012) compared different macroscopic and microscopic emission models (IMPACT, ARTEMIS, INST (EMIT)) coupled with a microscopic traffic model (AIMSUN). The three models provide very similar temporal evolution of $CO_2$ emissions in free-flow traffic. However, in congestion, the emissions of the instantaneous model (INST) are 2.5 times greater than those of the model based on average-speed (IMPACT) and 1.5 times greater than those of the model based on traffic-situation (ARTEMIS). Accordingly, the emission-averaged model cannot estimate correctly the emissions of $CO_2$ in stop & go situations.

- **Microscopic (microscopic traffic flow simulation and instantaneous emission model)**

Emission rates for vehicle operation during a series of short time steps can be predicted by coupling a microscopic traffic model with an instantaneous emission model. The main advantages are the prediction of individual vehicle emission rates as a function of time and the use of driver behaviour. Therefore, this coupling allows one to model traffic emissions at a great level of spatial and temporal detail. The drawback of this type of coupling is that detailed input data for instantaneous emission models are not usually provided by microscopic traffic models (vehicle category) and must be specified by the user. We present below several studies in which a microscopic traffic model has been combined with an instantaneous emission model.

One example is the coupling of VISSIM with PHEM. The instantaneous emission model (PHEM) calculates the emission of road vehicles with 1 s time steps for a given driving cycle

based on emission maps, that is emission level as a function of engine speed and engine power (Zallinger et al, 2008). The traffic flow model in VISSIM is a discrete, stochastic, time-step based microscopic model, with a psycho-physical car-following model. PHEM takes as input time, speed and vehicle characteristics of every single vehicle with other information defining vehicle location from VISSIM and calculates the emissions of each vehicle. The vehicle and engine data required by PHEM are taken from the data base developed from average vehicle data. The classification into Euro classes is chosen automatically in PHEM according to the fleet composition defined by the user. Hirschmann et al, (2010) have proposed to calibrate the traffic data calculated by VISSIM. For example, the maximum acceleration rates have been calibrated to perform the simulation. They assumed that the majority of the calibration effort carried out within their research project can be used also in other urban applications. The time resolution in the VISSIM simulation should be at least 0.3 s to achieve realistic speed profiles (Fellendorf and Vortisch, 2011).
The integrated VISSIM-CMEM traffic emission coupling was developed by Nam et al (2003), Chevallier (2005), Noland and Quddus (2006), Chen and Yu (2007), Stevanovic et al. (2009). The output of VISSIM is converted into the required input file for the CMEM and US vehicle emission standards are converted into European Union standards. VISSIM is currently the most widely used package. Beside this model, PARAMICS (Quadstone, 2002), AIMSUN (Bacelo and Casas, 2005) and DRACULA (Liu, 2005) have been used. Recently, a new microscopic model, Symuvia (Leclercq et al., 2007), has been developed to provide location, speed, and acceleration of each vehicle on a network at any simulation time. This model takes into account initial acceleration, line changing, and vehicle interaction and changes inputs over time. Other similar model coupling studies have been done by Park et al. (2001) with VISSIM and MODEM, Barth et al. (2001) and Boriboonsomsin and Barth (2008) with PARAMICS and CMEM, Tate et al. (2005) with DRACULA and CMEM, and Panis et al. (2006), with DRACULA and emission functions for each vehicle as a function of instantaneous speed and acceleration, Lin et al. (2011) with Dynust and MOVES, Madireddy et al. (2011) with PARAMICS and VERSIT+, and Xie et al. (2012) with PARAMICS and MOVES.

#### *3.3.1.1 Case study coupling traffic and emissions*

A coupling between microscopic traffic models and both macroscopic and microscopic emission models was conducted. The results of the two couplings are compared to understand the difference between each coupling. In the first coupling, the dynamic microscopic traffic model, Symuvia, is coupled with an instantaneous emission model, PHEM. PHEM calculates the emission rates of individual vehicles by taking into account the vehicle kinematic parameters with time resolution of 1 s. The second coupling is between the same microscopic traffic model and a macroscopic emission model, CopCETE (CETE Normandie, 2010). In this case, the average speed and number of vehicles on each road segment are obtained from the traffic model. CopCETE is based on the COPERT4 methodology (Ntziachristos et al., 2009) with the same methods and equations but with a mesoscopic approach that considers each road category separately. The simulations were performed for an urban boulevard, Cours Lafayette, and its associated street network in Lyon, France. The network is divided into 84 segments with a total distance of 2.87 km. These different segments include the street intersections and the distinct lanes for passenger cars and buses (Figure 3.3).

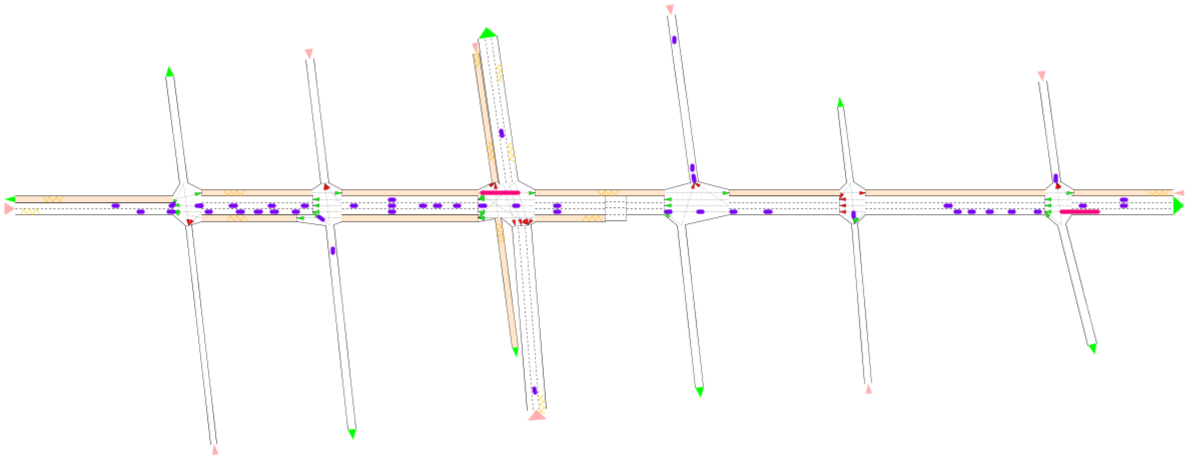

Figure 3.3. Schematic representation of Cours Lafayette; orange lines are bus lanes. The dark blue dots represent individual vehicles, the elongated red dots represent buses.

There are six common pollutants in the two emissions models, which are $NO_x$, $PM_{10}$, CO, $CO_2$, $SO_2$, and benzene. The exhaust emissions calculated with both model couplings for a 15 min simulation are illustrated in Figure 3.4. For all pollutants except benzene, emissions are greater with the instantaneous emission models i.e., Symuvia-PHEM. The results are in agreement with the study of Chanut and Chevallier (2012) who compared emissions of $NO_x$, $PM_{10}$, CO, $CO_2$, and hydrocarbons (HC) calculated with three emission models, an average-speed model (IMPACT), a traffic-situation model (ARTEMIS), and an instantaneous model (INST). Emissions of $NO_x$, $PM_{10}$, CO, and $CO_2$ were greater with the coupling of the traffic microscopic model (AIMSUN) and the instantaneous emission model (INSTA), but this was not the case for HC. The reason for theses results is that the driving cycle of the average-speed emission model does not represent the actual movement of vehicles, which includes a stop & go behaviour over short distances between intersections. The example of Chanut and Chevallier (2012) (Figure 3.5) shows for a situation of stop & go that the emissions of $CO_2$ for diesel passenger cars calculated with the average-speed model are 3 times smaller than those of the instantaneous emission model.

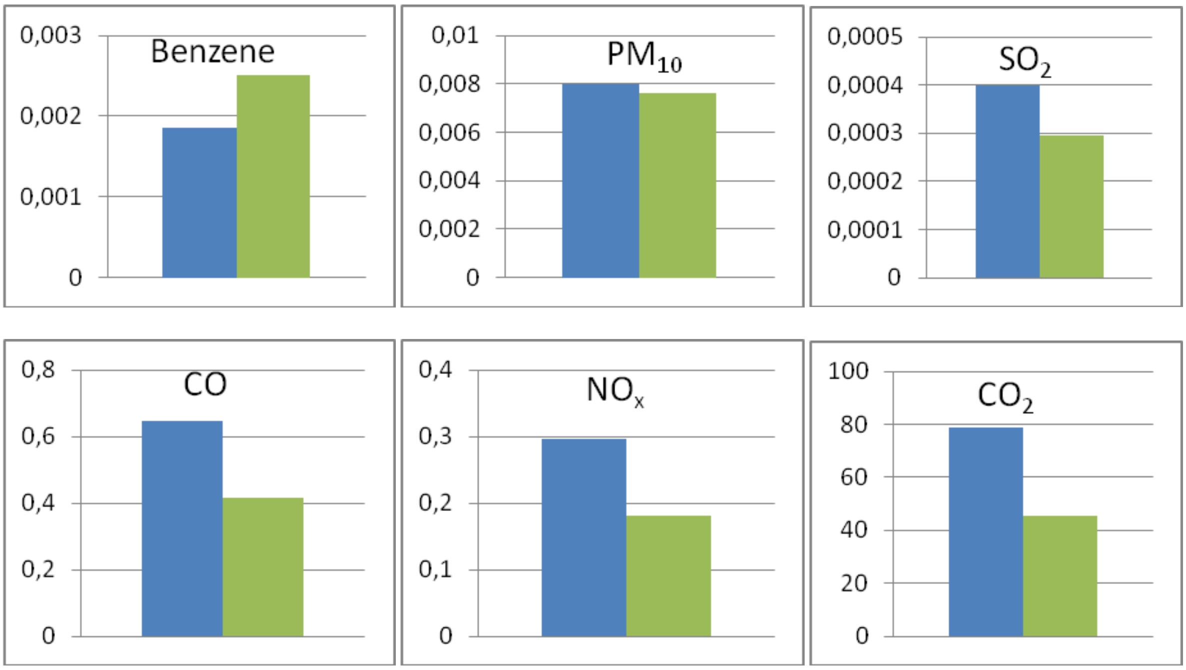


Figure 3.4. Emissions of pollutants (kg/15 min) with a Symuvia simulation for the Cours Lafayette network and the PHEM (blue) and CopCETE (green) emission models.

In our case study, the ratio of the macroscopic and microscopic models are 134%, 96%, 74%, 65%, 61%, 58% for benzene, $PM_{10}$, $SO_2$, CO, $NO_x$, and $CO_2$, respectively. The fuel consumption ratio is 59%. The emission of benzene depends on cold-start emissions and increases during the warm-up phase (Boulter and Latham, 2009). It is difficult to estimate cold-start emissions for short-time simulations that depend strongly on ambient temperature and the engine conditions. Furthermore, the approaches for estimating cold-start emissions in CopCETE and PHEM are very different. PHEM is based on a heat balance in the engine and the exhaust system; whereas CopCETE uses a method, which is a function of the aggregated value (e.g., average national value of trip length). It should be noted that we tried to match the fleet composition in both models but different definitions of vehicle categories did not allow us to obtain exactly the same fleet compositions.

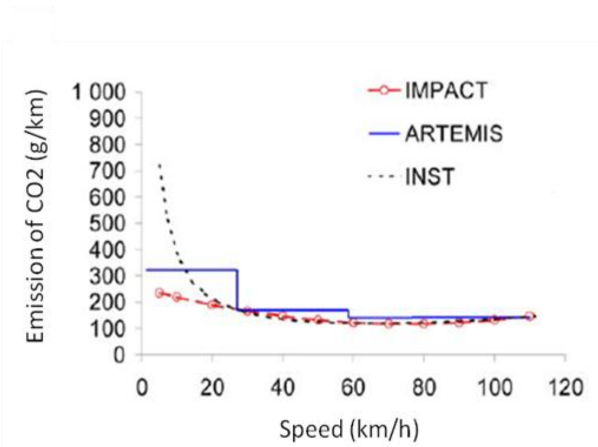


Figure 3.5. Comparison of $CO_2$ emissions calculated with an average speed model (IMPACT), a traffic-situation model (ARTEMIS) and an instantaneous model (INST) for diesel passenger cars (Source: Chanut and Chevallier, 2012).

The ratio of the emissions calculated with the average-speed model and the instantaneous model for street segments and intersections provides information on the impact of acceleration and deceleration on pollutant emissions. These results (Table 3.5) show that the emission ratio is smaller for intersections than for street segments, which suggests that acceleration in intersections can increase emissions twice as much as in street segments.

Table 3.5. Ratio of pollutant emissions calculated with the CopCETE and PHEM models using a 15-min Symuvia simulation of Cours Lafayette, Lyon, France.

| Emission ratio CopCETE/PHEM | Benzene | $PM_{10}$ | $SO_2$ | CO | $NO_x$ | $CO_2$ |
|---|---|---|---|---|---|---|
| Street segment | 1.5 | 1.05 | 0.82 | 0.72 | 0.66 | 0.64 |
| Intersection | 0.65 | 0.54 | 0.39 | 0.32 | 0.37 | 0.3 |

### 3.3.2 Coupling of emission models and atmospheric models

Understanding vehicle traffic flow and induced emissions alone is not sufficient to predict air pollution in an urban area; hence, an atmospheric dispersion model is needed to predict the temporal and spatial variation of air pollutant concentrations. The major input data necessary for the air quality model are spatially-distributed and temporally-resolved emissions provided by the emission model, meteorological inputs and background concentrations of air pollutants. It is also useful to have input data from a traffic model for dispersion models that account for vehicle-induced turbulence (VIT). The emissions inventory must be compatible with the dispersion model to facilitate data transfer between the two (Lim et al., 2005).

Atmospheric dispersion in urban areas is complex because of street and building geometry effects. CFD modeling techniques provide a detailed representation of the air flow and turbulence, including vehicle-induced turbulence, which is particularly useful in areas with complex geometries such as street canyons and areas with noise barriers. However, the large computational requirements limit their applications to small areas for limited periods. Wang and Zhang, (2009) demonstrated that the results of Gaussian models for atmospheric dispersion of traffic emissions near a road can be better than those of a CFD model without considering VIT and RIT (road-induced turbulence). However, a CFD model with VIT and RIT can be a valuable tool thanks to the rigorous representation of the turbulent mixing mechanisms. The output frequency of instantaneous emission models, which can be on the order of 1 s, can only be taken into account by CFD model. It is, however, possible to average the emission rates over time if one is only interested in concentrations averaged over time. For example, Misra et al. (2013) used hourly average results of microscopic traffic and emission models with a Gaussian model.

The Gaussian models are suitable for local-scale applications and their computational efficiency makes them attractive for applications to large road networks over long time periods. Typically, the input and output frequencies of Gaussian models are 1 h with a receptor resolution or grid size ranging from a few meters to several hundred meters.

Sahlodin et al. (2007) developed a mathematical model that incorporated VIT into a Gaussian dispersion model. Also, the effect of air flow around buildings can be approximated by modifying the dispersion coefficient in the Gaussian equation (Huber, 1991). In the most commonly used models (Gaussian and CFD models), roads are divided into segments which are considered as line (or elongated surface) sources and emissions from vehicles are estimated individually for each road segment. A comparison of air pollutant concentrations obtained from Gaussian and urban CFD models has been conducted by Pullen et al. (2005). Their study shows that the results of the Gaussian puff model are satisfactory in the far field.
Lagrangian and Eulerian models allow one to compute the transport and dispersion of pollutants at a large spatial scale. In the case of Eulerian air quality models, the emissions must be defined for the 3D grid-mesh and for each pollutant. They have been widely applied to simulate air pollution from all sources including roadways. However, they are not able to provide fine spatial resolution near sources. Thus, it is useful to combine regional-scale models such as Eulerian models and local-scale models such as Gaussian models. For example, Beevers et al. (2012) added the urban background concentrations calculated by an Eulerian model CMAQ to roadside concentrations obtained from the ADMS Gaussian model. Karamchandani et al. (2009) and Briant and Seigneur (2013) used a Gaussian puff or plume model, respectively embedded within the Eulerian model Polair3D. This coupling includes the transfer of pollutants between the Gaussian model and the Eulerian model at each time step thereby providing a more accurate representation of air pollutant transport and transformation and leading to better model performance.

One issue with the coupling of an emission model with an air quality model is the time scales involved, because the results of most emission models are not currently valid for short time scales. The output frequency of macroscopic emission models can be adapted to the input requirements of most air quality models, which are on the order of 1 h. To make full use of the advantages of microscopic emission models for simulation with time steps less than 1 h, e.g., on the order of 1 min, one should use CFD models or Gaussian puff models.

#### *3.3.2.1 Case study coupling emission and atmospheric models*

This case study corresponds to the atmospheric dispersion and deposition of pollutants emitted from traffic on a freeway in eastern France. Measurements of cadmium (Cd) particulate deposition were conducted by Promeyrat (2001). The measurements were performed at 5, 20, 40, 80, 160, and 320 meters on both side of the freeway in 1997. The A31 freeway segment is located between Metz and Maizières-lès-Metz. Due to difficult access, the measurement sites on each side of the road are distant by about a kilometer but correspond to the same road segment. The traffic data and meteorological conditions were recorded daily.

In this study, we focus on Cd deposition near the freeway in February 1997. The exhaust and non-exhaust emissions were calculated with the average-speed emission model CopCETE. This emission model seemed appropriate because traffic flow on the freeway was at nearly constant speed without congestion and was measured daily. Figure 6 shows the Cd daily emissions during February. The minimum values of emissions in the time series represent the light traffic on sundays and the maximum emissions are due to heavy traffic on fridays.

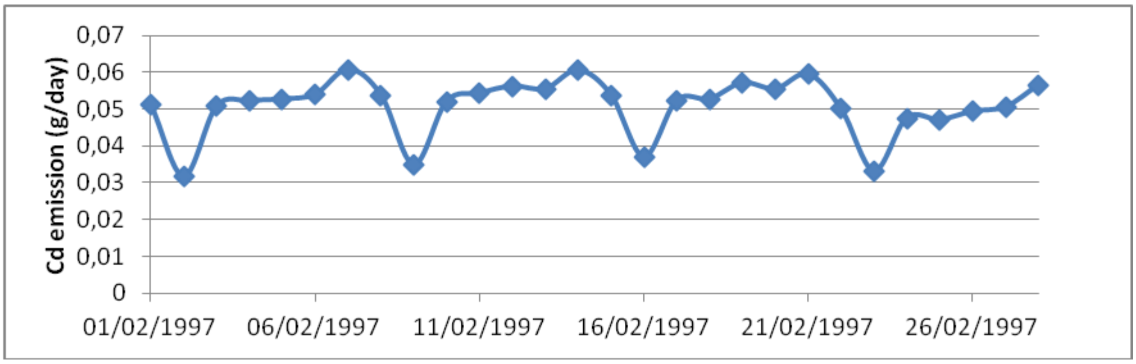


Figure 3.6. Cadmium emissions calculated with CopCETE during February 1997.

Following the calculation of the traffic emissions and the preparation of the other necessary inputs (meteorological data, receptor and source coordinates), the dispersion of pollutants was calculated at the receptor points with the Polyphemus Gaussian plume model (Briant et al., 2011).

Atmospheric deposition was calculated from the pollutant concentrations and compared with the experimental results. Atmospheric deposition occurs via dry processes (i.e., when gas molecules and aerosol particles get into contact with surfaces) and wet processes (i.e., when gases and particles are scavenged by precipitation, mostly by rain). Several studies have experimentally quantified atmospheric deposition of metals near roadways (Viard et al., 2004; Azimi et al., 2005; Sabin et al., 2006; Loubet et al., 2010). These studies show that the deposition fluxes decrease rapidly as the distance increases from the roadway, which is consistent with the spatial gradients observed for atmospheric concentrations.

Theoretical models have been developed for dry deposition (e.g., Zhang et al. (2001), Wesely (2000), Sportisse (2007)) and wet deposition (e.g., Duhanyan and Roustan, 2011).

The dry deposition flux is typically computed using the following formulation:

$$F_{dry}(x,y) = V_d . C(x,y,z_{ref}) \quad 3.1$$

where $V_d$ is the dry deposition velocity, which is a function of meteorology, land use, and particle size and $z_{ref}$ is the reference height for the pollutant concentration measured or modelled near the surface. The deposition velocities used here were obtained from Roustan (2005). The Cd mass distribution in $PM_{10}$ particles was assumed to be 74% in particles with a diameter less than 1 µm, 10% in particles between 1 and 2.5 µm, and 16% in particles with a diameter between 2.5 and 10 µm. Coarse particles with diameter >10 µm were not considered here. The dry deposition velocities were estimated as a function of an average wind speed (5 m/s) representation of conditions at the site.

Wet deposition was assumed to be homogeneous over the measurement area. The wet deposition scavenging coefficient was calculated following the Andronache (2004) formulation for rural areas.

Figure 3.7 shows the comparison of Cd deposition fluxes modeled and measured on both sides of the freeway. The results are satisfactory on the eastern side of the freeway from 20 m from the roadside onward. There is same overestimation on the western side between 50 and 200 m from the freeway. The underestimation in close vicinity of the freeway may be due to the fact that particles with diameter greater than 10 µm were not included in the emission estimates. These larges particles, which can be emitted from tyre and brake wear have greater sedimentation velocity than $PM_{10}$ particles and, therefore, deposit rapidly near the roadside.

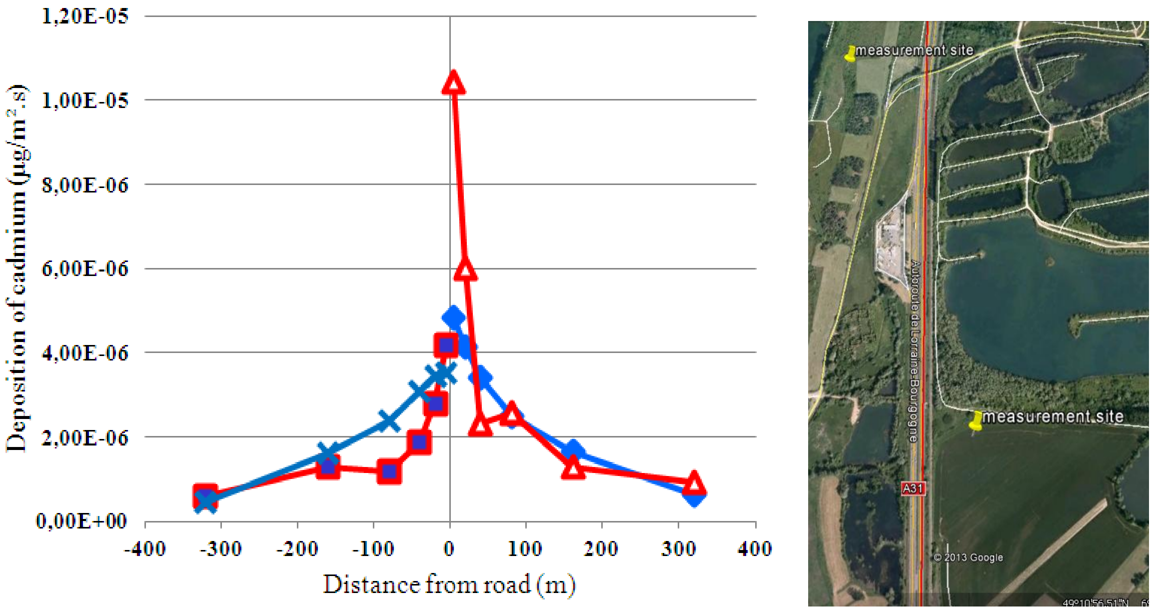


Figure 3.7. Cadmium deposition fluxes modeled (blue) and measured (red) on both sides of the A31 freeway.

### 3.3.3 Coupling of atmospheric models and stormwater runoff models

The estimation of the traffic impact on water quality is often based on measurements of pollutant concentrations in air and water. However, this method is site-specific and does not allow one to evaluate the impact of traffic at any point of an urban catchment or to estimate water contamination for future road projects. The effect of the atmospheric deposition of pollutants is important to predict water quality when major sources are located near or within a catchment. Therefore, the outputs from air quality models should be used as data inputs for stormwater models. Deposition fluxes of atmospheric pollutants can be estimated for dry and wet deposition as a function of time and location. Deposition near roadways of atmospheric pollutants emitted by traffic is mostly due to dry deposition. Wet deposition scavenges the entire atmospheric column and, therefore, includes background pollutants. Sabin et al. (2005) calculated that in Los Angeles, California, annual wet deposition fluxes were significantly lower than dry deposition fluxes with wet deposition, comprising only 1-10% of the total deposition flux. Nevertheless, air pollution models must estimate both dry deposition to determine pollutant buildup (mass per unit area) during dry periods and washout during rainfall events.

A major scientific stumbling block is that air quality models typically consider only those particles smaller than 10 µm in aerodynamic diameter (e.g., see case study above) because coarser particles are not subject to air quality regulations, which are driven mainly by inhalation-based health concerns. There is, therefore, a lack of an integrated multi-media environmental approach (Hidy et al., 2014). However, the mass of particles greater than 10 µm is significant and relevant to water quality and should be taken into account (Kakooei and Kakooei, 2007). Although the smaller fraction of particles may have a higher concentrations of some pollutants, the fraction of pollutants contained in particles of larger sizes may not be negligible (Gunawardena et al., 2012). Improving emission models as requested by regulations such as the EU Water Framework Directive and the EU Environmental Quality Standard Directive should be an objective to address multi-media issues.

Several studies coupling air and watershed models at the regional scale already exist (e.g., Burian et al., 2002; Schwede et al., 2009; Vijayaraghavan et al., 2010). These coupled models are able to read a processed gridded output of atmospheric deposition from the air quality model, and calculate average fluxes per unit area. Most of the work conducted so far on the coupling of atmospheric models and stormwater models was done at regional scales for long time periods, such as annual or seasonal budgets of atmospheric pollutant loadings to address environmental issues such as acid or mercury deposition. However, the dynamics of multimedia pollutant transfer is of interest for urban applications. Therefore, there is a real need for the development of a modelling chain that can address both urban air and water quality issues in an integrated fashion. The evaluation of this new modelling chain will need to distinguish between pollutants linked to traffic emissions and other pollutant sources in urban areas.

The main limitation is coupling of spatial scales between air quality and stormwater models. The air quality models provide spatially-distributed deposition fluxes. These fluxes must be used by stormwater models, but it is generally necessary to adapt the spatial scale to the semi-distributed water quality models (Fallah Shorshani et al., 2014). Therefore, the deposition fluxes must be calculated by averaging deposition over each subcatchment. The fully-distributed stormwater models may simulate water quality on the same grid resolution as the air quality model, however, the description of land use may not be detailed enough, because different land use types may be present in each model grid cell. This difficultly can be solved by using high grid resolution.

Finally, the evaluation of integrated air and water quality models remains challenging because of the variety of sources of pollutants in stormwater, which make source attribution difficult and may lead to compensation of errors (Vezzaro et al., 2012).

#### *3.3.3.1 Case study of the effect of air pollution on water quality*

This case study addresses the impact of traffic emissions on water quality via atmospheric deposition in an area located in the Paris region. The whole modelling chain has been treated by Fallah Shorshani et al. (2014); here, we focus on the atmosphere/water interface. Therefore, instead of using model outputs from traffic, emission and air quality models, experimental data on pollutant deposition fluxes are used to estimate roadside impacts.

The Grigny catchment is located 20 km south of Paris. The catchment area of 365.7 ha is covered by several municipalities. This area is impacted by two main roads (D310 and D445) and the A6 highway, having annual average daily traffic volumes of 17,000, 21,000 and 125,300 vehicles per day respectively.

The present study focuses on three trace metals (Cd, Zn, and Pb) emitted from traffic and deposited to the Grigny catchment during 2009 and 2010. The model used to perform the stormwater runoff analysis is SWMM 5 (Rossman, 2010). This model is an open-source modelling software, which is appropriate for this study as it allows rainfall-runoff simulations (quantity and quality) over long periods with short time steps. The water quantity modelling and the flow-rate calibration were performed using a genetic algorithm to maximize the Nash criteria, as described in detail by Petrucci et al. (2013).

The dispersion of atmospheric pollutants is calculated using wind direction data covering two years, 2009 and 2010. The wind rose is based on observations at the nearest station (Orly airport, 8 km from the catchment). The use of the wind rose from a close but different location is appropriate in this case because of the relatively flat terrain and the surrounding land use (i.e., suburban residential area). Total concentrations of Cd, Pb, and Zn are simulated in runoff from the Grigny catchment during 23 months (01/01/2009-01/12/2010) with a 5 min reporting time step. The aim of such a long-term simulation is to determine the effects of traffic on the pollutant levels at the outlet of the catchment within this period. To that end, two cases were studied. The first case takes explicitly into account background deposition and the local pollutant deposition due to the three main roadways of this heavy-traffic area; the latter is spatially variable. The second case uses only a uniform deposition flux corresponding to an averaged urban pollution background typical of low-volume surface roads (<2000 vehicles/day). The study by Wicke et al. (2011) was used to estimate the following background deposition fluxes of Cd, Pb, and Zn: 0.13, 8, and 140 µg $m^{-2}$ $day^{-1}$, respectively.

Water quality simulations include the pollutant buildup during dry periods and washoff during rainfall events. Different mathematical approaches are available to represent the processes governing pollutant accumulation and washoff. The exponential buildup and power washoff equations are used in this study (Hossain et al. 2010). The daily accumulation rates are calculated according to the deposition flux of each pollutant source (i.e., the two roads and the highway), the associated level of traffic, and the wind direction. Pollutant deposition exhibits well-defined linear relationships with traffic volume (Brett and Gavin, 2011). Therefore, the traffic effect can be calculated based on the measurement data of highway A31 with the proper traffic scaling. The spatial distribution of deposition fluxes is estimated for each road or highway based on the wind rose. According to previous work (Azimi et al., 2005; Sabin et al., 2006; Loubet et al., 2010), the daily accumulation rates for each sub-catchment are calculated over areas impacted by road traffic that extend up to about 240 m from the road. Then, traffic emissions for each road impact a fraction of the sub-catchment area based on road location with respect to the sub-catchment and wind direction. The background deposition level was attributed to all sub-catchments. Next, based on those input parameters for stormwater modelling, the pollutant concentrations in water were calculated with SWMM.

The comparison of two simulations (heavy traffic and low-level traffic) shows a significant effect of traffic on water contamination. The results presented in Figure 8 show the relative load of Zn in each sub-catchment for both simulations: i.e., with an explicit description of the contribution of traffic and considering only the effect of a background residential contamination. Some sub-catchments present low pollutant concentrations because they do not produce any runoff due to a large amount of pervious surface (vegetation-covered areas) in the sub-catchment. Figure 3.8 shows that the traffic emissions can increase the water contaminant concentrations on highly exposed sub-catchments by up to 3 times in comparison with the case without traffic.

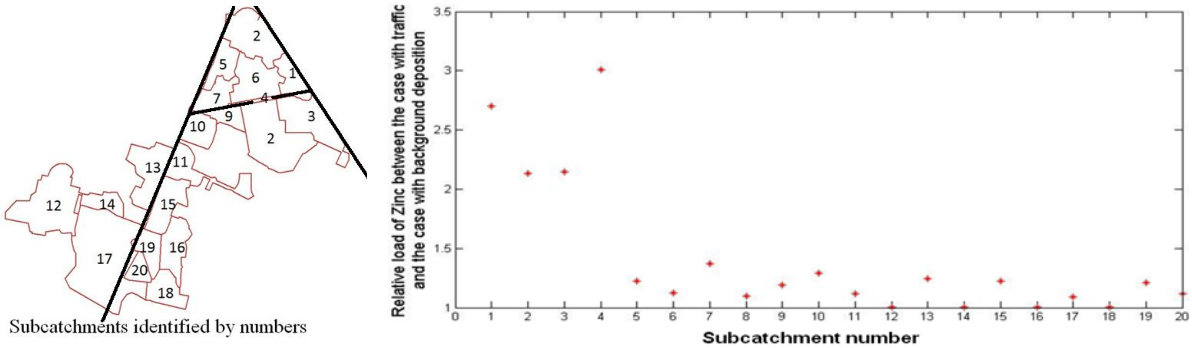


Figure 3.8. Relative load of Zn in each sub-catchment between the case with explicit treatment of traffic on main roads and the case with background deposition only.

The results of Zn concentrations at the outlet between the case with background deposition and with traffic during 6 days are shown in Figure 3.9. The relative variation between daily and period-averaged Zn concentrations was simulated over two years for both cases. The highest concentration peak compared to the average Zn concentration is about twice greater in the case with explicit traffic treatment than in the case with urban background deposition. The highest concentrations of Cd, Pb, and Zn at the outlet are respectively 2.12, 285, and 1758 µg $L^{-1}$. Cases without traffic reach a maximum of 0.78 µg-Cd-$L^{-1}$, 47.7 µg-Pb-$L^{-1}$, and 835 µg-Zn-$L^{-1}$. These important differences are related to the pollution peaks. The average concentrations over the two-year period (2009-2010) are 0.08 µg-Cd-$L^{-1}$, 6.33 µg-Pb-$L^{-1}$, and 79 µg-Zn-$L^{-1}$ with the explicit treatment of traffic. These values in the case without explicit treatment of traffic impact are 0.06 µg-Cd-$L^{-1}$, 4.0 µg-Pb-$L^{-1}$, and 70.2 µg-Zn-$L^{-1}$. These results show that an explicit description of local atmospheric pollution sources such as traffic has a strong impact on pollution peaks observed at the outlet of an urban catchment.

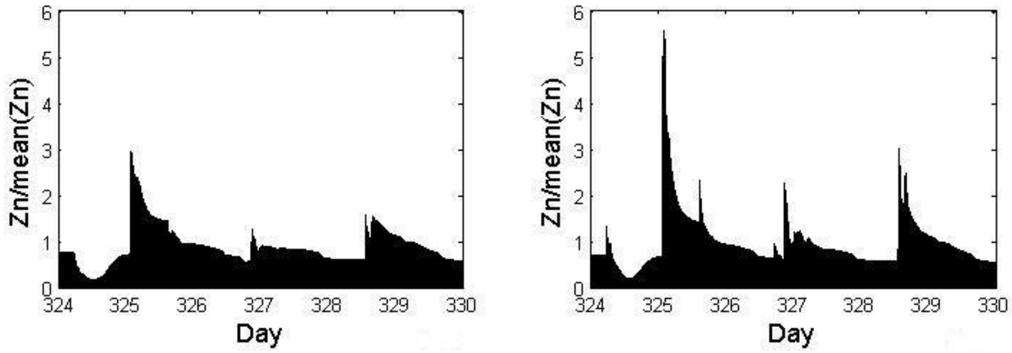


Figure 3.9 . Relative Zn concentration (ratio between daily and period- averaged concentrations of zinc) over 6 days for the case with background deposition (left) and the case with explicit traffic treatment on main roads (right).

## 3.4 Conclusion and Recommendations

In this study, the various modeling approaches available for traffic, emissions, atmospheric pollution, and stormwater pollution were presented and discussed in terms of their advantages, shortcomings, and compatibility. This review aimed at providing relevant information to facilitate the selection of the most appropriate models to be coupled in order to implement an integrated and efficient modelling chain for the simulation of air and water quality in urban areas. The importance of input and output data, compatibility among models, spatial and temporal scales were discussed. Most available models are based on temporally and spatially averaged input data. These average-based models are useful for many particular problems. However, the use of dynamic models is recommended for some applications and their use is feasible with current computing resources. As examples, we propose below two modelling chains to simulate the environmental impacts of traffic at the local urban scale for both average-based and dynamic models (see Figure 3.10).

1) Regarding the special requirements and level of details needed for a mesoscopic scale such as a city or neighbourhood, the modelling chain may consist of a static traffic model or a macroscopic dynamic model. These models provide the flow and speed of vehicles for an average-speed emission model such as Copert or CopCETE. A Gaussian or street-canyon model will then be appropriate to simulate the atmospheric dispersion of vehicle emissions at the mesoscopic scale. A semi-distributed water quality model can simulate the transfer of pollutants to the wastewater system. If a large number of pollutants and emission phenomena (fuel evaporation and non-exhaust emissions in addition to exhaust emissions) must be treated, such a modelling chain may be needed, because emission factors may not be available for more detailed models (see below).

2) A microscopic modelling chain can be used at a local scale, but only for exhaust emissions, because instantaneous emission models cannot estimate fuel evaporation and non-exhaust particle emissions. These models are able to represent the dynamic phenomena occurring in the traffic flow. The microscopic dynamic (car-following) models require many parameters and such models are data and computation demanding. The microscopic models with macroscopic law models (such as Symuvia) are an alternative because they are well suited for a dynamic representation of urban traffic with manageable data needs. For air quality, the CFD models can be used to calculate the dispersion of vehicle emissions at fine spatio-temporal scales. For water quality, a fully-distributed model can be coupled with a CFD model using compatible spatial grids. However, the limitations of instantaneous emission models do not allow one to treat non-exhaust emissions, which can be an important source of pollutants relevant to water contamination.

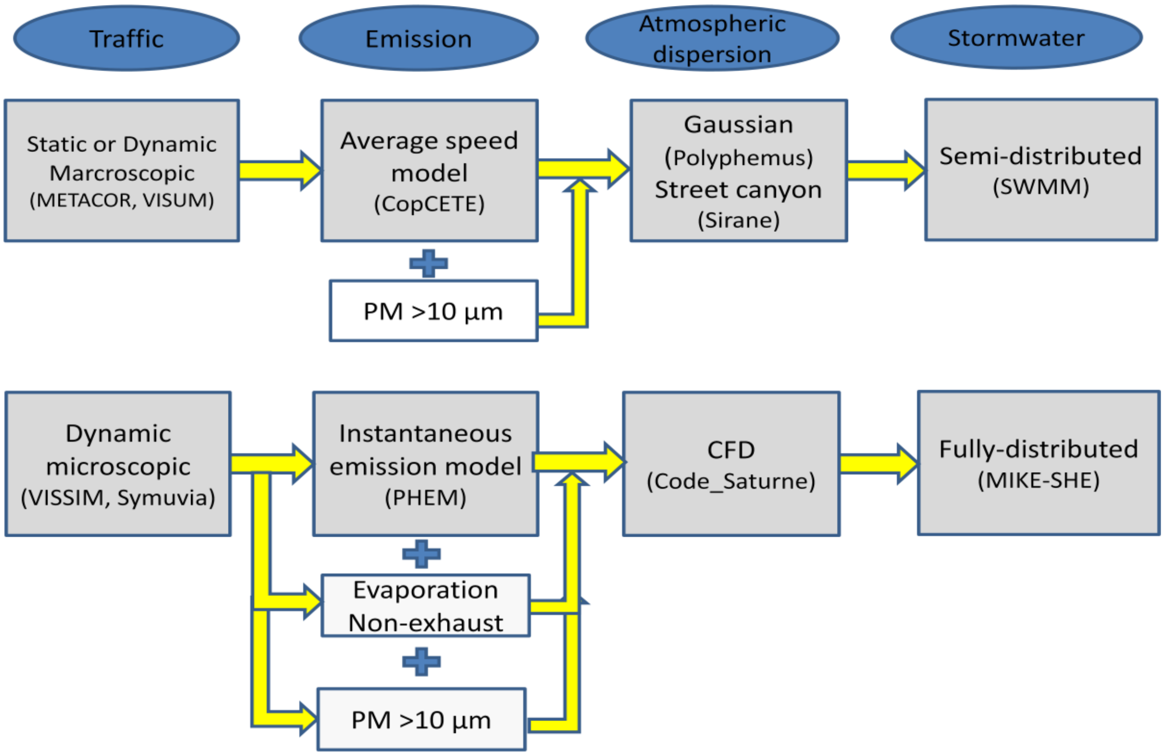


Figure 3.10. Schematic representation of the modelling chains for mesoscopic (top) and microscopic (bottom) scales with examples of models for each component of the modeling chain. Note that the list of models is not exhaustive and that other model choices are possible.

Case studies were provided to explain model integration between traffic, emission, atmospheric dispersion and stormwater quality. These examples underlined the strengths and limitations of the different models in terms of their ability to represent physical processes and demonstrated the importance of the environmental impacts of traffic at the local scale.

In summary, a modelling chain must be able to handle the various aspects enunciated above in a realistic, yet computationally efficient manner. Existing models will, therefore, need to be improved and adapted to address all these issues.