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Estudo da interação entre o transporte de compostos orgânicos voláteis biogênicos e química dentro de um dossel da floresta tropical utilizando Large Eddy Simulation

Large eddy simulation of the interaction between biogenic volatile organic compound transport and chemistry within a tropical forest canopy

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Resumo

Florestas tropicais emitem um grande número de compostos orgânicos voláteis biogênicos (COVB), que podem reagir com oxidantes atmosféricos (como por exemplo radicais Ozônio O_3, nitrato NO_3 ou hidroxila OH, normalmente originados acima do dossel) e os produtos da reação podem condensar formando aerossóis orgânicos secundários. Simulações de Grandes Vórtices (LES, da sigla em inglês) que resolvem o dossel, combinadas com uma representação da química da atmosfera, são uma poderosa ferramenta para um melhor entendimento da interação entre os processos químicos e de transporte. Para tanto, uma resolução adequada do campo de concentração dos reagentes (COVB e oxidantes), assim como do escoamento dentro do dossel são necessários. Nesse trabalho são apresentados os resultados de um estudo utilizando LES com 17 camadas dentro da floresta (resolução vertical de 2 m), incluindo uma química simplificada de COVB, para estimar o transporte através do topo da floresta de COVBs e de seus principais produtos, como o metil vinil cetona (MVC) e a Metacroleína (MACR). Os resultados são comparados com medições de campo de ozônio, óxidos de nitrogênio, isopreno, monoterpenos, assim como MVC e MACR observados durante uma campanha na torre K34 da Reserva Biológica Cuieiras (2°36'32" S, 60° 12'33" W) de Abril/2014 a Janeiro/2015.

***Palavras-chave**: simulação de grandes vórtices, química atmosférica, COVB, ozônio, dosséis de floresta*

Abstract

A multitude of biogenic volatile organic compounds (BVOCs) are emitted within the canopy air-space of tropical forests. These compounds undergo reactions with atmospheric oxidants (eg. Ozone O_3, the nitrate NO_3 or the hydroxyl OH radicals), which mainly originate above the canopy, and reaction products can subsequently condense to form secondary organic aerosols. Canopy resolving Large Eddy Simulation (LES) combined with a representation of atmospheric chemistry presents a valuable tool for a better understanding of the interaction between chemistry and transport processes. This requires the adequate resolution of concentration fields of reactants (BVOCs and oxidants) as well as the flow field inside the canopy. We present the results of an LES study with 17 layers inside the forest (2 m vertical resolution), which includes a simplified BVOC chemistry in order to estimate the export of BVOCs and their principal reaction products such as methyl vinyl ketone (MVK) and methacrolein (MACR) from a tropical canopy. These results are compared to field measurements of ozone, nitrogen oxides, isoprene, monoterpenes as well as MVK and MACR observed during a field campaign at the Cuieiras Biological Reserve K34 (2°36'32" S, 60° 12'33" W) tower from April 2014 to January 2015.

***Keywords**: large eddy simulation, atmospheric chemistry, BVOC, ozone, forest canopies*

1 Introduction

Tropical forests, which cover large areas, emit a plethora of biogenic volatile organic compounds (BVOC), including isoprene and monoterpenes. These hydrocarbons react with atmospheric oxidants such as ozone (O3), the nitrate radical (NO3) or the hydroxyl radical (OH) and the resulting products can subsequently condense to form secondary organic aerosols (SOA) (i.e., Andreae, 2008). Due to the typically clean tropical air masses, SOA can make up a large portion of the total aerosol loading and may thus affect cloud development and climate. Consequently, there is a growing research interest in estimating the amount of BVOCs and their reaction products, which are exported from tropical forests to the free atmosphere. Once emitted on the leaf-level, BVOCs in the canopy air-space are subject to the interplay between turbulent transport processes and reactions with atmospheric oxidants, which primarily originate from above the canopy, before they are released into the atmospheric surface layer (Figure 1). Air parcel residence times and thus reaction time-scales within the dense Amazon canopies can range from a few seconds (near the canopy top and through fast acting coherent ejections) to several minutes (small flow velocities near the surface). It is therefore critical to not only resolve in-canopy velocities, but also concentration fields of BVOCs and atmospheric oxidants, which vary in space and time.

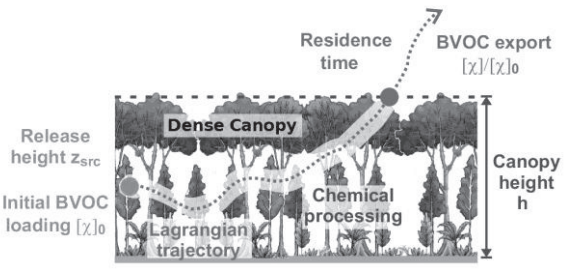

Figure 1: Illustration of the interplay between transport and chemistry within forest canopies.

Canopy resolving Large Eddy Simulation (LES) coupled with a chemical model, can be an important tool to expand our knowledge about these in-canopy processes.

2 Methodology

From March 2014 to January 2015 a field campaign took place at the Cuieiras Biological Reserve K34-tower (2°36′32″ S, 60° 12′33″ W) 60 km north-northwest of Manaus as part of the GoAmazon 2014/5 project. The canopy height (h) is approximately 35 m. Turbulence data were collected at 9 levels within and above the canopy ($z\ h^{-1}$ = 0.20, 0.39, 0.52, 0.63, 0.70, 0.90, 1.00, 1.15, and 1.38). Additionally, ozone, NO_x, isoprene and monoterpenes were continuously recorded with inlets located at $z\ h^{-1}$ = 1.14.

The LES model used for this work is described in Chamecki et al. (2008). The LES is canopy resolving in the sense that grid cells within the canopy are subject to drag forces that represent canopy influences following Shaw and Schumann (1992).

The simulations are set-up with a grid resolution of 8 m x 8 m x 2 m in the x, y, and z direction with 144 x 96 x 192 grid points. This equates to approximately 10 canopy heights in the vertical dimension and gives 17 layers inside the canopy. The LES is forced with a pressure gradient force corresponding to a friction velocity of $u_* = 0.4\ m\ s^{-1}$ and includes a leaf area distribution following Tóta et al. (2012). Buoyancy effects are neglected in the LES.

Chemical species are included in the LES as reactive tracers. Isoprene oxidation processes related to ozone, the nitrate and hydroxyl radicals are included by using the atmospheric chemistry module from the Dutch Atmospheric LES (DALES) (Ouwersloot et al., 2013).

3 Preliminary Results

The LES is capable of reproducing the most important features of observed turbulence statistics at the K34-tower (Figure 2). Simulated wind speeds in the upper canopy and above match observations closely. Similarly, turbulent quantities such as the vertical momentum flux

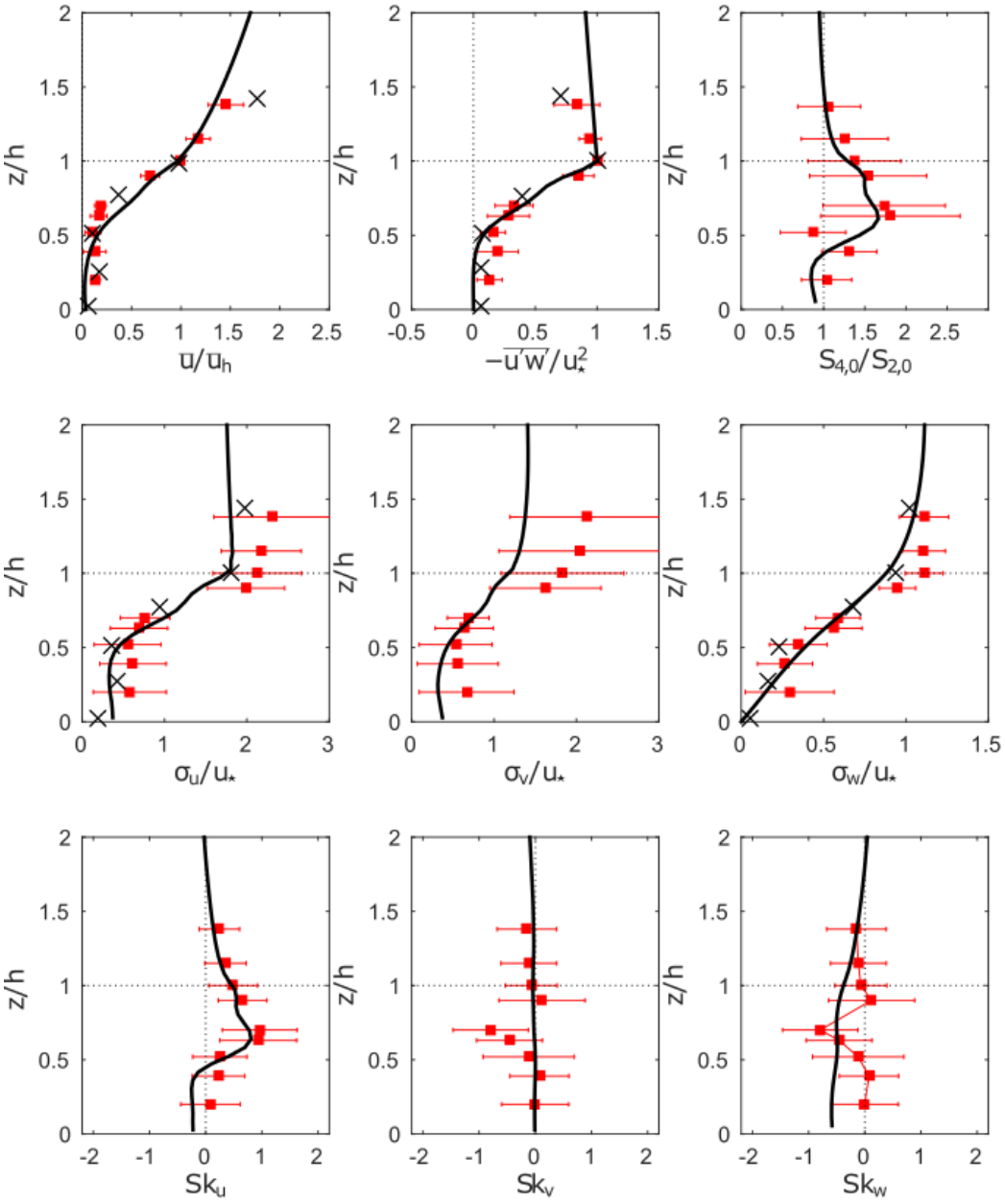

Figure 2: Vertical profiles of turbulence statistics inside and above the forest. LES results (solid line) and field observations (red squares for K34 data and black crosses for data reported in Kruijt et al. (2000)

$\overline{u'w'}$ standard deviations of horizontal and vertical velocities σ_u, σ_w demonstrate that the model reliably reproduces turbulent conditions. Additionally, the model captures the impact of coherent motions in the momentum transport such as sweeps ($w'<0$; $u'>0$) and ejections ($w'>0$; $u'<0$) well as shown by the ratio of sweeps and ejections ($S_{4,0}/S_{2,0}$) and the skewness of horizontal wind Sk_u. The LES, used in conjunction with a Lagrangian particle tracking algorithm, also demonstrated that air parcel residence times within the dense forest canopy spanned a range from seconds near the canopy top and to minutes near the surface, which can exceed the oxidation timescales for reactive trace gases (such as β-caryophyllene) and also impact the canopy export of less reactive gases such as isoprene.

Final Considerations

Based on the preliminary results from the LES simulations and the documented performance of the atmospheric chemistry model from DALES, we investigate the interactions between transport and chemical processing for plant emitted hydrocarbons within an Amazon canopy. Subsequently we estimate the export of isoprene and primary reaction products, such as methyl vinyl ketone (MVK) and methacrolein (MACR) from the canopy and present the simulated export of BVOCs from the forest's canopy. These results will be compared to field measurements from the K34 tower.

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