

Advancing the BRAMS wildfire–atmosphere modelling system: application to an extreme wildfire event

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Abstract. Wildfire smoke significantly perturbs atmospheric composition and radiative balance, with implications for air quality, weather, and climate. Accurately simulating smoke–radiation–convection interactions remains a scientific challenge, particularly at meso-local scales. This study presents developments in the BRAMS v6.0 modelling system, including the integration of crown fire spread into SFIRE and dynamic coupling of fire-emitted smoke fluxes. These enhancements enable physically consistent simulations of wildfire behaviour, smoke emissions, and their radiative impacts.

~~The model couples fire spread and heat release~~ are used to compute Fire Radiative Power, which drives smoke emissions in real time. These emissions are fully integrated with aerosol–radiation interactions and atmospheric dynamics. The system was applied to the 15 October 2017 wildfire in central Portugal using high-resolution simulations.

Model performance was evaluated by comparing a diagnostic Smoke Optical Depth (SOD), computed offline from BRAMS-simulated PM_{2.5} using a Mie-based framework, ~~with~~ against MERRA-2 Aerosol Optical Depth (AOD). ~~The SOD fields reproduced the main spatial and temporal patterns of smoke transport and the wavelength-dependent optical behaviour, including extinction and absorption at 400, 550, and 700 nm.~~

25 Statistical comparison shows that SOD and MERRA-2 AOD share a coherent spatiotemporal structure, with correspondence maximised during the active fire phase. Statistical comparison confirmed a physically consistent agreement between simulated smoke optical depth (SOD) and satellite AOD, particularly during the active fire phase. Extinction reached 67 m⁻¹ at 400 nm, while absorption peaked near 5 m⁻¹ at 550 nm, revealing the dominant role of organic carbon in visible-range scattering and of black carbon in shortwave absorption. Radiative heating within the plume induced upward displacements of the CIN layer by 100–200 m and partial erosion of thermal inversions, forming transient radiative lids that modulated boundary layer stability. CAPE was locally enhanced, indicating a radiative–convective feedback between smoke heating and near-surface buoyancy. Peak extinction reached ~67 m⁻¹ at 400 nm and absorption approached ~5 m⁻¹ at 550 nm in the near-source plume core, consistent with an OC-dominated scattering regime and localized BC-driven shortwave absorption. The resulting

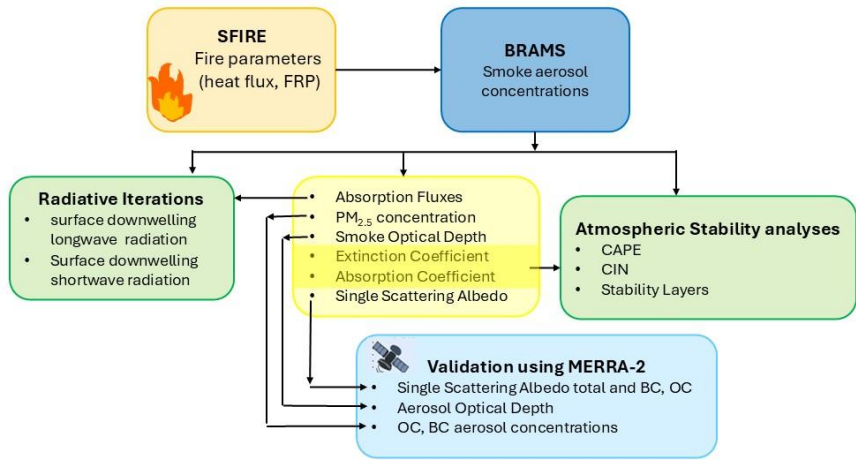
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radiative heating contributed to the upward displacement of the CIN layer ($\approx 100\text{--}200\text{ m}$) and to the partial erosion of low-level inversions, producing transient stability modifications.

Although the model occasionally produces very high near-source PM_{2.5} and optical-depth values confined to a small number of grid cells, additional diagnostics show that plume-integrated mass and optical properties remain physically consistent and are not dominated by boundary effects. These results demonstrate that the enhanced BRAMS system captures the coupled fire–atmosphere–radiation feedbacks of intense wildfires, improving the interpretation and prediction of smoke-induced thermodynamic and radiative perturbations.

~~These results demonstrate that the enhanced BRAMS model can realistically capture coupled fire–atmosphere–radiation processes at high resolution, improving both the interpretation and prediction of smoke-induced thermodynamic and radiative perturbations over complex terrain.~~

Graphical Abstracts.



1 Introduction

Understanding wildfire emissions is essential for accurately predicting air quality (Fernandes et al., 2022) and radiative impacts, particularly in complex terrains where local meteorological dynamics strongly influence smoke dispersion~~where smoke dispersion is strongly influenced by local meteorological dynamics~~. Recent European case studies have shown severe urban air-quality degradation during major wildfire episodes, including the August 2021 Athens fires (Osswald et al., 2023)

55 and the October 2017 north centre of Portugal wildfires (Lopes et al., 2024). Wildfires release large quantities of trace gases and aerosols that interact with atmospheric chemistry (Andreae et al., 2001; Jaffe et al., 2008; Monks et al., 2012), modulate radiative transfer (Clinton et al., 2006; Menezes et al., 2024), reduce visibility (Valente et al., 2007), and severely affect human health (Apte et al., 2018; Lopes et al., 2024; Miranda et al., 2010). These impacts further highlight the growing importance of high-resolution, community-based air-quality monitoring and citizen engagement initiatives (Relvas et al., 2025), which
60 complement modelling and satellite approaches by improving local understanding and response capacity during wildfire events. These challenges are especially difficult to quantify under the rapidly changing conditions typical of wildfire episodes, requiring dynamic models capable of resolving fire–atmosphere feedback at high spatial and temporal resolutions.

Traditional approaches for estimating biomass-burning emissions in operational air-quality and climate models often rely on semi-empirical methods, including precompiled inventories such as the Global Fire Emissions Database (GFED) and satellite-derived Fire Radiative Power (FRP) products assimilated in systems like the Copernicus Atmosphere Monitoring Service, Global Fire Assimilation System (CAMS-GFAS) ~~(CAMS (CAMS, 2015))~~. While these frameworks provide valuable large-scale emission estimates, their relatively coarse spatial resolution and simplified fire parameterizations limit their ability to capture the rapid evolution and spatial heterogeneity of active wildfires. This limitation is particularly critical in forested regions, where intense crown fires coexist with patchy surface burning and smouldering phases. As demonstrated by Oliveira
70 et al. (2025), coarse FRP retrievals often miss or underestimate localized high-intensity combustion in complex terrain, introducing systematic biases in both the magnitude and timing of smoke emissions. While computationally efficient, these methods do not simulate fire spread or associated heat release, limiting their capacity to resolve the dynamic feedbacks that modulate local atmospheric stability and pollutant dispersion. The Brazilian Biomass Burning Emission Model (3BEM) ~~(Freitas et al. (Freitas et al., 2009; Longo et al., 2010); Longo et al.)~~ coupled to BRAMS (Brazilian Regional Atmospheric
75 Modeling System) follows this approach, estimating smoke emissions based on FRP, surface type, and meteorology, but without explicit coupling to fire dynamics. This framework is suitable for regional or long-term assessments but lacks physical consistency under rapidly evolving fire conditions.

Wildland fire behaviour models developed historically within the forestry community have been primarily designed to predict two-dimensional surface fire spread rates and heat release under prescribed fuel types, slope conditions, and wind fields, with
80 a primary focus on fire danger assessment and surface fire behaviour. These operationally oriented semi-empirical models are not intended to resolve highly dynamic or plume-driven fire behaviour, nor the onset of extreme fire development beyond the incipient stage.

Fully coupled atmosphere–surface fire models, such as AIRFIRE (Miranda, 2004), WRF-SFIRE (Mandel et al., 2011), CAWFE (Clark et al., 1996; Coen, 2005), or BRAMS-SFIRE (Menezes et al., 2021) and ForeFire/Meso-NH (Filippi et al.,
85 2013), integrate a mesoscale non-hydrostatic, large-eddy numerical weather prediction core with a semi-empirical fire surface spread module (typically based on Rothermel (1972) and McArthur (1967)). In such systems, the fire and atmosphere evolve as a single dynamically coupled entity, allowing simulation of small-scale fire–atmosphere interactions, vorticity-driven dynamics, fire-induced buoyancy, and turbulence feedback. These models explicitly represent fire-generated kinetic and

potential energy via resolved sensible and latent heat fluxes, and predict fire perimeter evolution, fuel consumption, fireline intensities, and rate of spread. Model initialization requires fuel load and fuel moisture content, fuel burn rate, combustion heat release, and treatment of canopy ignition when heat flux exceeds a critical threshold, in addition to terrain and local wind forcing.

In addition to the large variability in fire intensity and fuel structure, the chemical and physical characteristics of smoke particles evolve rapidly as they are transported away from the source, altering their optical behaviour and radiative impacts in ways that are not captured by simplified bulk-emission schemes.

Forest fires, during their propagation, consume the available biomass as characterized by the different NFFL fire behaviour fuel models (Anderson, 1982), which represent the landscape, and release high concentrations of particles and trace gases into the atmosphere. Primary aerosols are emitted throughout combustion, during both the flaming and smouldering phases, while secondary aerosols form in the atmosphere through chemical reactions involving precursor gases. However, primary particles can serve as condensation nuclei or "seeds" for secondary particle formation through aging processes, resulting in internally mixed aerosols with complex and evolving chemical compositions as they are transported within the smoke plume.

Primary particles include soot, predominantly composed of elemental carbon (BC), along with ash and mineral components derived from the burned biomass. These materials may exist as distinct particles or aggregate into larger mixed particles during combustion. Depending on their composition and surface properties, these aerosols can be hydrophilic (attracting water, enhancing growth in humid conditions) or hydrophobic (repelling water), affecting their interaction with radiation and their ability to act as cloud condensation nuclei (CCN).

As these particles are transported within the smoke plume, they undergo aging processes that alter their physical and chemical properties. These include: (1) Coagulation — collisions and merging with other particles, leading to increased size and complexity; (2) Surface reactions – interactions with atmospheric gases such as SO₂, NO_x, and volatile organic compounds (VOCs), including terpenes and isoprenes (emitted by vegetation during natural biological processes) and aromatic compounds (from biomass combustion). These reactions lead to the formation of sulfates, nitrates, and organic coatings; (3) Oxidation — particularly of BC, resulting in the acquisition of oxygen-containing functional groups that modify its optical properties and enhance hydrophilicity.

In parallel, VOCs are oxidized in the atmosphere to produce oxygenated organic compounds, such as carboxylic acids (e.g., formic acid, acetic acid) and aldehydes (e.g., formaldehyde), which contribute to the formation and growth of secondary organic aerosols (SOA). These compounds can condense onto primary particles, forming coatings that significantly modify their optical and hygroscopic properties.

Moreover, photochemical reactions involving VOCs and oxidants such as ozone (O₃) and hydroxyl radicals (OH) also lead to secondary particle formation. Not all secondary aerosols are of local fire origin; VOCs and precursor gases transported from urban pollution sources or natural vegetation in other regions may also contribute further to increasing the complexity of the smoke plume and its optical properties.

Both primary and secondary aerosols interact with solar radiation through scattering and absorption of shortwave (visible and near-infrared) radiation, reducing direct sunlight at the surface while enhancing diffuse radiation (Yamasoe et al., 2006). These particles also absorb and re-emit longwave (thermal infrared) radiation. While BC strongly contributes to absorption, sulfates and organic aerosols primarily enhance scattering, collectively influencing the atmospheric radiative energy balance (Yamasoe et al., 2006). The net result often includes local atmospheric heating, particularly in layers rich in BC.

These radiative interactions are governed by Mie theory, as most smoke particle sizes fall within the Mie regime (approximately 0.1 μm to 1 μm), where the particle diameter is comparable to the wavelength of incident radiation. Smaller particles ($\ll 0.1 \mu\text{m}$) scatter more efficiently at shorter wavelengths (e.g., blue light) and are better described by Rayleigh theory, which assumes particle sizes much smaller than the radiation wavelength. In contrast, larger particles exhibit non-selective scattering and remain within the Mie regime, with their radiative behaviour less dependent on wavelength.

As these primary and secondary aerosols interact with radiation through wavelength-dependent scattering and absorption, their evolving size distribution, mixing state and refractive index directly determine the radiative forcing exerted by the plume. This motivates the need for models capable of explicitly representing both fire behaviour and the microphysical processes that govern smoke optical properties.

Smoke aerosols strongly perturb the atmospheric energy balance through wavelength-dependent scattering and absorption, governed by their size distribution, complex refractive index, mixing state, and ageing (Pueschel et al., 1988; Reid et al., 2005). These properties determine aerosol optical depth (AOD), single-scattering albedo, and vertical extinction structure, thereby influencing surface heating, atmospheric stability, and fire-atmosphere feedback. Curci et al. (2015) showed that neglecting aerosol mixing state can alter simulated AOD by more than a factor of two for identical aerosol mass, emphasising the need for physically based optical treatments in coupled fire-atmosphere systems. Regional studies have documented wide variability in smoke optical behaviour. Procopio et al. (2003) analysed AERONET observations over Brazil using Mie theory and validated a radiative forcing model across multiple optical thickness regimes and wavelengths. Reid and Hobbs (1998) found that Brazilian smoke exhibits about 15 % lower scattering coefficients and reduced single-scattering albedo relative to North American fires, attributed to combustion efficiency differences. Reid et al. (1999) further reported pronounced temporal variability in AOD over diurnal and multi-day cycles. Yumimoto et al. (2018) demonstrated that assimilating Himawari-8 aerosol observations improves the representation of Siberian smoke transport, correcting emission underestimations and capturing the distinctive C-shaped dispersion pattern over Japan. Finally, Ferrare et al. (1990), using NOAA-7 AVHRR data, characterized large-scale smoke transport from Canadian forest fires, with optical thickness ranging from < 0.1 to > 3.7 , particle radii of 0.3–0.9 μm , and lifetimes of 15–20 days, evidence of persistent, long-range smoke layers influencing regional radiative forcing. Makar et al. (2021) additionally demonstrated that wildfire smoke can cool the surface and stabilise the lower troposphere, altering plume dynamics and atmospheric circulation.

Recent advances in operational smoke forecasting systems, such as the HRRR-Smoke model (Ahmadov, 2017; Ye et al., 2021), have improved the coupling between fire activity, emissions, and atmospheric transport. Similar developments in regional and global frameworks (Anderson et al., 2024; Kochanski et al., 2021; Kochanski et al., 2015) have enhanced the representation

of plume rise, aerosol–radiation interactions, and smoke dispersion. However, these systems generally rely on semi-empirical plume-injection schemes and parameterized fire emissions, without resolving crown-fire propagation or the thermodynamic feedbacks associated with combustion heat release. Fully physically coupled fire–atmosphere models capable of simultaneously representing fuel consumption, surface- and canopy-fire spread, heat fluxes, and the resulting smoke optical effects remain rare in European wildfire contexts, particularly in complex mountainous terrain.

Addressing this gap, the present study employs a BRAMS–SFIRE configuration that explicitly resolves both surface and crown fire propagation and dynamically couples sensible and latent heat release to plume rise and vertical smoke transport. The main purpose of this paper is to describe the improvements implemented in the BRAMS-SFIRE (Freitas et al., 2017; Menezes et al., 2021; Menezes, 2015a) modelling system to enhance the physical realism of wildfire representation beyond surface-fire-only approaches, by including an explicit crown–fire propagation scheme. With this explicit treatment of crown-fire propagation, the model is expected to generate a more physically consistent smoke plume evolution, particularly under high-intensity fire conditions. By resolving fire–atmosphere interactions at fine spatial scales, the resulting smoke injection height, plume structure, and downwind dispersion are anticipated to more closely resemble observed plume behaviour, thereby improving the realism of high-resolution wildfire smoke simulations. Moreover, this integration enables simulations that explicitly resolve surface and canopy fire spread, fuel consumption, and the associated release of heat and smoke over heterogeneous terrain. Fire Radiative Power (FRP) is not prescribed but internally computed from model-resolved sensible heat fluxes, allowing smoke emissions to evolve dynamically with fire intensity and meteorological conditions. The two-way coupling supports feedback between combustion processes and local thermodynamics, which are critical for reproducing vertical smoke transport and smoke–radiation–convection interactions.

~~Compared to the WRF-SFIRE system (Allen et al., 2021; Kochanski et al., 2021; Mandel et al., 2014; Mandel et al., 2011), BRAMS shares a similar physical coupling architecture for simulating surface fire-atmosphere interactions. BRAMS originated from the RAMS model, a globally applicable mesoscale model initially developed in the United States. Over time, RAMS was adapted with physical parameterizations better suited to represent processes relevant to tropical regions, leading to the development of BRAMS.~~

~~BRAMS has been extensively applied in South America, it remains a versatile model capable of simulating atmospheric processes across a wide range of latitudes, from tropical to mid-latitude conditions, in both hemispheres. The main differences between BRAMS and WRF lie in their physical parameterizations, vertical coordinate systems, and the way they resolve the atmospheric base state. These structural differences influence how each model represents radiation, microphysics, turbulence, and surface-atmosphere interactions, particularly under conditions of strong vertical development such as those driven by wildfires. The improved modelling system was tested through its application to the Sertão extreme wildfire of 15 October 2017 in central Portugal (Menezes et al., 2024). The event occurred in a mountainous region with strong mountain-valley circulations, which strongly modulate smoke dispersion and vertical mixing, providing a demanding yet scientifically valuable testbed for model evaluation.~~ Section 2 describes the modelling developments and experimental design, including the treatment of crown-fire initiation and vertical injection of emissions. Section 3 presents the simulated fire-spread behaviour, plume

190 injection heights, PM_{2.5} loadings, and the resulting radiative and thermodynamic impacts, highlighting the value of fully two-way fire-atmosphere coupling for advancing understanding of wildfire-induced air-quality degradation and atmospheric feedback processes.

2 Methodology

195 This section details the advancements made in the BRAMS-SFIRE modelling system, including the integration of a crown fire spread behaviour model and the implementation of FRP calculations within SFIRE. The processes for assimilating National Fuel Fire Laboratory (NFFL) fuel behaviour models and high-resolution terrain elevation data are also described, ensuring accurate nesting of the SFIRE grid within the BRAMS grid for two-way coupling of wildfire fluxes and emissions. Furthermore, the methodology used to characterize particulate matter with an equivalent diameter less than 2.5 µm (PM_{2.5}) released during the Sertão wildfire episode on 15 October 2017, as simulated by BRAMS, is thoroughly explained. This includes
200 the validation and interaction of smoke with atmospheric radiation, as well as the specification of surface conditions required by the SFIRE simulation. For a better understanding of the improvements that have been made, the section starts with a description of the original BRAMS-SFIRE modelling system.

2.1 The BRAMS-SFIRE modelling system

2.1.1 The BRAMS model

205 The BRAMS is based on the Regional Atmospheric Modeling System (RAMS) developed at Colorado State University (CSU/USA). It is free software (CC-GPL), maintained by the Centre for Weather Forecasting and Climate Studies from the National Institute for Space Research (CPTEC/INPE), the University of São Paulo (USP), and other institutions in Brazil and abroad. BRAMS and RAMS are versatile numerical weather prediction models, capable of simulating atmospheric circulations across a wide range of scales, from hemispheric to large eddy simulations (LES) of the planetary boundary layer. Significant
210 improvements have been made to BRAMS to better represent key physical processes in tropical and subtropical regions, alongside integrated atmospheric chemistry and aerosol processes. It also includes a state-of-the-art model for simulating the exchange of water, energy, momentum, and biogeochemical tracers between the atmosphere and the surface (Freitas et al., 2017). BRAMS solves the compressible, non-hydrostatic atmospheric equations described by Tripoli and Cotton (1982). It uses a one-way nesting scheme to perform downscaling on computational grids with increasing spatial resolution (Freitas et
215 al., 2017).

Additionally, BRAMS incorporates a real-time assimilation method for the CCATT, focusing on the assimilation of trace gas and aerosol emissions from biomass burning, using FRP data derived from MODIS and GOES satellite products (Pereira et al., 2022; Pereira, 2013). Although the model typically underestimates emissions by up to 25%, it successfully captures around 90% of biomass burning activity, demonstrating high potential for near real-time monitoring of gases and aerosols emitted

220 during biomass combustion. The FRP-based method improves emission estimations by 25% compared to traditional methods, accurately capturing regional and local burning of biomass patterns (Pereira, 2013).
BRAMS has been extensively applied in South America; it remains a versatile model capable of simulating atmospheric processes across a wide range of latitudes, from tropical to mid-latitude conditions, in both hemispheres. To better evaluate its behaviour in complex topography and dynamically evolving mountain–valley breezes, estimated burned area values for the wildfire episode in Sertão, as simulated by BRAMS-SFIRE and WRF-SFIRE, were compared. The WRF-SFIRE and the BRAMS-SFIRE systems share a similar physical coupling architecture for simulating surface fire–atmosphere interactions.

2.1.2 The surface fire model (SFIRE)

230 A detailed description of the SFIRE surface-fire module, including its ignition strategy, level-set front propagation, fuel-consumption algorithms, and coupling to atmospheric forcing, was originally documented in Annex C of Menezes Isilda (2015b)(2015). For completeness and clarity, we provide ~~here~~ a concise summary of the key elements relevant to the present study below.

235 2.1.2.1 Ignition and initial conditions

SFIRE initializes combustion from a user-specified point or line ignition. To avoid singular behavior at time $t = t_0$ and to seed a finite front, the code creates an initial burned kernel (small disc/segment) around the ignition locus. The advancing fireline is represented by a level-set function $\psi(x, t)$, with $\psi < 0$ inside the burning region, $\psi = 0$ at the fireline, and $\psi > 0$ outside.

240 2.1.2.2 Front kinematics via level sets

The fireline evolves according to a Hamilton–Jacobi equation:

$$\frac{\partial \psi}{\partial t} + R(x, t) \|\nabla \psi\| = 0 \quad (1)$$

where R is the local rate of spread (ROS, m s^{-1}) evaluated along the outward normal to the front. Time stepping uses a two-stage Heun (second-order Runge–Kutta) scheme. Spatial derivatives are computed with upwind-consistent reconstructions (standard upwind, Godunov, ENO, or Sethian formulations), which preserve the correct upwind direction and suppress
 245 spurious oscillations. Standard reinitialization keeps ψ close to a signed-distance function, stabilizing $\|\nabla \psi\|$. At the grid scale, a cell transitions to burning when ψ changes sign within the cell; hence, propagation between cells is governed by the zero-crossing of ψ , not by explicit geometric “jumps”.

250 **2.1.2.3 Rate of spread and directional dependence**

In the default configuration, the no-wind/no-slope ROS comes from the semi-empirical Rothermel (1972) formulation. Directional amplification by wind and slope is applied via multiplicative factors projected on the front normal. The model framework allows the user to select alternative spread formulations when appropriate for the dominant fuel type or regional fire regime. Available parameterizations include the McArthur (1966, 1967) law, commonly used for Australian forest fuels, and the Clark et al. (2004) spread formulation for chaparral and shrubland ecosystems. These options are user-defined in the configuration namelist.

2.1.2.4 Atmospheric forcing and topographic effects

The horizontal wind from the host atmosphere model is horizontally interpolated to the fire grid and vertically adjusted to mid-flame height using a logarithmic profile. Optionally, a mid-flame wind reduction factor (Baughman and Albini, 1980) is applied, conditioned on the fuel category, to represent drag within the fuelbed. Slope enters through the local terrain gradient projected onto the propagation direction, providing the Rothermel (1972) slope factor.

2.1.2.5 Fuel consumption and heat release

Each fire-grid cell carries a non-dimensional available-fuel fraction $F \in [0,1]$ that decays after ignition according to the cell's flame residence time and fuel moisture. Two consistent algorithms compute within-cell fuel loss using bilinear interpolation of ψ and ignition time at cell vertices/edges: (i) a fast algebraic approximation and (ii) a more accurate quadrature/least-squares method for partially burning cells (Fig. 1). Sensible and latent heat fluxes (W m^{-2}) are then diagnosed from the burning rate and fuel properties and coupled back to the atmosphere.

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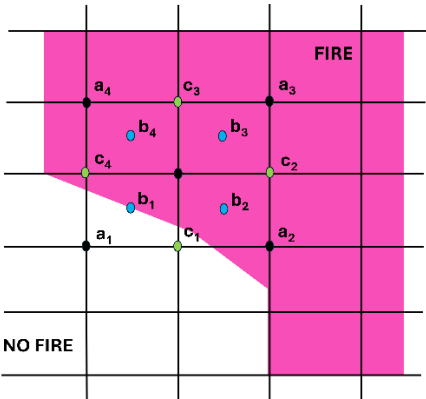


Figure 1: Schematic of fire-front propagation on the fire mesh. Black markers denote the high-resolution fire grid where the level-set function ψ and the burn time τ are advanced. Blue markers indicate bilinear interpolation of ψ and τ to the cell-center vertices using a four-point stencil. Green markers indicate bilinear interpolation of ψ and τ to the midpoints of each cell edge using a 1-D edge stencil. These interpolated values drive the fuel-consumption update (remaining-fuel calculation) at sub-cell locations. The magenta area marks cells classified as FIRE, while the white area corresponds to NO FIRE.

2.1.2.6 Fuel-moisture diagnosis

Fuel moisture responds to ambient humidity, temperature, and precipitation using established wetting/drying laws (after Van Wagner and successors), with appropriate lags for different timelag classes. Atmospheric scalars are interpolated from the host grid to the fire grid with distance-weighted schemes; precipitation and relative humidity modulate both consumption and diagnosed heat fluxes.

2.1.2.7 ~~Why grid resolution matters and what we mean by “overpropagation.”~~ Fire-grid stability and definition of overpropagation

Let Δx be the fire-grid spacing and Δt the integration step used for the level-set update. The distance a front element advances in one step is $d \approx R\Delta t$. If d becomes comparable to or exceeds Δx anywhere on the mesh, the front can traverse multiple cells in a single update, producing a numerically accelerated spread that is not physically warranted by the resolved fields. We refer to this violation of the fire-CFL condition: $R\Delta t \lesssim c\Delta x$ ($0 < c \leq 1$) as overpropagation. The risk increases (i) when a coarse Δx is advanced with too large a Δt (e.g., if fire is stepped only at the atmospheric time step), and (ii) locally where R spikes due to strong winds are projected at mid-flame height or steep terrain slopes (especially if wind reduction or terrain resolution are not consistent with the fire grid).

2.1.2.8 Numerical and physical controls to avoid overpropagation

SFIRE employs several safeguards:

- temporal subcycling of the fire solver. Within each atmospheric step, the level-set is advanced with one or more fire substeps Δt_{fire} chosen to satisfy $R\Delta t_{fire} \leq c\Delta x$ across the grid.
- Physically plausible ROS caps. Upper bounds on R per fuel type and environmental state prevent unrealistically large local advances (e.g., under transient gusts or extreme slopes).
- Level-set reinitialization. Periodic signed-distance reinitialization stabilizes $\|\nabla\psi\|$ and the speed function.
- Consistent forcing. Application of mid-flame wind reduction factors and the use of terrain data at a resolution commensurate with the fire grid mitigate artificial inflation of the wind and slope multipliers.

- Realistic ignition seeding. A finite initial burned kernel aligned with observed perimeters avoids spuriously rapid early-time expansion from a point-like ignition on coarse meshes.

Together, these measures keep front advancement physically consistent across grid sizes and explain why resolution-aware tuning (choice of subcycling, ROS caps, and forcing options) is necessary and justified.

2.1.3 BRAMS-SFIRE interface integration

BRAMS was coupled with the SFIRE model to simulate atmosphere and fire interactions (Menezes et al., 2021). The communication between the BRAMS model and the SFIRE model is facilitated through an interface program. In this process, variables from BRAMS related to the basic state of the atmosphere are assimilated through this interface with SFIRE. These variables include surface pressure, air moisture at 2 m, air temperature at 2 m, zonal and meridional wind components at the lowest vertical model levels, geopotential height, air density, microphysics, vegetation cover (including roughness and vegetation type), and heat fluxes.

When SFIRE is called for the first-time step, the driver initializes the SFIRE model by reading SFIRE's parameters from a name list, configuring flags, and setting the grid spacing. The high-resolution SFIRE domain is then integrated into the BRAMS model domain by creating a grid centred on the ignition points, with a radius that encompasses the area predicted to be burned by the fire. Detailed input on fuel behaviour models and terrain height at high resolution must be provided, which are then read and interpolated onto the SFIRE grid domain. After the ignition time, SFIRE injects sensible and latent heat fluxes, along with FRP, into BRAMS, explicitly forcing the atmospheric energy and thermodynamic fields and driving the production and transport of smoke-related aerosol mass. These heat fluxes are directly coupled to the BRAMS turbulence and boundary-layer parameterizations, ensuring dynamic consistency in the representation of fire-induced buoyancy and energy transfer within the atmospheric column.

The BRAMS model offers two approaches for simulating smoke pollution, (1) the dispersion of smoke particulate matter derived from FRP, simulated by SFIRE and used as a passive tracer for atmospheric transport; and (2) a chemistry-coupled approach that integrates smoke particulate matter from SFIRE with emissions from the Biomass Burning Emission Model (3BEM), anthropogenic and biogenic inventories, and analysis data from the Copernicus Atmosphere Monitoring Service (CAMS). This latter approach is implemented through the CCATT module of BRAMS, enabling more comprehensive simulations of atmospheric composition, pollutant transport, and concentration patterns. These dual methodologies enhance the model's capability to accurately represent the complex interactions between fire emissions and atmospheric chemistry.

2.1.4 Plume-rise and vertical injection of fire emissions in BRAMS

In BRAMS, fire-emitted aerosols and gases are not injected solely at the surface. Instead, the model employs an online, physically based plume-rise scheme implemented within the CCATT-BRAMS chemistry and aerosol module (Freitas et al.,

2006; Freitas et al., 2007; Freitas et al., 2010). ~~At each timestep~~At every model timestep, the sensible heat flux released by the fire is used to ~~provides the buoyant energy diagnose the buoyant energy that drives vertical transportthat drives of~~ the plume, which determines the plume-top height dynamically by applying a 1-D time-dependent cloud model. The diagnosed injection height is then projected onto the model's σ -coordinate system, and the emitted mass is vertically distributed across multiple
340 layers, rather than being confined to a single surface level.

Accordingly, BRAMS follows a surface emission plus dynamic plume-rise approach, in which the vertical distribution of smoke is determined interactively at runtime by the evolving fire heat release (Q), atmospheric stability, and convective turbulence, rather than by any fixed or user-defined injection layer. This ensures that the injection height and profile evolve consistently with the meteorological state and the fire intensity.

345 The BRAMS-SFIRE modelling system was evaluated through its application to the Sertã extreme wildfire occurred on 15 October 2017 in central Portugal (Menezes et al., 2024). This event unfolded over complex mountainous terrain dominated by strong valley-mountain circulations, providing a demanding testbed for assessing plume-dynamics realism. Figure 2 shows the simulated smoke column for this case, with PM_{2.5} lofted several hundred metres above the surface. This vertical structure arises directly from the SFIRE-resolved heat fluxes and the associated FRP-derived emissions. The plume-rise diagnosis, after
350 which the smoke is advected, mixed and transformed by the model's dynamical, turbulent and chemistry-aerosol processes described in the following subsections.

~~As an example, Fig. 2 shows the simulated smoke column on 15 October 2017 over complex terrain, with PM_{2.5} lofted well above the surface. This vertical structure is generated online by the SFIRE heat fluxes and the associated FRP derived emissions, which determine the diagnosed plume top height before the mass is subsequently mixed and transported by the model dynamics, turbulence, and the chemistry-aerosol processes described~~
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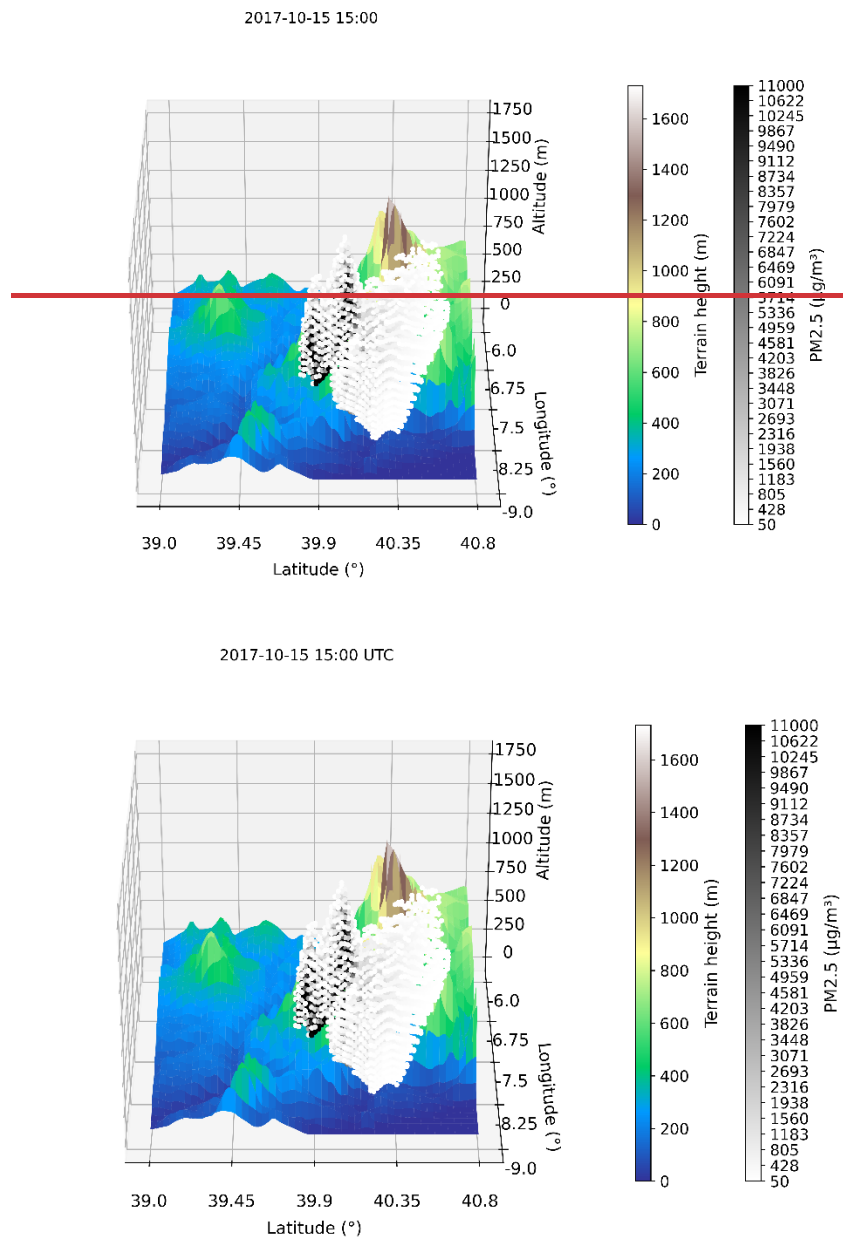


Figure 2: 3-D view of BRAMS-SFIRE smoke injection on 15 Oct 2017 (15:00 UTC); plume-top height and vertical allocation are computed online from SFIRE heat release/FRP using the CCATT-BRAMS plume-rise scheme.

2.1.5 New improvements on BRAMS-SFIRE

Several enhancements were made to this coupled BRAMS-SFIRE system. Fig. 3 schematically shows these improvements.

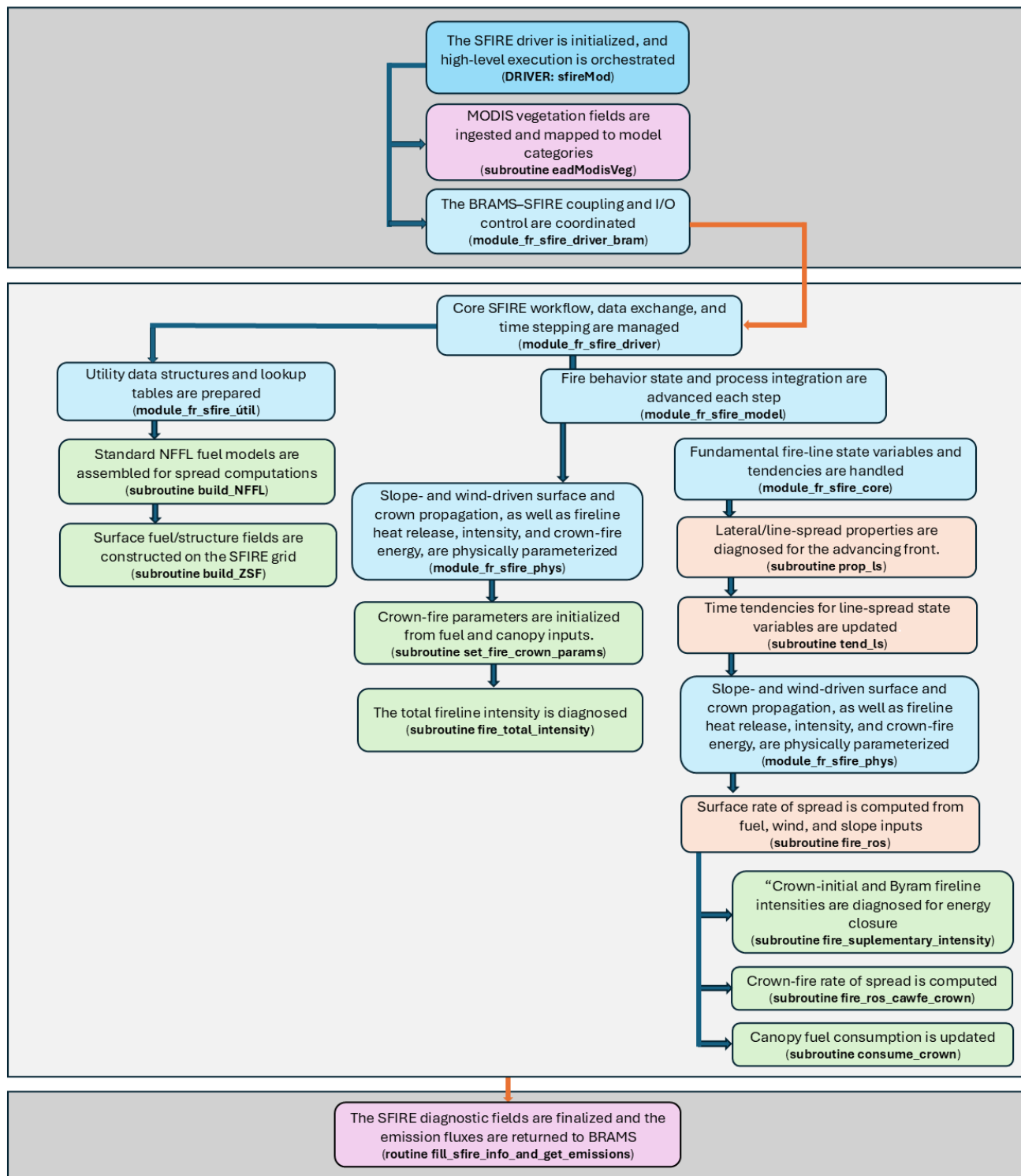


Figure 3: Diagram illustrating the structure of the SFIRE model, with newly integrated subroutines denoted in light green boxes and called within the subroutines highlighted in light orange. The light blue boxes indicate the modules where these subroutines are implemented. The light pink boxes represent the subroutines responsible for integrating the BRAMS and SFIRE models in the context of the wildfire emissions.

[Further details on the improvements and the new subroutines integrated in the modelling system are provided in the following subsections.](#)

2.1.5.16 Implementation of the Crown Fire Behaviour Model

The SFIRE model (Mandel et al., 2009; Mandel et al., 2011), coupled with BRAMS (Freitas et al., 2017) by Menezes et al. (2021) and Menezes (2015a), enables the analysis of surface fire behaviour, accounting for fuel bed type along with its thermal, mineral, and dendrometric characteristics, moisture content, topography, and atmospheric wind conditions. Significant improvements were made to this coupled model based on the work of Scott and Reinhardt (2001), by integrating a numerical model that predicts the spread and intensity of crown fires. This enhancement was incorporated into the SFIRE surface fire spread subroutines, as is illustrated in the scheme shown in Figure 3. The new subroutines were developed to improve the prediction of fire spread and intensity in tree canopies and to perform the interpolation of NFFL fuel behaviour models and terrain elevation onto the SFIRE grid.

In the 'set_fire_crown_params' subroutine, the quasi-steady rate of spread is calculated for fuel behaviour model 10, which is a standardized vegetation fuel description. This model defines the physical and chemical properties of the fuel that are essential for computing fire spread rate, intensity, and overall fire behaviour. In the 'consume_crown' subroutine, the rate of active crown fire spread and the fraction of the canopy fuels consumed are computed. To determine these parameters, the subroutine calculates the equivalent rate of spread $R_{initialization}$ (Eq. (2), concepts in Forestry Canada Fire Danger Group (1992) and Van Wagner (1977)), which depends on the critical (minimum) fireline intensity $I_{initialization}$ of the surface fire, and the heat yield of fuel release per unit area H . It is important to note that SFIRE is implemented using the International System of Units (SI).

$$R_{initialization} = \frac{60I_{initialization}}{H} \quad (2)$$

Where 60 is a conversion factor so that the units for I reduce from $\text{kJ m}^{-1} \text{min}^{-1}$ to kW m^{-1} , and H (Andrews and Rothermel, 1982):

$$H = I_{r10} t_r \quad (\text{in } \text{kJ m}^{-2}) \quad (3)$$

400 The symbol $I_{r_{10}}$ represents the reaction intensity for NFFL fuel behaviour model 10, while t_r (Eq. (4)) represents the residence time for the same model (in minutes). The latter variable is a function of the surface-area-to-volume ratio (σ_{10}), as described below,

$$t_r = \frac{12.595}{\sigma_{10}} \quad (4)$$

405

The rate of active crown fire spread R_{active} (Eq. (5)), set to 40 % of the observed 6.1-meter windspeed at midflame height (Rothermel, 1991), i.e., the average height within the flaming combustion zone where wind directly influences fire behavior. This height is commonly used in fire behavior modeling for standardization, particularly in the context of surface and crown fire interactions. Active crown fire spread varies with wind speed, but is also influenced by slope and foliar moisture content (FMC, measured in percent), through the foliar moisture effect (FME) as defined by Van Wagner (Van Wagner, 1974, 1977, 1989),

410

$$R_{active} = 3.34 \left(\frac{FME}{FME_0} \right) (R_{10})_{40\%} \text{ (in ms}^{-1}\text{)} \quad (5)$$

415 with,

$$FME = \frac{(1.5 - 0.00275FMC)^4}{460 + 25.9FMC} \quad (6)$$

420

considering the ratio of FME to a reference value $FME_0 = 0.0007383$, established for a foliar moisture content (FMC) of 100 percent (Scott and Reinhardt, 2001).

Building upon the transition function concept proposed by Van Wagner (1989) that provides a scaling mechanism between surface and crown fire spread predictions, the model accounts for this process using Eq. (7).

425

$$R_{surface} \geq R_{initialization} + 32.8084 \text{ (in m s}^{-1}\text{)} \quad (7)$$

CFB (Eq. (8)) is a transition function known as the crown fraction burned, representing the fraction of available canopy fuels consumed during a fire. It is used to estimate the degree of crowning (Van Wagner, 1989) and to predict the resulting spread rate in fire behaviour simulations. CFB values range from 0 for a surface fire to 1 for a fully active crown fire.

430

$$CFB = 1 - e^{-0.23(R_{surface} - R_{initialization})} \quad (8)$$

The 'fire_ros' subroutine applies criteria to determine the initiation and sustained spread of crown fires, classifying a fire as either surface fire or crown fire, without differentiating between passive and active crown fire. The approach is based on a threshold criterion (Eq. (9)) involving the fireline intensity required to sustain crown fire behaviour (Classification based on Van Wagner (1977) and Alexander (1988), as described in Figure 6 of Scott and Reinhardt (2001)),

$$I_{surface} > I_{initialization} \quad (9)$$

with $I_{surface}$ representing the Byram fireline intensity, which is the rate of heat release per unit length of fire front (kW m^{-1}), and $I_{initialization}$ (Van Wagner, 1977) calculated within the fire_supplementary_intensity subroutine, as defined in Eq. (10).

$$I_{initialization} = \frac{CBH(460+25.9FMC)^{3/2}}{100} \quad (\text{in W m}^{-1}) \quad (10)$$

where CBH represents the canopy base height. R_{10} refers to the surface fire spread rate for fuel behaviour model 10 (Mandel et al., 2011; Rothermel, 1972), with its components calculated within the 'fire_ros_cawfe_crown' subroutine, as defined in Eq. (11).

$$R_{10} = R_{back_{10}} + R_{wind_{10}} + R_{slope_{10}} \quad (\text{in m s}^{-1}) \quad (11)$$

By substituting Eq. (11) into Eq. (5) from the 'consume_crown' subroutine and incorporating Eq. (8) for crown fraction burned (CFB) from the same subroutine, Eq. (12) can be derived to calculate the total fire spread following Van Wagner (1989, 1993) and the Forestry Canada Fire Danger Group (1992), considering Eq. (9).

$$R_{final} = \begin{cases} R_{surface} + CFB(R_{active} - R_{surface}) & \text{with crown spread} \\ R_{surface} & \text{otherwise} \end{cases} \quad (\text{in m s}^{-1}) \quad (12)$$

The fire_total_intensity subroutine calculates the fire energy flux (ϕ) (W m^{-2} , Mandel et al. (2011)) originating from the combustion of dried fuel, as defined in Eq. (13),

$$\phi = \frac{W_{surface}}{dt} R_{final} \left(1 - \frac{FMC}{1-FMC}\right) H_{Low} \quad (13)$$

where $W_{surface}$ represents the initial total mass of surface fuel (kg m^{-2}), and H_{Low} denotes the lower heat content of the fuel. This calculation, defined in Eq. (14), is performed to predict the fire intensity, I_{final} (Scott and Reinhardt, 2001), accounting for the integration between the shrub/herbaceous layer and the tree canopy.

$$I_{final} = \frac{(H + \phi \cdot CFB) R_{final}}{60} \quad (\text{in W m}^{-1}) \quad (14)$$

2.1.5.27 Implementation of FRP in SFIRE

The following equations, implemented in module_fr_sfir_model, are used to estimate the radiative power emitted from a burning area A , based on the Stefan-Boltzmann law and the sensible-heat (calorimetry) relation. The radiative power P (Eq. (15)) is proportional to the emissivity ϵ , the Stefan-Boltzmann constant σ , the burnt area A , and the fourth power of the temperature T (K).

Alternatively, the equation can also be expressed in terms of the sensible heat flux Q_s (W m^{-2}), the mass of the burned material m , and the specific heat capacity c of dry wood, as shown in Eq. (16).

$$P = 10^{-6} (\epsilon \cdot \sigma \cdot A \cdot T^4) \quad (\text{in MW}) \quad (15)$$

$$P = 10^{-6} \left(\epsilon \cdot \sigma \cdot A \cdot \left(\frac{Q_s}{m \cdot c} \right)^4 \right) \quad (\text{in MW}) \quad (16)$$

The parameters used in this study are as follows: an emissivity value of 0.85 (Àgueda et al., 2010; Riggan et al., 2004), a specific heat capacity for dry wood estimated as $c = 1500 \text{ J (kg K)}^{-1}$ (Radmanović et al., 2014), and the Stefan-Boltzmann constant as $\sigma = 5.67 \cdot 10^{-8} \text{ W (m}^2 \text{ K}^4)^{-1}$.

2.1.5.38 Fuel Models and Terrain Data Assimilation Subroutine Implementation

The build_NFFL and build_ZSF subroutines are responsible, respectively, for the integration of NFFL fuel behaviour models and high-resolution terrain elevation data into the SFIRE computational domain. This process is carried out following the procedure detailed below:

- **Data Input and Configuration:** The subroutines read user-provided input files, generated in accordance with the methodology described by Menezes et al. (2021) and Menezes (2015a). One file contains categorical information on NFFL fuel models, while the other provides terrain elevation data. During this step, key parameters such as grid resolution, initial coordinates, geospatial constants, and the dimensions of both datasets are defined.

- 490
- Coordinate Calculation: Geodetic coordinates (latitude and longitude) corresponding to the input data grids are calculated based on the predefined cell size.
 - Data Interpolation: The input fuel and terrain data are interpolated onto the SFIRE grid by identifying the nearest neighbouring grid nodes. This interpolation employs the Haversine formula to calculate geodesic distances, ensuring that the curvature of the Earth is properly accounted for in the spatial mapping.
- 495
- Result Storage: The resulting interpolated datasets are saved in binary format for efficient access and subsequent use during the simulation workflow.

2.1.5.49 Coupling SFIRE Outputs with the BRAMS Framework for Wildfire Emissions Simulation

The fill_sfire_info_and_get_emissions subroutine integrates the FRP generated by the SFIRE domain simulation into the coarse-resolution grid of the BRAMS model, enabling the calculation of wildfire emissions. It performs the following key tasks:

- 500
- ~~Aggregated radiative power: The FRP, calculated from the SFIRE grid-cell sensible heat flux, is spatially aggregated (summed) into the corresponding BRAMS atmospheric grid cells.~~
 - ~~Iterates over the SFIRE grid to identify cells with positive FRP, burned area and burn duration. These cells are classified as valid active fire points.~~
- 505
- Stores fire data: For each valid fire point, the corresponding information is stored in an array, indexed by geographic coordinates.
 - Calls the subroutine “get_emission_in_global_brams_grid”, which:
 - ~~Maps each fire point from the SFIRE grid onto the global BRAMS grid. BRAMS grid cells exhibiting positive FRP, burned area, and finite burn duration are identified and classified as active fire points.~~
 - ~~Associates each fire point with a vegetation type based on MODIS land cover data within the BRAMS grid. Associates each fire point with a vegetation type, based on land cover (COS) data provided within the BRAMS grid.~~
 - Calculates burned biomass and emissions of various particulate matter species (e.g., PM10, PM2.5), using emission factors and the flaming fraction, which distinguishes between flaming and smoldering phases.
- 510
- Aggregates emissions: The calculated emissions are summed into the respective BRAMS grid cells.
 - Performs statistical calculations: Computes emission statistics, such as the mean and standard deviation of FRP and burned area for each BRAMS grid cell.
- 515

This workflow ensures a seamless integration between fire dynamics modelled by SFIRE and the atmospheric process represented in BRAMS, enabling accurate simulation of wildfire emissions and their atmospheric impacts. In this study, only

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BRAMS passive tracer dispersion capabilities are used, focusing on the transport and dispersion of tracers without engaging

the full atmospheric chemistry module. This approach allows for detailed analysis of pollutant transport patterns while minimizing computational costs.

2.1.5.10 Fire Mesh Refinement and Coupling Strategy within the SFIRE–BRAMS Framework

In SFIRE–BRAMS, the fire module does not operate on an independent or arbitrary domain but rather on a refined computational mesh dynamically generated around the ignition point(s) specified by the user (Fig. 4). The horizontal extent of this refined mesh is defined in degrees of latitude and longitude and determines the size of the nested fire grid within the parent BRAMS domain. The atmospheric grid resolution (typically 2–1 km down to 200 m) and an integer refinement factor (even-valued) jointly control the local fire-grid spacing, which usually ranges from 200 m to 10 m depending on factor the user specifications.

Within this refined sub-domain, SFIRE resolves ignition, flame propagation, and perimeter evolution using the level-set method coupled with the Rothermel (1972) spread-rate formulation. The refinement must, however, remain physically consistent with the expected fire behaviour: excessively coarse fire meshes tend to smooth the flaming front and underestimate fire radiative power (FRP) and burned area, whereas overly fine meshes may become computationally prohibitive without a commensurate gain in accuracy.

Thus, the FRP/active-area/perimeter dynamics are not “scaled” but explicitly resolved at the SFIRE resolution inside the BRAMS parent cell. In this study, we selected the refinement factor by balancing physical realism with the maximum computational user capacity allowed on the available HPC infrastructure (memory per node and MPI task limits), ensuring that SFIRE could explicitly resolve fire-front geometry while maintaining BRAMS time-step stability and tractable wall-clock cost.

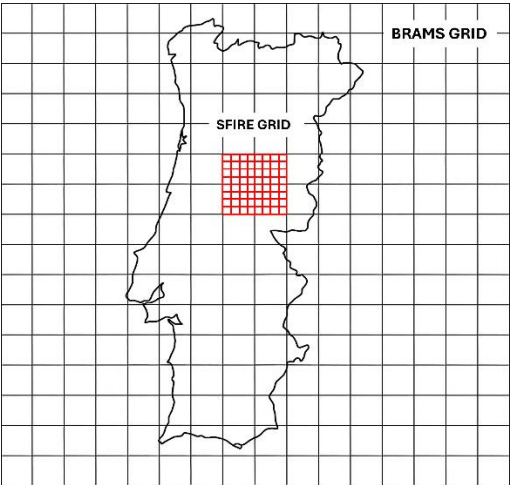


Figure 4: Schematic representation of the SFIRE–BRAMS grid nesting approach. Only for illustration a regular 14×14 coarse-resolution BRAMS grid is superimposed on the outline of mainland Portugal, showing illustrating the atmospheric model domain onto which the finer-resolution SFIRE fire grid can be dynamically embedded.

The simulation domains used in this study are shown in Fig. 5. The coarser domain, corresponding to the BRAMS grid, was configured with a 2 km resolution, while the inner SFIRE domain was nested at a finer resolution of 200 m.

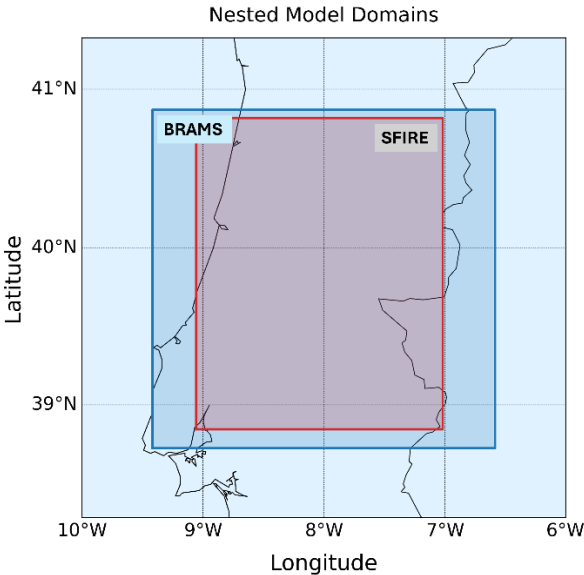


Figure 5: Nested simulation domains over central–northern Portugal. The dark-blue region represents the coarse BRAMS domain (2 km resolution), while the red–cyan region corresponds to the inner high resolution SFIRE domain (200 m resolution).

2.1.5.6H Representation of Aerosol–Radiation Interactions in BRAMS for Iberian Applications~~**Radiative–Aerosol Coupling within BRAMS for Applications over the Iberian Peninsula**~~

Having established the mesh-refinement configuration and the two-way fire–atmosphere coupling, the representation of aerosol-radiation interactions in BRAMS, which shapes wildfire-driven thermodynamic responses over the Iberian Peninsula, is described. The incorporation of regionally tuned Aerosol Spectral Optical Properties (ASOP) models into the BRAMS radiative framework is first outlined, followed by the diagnostic derivation of spectrally resolved smoke optical properties from BRAMS–SFIRE prognostic PM_{2.5} fields. This enables a physically consistent evaluation of wildfire smoke optical behaviour and its radiative feedbacks on the lower troposphere.

2.1.5.6.1 Improvement of Regional Aerosol Spectral Optical Properties into BRAMS

Given the limited spatial-temporal coverage of satellite aerosol products (e.g., MODIS, VIIRS) and reanalysis datasets such as MERRA-2, particularly under cloudy, or nighttime conditions, physically based models such as BRAMS offer both a complementary and, when required, a fully self-contained alternative. BRAMS can ingest satellite information for constraint and evolution, but it also runs in a physically based, coupled fire-atmosphere mode that explicitly simulates fire spread from fuel properties and meteorological conditions, prognoses fire radiative power (FRP), and resolves smoke concentration fields alongside meteorological and thermodynamic variables. Because the realism of these simulations depends critically on how the model represents aerosol optical behaviour, regional parametrisations tailored to Iberian aerosol regimes have become increasingly necessary. In this context, Rosário et al. (2025) developed seasonal Aerosol Spectral Optical Properties (ASOP) models for Iberian aerosol mixtures to improve the representation of radiative and aerosol processes in BRAMS, affecting the atmosphere over the Iberian Peninsula. These models were implemented within the BRAMS framework for improved optical properties of particulate material emitted by a wildfire simulation using the SFIRE model coupled to BRAMS. These ASOP models were subsequently incorporated into BRAMS to enhance the optical characterisation of particulate matter emitted in wildfire simulations performed with the coupled BRAMS-SFIRE system.

Based on a long-term (2003–2023) characterization of aerosol microphysical properties, optical parameters, such as spectral AOD, Angstrom Exponent (AE), SSA asymmetry parameter, and refractive indices, were derived using Mie theory applied to AERONET sun photometer data. The ASOP models represent typical regional aerosol scenarios, including smoke, dust, and background aerosol mixtures. Spatial representativeness was evaluated through monthly correlations between MERRA-2 and AERONET data, including AOD and SSA, enabling the identification of areas predominantly influenced by each model. This approach enhances aerosol-radiative transfer simulations in BRAMS over the Iberian Peninsula, improving predictions of thermodynamic profiles and surface temperatures, while reducing uncertainties in the representation of aerosol optical properties.

2.1.5.6.2 Diagnostic Derivation of Smoke Optical Properties from BRAMS-SFIRE Aerosol Field Output

Given the limited spatial-temporal coverage of satellite aerosol products (e.g., MODIS, VIIRS) and reanalysis dataset such as MERRA-2, particularly under cloud, or nighttime conditions and for short-lived, small-scale agricultural burns (Oliveira et al., 2025), physically based models such as BRAMS, offers both a complementary and, when required, a fully self-contained alternative. BRAMS can ingest satellite information for constraint and evolution, but it also runs in a physically based, coupled fire-atmosphere mode that explicitly simulates fire spread from fuel properties and meteorological conditions, prognoses fire radiative power (FRP), and resolves smoke concentration fields alongside meteorological and thermodynamic variables.

Although BRAMS ~~output~~ ~~does~~ not directly provide aerosol optical properties, in this work, ~~they are, we~~ diagnostically derived ~~them~~ from ~~the~~ prognosed aerosol mass and thermodynamic fields (e.g., temperature and relative humidity). Using Mie theory and radiative-transfer formulations, ~~we obtain~~ spectrally and vertically resolved extinction, scattering, and absorption coefficients ~~are obtained~~, from which ~~we compute~~ integrated optical metrics such as aerosol optical depth (AOD), single-scattering albedo (SSA), and the asymmetry factor ~~are computed~~. This physically consistent offline radiative post-processing ~~enables the allows us to assessment how of~~ wildfire smoke ~~enables the modifications to~~ radiative fluxes and lower-tropospheric thermodynamics (e.g., heating/cooling rates, static stability, boundary-layer evolution), while ~~also facilitating enabling~~ robust comparison with satellite-retrieved AOD.

~~Rosário et al. (2025) developed seasonal Aerosol Spectral Optical Properties (ASOP) models for aerosol mixtures affecting the atmosphere over the Iberian Peninsula. These models were implemented within the BRAMS framework for improved optical properties of particulate material emitted by a wildfire simulation using the SFIRE model coupled to BRAMS. Based on a long-term (2003–2023) characterization of aerosol microphysical properties, optical parameters, such as spectral AOD, Angstrom Exponent (AE), SSA asymmetry parameter, and refractive indices, were derived using Mie theory applied to AERONET sun photometer data. The ASOP models represent typical regional aerosol scenarios, including smoke, dust, and background aerosol mixtures. Spatial representativeness was evaluated through monthly correlations between MERRA-2 and AERONET data, including AOD and SSA, enabling the identification of areas predominantly influenced by each model. This approach enhances aerosol radiative transfer simulations in BRAMS over the Iberian Peninsula, improving predictions of thermodynamic profiles and surface temperatures, while reducing uncertainties in the representation of aerosol optical properties.~~

2.2 Data requirements

2.2.1 Surface data used as input in SFIRE

To simulate the spread of surface and crown fires using SFIRE, high-resolution Northern Forest Fire Laboratory (NFFL) fire behaviour fuel models and terrain elevation data on a regular grid are required. The NFFL fuel behaviour models are a set of 13 canonical fuel categories developed by the US Forest Service's Northern Forest Fire Laboratory (Albini, 1976; Anderson, 1982) to parameterize surface fuel characteristics for operational fire spread modelling (Rothermel, 1972). Each model specifies representative fuel properties, such as fuel load partitioned by size class, surface-area-to-volume ratio, fuelbed depth, heat content, moisture-of-extinction, and live/dead fractions, that together determine ~~the~~ rate of spread, fireline intensity, and flame length under given wind and slope. The NFFL ~~fuel behaviour~~ models provide a standardised mapping between vegetation/fuel types and the inputs required by semi-empirical fire ~~spread behaviour~~ equations; they are widely used for case studies, fire danger rating, and coupled fire–atmosphere applications. While subsequent schemes expanded and refined these categories (e.g. the 40 “standard” fuel models of Scott and Burgan (2004)), the original 13 NFFL models remain a common

reference and are frequently denoted as NFFL 1–13. ~~(e.g. “NFFL 10—timber litter and understory”).~~ Among them, NFFL 10 (timber litter and understory) is particularly relevant because it represents dense surface fuels that readily support high-intensity surface fire, making it one of the canonical fuel types used to evaluate the potential for surface-to-crown fire transition. In this study, NFFL fuel behaviour model data were derived from the Portuguese National Forest Inventory 6 (Menezes et al., 2021). Additional inputs are also needed for the “namelist.fire” file, including physical, thermal, chemical, and mineral specifications of surface vegetation (Menezes et al., 2021; Menezes, 2015a), as well as of tree canopy fuel within the simulation domain (such as canopy base height (CBH) and crown foliar moisture content (FMC)) for the 13 NFFL fuel behaviour models. CBH and FMC values were assigned using GIS methods by intersecting primary and secondary land data with five dominant forestry species (Table 1) and cross-referenced with the 13 NFFL fuel models. These data were part of 7,964 field plots of the 2006 National Forest Inventory, provided by the Portuguese Institute for Nature Conservation and Forests (ICNF, 2015), and adopted from the work of Menezes (Menezes, 2015a) based on measurements conducted in October 2010 in the Évora district, part of the Alentejo region in southern Portugal, characterized by agro-silvopastoral landscapes known as Montado. Although FMC values from international literature were considered, they were ultimately excluded from this study, because ~~as~~ they may not accurately represent the climatic, edaphic, and physiological conditions of Portuguese ecosystems. The FMC values presented in Table 1 were therefore used to do this classification.

Table 1: Average crown foliar moisture content (in %) for the 13 NFFL fuel behaviour models based on field data from five dominant forestry species (Alentejo, Portugal; October 2010) (Menezes, 2015a).

Tree species	FMC
<i>Pinus pinaster</i> Aiton	126.89
<i>Pinus pinea</i> L.	129.62
<i>Eucalipto globulus</i> Labill	118.51
<i>Quercus rotundifolia</i>	63.37
<i>Quercus suber</i> L.	72.32

Following the same methodology, CBH was determined. CBH is influenced by factors such as forest management practices, stand density, tree age, and species composition. In Portugal, CBH values can vary significantly. The specific average ranges, calculated using only the same five tree species, for each of the 13 NFFL fuel models, are detailed in Table 2.

Table 2: Average canopy base height (in meters) for the 13 NFFL fuel behaviour models based on field data from five dominant forestry species (Alentejo, Portugal; October 2010) (Menezes, 2015a).

Fuel Models	CBH
-------------	-----

NFFL 1	6.43
NFFL 2	8.28
NFFL 3	8.11
NFFL 4	8.02
NFFL 5	10.04
NFFL 6	8.94
NFFL 7	9.67
NFFL 8	7.36
NFFL 9	7.32
NFFL 10	7.60
NFFL 11	7.02
NFFL 12	3.02
NFFL 13	0.62

2.2.2 Surface and meteorological data used as input in BRAMS

655 Having detailed the surface datasets used to characterise the SFIRE grid, namely the high-resolution terrain, the land-cover classification, and the associated fuel models and their physical properties that govern fire spread and heat release, the description now turns to the surface and meteorological fields that provide the initial and boundary conditions for the BRAMS grid, thereby ensuring dynamical consistency between the fire module and the atmospheric environment in which it evolves.

To establish the initial atmospheric state, BRAMS incorporated several datasets, including land cover type, soil type, the Normalized Difference Vegetation Index (NDVI), weekly sea surface temperatures, daily soil moisture, and soil temperature.

660 The NDVI was derived from 15-day MODIS composite images spanning 2001 to 2002 (Moreira et al., 2013), while weekly sea surface temperature data were obtained from datasets distributed by [Reynolds et al.](#) (2002). Daily soil moisture, an operational product of CPTEC/INPE based on rainfall estimated from TRMM (Gevaerd and Freitas, 2006), was also integrated. The initialization of soil temperature was based on air temperature values from the first level of the BRAMS atmospheric model.

665 Terrain elevation data with a spatial resolution of 30 arc seconds (approximately 1 km) in latitude and longitude were sourced from the United States Geological Survey's Earth Resources Observation Systems data centre (Gesch et al., 1999) and assimilated during the model initialization.

The atmospheric fields, including zonal and meridional wind, air temperature, geopotential height, and relative humidity, used for both the initialization and boundary conditions, were obtained from the ECMWF Reanalysis v5 (ERA5, 2019). These data

670 were available at 37 vertical pressure levels and 6-hour intervals on a regular grid and were interpolated to the BRAMS grid to ensure consistency between the initial and boundary conditions.

2.2.3 Data used for model validation

675 Having outlined the initial and boundary conditions for the BRAMS grid, the following paragraphs describe the reanalysis datasets used for model validation, which provide an external benchmark for assessing the realism of the simulated fine particulate matter (PM_{2.5}) generated by fire smoke–atmosphere interactions.

Aerosol concentration, extinction coefficients, and AOD values were retrieved from the Modern-Era Retrospective analysis for Research and Applications, version 2 (MERRA-2, 2015) dataset. This dataset assimilates observations from a variety of instruments, including satellite-based radiometers, to provide global, long-term atmospheric reanalysis data.

680 MERRA-2 offers a spatial resolution of $0.5^\circ \times 0.625^\circ$ and includes 72 hybrid-eta vertical levels extending from the surface to 0.01 hPa (Gelaro et al., 2017). Its temporal resolution is 3 hours, consistent across the various atmospheric and aerosol variables. The MERRA-2 collections used in this study were obtained from the Global Modeling and Assimilation Office (GMAO) (MERRA-2, 2015).

685 MERRA-2 uses the GEOS-5 model (~50 km horizontal resolution, 72 vertical levels) coupled to the GOCART aerosol module and a 3-hourly aerosol analysis system (GAAS). Column AOD at 550 nm is assimilated through three-dimensional variational data assimilation. The resulting AOD increments are mapped to three-dimensional aerosol mixing-ratio increments using analysis (Kalman) gain matrix $K = P_f H^T (H P_f H^T)^{-1}$, where H is the linearised observation operator relating model aerosol profiles to column AOD (i.e., $H(x) = \text{AOD}$), and P_f is the forecast-error covariance matrix. This gain distributes the AOD innovation vertically and across aerosol species according to their optical sensitivities and prescribed background-error correlations, yielding dynamically and optically consistent updates of black carbon (BC) and organic carbon (OC) by level and species. BC and OC are not directly observed; rather, they are inferred from the assimilated AOD constraint combined with model modelled radiation, transport, and assumed aerosol optical and microphysical properties (externally mixed tracers; hygroscopic growth as a function of relative humidity (RH); OPAC optical properties and non-spherical dust treatment). Emissions for carbonaceous aerosols include QFED (Quick Fire Emissions Dataset, FRP-based) biomass-burning sources as well as fossil and biofuel emissions, while removal processes comprise dry and wet deposition and scavenging. Oxidant fields follow monthly climatological values. A background-state correction and averaging-kernel diagnostic are applied to ensure consistency between the 3-hour AOD analyses and the 6-hour meteorological assimilation cycle.

690 In summary, MERRA-2 BC and OC fields arise from AOD assimilation constrained by radiative transfer and transport, under fixed assumptions regarding particle size distribution, mixing state, vertical structure, and emissions (Buchard et al., 2015; Buchard et al., 2016; Darmenov and da Silva, 2015; Randles et al., 2017).

700 MERRA-2 uses the GEOS-5 model (~50 km, 72 levels) with the GOCART aerosol module and a 3-hourly aerosol analysis (GAAS). Column AOD at 550 nm is assimilated via three-dimensional variational data assimilation; the analysed AOD

increments are projected to 3-D mixing-ratio increments for each species through $P_f H^T (H P_f H^T)^{-1}$ i.e., the analysis gain that maps an AOD increment into consistent black carbon (BC) and organic carbon (OC) updates by level and species, weighted by optical sensitivities and the model's background error uncertainties. BC and OC are not observed directly; they are inferred from the AOD constraint combined with model radiation/transport and assumed optical/mixture properties (externally mixed tracers; hygroscopic growth vs RH; OPAC optics; non-spherical dust). Emissions for carbonaceous aerosols include QFED (Quick Fire Emissions Dataset, FRP-based) biomass burning plus fossil/biofuel sources; losses include dry/wet deposition and scavenging. Oxidant fields use monthly climatology. A background state correction and an averaging kernel diagnostic are applied for consistency of the 3-h AOD analyses within the 6-h met cycle. In short, MERRA-2 BC/OC arise from AOD assimilation + radiative transfer with fixed assumptions on size, mixing state, vertical profiles, and emissions (Buchard et al., 2015; Buchard et al., 2016; Darmenov and da Silva, 2015; Randles et al., 2017).

2.3 Comprehensive Study of SOD and Atmospheric Properties

In this study, BRAMS simulations were used to provide aerosol mass concentration fields (e.g., PM_{2.5}) associated with wildfire smoke. Since BRAMS does not explicitly calculate aerosol optical properties, these were derived off-line through additional post-processing. To link simulated aerosol mass with size distributions and optical characteristics relevant for biomass burning smoke, a set of representative assumptions and parameters was adopted, as summarized in Table 3. These choices ensure physical consistency with observed smoke properties and provide transparency and reproducibility for the optical analysis presented in the following sections. This section describes the methodology used to derive the optical and microphysical properties of wildfire smoke from the BRAMS-simulated PM_{2.5} field. Although BRAMS-SFIRE internally represents aerosol-radiation interactions, the corresponding optical diagnostics are not available in the analysis output fields. For this reason, all radiative quantities examined in this study were obtained through offline post-processing. A set of microphysical assumptions, including particle size distribution, hygroscopic growth, refractive index, and ageing state, was adopted to translate PM_{2.5} mass into wavelength-dependent extinction and absorption. These choices (summarised in Table 3 described in the Subsection 2.3.6) ensure physical consistency with observed biomass-burning aerosols and provide a coherent framework for the multi-stage optical analysis presented in Subsections 2.3.1–2.3.8.

To enable a consistent comparison between SOD and AOD, it is also necessary to clarify the spectral behaviour of smoke aerosols and the physical interpretation of column optical depth, both in the BRAMS framework and in the MERRA-2 reanalysis.

2.3.1 Spectral SOD analysis and validation

This subsection introduces the definition of smoke optical depth (SOD) and the methodology used to compute its spectral dependence from the BRAMS-simulated PM_{2.5} fields. It establishes the optical formulation, extinction, absorption, and scattering, that forms the basis for the microphysical refinements developed in the subsequent subsections.

In this study, the SOD associated with the Sertã wildfire is quantified in terms of its magnitude, spectral dependence, and sensitivity to atmospheric conditions. SOD is defined as the vertical integral of the aerosol extinction coefficient, combining wavelength-dependent scattering and absorption (Seinfeld and Pandis, 2016). To compute SOD from the BRAMS PM_{2.5} output, the aerosol population is represented using a lognormal dry-size distribution whose wet radius is modified through κ -Köhler hygroscopic growth, and optical efficiencies are evaluated using Mie theory. Meteorological variables such as temperature, relative humidity, and wind field, interact with the aerosol thermodynamic state and transport, conditioning hygroscopic growth and spatial redistribution, thereby influencing the computed spectral extinction. In this study, the smoke optical depth (SOD) generated during the Sertã wildfire is characterized in terms of its magnitude, spectral dependence, and interaction with atmospheric radiation. The influence of meteorological conditions on SOD was also examined, considering variables such as temperature, relative humidity, and wind speed. SOD is defined as the vertical integral of the aerosol extinction coefficient, i.e. the sum of absorption and scattering contributions along the column (Seinfeld and Pandis, 2016). To estimate SOD from simulated wildfire smoke, we combined BRAMS PM_{2.5} concentrations with a physically-based representation of particle size and hygroscopic growth.

The aerosol population is assumed to follow a lognormal size distribution characterized by a geometric mean radius and geometric standard deviation, with size evolution constrained by effective radii reported in field studies of biomass burning smoke (Reid et al., 2005). Hygroscopic growth is parameterized with the κ -Köhler approach (Petters and Kreidenweis, 2007), using κ values representative of fresh and mixed smoke conditions (Carrico et al., 2008; Engelhart et al., 2012). These parameterizations ensure consistency between modelled particle growth and observed microphysical properties reported in biomass burning studies. Under these assumptions, the extinction coefficient at wavelength λ and height z is given by Eq. (17), and the smoke optical depth follows as its vertical integral:

$$\beta_{ext}(z, \lambda) = \int_{r_{min}}^{r_{max}} Q_{ext}(m_{eff}(z, \lambda), r_{wet}, \lambda) \cdot \pi r_{wet}^2 n_{dry}(r_{dry}, z) dr_{dry} \quad (17)$$

$$SOD(\lambda) = \int_{z_0}^{z_t} \beta_{ext}(z, \lambda) dz \quad (18)$$

Where $r_{wet} = g(t, RH)r_{dry}$. Here, Q_{ext} is the Mie extinction efficiency (dimensionless), m_{eff} is the effective complex refractive index, r_{wet} is the physical (wet) particle radius “seen” by the light, and $n_{dry}(r_{dry}, z)$ is the differential number

distribution with respect to dry radius [cm^{-4}] such that $\int n_{dry} dr_{dry} = N(z)$ [cm^{-3}]. Unit consistency is enforced internally (radii converted to a consistent length unit before evaluating πr^2). Because both Q_{ext} and πr^2 depend on the instantaneous particle size, all optical terms are evaluated with the wet radius r_{wet} .

2.3.2 Hygroscopic growth

Having established the optical formulation for SOD, the analysis turns to the hygroscopic growth of smoke particles, a key process that links ambient relative humidity to changes in particle size and refractive index. Because condensation and coagulation are not represented in the BRAMS-SFIRE output used in this research, hygroscopic growth is applied offline using the κ -Köhler framework, ensuring physically consistent wet-radius estimates for the extinction calculations.

Since condensation and coagulation are not explicitly modeled, hygroscopic growth is parameterized with the κ -Köhler approach (Petters and Kreidenweis, 2007):

$$g(t, RH) = \left(1 + \kappa \frac{RH}{1-RH}\right)^{\frac{1}{3}} \quad (19)$$

where κ is the hygroscopicity parameter. ~~Reported values in the literature suggest~~ Literature-based ranges adopted here are:

- fresh/organic-dominated smoke: $\kappa \approx 0.06 - 0.30$ (Carrico et al., 2008).
- mixed/transitioning smoke: $\kappa \approx 0.08 - 0.30$ centered ≈ 0.2 (Engelhart et al., 2012).

These ranges reflect the variability observed across biomass-burning aerosol types and combustion conditions. In this study, the specific κ values adopted for the diagnostic optical calculations are described in Subsection. 2.4.5. Within each scenario (fresh or mixed), κ is treated as a composition-dependent physical parameter and- it taken to be constant across the aerosol size distribution, following common practice in previous observational and modelling studies. the size distribution within each scenario (fresh, mixed), consistent with prior studies.

2.3.3 Size-distribution support and quadrature

The integration bounds are defined in dry radius space as:

After defining the hygroscopic growth treatment, this subsection describes how the underlying dry aerosol size distribution is represented for the subsequent Mie extinction and scattering calculations. The aerosol population is described by a lognormal distribution characterised by a geometric mean (modal) dry radius r_g and geometric standard deviation σ_g .

To ensure full numerical support of the distribution, the integration bounds for the dry radius are defined as:

$$r_{dry} \in [r_{min}, r_{max}] = [r_g \sigma_g^{-k}, r_g \sigma_g^k] \quad (20)$$

with $k \approx 3 - 4$. Here r_g is the geometric mean (modal) dry radius and σ_g is the geometric standard deviation. Choosing $k \approx 3 - 4$ ensures that virtually the entire lognormal number/mass is captured (Hinds, 1999; Seinfeld and Pandis, 2016). The integral is evaluated using a logarithmic discretization of the dry radius interval. While $n = 60 - 100$ bins are commonly recommended to adequately resolve lognormal size distributions for Mie calculations (Bohren and Huffman, 2008; Seinfeld and Pandis, 2016), a grid convergence test performed here ($n = 30$ vs. $n = 80$) yielded negligible differences in bulk and spectral moments (e.g., number, extinction, SSA, AOD). We therefore adopt $n = 30$ to reduce computational costs without loss of accuracy for the present application.

with $k \approx 3$. Values in the range $k \approx 3 - 4$ are commonly recommended (Hinds, 1999; Seinfeld and Pandis, 2016), as they capture virtually all number and mass contained in a lognormal mode. The chosen value ensures that the optical integration fully resolves the aerosol population relevant to biomass-burning smoke.

The radius interval is discretised logarithmically. Although 60–100 bins are traditionally advised for Mie calculations (Bohren and Huffman, 2008; Seinfeld and Pandis, 2016), a grid-convergence test conducted here (30 vs. 80 bins) showed negligible differences in bulk and spectral moments (extinction, SSA, AOD). Therefore, $n = 30$ bins were adopted to reduce computational cost without compromising accuracy.

To evaluate the Mie integrals numerically, the continuous radius interval $[r_{min}, r_{max}]$ is discretised into n logarithmically spaced nodes, defined as:

$$r_j = r_{min} \left(\frac{r_{max}}{r_{min}} \right)^{\frac{j-1}{n-1}}, \quad j = 1, \dots, n \quad (21)$$

2.3.4 Relating r_e to (r_g, σ_g)

Since most field observations report effective radii rather than lognormal parameters, this subsection links the observed effective radius r_e to the geometric mean radius r_g and geometric standard deviation σ_g which are required for the size-distribution model. This conversion ensures consistency between observational constraints and the microphysical inputs used in the extinction calculations.

Most field studies provide the ambient effective radius r_e , not the pair (r_g, σ_g) . Because the single r_e does not uniquely identify both parameters, (i) the ambient r_e was converted to dry effective radius using the hygroscopic growth factor $g(RH)$, and (ii) σ_g was prescribed within literature-based ranges for biomass-burning fine mode aerosols ($\sigma_g \approx 1.5 - 1.9$, typically narrowing with aging; Reid et al. (2005), see Subsection 2.4.5). The corresponding dry r_g then follows from the lognormal moment relation (Hinds, 1999; Seinfeld and Pandis, 2016):

Most field studies report the (ambient) effective radius r_e , not (r_g, σ_g) . Since a single r_e does not identify both r_g and σ_g , we (i) convert ambient r_e to dry conditions via $g(RH)$, and (ii) prescribe σ_g within literature ranges for biomass burning fine mode

($\sigma_g \approx 1.5 - 1.9$, narrowing with aging; Reid et al. (2005)). The dry r_g then follows from the lognormal moment relation (Hinds, 1999; Seinfeld and Pandis, 2016):

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$$\langle r^k \rangle = r_g^k \exp\left(\frac{1}{2} k^2 \ln^2 \sigma_g\right), \quad r_e = \frac{\langle r^3 \rangle}{\langle r^2 \rangle} = r_g \exp\left(\frac{5}{2} \ln^2 \sigma_g\right) \quad (22)$$

Yielding,

825

$$r_g = \frac{r_e}{\exp\left(\frac{5}{2} \ln^2 \sigma_g\right)} \quad (23)$$

A sensitivity analysis across plausible σ_g values quantify the uncertainty in the retrieved r_g and in all subsequently derived optical properties.
~~A sensitivity analysis across plausible σ_g values quantify uncertainty in r_g and derived optics.~~

2.3.5 Mass-consistent normalization and mass fractions ~~(no circularity)~~

830

With the size-distribution framework established, the next step was the partition of the simulated PM2.5 mass consistently across the discretised radius bins. This subsection introduces the mass-fraction formalism used to distribute dry mass, derive bin-resolved number concentrations, and construct internally consistent lognormal sub-populations for Mie calculations. Let $\tilde{n}(r)$ denote the unnormalized lognormal shape (any proportional form is acceptable because the normalisation cancels in fractions). The mass fraction in bin j over $[r_j^-, r_j^+]$ is

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~~Let $\tilde{n}(r)$ denote the unnormalized lognormal shape (any proportional form; the overall scale cancels in fractions). The mass fraction in bin j over $[r_j^-, r_j^+]$ is~~

$$f_j^{(M)} = \frac{\int_{r_j^-}^{r_j^+} r^3 \tilde{n}(r) dr}{\int_{r_{min}}^{r_{max}} r^3 \tilde{n}(r) dr} \quad (24)$$

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Thus, $f_j^{(M)}$ is independent of the total number concentration N since the normalization cancels. Given the bulk dry PM25 mass $C_m(t)$ in a model layer, the -resolved masses follow $M_j = f_j^{(M)} C_m(t)$. If bin-wise number concentrations are required, they can be obtained from the third-moment closure of a lognormal distribution (Curci et al., 2015),
~~so $f_j^{(M)}$ does not require N (the normalization cancels). Given bulk dry PM25 mass $C_m(t)$ in a layer, bin masses are $M_j = f_j^{(M)} C_m(t)$. If desired, bin-wise number follows from the third moment closure (Curci et al., 2015):~~

$$N_j = \frac{M_j}{\rho_j \frac{4}{3} \pi r_{gj}^3 \exp\left(\frac{9}{2} \ln^2 \sigma_{gj}\right)} \quad (25)$$

845 where ρ_j is the dry effective density associated with the aerosol composition in bin j .
The bin-resolved lognormal number distribution is then,
and the bin lognormal is

$$n_j(r) = \frac{N_j}{\sqrt{2\pi} r \ln \sigma_{gj}} \exp\left[-\frac{\ln^2(r/r_{gj})}{2 \ln^2 \sigma_{gj}}\right] \quad (26)$$

850 This ensures that each bin possesses an internally consistent lognormal sub-population whose mass, number, and spectral moments match those used in the optical calculations.
(Here ρ_j is the effective dry density per bin or scenario.)

2.3.6 Aging scenarios

855 To represent the temporal evolution of smoke microphysics during the fire, two plume-age scenarios were adopted, following established observational classifications. This subsection defines the ‘fresh’ and ‘mixed’ smoke regimes, specifies their associated microphysical properties, and links these to the simulation setups described later in Section 2.4.5.

~~We consider~~ two plume-age scenarios were considered (Andreae and Rosenfeld, 2008; Reid et al., 2005), since the studied fire lasted ~11 h and did not reach plume ages representative of aged/scattering conditions:-

$$t = \{t_1: \text{fresh/absorbing}; t_2: \text{mixed}\}$$

860 These scenarios are summarized in Table 3. The ~~smoke optical depth (SOD)~~ was integrated hourly within each phase, with phase durations taken as ~6 h intervals.

Table 3. Classification of smoke-plume aging scenarios adopted in this study based in Reid et al., 2005

Phase	Plume age	Classification	σ_g	GMD (μm)	$r_g = \frac{GMD}{2}$ (μm)	$[r_{min}, r_{max}]$ ($k=3, \sigma_g = 1.7$) (μm)	Notes
t_1	0–6 h (Local time: 13:00h–19:00h)	Fresh / flaming (absorbing)	1.6–1.8 (typ. 1.7)	0.10–0.16 (centre ~0.13)	0.05–0.08 (typ. 0.065)	[0.013, 0.319] for ($r_g = 0.065$)	Fresh cores; very high number; rapid early growth observed.
t_2	6–12 h (Local time: 19:00h –23:00h)	Mixed / transition (incl. smouldering)	1.6–1.9 (typ. 1.7)	0.12–0.30 (most common ≈0.18)	0.06–0.15 (typ. 0.09)	[0.012, 0.442] for ($r_g = 0.09$)	Transition with smouldering + coagulation + some hygroscopic growth.

(Note: For a strictly lognormal distribution, the Count Median Diameter (CMD) and the Geometric Mean Diameter (GMD) are equivalent)

The microphysical characteristics (κ) and bounds (σ_g , $r_{g,dry}$) defined for the t_1 and t_2 phases, used in the Baseline, Conservative, and Lower-Envelope setups for all SOD, SSA, extinction, and absorption calculations, were selected from the hygroscopic growth definitions in Section 2.3.2 and from Table 3, and are formally presented in Section 2.4.5.

2.3.7 Derivation of MERRA-2 single-scattering albedo

Since modelled optical properties are compared against MERRA-2 reanalysis, this subsection describes how single-scattering albedo (SSA) is derived from the species-resolved extinction and scattering optical depths provided by MERRA-2. The same diagnostic formulation is then applied to the BRAMS–SFIRE output to ensure strict consistency in the comparison.

MERRA-2 provides column-integrated aerosol optical extinction and scattering optical depths (AOD) at 550 nm, resolved by process and by species (BC, OC, and total). The single-scattering albedo (SSA) is defined as the ratio of scattering to total extinction:

$$SSA = \frac{\tau_{sca}}{\tau_{ext}} \quad (27)$$

From the MERRA-2 fields and from the model outputs, ~~we computed~~ species-specific SSA were computed as:

$$SSA_{BC} = \frac{\tau_{sca}^{BC}}{\tau_{ext}^{BC}}, \quad SSA_{OC} = \frac{\tau_{sca}^{OC}}{\tau_{ext}^{OC}}, \quad SSA_{tot} = \frac{\tau_{sca}^{tot}}{\tau_{ext}^{tot}} \quad (28)$$

A combined smoke SSA representative of the fine-mode carbonaceous fraction was also derived as:

$$SSA_{BC+OC} = \frac{\tau_{sca}^{BC} + \tau_{sca}^{OC}}{\tau_{ext}^{BC} + \tau_{ext}^{OC}} \quad (29)$$

This same formulation was applied to the BRAMS–SFIRE simulations to ensure consistency with the MERRA-2 diagnostic structure and to enable a direct comparison of modelled and reanalysis optical properties.

2.3.8 Optical properties and spectral dependence of smoke aerosols

The specific extinction efficiency was computed using Mie theory as a function of particle radius, wavelength, and complex refractive index. A wavelength-dependent refractive index was prescribed following observational and review studies on biomass burning aerosols (Andreae and Gelencsér, 2006; Bond and Bergstrom, 2006; Kirchstetter et al., 2004; Reid et al., 2005). In this parameterization, the real part was held approximately constant at -1.55 , consistent with values typically reported for smoke particles, while the imaginary part was assumed to decrease with wavelength, reflecting stronger absorption in the blue due to brown carbon. The refractive indices applied in the simulations were $1.55 + 0.04i$ at 400 nm, $1.55 + 0.02i$ at 550 nm, and $1.55 + 0.01i$ at 700 nm. The Mie computations were used to derive the wavelength-dependent extinction and scattering efficiencies applied in the BRAMS-SFIRE radiation parameterization. However, the single scattering albedo (SSA) itself was diagnosed from the ratio of scattering to total extinction optical depth in both the model and the MERRA-2 data, ensuring consistency between modeled and reanalysis optical properties.

This study analysed three representative wavelengths from the visible spectrum: 400 nm (blue), 550 nm (green), and 700 nm (red). Aerosol particles produced during flaming combustion and from internal combustion engines are largely composed of BC and OC, both of which affect the Earth's radiative balance by reducing visibility and surface irradiance (Bond et al., 2004).

Black carbon is commonly used synonymously with soot, the major light-absorbing component of combustion aerosols in the visible spectrum (Bond and Bergstrom, 2006; Kirchstetter et al., 2004). BC consists of aggregates of nearly pure carbon spherules, with minor amounts of heteroatoms such as hydrogen and oxygen (Andreae and Gelencsér, 2006). Its microstructure is often described as onion-like, with an outer shell of disordered graphitic platelets surrounding a more amorphous carbonaceous core. Unlike crystalline graphite, the platelet layers are turbostratic, meaning that they are misaligned and wrinkled rather than parallel (Bischoff and Warren, 1942; Bond and Bergstrom, 2006). These morphological and chemical characteristics explain the nearly wavelength-independent absorption of BC across the visible spectrum.

In contrast, organic carbon, particularly in the form of brown carbon, exhibits stronger absorption at shorter wavelengths in the near-UV and blue regions, with absorption efficiency decreasing rapidly toward the visible and near-infrared (Andreae and Gelencsér, 2006; Kirchstetter and Novakov, 2004). This motivated the choice of 400 nm in the present analysis. The 550 nm band is a commonly used reference in atmospheric studies and satellite retrievals. At 700 nm, absorption by OC is already weak, while BC, with its nearly wavelength-independent absorption across the visible range, remains the dominant absorber. Although the absolute absorption by BC decreases with wavelength, its relative contribution becomes more important at longer wavelengths such as the red region (Bond and Bergstrom, 2006; Lack and Cappa, 2010).

SOD was calculated for each wavelength by vertically integrating extinction and absorption coefficients along both meridional and zonal cross-sections. The resulting SOD values were analysed in relation to thermodynamic parameters. Additionally, the influence of spectrally resolved smoke absorption on radiative transfer was examined, with emphasis on the visible to near-infrared range, to better understand the wavelength-dependent radiative impacts of smoke aerosols.

To ensure consistency with observational data, simulated SOD at 550 nm was directly compared with MERRA-2 AOD at the same wavelength. This spectral band is widely adopted as a standard reference in aerosol monitoring and ensures compatibility between model output and satellite-derived products.

Simulated SSA was compared with MERRA-2 SSA for BC and OC (Aerosol Optical Depth (AOD) at 550 nm), as well as with the total aerosol SSA from MERRA-2. Although the MERRA-2 files label BC and OC variables as Aerosol Optical Thickness (AOT), we refer to them as Aerosol Optical Depth (AOD) throughout the manuscript for consistency with the literature. Furthermore, SOD at 550 nm was evaluated against MERRA-2 BC and OC extinction AOD. Simulated PM_{2.5} concentrations were also compared with MERRA-2 BC and OC mass concentrations.

Having defined the microphysical and radiative components of the smoke model, this subsection details the spectral behaviour of extinction and absorption across the visible wavelengths. It outlines the refractive-index parameterisation, motivates the selected wavelengths (400, 550, 700 nm), and presents the resulting spectral signatures relevant for the radiative impacts examined later.

The specific extinction efficiency was computed using Mie theory as a function of particle radius, wavelength, and complex refractive index. A wavelength-dependent refractive index was prescribed following observational and review studies on biomass-burning aerosols (Andreae and Gelencsér, 2006; Bond and Bergström, 2006; Kirchstetter and Novakov, 2004; Reid et al., 2005). In this parameterisation, the real part was held approximately constant at ~1.55, consistent with values typically reported for smoke particles, while the imaginary part decreases with wavelength, reflecting the stronger absorption of chromophoric organics (brown carbon) in the near-UV and blue. Although the refractive-index formulation adopted here reflects the dominant OC-rich composition of the plume, the wavelength-independent absorption behaviour of black carbon and its implications for radiative transfer are analysed separately in Section 2.3.8.3.

2.3.8.1 Refractive-index values used and justification

In this study, the complex refractive index was chosen to represent the plume-integrated optical properties of organic-dominated fine-mode smoke, consistent with the carbonaceous composition diagnosed for the Sertã plume. The imaginary component k was set to 0.01–0.03 across 400–700 nm, representing weak absorption characteristic of primary and secondary organic aerosol (Chakrabarty et al 2016; Kirchstetter and Novakov, 2004). These values are substantially lower than those of fresh black carbon, for which k typically ranges from 0.44 to 0.71 in the visible spectrum (Bond and Bergström, 2006; Curci et al., 2015).

2.3.8.2 Rationale for Departing from BC-Like Optical Properties

BRAMS-SFIRE provides bulk PM_{2.5} mass, not speciated BC/OC fields. Because BC constitutes only a small fraction of the simulated carbonaceous mass (see Fig. 9 described in Subsection 3.3) and is confined to a narrow region near the flaming core, prescribing a BC-like refractive index would artificially amplify absorption across the broader plume. The weaker k values

955 therefore represent the plume-average optical behaviour, governed primarily by scattering from OC-rich aerosols, consistent with the MERRA-2 OC extinction fields (see Figs. 10–11 described in Subsection 3.3).

For transparency, the wavelength-specific values used in the optical solver were $1.55 + 0.04i$ at 400 nm, $1.55 + 0.02i$ at 550 nm, $1.55 + 0.01i$ at 700 nm. These parameters were used in the Mie computations to derive the wavelength-dependent extinction and scattering efficiencies.

960 **2.3.8.3 Sensitivity to more absorbing BC-like refractive index**

Sensitivity tests performed with a BC-like refractive index ($k \approx 0.4$) showed enhanced absorption only near the fire front but minimal impact on domain-integrated SOD, SSA, or the SOD–AOD coupling. This behaviour is consistent with previous findings that BC strongly influences absorption in small source-proximal regions but contributes far less to plume-integrated optical depth when OC dominates the aerosol mass (Bond et al., 2013; Lack and Cappa, 2010).

965 Thus, the refractive-index values adopted here should be interpreted as plume-representative rather than BC-representative, while acknowledging that absorption by fresh BC is likely underrepresented, a structural limitation reflected in the optical diagnostics discussed in Sect. 3.1 and in the thermodynamic response analysed in Section 3.6

2.3.8.4 Spectral dependence motivating the choice of wavelengths

Aerosols produced during flaming combustion are largely composed of OC and BC, both of which influence radiative transfer by reducing visibility and surface irradiance (Bond et al., 2004).

970 Black carbon, consisting of turbostratic graphitic aggregates (Bischof and Warren, 1942), exhibits nearly wavelength-independent absorption across the visible range (Bond and Bergstrom, 2006).

Organic carbon, especially brown carbon, absorbs strongly at short wavelengths, with absorption efficiency decreasing rapidly from the near-UV/blue toward the red and near-infrared (Andreae and Gelencsér, 2006; Kirchstetter and Novakov, 2004).

975 These properties motivated the three wavelengths used:

- 400 nm: strong OC/BrC absorption, strong refractive-index contrast
- 550 nm: standard reference band used in satellite retrievals and aerosol studies
- 700 nm: absorption dominated by BC as OC becomes optically weak

Although the absolute absorption by BC decreases slowly with wavelength, its relative importance increases at longer wavelengths.

980 **2.3.8.5 Diagnostic quantities**

Smoke Optical Depth (SOD) was computed at each wavelength by vertically integrating the extinction and absorption coefficients along meridional and zonal cross-sections. In this study, SOD represents the column-integrated smoke burden produced by the BRAMS–SFIRE system and is therefore used both as a physically meaningful depiction of plume structure

985 and as the primary variable for comparison with satellite- and MERRA-2-derived AOD. This comparison was performed at
the same wavelength (550 nm) to ensure compatibility with satellite retrievals. Single-scattering albedo (SSA), diagnostically
derived from the modelled extinction and scattering fields, was compared with MERRA-2 SSA for the BC, OC, and total
aerosol channels. Although the MERRA-2 files label BC and OC variables as AOT, we refer to them as AOD for consistency
with standard aerosol terminology. Additionally, SOD at 550 nm was compared with MERRA-2 BC and OC extinction AOD,
990 and simulated PM_{2.5} concentrations were evaluated against MERRA-2 BC/OC mass concentrations.
In contrast, the diagnosis of smoke–radiation–stability interactions was based on the spectrally resolved extinction and
absorption coefficients (SEC and SAC), which directly control radiative heating rates and thereby modulate the thermodynamic
response of the lower troposphere. Whereas SOD assesses how the model reproduces the large-scale optical signature and
spatial organisation of the plume, SEC and SAC quantify the local radiative forcing that drives changes in stability within the
995 boundary layer.

2.4 Gridding, Background Correction, and Sensitivity Tests

The evaluation of SOD against MERRA-2 products requires three methodological components: (i) a spatial harmonisation
procedure enabling point-to-point comparison, (ii) a background correction that isolates the fire-induced optical contribution,
and (iii) sensitivity tests that quantify how microphysical uncertainties affect the optical diagnostics.
1000 This section describes these three elements, highlighting their interconnections and significance. First, the regridding strategy
used to place the BRAMS grid and the MERRA-2 reanalysis fields onto a common spatial framework is described. Next, the
methodology adopted to remove the contribution from regional background aerosols present in MERRA-2, which is due to its
representation of large-scale sources, but absent in the BRAMS–SFIRE simulation that only contains fire-emitted smoke, is
defined. Finally, the diagnostic scenarios applied in the optical post-processing to assess the robustness of the results and their
1005 stability with respect to microphysical uncertainty, are outlined.
All variables were compared on the coarse BRAMS–SFIRE grid (2 km outer domain). The MERRA-2 fields were bilinearly
interpolated onto the BRAMS grid to enable grid-point matching and to preserve the higher spatial detail of the model fields.
This approach ensured a consistent spatial comparison while avoiding artificial smoothing that would result from regridding
the model data to the coarser MERRA-2 resolution. For each variable (AOD, SSA, BC, OC, and PM_{2.5} concentrations),
1010 collocated grid-point pairs were extracted and used to construct bivariate scatter plots and compute standard statistical metrics.
A detailed description of the analysis methodology is provided in the following subsections.

2.4.1 Apples-to-apples gridding

To enable a meaningful comparison between BRAMS–SFIRE and MERRA-2 aerosol fields, the MERRA-2 data were
remapped onto the native BRAMS grid using a consistent interpolation framework. All analyses were conducted on the 2-km
1015 BRAMS–SFIRE outer-domain grid to ensure spatial representativeness and to minimize interpolation-induced artifacts.
MERRA-2 aerosol variables were bilinearly interpolated onto the BRAMS latitude–longitude grid within the common sub-

domain (with longitudes wrapped to $[-180, 180]$), providing a one-to-one spatial pairing between datasets. Diagnostics included Total Aerosol Extinction AOD ($AOD_{Total_{ext}}$) and Total Aerosol Scattering AOD ($AOD_{Total_{scat}}$) at 550 nm, from which the MERRA-2 single-scattering albedo was computed as:

To ensure spatial representativeness and minimize interpolation artifacts, all comparisons were performed on the native BRAMS-SFIRE grid (2 km outer domain). MERRA-2 aerosol fields were bilinearly interpolated onto the BRAMS latitude-longitude grid within the common sub-domain (with longitudes wrapped to $[-180, 180]$). Diagnostics included Total Aerosol Extinction AOD ($AOD_{Total_{ext}}$) and Scattering AOD ($AOD_{Total_{scat}}$) at 550 nm from which the MERRA-2 single-scattering albedo was derived as:

$$SSA_{MERRA} = AOD_{Total_{scat}} / AOD_{Total_{ext}} \quad (30)$$

Where available, extinction and scattering contributions from BC and OC were also incorporated. Temporal matching used the nearest MERRA-2 timestamp corresponding to each BRAMS output time. Where available, BC/OC extinction and scattering components were also used. Temporal pairing employed the nearest MERRA-2 timestamp to the model output.

2.4.2 Upwind/background subtraction

Because MERRA-2 includes a regional aerosol load that is absent from the BRAMS fire-plume simulation, a background correction was applied to ensure that the comparison reflects only the fire-related contribution to AOD. The background field was estimated using an upwind method that identifies clean-air regions based on the inflow direction. This definition is physically consistent with the advection of background air entering the domain prior to interaction with the smoke plume. An upwind AOD field was computed on the BRAMS grid, and the plume-only optical depth was defined as:

$$AOD' = \max(AOD - AOD_{upwind}, 0) \quad (31)$$

Upwind boundaries were determined from near-surface winds (u_{10}, v_{10}) or, when unavailable, from the mean wind in the lowest five model layers. The upwind band spanned 18% of the domain along the inflow edges (W if $u > 0$, E if $u < 0$; S if $v > 0$, N if $v < 0$). Within this region, AOD_{upwind} was defined as the median of the lower half of AOD values, providing a robust estimate of the clean-air background while minimising contamination from the plume.

To isolate the fire plume contribution and minimize background bias, an upwind background AOD field was computed on the BRAMS grid, and the adjusted plume AOD was defined as:

$$AOD^L = \max(AOD - AOD_{upwind}, 0) \quad (31)$$

Upwind edges were diagnosed from near surface flow (u_{10}, v_{10}) or, when unavailable, from the median wind in the lowest five model layers (u_g, v_g). The upwind band width was set to 18 % of domain size along the inflow boundaries (W if $u > 0$, E if $u < 0$; S if $v > 0$, N if $v < 0$). Within that band, AOD_{upwind} was estimated as the median of the lower half of AOD values, ensuring robustness to residual plume contamination.

2.4.3 Phase windows vs. diagnostic scenarios (~~orthogonality~~)

The optical analysis distinguishes between physical plume-age phases (t_1 : 13–19 UTC “fresh”, t_2 : 19–24 UTC “mixed”) and diagnostic perturbation scenarios. The plume-age phases define the baseline microphysical parameters used in the optical calculations ($\sigma_g, \kappa, r_{g,dry}$). The diagnostic scenarios (BASE, ABSORBING, WIDE SIGMA, SMALL RG, LARGE RG) are then applied within each phase as controlled perturbations to these baseline parameters, while keeping the aerosol mass fixed. For each phase and each diagnostic scenario, an independent set of statistical validation analyses is performed, as described in the following subsection.

The phase windows (t_1 : 13–19 UTC “fresh”, t_2 : 19–24 UTC “mixed”) are temporal subsets used to stratify the analysis and to assign phase-specific optical parameters ($\sigma_g, \kappa, r_{g,dry}$). The scenario labels in the statistical tables (BASE, ABSORBING, WIDE SIGMA, SMALL RG, LARGE RG) denote diagnostic post-processing optical variants applied to the Mie/closure calculator at fixed aerosol mass within each phase. Accordingly, for each simulation and for each phase (t_1/t_2), we report statistics under multiple diagnostic scenarios as described in Subsection 2.4.6.

2.4.4 Phase selection and scope

Since the fire plume evolves rapidly during daytime and becomes more spatially coherent after sunset, selecting an appropriate evaluation window is essential. This subsection provides the rationale for focusing the primary analysis on the mixed-phase period and explains how this choice improves statistical stability.

To reduce diurnal aliasing and ensure stable grid-point pairing, the main evaluation focuses on the mixed phase period (19–24 local time), when the plume is more slowly~~less rapidly~~ evolving and spatial gradients are weaker. This choice minimizes sensitivity to sub-grid plume meandering and transient emission spikes that are more pronounced during early-afternoon hours, providing more stationary conditions for statistical comparison with the reanalysis. Domain-wide all-hours aggregates are also included for completeness.

2.4.5 Microphysical phase windows and simulation setups

In addition to temporal stratification, optical analysis requires specifying phase-dependent microphysical parameters. This subsection defines the microphysical configurations associated with fresh-smoke and mixed-smoke periods and describes how

these parameters are used to diagnostic scenarios (BASE, ABSORBING, WIDE SIGMA, SMALL RG, LARGE RG) described in Subsection 2.4.6.1, which are designed to bracket the Mie-based optical calculations.

To represent plausible within-plume microphysical evolution while preserving mass consistency, two temporal phase windows (t_1 and t_2) were considered. For each phase and scenario, a representative set of microphysical parameters was selected within the ranges defined in Table 3 (Subsection 2.3.6), based on physically plausible values of the lognormal size distribution and hygroscopicity. One-at-a-time sensitivity perturbations were then applied. These scenarios span conservative and lower-bound microphysical states:

- Baseline:

t_1 - fresh/absorbing: $\sigma_g = 1.70, \kappa = 0.12, r_{g,dry} = 0.065 \mu m$

t_2 - mixed: $\sigma_g = 1.70, \kappa = 0.20, r_{g,dry} = 0.090 \mu m$

- Conservative (narrower/less hygroscopic):

t_1 - fresh/absorbing: $\sigma_g = 1.60, \kappa = 0.08, r_{g,dry} = 0.060 \mu m$

t_2 - mixed: $\sigma_g = 1.60, \kappa = 0.14, r_{g,dry} = 0.080 \mu m$

- Lower envelope (most conservative bounds used):

t_1 - fresh/absorbing: $\sigma_g = 1.60, \kappa = 0.06, r_{g,dry} = 0.055 \mu m$

t_2 - mixed: $\sigma_g = 1.60, \kappa = 0.10, r_{g,dry} = 0.070 \mu m$

For all scenarios and wavelengths used in the SOD, SSA, and extinction/absorption calculations, the complex refractive index was prescribed as:

$$m(\lambda) = \{400:1.55+0.04i; 550:1.55+0.02i; 700:1.55+0.01i\} \quad (32)$$

No additional spectral perturbations were applied beyond these baseline values. Mie calculations were evaluated at 400, 550, and 700 nm wavelengths. The geometric integration bounds for the lognormal distribution were fixed at $k = 3$, ensuring consistent coverage ($\sim \pm 3 \sigma$) radius coverage across all cases. Consequently, the sensitivity analysis isolates the effects of σ_g , κ and $r_{g,dry}$ without modifying the prescribed refractive indices $m(\lambda) = n(\lambda) + ik(\lambda)$. In particular, no additional increment of the imaginary refractive indices part (e.g., no +0.02 at 550 nm) and no changes to the spectral slope of $k(\lambda)$ were introduced. All statistical metrics (correlation, bias, RMSE, etc.) were computed from the same Mie-derived optical fields, consistently evaluated at 550 nm using the wavelength-dependent refractive index $m(550) = 1.55+0.02i$.

To capture plausible within-plume microphysical evolution while preserving mass consistency, two temporal phase windows were defined:

- a daytime fresh smoke period (t_1 : fresh/absorbing, 13–19 UTS, dominated by recently emitted, BC/OC rich smoke) and,
- an evening mixed period (t_2 : mixed, 19–24 UTS, representing more aged, diluted, and partially hygroscopic smoke),

For each phase, one at a time envelopes were applied to the lognormal parameters and hygroscopicity to represent conservative and lower-bound microphysical states:

- Baseline:
 - t_1 —fresh/absorbing: $\sigma_g = 1.70, \kappa = 0.12, r_{g, dry} = 0.065 \mu m$,
 - t_2 —mixed: $\sigma_g = 1.70, \kappa = 0.20, r_{g, dry} = 0.090 \mu m$
- Conservative (narrower/less hygroscopic):
 - t_1 —fresh/absorbing: $\sigma_g = 1.60, \kappa = 0.08, r_{g, dry} = 0.060 \mu m$
 - t_2 —mixed: $\sigma_g = 1.60, \kappa = 0.14, r_{g, dry} = 0.080 \mu m$
- Lower envelope (most conservative bounds used):
 - t_1 —fresh/absorbing: $\sigma_g = 1.60, \kappa = 0.06, r_{g, dry} = 0.055 \mu m$
 - t_2 —mixed: $\sigma_g = 1.60, \kappa = 0.10, r_{g, dry} = 0.070 \mu m$

For all runs presented in the plots of SOD, SSA, and extinction or absorption coefficients, the complex refractive index was prescribed as wavelength dependent:

$$m(\lambda) = \{400:1.55+0.04i; 550:1.55+0.02i; 700:1.55+0.01i\} \quad (32)$$

No additional spectral perturbation was applied beyond this baseline, and the Mie calculations were evaluated at 400, 550 and 700 nm wavelengths. The geometric integration bounds for the lognormal distribution were fixed at $k = 3$, ensuring consistent coverage ($\pm 3 \sigma$) coverage across all cases. Consequently, the sensitivity analysis isolates the effects of σ_g, κ and $r_{g, dry}$ without altering the prescribed refractive indices $m(\lambda) = n(\lambda) + ik(\lambda)$, in particular, no additional increment of the imaginary refractive part (e.g., no $+0.02$ at 550 nm) and no changes to the spectral slope of $k(\lambda)$ were introduced. All statistical metrics (correlation, bias, RMSE, etc.) were derived from the same Mie calculated optical fields, evaluated at 550 nm using the wavelength dependent refractive index $m(550) = 1.55 + 0.02i$.

2.4.6 Diagnostic post-processing experiments for optical sensitivity and background treatment

To assess how uncertainties in aerosol microphysics and background aerosol load affect the optical diagnostics, a suite of controlled post-processing sensitivity experiments was performed. These experiments modify only the microphysical

parameters used by the Mie optical calculator and the background treatment applied to AOD, while the simulated aerosol mass fields (PM25) remain unchanged. This design isolates the optical response to microphysical assumptions and background biases without altering the underlying BRAMS–SFIRE plume dynamics.

2.4.6.1 Microphysical perturbation scenarios

- Let $\sigma_g, \kappa,$ and $r_{g,dry}$ denote the phase-dependent baseline parameters defined in Section 2.4.5. Each diagnostic scenario perturbs these parameters through multiplicative scaling factors ($s_g, s_\kappa,$ and s_r) and/or an additive increment in the imaginary part of the refractive index $k(\lambda)$: BASE: reference optics for the active phase, using the unmodified microphysical parameters;
- ABSORBING: enhanced intrinsic absorption and reduced hygroscopicity ($k(\lambda) = +0.02$ at 550 nm; $\kappa \times 0.6$);
- WIDE SIGMA: broader size distribution ($\sigma_g \times 1.10$) with the lognormal grid discretised over $n = 30$ radius bins $[r_g \sigma_g^{-3}, r_g \sigma_g^3]$;
- SMALL/LARGE RG: reduced or increased dry geometric radius ($r_{g,dry} \times 0.80$ or 1.2), representing plausible bounds for each phase rather than arbitrary $\pm 20\%$ variations.

These perturbations are purely diagnostic and are applied independently to quantify how variations in $\sigma_g, \kappa, r_{g,dry}$, and $k(\lambda)$ influence extinction, scattering, absorption, SOD, and SSA.

2.4.6.2 Background-subtracted anomaly fields

Depending on the diagnostic objective, comparisons may be performed using either the raw optical depth fields or background-subtracted anomaly fields. A binary flag (TRUE/FALSE) indicates whether background removal is applied before computing the statistical metrics:

- FALSE -no background subtraction:
Statistics are computed from the raw fields, $X = \text{AOD}$, $Y = \text{SOD}$
- TRUE -with background subtraction:
A background level is diagnosed for each hourly field to isolate the smoke-related anomaly.

2.4.6.3 Background estimation

The background AOD (AOD_{bg}) is obtained using the upwind clean-air region identified according to Subsection 2.4.2. For each hour:

1. The inflow direction is determined from the near-surface winds (10 m) or, when unavailable, from the mean wind in the lowest five model layers.

2. An upwind band corresponding to 18% of the domain width is extracted along the inflow boundary.

3. AOD_{bg} is defined as the median of the lower half of AOD values within this upwind band, a conservative estimator designed to minimize residual plume influence.

The same methodology is applied to obtain SOD_{bg} , although in practice BRAMS has negligible regional aerosol loading and $AOD_{bg} \approx 0$.

Anomaly fields are:

$$AOD' = \max(AOD - AOD_{bg}, 0)$$

$$SOD' = \max(SOD - SOD_{bg}, 0)$$

Statistical comparison is then computed using $X = AOD'$, $Y = SOD'$

This procedure removes the nearly constant regional aerosol offset present in MERRA-2 but absent from the simulated plume, typically reducing bias, lowering the regression intercept, and strengthening correlation and linearity in the SOD–AOD relationship.

2.4.6.4 Workflow of the diagnostic post-processing

The full statistical diagnostics for all microphysical sensitivity scenarios (BASE, ABSORBING, WIDE_SIGMA, SMALL_RG, LARGE_RG), spatial masks (ALL, P70, P80, P90), and background configurations (AOD vs. AOD') are computed using this post-processing workflow. These results are presented in Tables 5 and 6 of Section 3.3, with the full set of diagnostics provided in the Supplementary Material (Tables S1–S3) and are further discussed in Section 3.2 and 3.3 of the Results and Discussion.

2.4.6 Post-processing optical sensitivity scenarios (diagnostic only)

To explore the optical closure sensitivity at fixed aerosol mass, a set of diagnostics, one at a time optical scenarios was applied in post processing. These scenarios modify only the parameters used by the optical calculator (Mie/closure efficiencies Q_{ext} , Q_{abs} , Q_{scat}) while keeping the simulated aerosol fields unchanged.

Let σ_g , κ and $r_{g, dry}$ denote the base parameters defined for phase t (fresh or mixed). Each scenario perturbs these parameters through multiplicative scaling factors (s_g , s_κ and s_r) and/or an additive increment in the imaginary refractive index $k(\lambda)$:

- BASE: reference optics for the active phase, using the absolute microphysical parameters defined for each phase window (no additional perturbation applied).
- ABSORBING like: increased intrinsic absorption and reduced hygroscopic growth ($k(\lambda) = +0.02$ at 550 nm; κ scaled by 0.6).
- WIDE_SIGMA: implemented by increasing the lognormal width (σ_g) relative to the phase baseline, conserving column mass. The particle size grid is logarithmically spaced with $n = 30$ bins over $[r_g \sigma_g^{-3}, r_g \sigma_g^3]$.

- ~~SMALL/LARGE RG: smaller or larger dry geometric radius ($r_{g, dry}$ scaled by 0.8 / 1.2), representing discrete phase-specific configurations rather than $\pm 20\%$ perturbations.~~

~~The absolute optical values therefore depend on the phase-specific baseline, while the scaling factors define the relative perturbation applied in each diagnostic scenario. Percentile masks (P70–P90) were computed for exploratory statistics, while the main analysis and figures report domain-wide (all-hours) results.~~

2.4.7 Evaluation metrics and visualization

A consistent set of statistical metrics is required to quantify differences between simulated and reanalysis optical properties. This subsection describes the evaluation framework used for the main BRAMS–MERRA-2 comparison, including the metrics, temporal pairing, and visualisation strategy.

Model–reanalysis pairs were formed on the native BRAMS grid after bilinear interpolation of MERRA-2 and nearest-hour temporal pairing. Statistics were computed both for the raw AOD and for the background-corrected field,

$$AOD' = \max(AOD - AOD_{upwind}, 0) \quad (33)$$

using all valid grid-point pairs over the common domain (i.e., no percentile-based plume masks were applied).

The diagnostic set comprised means of X and Y, bias (X–Y), mean absolute error (MAE), root-mean-square error (RMSE), Pearson correlation coefficient (r), and Spearman’s rank correlation coefficient (ρ), and ordinary-least-squares (OLS) linear fit $Y = aX + b$ with coefficient of determination (R^2). The primary evaluation used $X = SOD_{550}$ and $Y \in \{AOD_{550}, AOD'_{550}\}$. The same framework was applied to SOD vs. BC/OC extinction and to model-diagnosed SSA vs SSA from MERRA-2. Hourly diagnostics were subsequently aggregated into all-hours statistics.

Scatter plots were rendered as log-density hexbin diagrams to avoid overplotting. Each diagram was rendered as log-density hexbin plots, including the 1:1 reference line, the OLS regression, and annotated values of the key statistics (e.g., r, ρ , RMSE, bias and R^2) ensuring visual and quantitative consistency with the tabulated metrics.

All hourly statistical results derived from this evaluation framework, are presented in Table 4 and scatters of Fig. 8, discussed in Section 3.2, and scatters of Fig. 11 and 13, discussed in Section 3.3 of the Results and Discussion.

2.4.7 Evaluation metrics and visualization

~~Model–reanalysis pairs were formed on the native BRAMS grid after bilinear interpolation of MERRA-2 and nearest-hour temporal pairing. Statistics were computed for both the raw AOD and the background-corrected field:~~

$$AOD^t = \max(AOD - AOD_{upwind}, 0) \quad (33)$$

No percentile (“in plume”) masks were applied; all valid grid point pairs over the common domain were used.

The diagnostic set comprised means of X and Y , bias ($X - Y$), mean absolute error (MAE), root mean square error (RMSE), Pearson correlation coefficient (r) and Spearman’s rank correlation coefficient (ρ), and ordinary least squares (OLS) linear fit $Y = aX + b$ with R^2 . We evaluate $X = SOD_{550}$ against $Y \in \{AOD_{550}, AOD_{550}^t\}$, and applied the same framework to SOD vs. BC/OC extinction and to SSA (model) vs SSA (MERRA-2). Hourly results were aggregated into all-hours summaries. Scatter plots were rendered as log-density hexbin diagrams to avoid overplotting, showing the 1:1 reference and the OLS fit; with key metrics (e.g., r , ρ , RMSE, bias) annotated on each panel.

2.4.8 Physical background (AOD-upwind)

In this approach, the background optical depth (AOD_{bg}) is computed upwind of the smoke plume, that is, within grid cells located in the direction opposite to the plume advection, where the smoke has not yet arrived. These regions represent the true clean air background entering the domain before interacting with the fire emissions.

Formally,

$$AOD_{bg} = \text{mean}(AOD_{upwind\ region}) \quad (34)$$

where the upwind region is defined according to the 10-m wind field or the mean flow within the mixed layer. This approach has the advantage of being physically consistent, as it represents the incoming air mass prior to smoke influence. Its main limitation is that it requires an accurate estimate of wind direction and a well-defined upwind spatial mask to exclude partially affected cells.

2.4.9 Computation of background-subtracted fields

The background flag (TRUE/FALSE) in Tables S1–S3 of supplementary material indicates whether a spatial background removal was applied before computing the statistical metrics:

- FALSE (no background subtraction):

Statistics are computed directly from the raw fields, $X = AOD$, $Y = SOD$

- TRUE (with background subtraction):

A background level is estimated for each hourly field to isolate the smoke-related anomaly.

1. Background estimation:

AOD_{bg} is taken as the spatial median (or a low quantile, e.g. P10–P25) of “clean air” grid cells within the domain for that hour.

The same approach is applied to SOD_{bg} (often ~ 0 in the model).

2. Anomaly computation:

$$AOD^t = \max(AOD - AOD_{bg}, 0)$$

$$SOD^t = \max(SOD - SOD_{bg}, 0)$$

3. Statistical comparison:

The diagnostics are then computed using $X = AOD^t, Y = SOD^t$

This procedure removes the nearly constant regional aerosol offset present in MERRA-2 but not in the simulated plume, thereby reducing bias and intercept values and typically improving correlation. In some experiments, the background may alternatively be derived from the corresponding no-fire run; the principle, using anomaly fields to represent fire-related optical depth, remains the same.

2.4.8 PM2.5 Quality Assurance and Plume-Evolution Diagnostics

In addition to the optical and microphysical diagnostics, a set of supplementary procedures was implemented to verify the physical consistency of the simulated aerosol fields and to examine their spatial and temporal evolution during the wildfire event. These quality-assurance analyses were performed independently from the optical post-processing and serve to document the behaviour of the PM2.5 mass field that underpins the SOD calculations.

2.4.8.1 Distribution checks and hourly histograms

To examine the spatial distribution of simulated surface PM2.5 concentrations, two complementary histogram-based diagnostics were used.

The first diagnostic, shown in Fig. 14 (Section 3.4), consists of hourly histograms constructed from all PM2.5 surface values at selected times. These histograms use a fixed number of concentration bins and a logarithmic frequency axis, providing an instantaneous view of the spatial distribution at those specific hours. They are intended to highlight features such as broad upper tails or isolated high-value spikes that may influence the interpretation of the optical fields.

The second diagnostic, illustrated in Fig. 15 (Section 3.4), is a histogram representative of a particular hour extracted from a continuous, hour-by-hour quality-assessment procedure applied throughout the simulation period. While the binning strategy is similar to that used in Fig. 14, this diagnostic serves a different purpose: it documents the distribution of PM2.5 at each hour as part of a systematic evaluation of numerical consistency, unit handling, and physical plausibility. The figure shown corresponds to one of these hourly distributions.

1295 Together, these two diagnostics provide complementary perspectives, Fig. 14 focuses on selected hours relevant to the optical analysis, while Fig. 15 represents the broader quality assessment-oriented evaluation conducted across all simulation times.

2.4.8.2 Column-integrated PM2.5 evolution north of the fire line

1300 A complementary plume-evolution diagnostic focused on the portion of the domain located north of a fixed latitude threshold (40.35° N). For each hourly output, the vertically integrated PM2.5 column mass was computed and summed over all grid cells north of this latitude. This metric serves as a bulk indicator of the amount of smoke crossing the latitude line and therefore provides insight into directional plume transport and the potential for dynamical trapping or stagnation.

1305 The corresponding time series is presented in Fig. 22 and described in Section 3.6 of the Results and Discussion. This diagnostic allows interpretation of whether the plume is steadily advected, transiently confined near the source, or intermittently re-accumulated under weak-wind conditions, behaviour relevant for understanding plume-background interactions, residence times, and the temporal structure of the optical evaluation.

2.4.8.3 Local accumulation and meteorological co-variability

1310 To characterize potential interactions between smoke loading and near-surface meteorology, PM2.5 column mass and sensible heat flux (H) were extracted at three representative locations along the plume pathway: a point near the fire origin, a midpoint within the valley corridor, and a downwind endpoint. For each site, hourly time series of column-integrated PM2.5 and sensible heat flux were constructed.

The PM2.5 series were accompanied by simple diagnostic indicators, namely the median, the p70–p90 range, and the hourly maximum, to highlight temporal fluctuations in column loading and to identify periods of enhanced local concentration. Sensible heat flux was co-plotted to document concurrent variations in surface forcing, enabling a qualitative assessment of the temporal co-variability between thermodynamic conditions and smoke loading.

1315 This procedure provides an auxiliary, location-specific diagnostic framework used to contextualize plume behavior and near-surface meteorological conditions. The interpretation of these series is presented separately in Fig. 23 and in Section 3.6 of the Results and Discussion.

2.4.9 Quality control

1320 Finally, to ensure reproducibility and physical consistency, all fields used in the analysis were subjected to systematic quality-control procedures. This subsection summarises the checks applied to meteorological, optical, and microphysical variables prior to statistical evaluation.

Relative humidity was clipped to the physically meaningful range [0, 0.999]. Heights were ingested directly in metres or, when stored as geopotential, converted using division by gravitational acceleration (g). Layer thicknesses were verified to remain within plausible atmospheric limits.

1325 All configurable parameters, such as the upwind-band width, statistical options, and microphysical sensitivity factors, were explicitly documented to guarantee transparency and reproducibility of the diagnostic workflow.

2.4.10 Quality control

1330 Relative humidity was clipped to the physical range [0, 0.999]. Heights are read directly in meters or derived from geopotential divided by gravitational acceleration (g), and column thickness was verified to lie within plausible atmospheric limits. All configurable parameters, including the upwind-band width, statistical options, and sensitivity factors, were documented to ensure reproducibility.

2.5 Absorption of Solar Radiation by Smoke and Radiative Budget Impacts

1335 Smoke aerosols modify the surface radiation budget through scattering and absorption of solar radiation. To quantify these effects, differences between simulations without and with fire emissions were evaluated using the accumulated surface downwelling shortwave (W m^{-2}) and longwave (W m^{-2}) radiative fluxes. This comparison provides a first-order estimate of how the presence of smoke alters the net radiative energy reaching the surface.

In addition to these broadband radiative diagnostics, the smoke-absorbed shortwave flux at 550 nm, $F_{abs}(550\text{nm})$ (W m^{-2}), was estimated by relating the vertically integrated aerosol absorption to the heating potential of the plume. The column absorption optical depth at 550 nm is computed as:

1340
$$\tau_{abs}(550) = \int_{z_0}^{z_t} Q_{abs}(m_{eff}(z, 550), g, r_{dry}, 550) \pi (g r_{dry})^2 n_{dry}(r_{dry}, z) dr_{dry} dz \quad (34)$$

where Q_{abs} is the Mie absorption efficiency for the effective refractive index m_{eff} , g is the hygroscopic growth factor, r_{dry} the dry particle radius, and n_{dry} the dry-number distribution.

1345 A simplified diagnostic estimate of smoke-absorbed radiant energy is then obtained as:

$$F_{abs}(550\text{nm}) = H_{sen} \tau_{abs}(550) \quad (35)$$

1350 where H_{sen} is the surface sensible heat flux associated with the fire. Although not a full radiative-transfer computation, this formulation provides a physically interpretable proxy linking absorption optical depth to the potential radiative heating within the plume.

The radiative balance was analysed by comparing simulations results with and without fire, specifically considering surface downwelling shortwave radiation (W m^{-2}), and surface downwelling longwave radiation (W m^{-2}). These accumulated energy fluxes are used to evaluate the radiation budget under smoke conditions at the surface. The smoke absorbed shortwave

1355 radiation at 550 nm ($F(550\text{ nm})_{\text{abs}}, \text{W m}^{-2}$) was estimated based on the heating potential of the fire plume and the vertical profile of aerosol absorption using the following relation expressed in Eq. (35):

$$\tau_{\text{abs}}(550) = \int_{z_g}^{z_t} \int Q_{\text{abs}}(m_{\text{eff}}(z, 550), g r_{\text{dry}}, 550) \pi [g r_{\text{dry}}]^2 n_{\text{dry}}(r_{\text{dry}}, z) dr_{\text{dry}} dz \quad (34)$$

$$1360 F(550\text{ nm})_{\text{abs}} = H_{\text{sen}} \tau_{\text{abs}}(550) \quad (35)$$

Where H_{sen} is the surface sensible heat flux associated with the fire.

2.6 Vertical Profiles of Aerosol Optical Properties and Atmospheric Stability

1365 Building on the radiative impacts examined in Subsection 2.5, this section investigates how smoke-induced heating interacts with the vertical thermodynamic structure of the atmosphere. The analysis focuses on the coupling between aerosol optical properties, namely extinction and absorption and atmospheric stability in smoke-affected layers.

1370 Atmospheric stability was evaluated using vertical profiles of potential temperature (θ) and relative humidity (RH), extracted along a longitudinal cross-section intersecting the plume. These profiles were displayed in paired panels, showing the differences between fire and no-fire conditions relative to the corresponding no-fire reference fields, thereby isolating smoke-induced thermodynamic modifications. Thermal inversions were identified from layers where θ increases with height ($d\theta/dz > 0$), indicating inhibited vertical mixing. Although RH is not used as a formal inversion criterion, its vertical structure provides a supplementary indicator: sharp RH transitions or inflection points often coincide with inversion layers and therefore help delineate the vertical extent of stratified regions.

1375 To relate thermodynamic modifications to aerosol–radiation interactions, vertical cross-sections of the smoke extinction coefficient (SEC) and smoke absorption coefficient (SAC) at 500 nm and 700 nm were analyzed together with CAPE and CIN diagnostics. CAPE and CIN were computed and displayed in paired panels for both the smoke and no-fire states. This layout provides a direct visual comparison between (i) the underlying thermodynamic structure, (ii) the radiative perturbations induced by smoke (via SEC and SAC), and (iii) the corresponding stability response under convectively favorable (CAPE) or suppressed (CIN) conditions.

1380 This combined framework, thermodynamic profiles, RH structure, and smoke optical properties, provides the basis for interpreting how absorption-driven heating may alter stratification and vertical mixing. The resulting cross-sections used in the analysis are presented in Figures 17-21 of Section 3.6 (Results and Discussion), where their implications are examined in detail.

1385 Atmospheric stability was assessed specifically within smoke-affected layers of the atmospheric column. The analysis focuses on detecting thermal inversions by examining vertical profiles of potential temperature and relative humidity in regions

influenced by simulated smoke, under both fire and no-fire scenarios. A thermal inversion is identified when both potential temperature and relative humidity increase with height.

To evaluate the impact of smoke on atmospheric stability, these thermodynamic profiles were analysed in conjunction with vertical distributions of smoke extinction and absorption coefficients at 550 nm. This approach highlights the interaction between radiation and fine particulate matter (PM_{2.5}), and the resulting effects on local temperature structure.

Furthermore, Convective Available Potential Energy (CAPE) and Convective Inhibition (CIN) were compared for smoke and non-smoke conditions. Differences in these parameters (Δ CAPE and Δ CIN) were computed and represented as vertical profiles, providing insights into how smoke alters convective dynamics and overall atmospheric stability.

3 Results and discussion

In the following sections, we first compare the burned area produced by the wildfire episode in Sertã as simulated by the BRAMS and WRF models, in order to evaluate fire-spread performance in a forested region with complex topography and dynamically evolving mountain-valley breezes. Second, the simulated Smoke Optical Depth (SOD) is evaluated against MERRA-2 AOD to assess spatial and temporal coherence over the region. Column-integrated extinction coefficients at 550 nm are also compared with extinction derived from MERRA-2 BC and OC aerosol components, to determine whether the simulated optical behaviour is consistent with the dominant aerosol types present during the event.

The simulated SSA is compared with MERRA-2 SSA, along with simulated and MERRA-2 aerosol mass concentrations, to validate whether the simulated aerosol composition, particularly the relative abundance of BC and OC, is consistent with observed radiative behaviour. This comparison also evaluates whether the simulated vertical mass profiles of BC, OC, and PM_{2.5} are consistent with the resulting optical properties. Frequency distributions of surface PM_{2.5} concentrations across the simulation domain are analysed to characterise the spatial variability of particulate loading and to identify the prevalence of low-, moderate-, and high-concentration regimes. In addition, the impact of smoke absorption on surface downwelling shortwave and longwave radiation is assessed to determine how the simulated aerosol burden modifies the local radiative budget. The optical effects on atmospheric stability are investigated through the analysis of CAPE and CIN, which provide complementary measures of convective potential and suppression. Vertical profiles of extinction and absorption coefficients are further examined together with the development of thermal inversion layers, enabling an assessment of whether the model accurately reproduces the radiative signature of smoke and its influence on local thermodynamic structure.

In the following sections, the burned area resulting from the wildfire episode in Sertã is compared between simulations using the BRAMS and WRF models, in order to assess fire spread performance under forested and complex topographic conditions. Simulated SOD is evaluated against MERRA-2 AOD to assess spatial and temporal coherence. Column-integrated extinction coefficients at 550 nm are also compared with extinction derived from MERRA-2 BC and OC aerosol components, in order to verify whether the simulated optical processes reflect the dominant aerosol types observed.

The simulated SSA is compared with MERRA-2 SSA, along with simulated and MERRA-2 aerosol mass concentrations, to validate whether the simulated aerosol composition, particularly the relative abundance of BC and OC, is consistent with observed radiative behaviour. This comparison also aims to verify whether the simulated mass profiles of BC, OC, and PM2.5 correspond to the resulting optical properties. Frequency distributions of particulate matter concentrations across the simulation domain are analysed to assess the spatial variability and intensity of aerosol loading. Additionally, the impact of smoke absorption on surface downwelling shortwave and longwave radiation is evaluated.

The optical effects on atmospheric stability layers are investigated through the analysis of CAPE and CIN. Vertical profiles of extinction and absorption coefficients are further examined in relation to the development of thermal inversion layers, in order to determine whether the model accurately reproduces the optical signature of smoke in radiative transfer simulations.

3.1 BRAMS and WRF model differences in burned area representation and their implications

Significant differences in the simulated burned area for the same Sertã wildfire event, as depicted in Fig. 6, were observed between BRAMS-SFIRE and the WRF-SFIRE results previously reported by Menezes et al. (2024). BRAMS-SFIRE simulated a broader westward spread, while WRF-SFIRE produced a more confined footprint; that extended, extending further north. These discrepancies arise from differences in model configuration, fire propagation schemes, and spatial resolution.

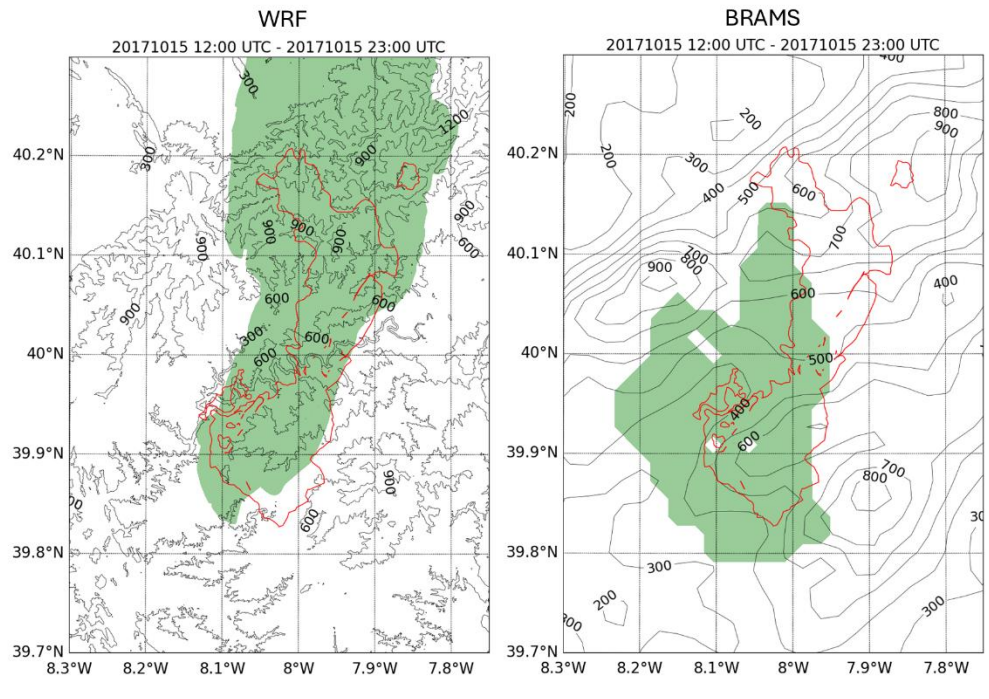


Figure 6: Comparison of simulated burned area over high-resolution topography from the (a) WRF-SFIRE and (b) RAMS-SFIRE models for the wildfire event on 15 October 2017, accumulated between 12:00 and 23:00 UTC. Green-shaded regions represent the cumulative burned area, while red contours delineate the observed fire perimeter.

First, although WRF-SFIRE resolves fire spread at a finer horizontal resolution (20 m) than RAMS-SFIRE (200 m), RAMS exhibits stronger sensitivity to terrain-induced effects due to its topographic assimilation and interaction with the atmospheric fields at coarser grid scales (2 km in diagnostics). This can amplify upslope spread, especially on west-facing slopes, where heating of unburned fuels by the flame front is intensified. Additionally, RAMS employed a default rate of spread approximately ten times greater than that used in WRF, resulting in more aggressive lateral fire expansion, particularly in regions where wind-driven constraints are weaker.

Second, resolution differences in output diagnostics further influence the apparent burned area. WRF's higher resolution (20m) output preserves more spatial detail, limiting the smoothing of the burned footprint. Conversely, the RAMS burned area (200 m resolution) was accumulated and plotted in the RAMS 2 km grid resolution, which introduces spatial averaging and may artificially enlarge the apparent extent of fire-affected regions.

Moreover, the delayed onset of burned area in RAMS-SFIRE when using lower propagation rates is not solely due to ignition misalignment, but rather a result of the interaction between the fire spread rate and the coarser fire grid resolution (200 m). Unlike WRF-SFIRE, which operates at a much finer 20 m resolution for fire propagation, RAMS requires the flame front to traverse larger grid cells to ignite neighbouring areas. This means that if the default rate of spread is reduced without compensating for grid size, the fire may fail to reach adjacent cells in a timely manner, leading to an underrepresentation of burned area in the early stages. Therefore, a balanced calibration is needed between the fire spread rate and grid resolution in RAMS to ensure that the ignition front progresses consistently with observed timelines. While finer resolution in WRF (20 m) inherently provides more accurate spatial detail in fire development (Menezes et al., 2024), RAMS relies on a more approximate representation, making it sensitive to how rate-of-spread parameters are tuned relative to its mesh scale.

In summary, while WRF-SFIRE offers finer-scale detail in fire perimeter shape, RAMS-SFIRE exhibits stronger coupling between fire dynamics, topography, and atmospheric feedbacks. For prognostic simulations of fire spread and smoke transport in complex terrain, RAMS-SFIRE may provide enhanced physical realism, provided its rate of spread is properly calibrated to avoid over propagation, particularly in orographically enhanced directions.

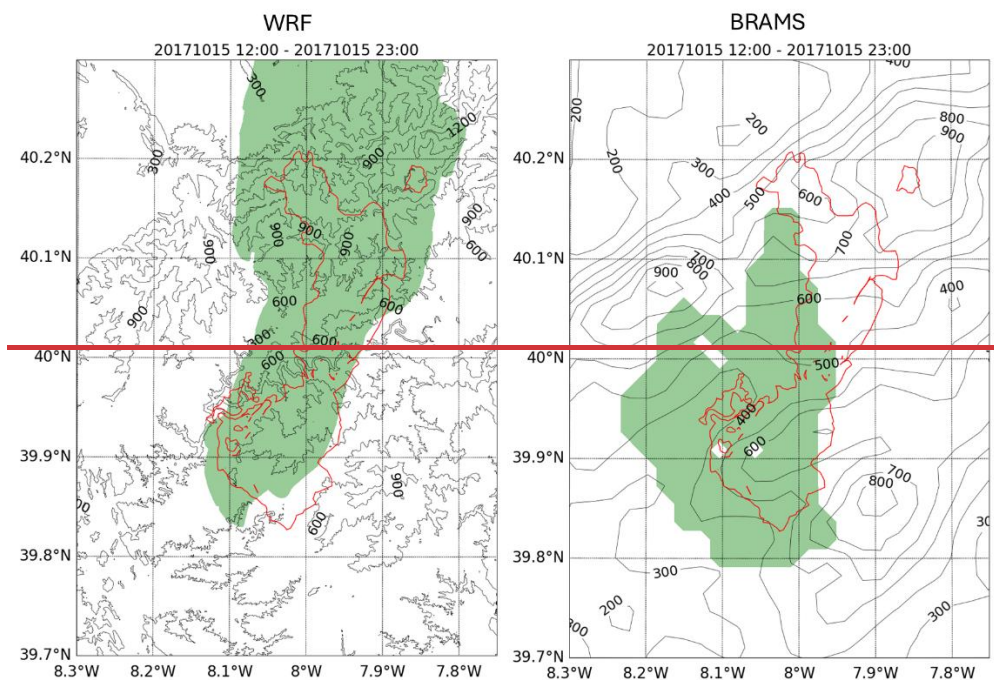


Figure 6: Comparison of simulated burned area over high-resolution topography from the (a) WRF-SFIRE and (b) RAMS-SFIRE models for the wildfire event on 15 October 2017, accumulated between 12:00 and 23:00 UTC. Green shaded regions represent the cumulative burned area, while red contours delineate the observed fire perimeter.

3.2 Optical properties comparison between SOD and AOD -from MERRA-2

Following the assessment of burned area estimates, the results for the optical properties of the smoke plume, are presented and discussed, starting with a comparison between simulated SOD and MERRA-2 AOD.

~~Forest fires, during their propagation, consume the available biomass as characterized by the different NFFL fire behaviour fuel models (Anderson, 1982), which represent the landscape, and release high concentrations of particles and trace gases into the atmosphere. Primary aerosols are emitted throughout combustion, during both the flaming and smouldering phases, while secondary aerosols form in the atmosphere through chemical reactions involving precursor gases. However, primary particles can serve as condensation nuclei or "seeds" for secondary particle formation through aging processes, resulting in internally mixed aerosols with complex and evolving chemical compositions as they are transported within the smoke plume.~~

~~Primary particles include soot, predominantly composed of elemental carbon (BC), along with ash and mineral components derived from the burned biomass. These materials may exist as distinct particles or aggregate into larger mixed particles during combustion. Depending on their composition and surface properties, these aerosols can be hydrophilic (attracting water,~~

enhancing growth in humid conditions) or hydrophobic (repelling water), affecting their interaction with radiation and their ability to act as cloud condensation nuclei (CCN).

As these particles are transported within the smoke plume, they undergo aging processes that alter their physical and chemical properties. These include: (1) Coagulation — collisions and merging with other particles, leading to increased size and complexity; (2) Surface reactions — interactions with atmospheric gases such as SO₂, NO_x, and volatile organic compounds (VOCs), including terpenes and isoprenes (emitted by vegetation during natural biological processes) and aromatic compounds (from biomass combustion). These reactions lead to the formation of sulfates, nitrates, and organic coatings; (3) Oxidation — particularly of BC, resulting in the acquisition of oxygen-containing functional groups that modify its optical properties and enhance hydrophilicity.

In parallel, VOCs are oxidized in the atmosphere to produce oxygenated organic compounds, such as carboxylic acids (e.g., formic acid, acetic acid) and aldehydes (e.g., formaldehyde), which contribute to the formation and growth of secondary organic aerosols (SOA). These compounds can condense onto primary particles, forming coatings that significantly modify their optical and hygroscopic properties.

Moreover, photochemical reactions involving VOCs and oxidants such as ozone (O₃) and hydroxyl radicals (OH) also lead to secondary particle formation. Not all secondary aerosols are of local fire origin; VOCs and precursor gases transported from urban pollution sources or natural vegetation in other regions may also contribute further to increasing the complexity of the smoke plume and its optical properties.

Both primary and secondary aerosols interact with solar radiation through scattering and absorption of shortwave (visible and near infrared) radiation, reducing direct sunlight at the surface while enhancing diffuse radiation (Yamasoe et al., 2006). These particles also absorb and re-emit longwave (thermal infrared) radiation. While BC strongly contributes to absorption, sulfates and organic aerosols primarily enhance scattering, collectively influencing the atmospheric radiative energy balance (Yamasoe et al., 2006). The net result often includes local atmospheric heating, particularly in layers rich in BC.

These radiative interactions are governed by Mie theory, as most smoke particle sizes fall within the Mie regime (approximately 0.1 μm to 1 μm), where the particle diameter is comparable to the wavelength of incident radiation. Smaller particles (< 0.1 μm) scatter more efficiently at shorter wavelengths (e.g., blue light) and are better described by Rayleigh theory, which assumes particle sizes much smaller than the radiation wavelength. In contrast, larger particles exhibit non-selective scattering and remain within the Mie regime, with their radiative behaviour less dependent on wavelength.

Understanding the spectral behaviour of smoke aerosol optical properties is essential for interpreting optical depth measurements. In this context, both the simulated SOD at 550 nm and the MERRA-2 AOD at the same wavelength represent the column-integrated attenuation of solar radiation due to the presence of aerosols in the atmosphere. However, there are conceptual differences that affect their comparison. SOD corresponds specifically to the fraction of AOD attributed to smoke particles generated by wildfires and biomass burning, while MERRA-2 AOD includes all aerosol types present in the atmosphere, such as mineral dust, sulfates, nitrates, sea salt, and soot.

When $SOD \leq AOD$, only a fraction of the total aerosol burden can be attributed to smoke. When $SOD \approx AOD$, the aerosol population is dominated by biomass-burning particles, as expected during intense fire activity with minimal influence from other sources. In contrast, situations where $SOD \ll AOD$ indicate that non-smoke aerosol types, such as mineral dust, industrial sulfate pollution, or marine aerosols (e.g., Saharan intrusions), contribute substantially to the observed optical depth. When $SOD \leq AOD$, it indicates that smoke aerosols constitute only a portion of the total aerosol load. In contrast, when $SOD \approx AOD$, it suggests that the majority of aerosols in the region and time analysed originate from biomass burning, which typically occurs during intense fire events with limited interference from other aerosol sources. Conversely, when $SOD \ll AOD$, it implies a significant contribution from non-smoke aerosol sources, such as mineral dust (e.g., Saharan intrusions), industrial pollution (sulfates), or marine aerosols. These physical considerations provide the basis for interpreting the spatial correspondence between simulated SOD and MERRA-2 AOD, shown in Figure 7.

Figure 7 presents the spatial distribution of SOD under the Baseline configuration, for both dry and wet conditions, compared with MERRA-2 AOD at 550 nm at 18:00 UTC on 15 October 2017, during the t_1 -fresh phase. Four fixed base classes between 0 and 4 (unitless) were defined for AOD, as this range is most representative of intense fire plumes. ~~At this time, both SOD and AOD show a marked enhancement relative to earlier afternoon conditions, reflecting the intensification and vertical deepening of the smoke plume associated with the major wildfires over central Portugal. The dry SOD contours delineate the plume core, whereas the wet configuration extends further downwind, suggesting hygroscopic growth and enhanced optical thickness under humid conditions. Overall, the model reproduces the main spatial pattern of MERRA-2 AOD, albeit with a thinner and slightly displaced plume.~~

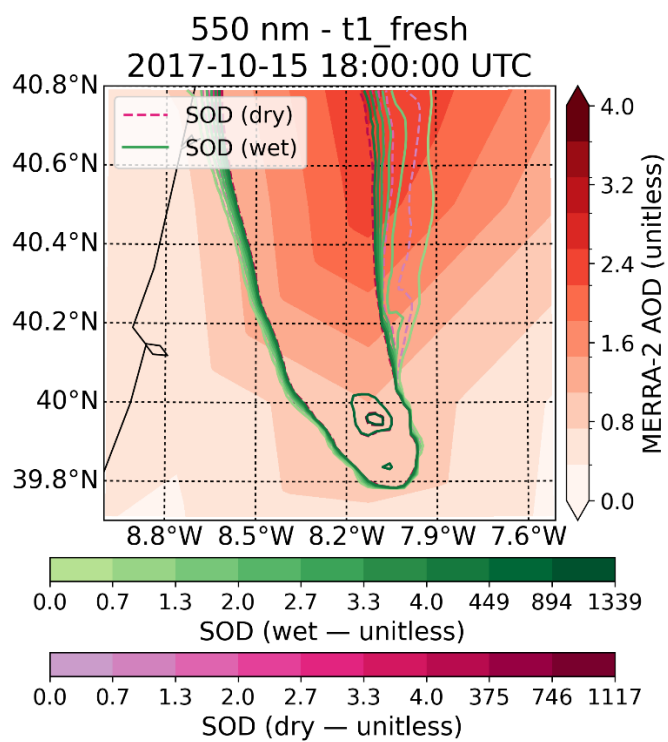
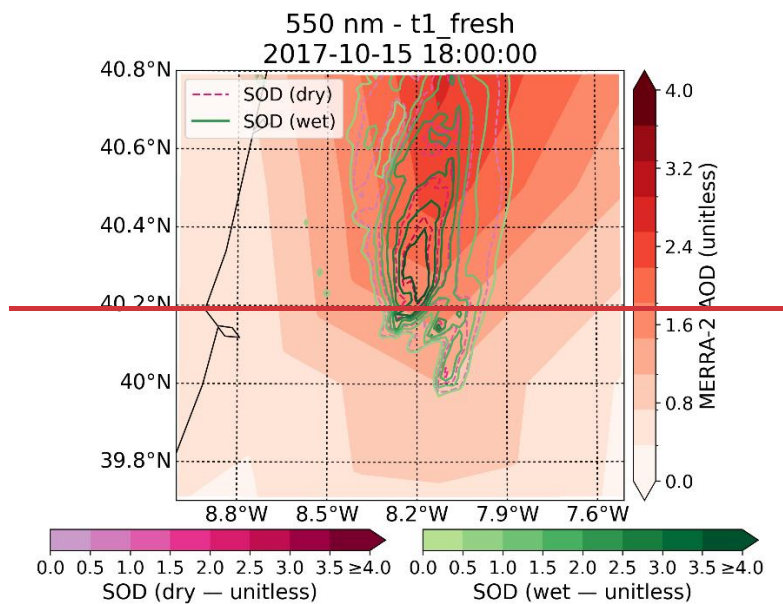


Figure 7: Spatial distribution of smoke optical depth (SOD) and MERRA-2 AOD (550 nm) over the study domain at 18:00 UTC on 15 October 2017, during the intense Sertão wildfire episode. AOD is shown as shaded colours; SOD (dry) and SOD (wet) are overlaid as dashed and solid contours, respectively.

At this time, both SOD and AOD show a pronounced increase relative to earlier afternoon conditions, reflecting the intensification and vertical deepening of the smoke plume over central Portugal. The dry SOD contours highlight the plume core, whereas the wet SOD field extends further downwind and attains higher values, indicating enhanced optical thickness driven by hygroscopic growth under humid conditions. The overall spatial pattern compares well with MERRA-2 AOD, with the model capturing the main plume structure and gradients, albeit with a somewhat narrower extension compared to the reanalysis. These results reinforce the strong aerosol load and plume development characteristic of the t₁-fresh phase. The highest SOD values fall within the expected range for intense wildfire plumes, although some amplification is likely due to plume retention within the limited model domain, which restricts northward dispersion.

In the Baseline configuration, between 13:00 and 17:00 UTC, a strong decoupling was found between the simulated SOD and the MERRA-2 AOD (Fig. 8a). The high regression intercepts (dry: 0.94–2.05; wet: 0.90–2.05) indicate a persistent background aerosol contribution (regional haze, dust, or pollution) captured by MERRA-2 but not associated with the simulated smoke plume. The steep slopes (dry: 1.39–3.03; wet: 0.55–2.84), together with a narrow SOD range (mostly below 0.5), reveal that AOD varied almost independently of SOD, suggesting a spatial or temporal offset between the modeled and observed plume positions. Beyond the spatial structure at 18:00 UTC, the temporal evolution of SOD and AOD provides further insight into model–reanalysis consistency. In the Baseline configuration, the comparison between simulated SOD and MERRA-2 AOD from 13:00 to 17:00 UTC reveals a persistent mismatch in both magnitude and spatial organisation, despite the progressive strengthening of the modeled plume. At 13:00 UTC, SOD remains confined and weak, whereas MERRA-2 depicts a broader, already well-developed smoke layer. This early underestimation reflects a timing offset, with the model delaying the onset of plume intensification relative to the reanalysis. From 14:00 to 16:00 UTC, both dry and wet SOD increase substantially, but the rate of increase is disproportionate relative to AOD. The simulated fields exhibit a much sharper spatial gradient and a narrower plume core, while MERRA-2 maintains a smoother, more diffused structure. This behaviour indicates that SOD responds primarily to the intense, locally concentrated core of the simulated plume, whereas MERRA-2 retains a broader regional aerosol contribution that is not present in BRAMS. Although an upwind background correction was applied to MERRA-2 AOD, it specifically removes only the inflow background and does not eliminate the wider regional AOD structure inherent to the reanalysis. As a result, MERRA-2 continues to exhibit a spatially smoother, regionally extensive optical depth, while SOD reflects only the fire-driven aerosol load. Consequently, the SOD–AOD relationship remains weakly constrained, with MERRA-2 showing elevated AOD even where SOD remains low or absent. By 17:00 UTC, SOD reaches its maximum values, particularly in the wet configuration, with magnitudes that fall within the physical range of dense wildfire smoke but exceed the AOD variability in the corresponding area. Part of this amplification is attributable to plume confinement within the limited model domain, which prevents northward dispersion and leads to artificial accumulation. In contrast, MERRA-2

retains a more spatially extensive plume, reflecting long-range transport that the regional simulation cannot capture. The very high SOD values, arising from the intense fuel burning confined to a subset of SFIRE grid cells, fall within the physical range of extreme wildfire plumes and accentuate the contrast with the smoother and lower AOD structure in MERRA-2. This discrepancy further weakens the SOD–AOD correspondence at this stage of the plume evolution. Part of the discrepancies between SOD and AOD across the domain arise from temporal offsets, differences in plume confinement, and the distinct spatial scales represented by the model and the reanalysis, which collectively limit their correspondence during the plume’s evolution.

From 18:00 to 23:00 UTC (Fig. 8b), the coupling between both datasets improves notably. The regression slopes decrease to 0.21–0.36 (dry) and 0.19–0.34 (wet), indicating that SOD variations begin to explain part of the AOD variability, although the model still underestimates the total column optical depth, producing a thinner smoke layer. The SOD (wet) configuration provides slightly better agreement ($r \approx 0.14$) than SOD (dry) ($r \approx 0.13$), while lower intercepts (dry: 0.66–0.78; wet: 0.65–0.77) denote improved representation of smoke-related aerosols and greater spatial consistency with MERRA-2. Visualisation of the SOD–AOD scatter relationships (Fig. 8a–b) representing the Baseline optical configuration (test 1), provides insight into how the simulated plume evolves relative to the MERRA-2 reanalysis throughout the afternoon. Between 15:00 and 19:00 UTC, the statistical coupling between SOD (wet configuration) and MERRA-2 AOD improves, although substantial differences remain in their absolute magnitudes and spatial structure. At 15:00 UTC, the regression fit derived from the scatterplot (slope = 0.56, $R^2 = 0.03$) shows weak correspondence, primarily because the AOD field retains a high regional background level (intercept ≈ 2.08) not represented by the localised smoke plume in BRAMS. By 19:00 UTC, the relationship strengthens somewhat (slope = 0.30, $R^2 = 0.36$), but a clear shift becomes apparent: the simulated SOD reaches much higher values than the MERRA-2 AOD across most of the range. This indicates that the model generates a more optically intense core of the plume, whereas MERRA-2 maintains a smoother and less concentrated aerosol structure. Hygroscopic growth in the wet configuration further amplifies the SOD, enhancing the optical depth relative to the reanalysis. The Conservative (test 2) and Lower-Envelope (test 3) optical configurations exhibit regression behaviour very similar to the Baseline test, with only minor quantitative differences. At 15:00 UTC, both tests 2 and 3 display weak statistical coupling between SOD (wet) and MERRA-2 AOD, with slopes near 0.55, intercepts around 2.1, and negligible explained variance ($R^2 \approx 0.02$ – 0.03). These metrics indicate that, as in the baseline case, MERRA-2 retains a substantial background AOD contribution that is not represented by the simulated plume, and that early-phase SOD variability accounts for only a small fraction of the observed optical depth.

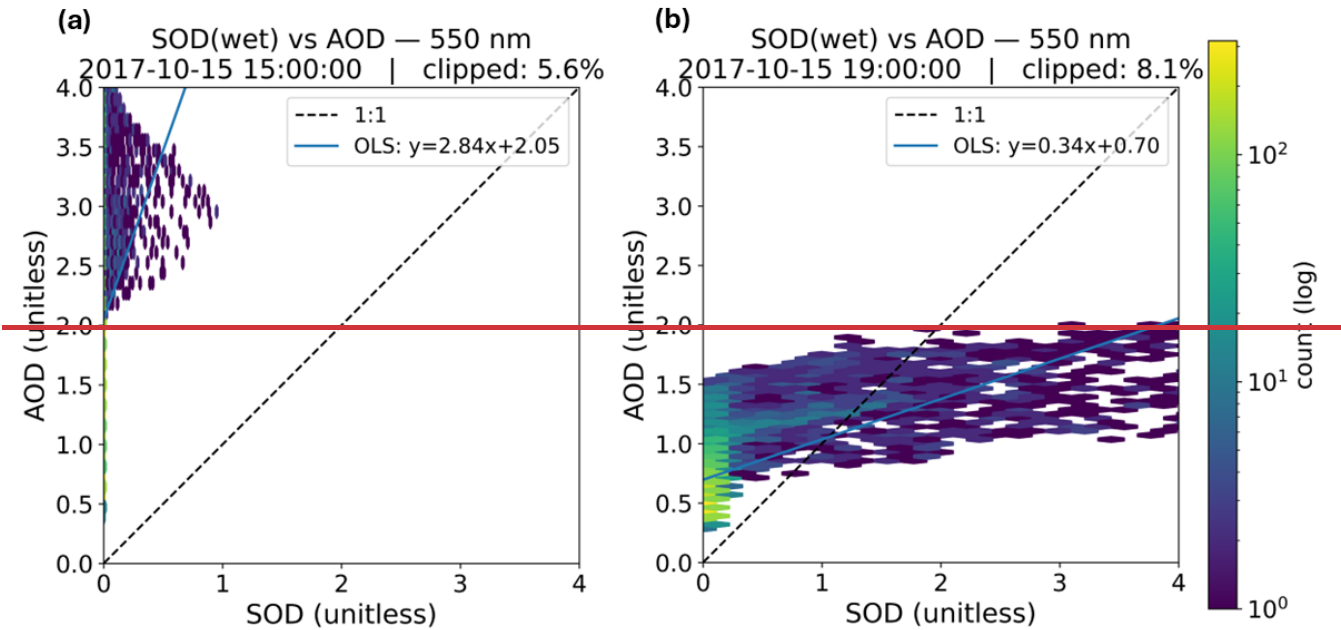
The Conservative (Test 2) and Lower Envelope (Test 3) configurations exhibit similar overall behavior. During the fresh phase, intercepts range between 0.89–2.05 (dry) and 0.90–2.05 (wet) for the Conservative setup, and 0.89–2.05 (dry) and 0.90–2.05 (wet) for the Lower Envelope setup. In the mixed phase, intercepts vary between 0.66–0.77 (dry) and 0.65–0.76 (wet) for the Conservative case, and 0.66–0.78 (dry) and 0.70–0.77 (wet) for the Lower Envelope case. Corresponding slopes range from 0.21–0.36 (dry) and 0.20–0.33 (wet) for the Conservative setup, and 0.21–0.36 (dry) and 0.20–0.34 (wet) for the Lower

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Envelope. These variations indicate that reducing κ and $r_{g,dry}$ or narrowing σ_g produces only moderate changes in the regression metrics, confirming that the optical results are relatively insensitive to plausible microphysical perturbations. Overall, all configurations consistently reproduce the main spatial structure of the observed plume but underestimate its total optical depth. The wet runs yield the best correspondence with MERRA 2, emphasizing the importance of hygroscopic growth in reproducing observed AOD magnitudes during the plume's mature stage.

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By 19:00 UTC, the coupling strengthens in both configurations: slopes decrease to roughly 0.29–0.30, intercepts fall to ~0.65 (as in test 1), and R^2 increases to 0.35–0.36. This convergence across the three tests demonstrates that modifying κ , $r_{g,dry}$, or narrowing σ_g leads to only modest changes in the regression behaviour. The similarity of the results confirms that the optical response is relatively insensitive to plausible microphysical perturbations within the tested parameter space.



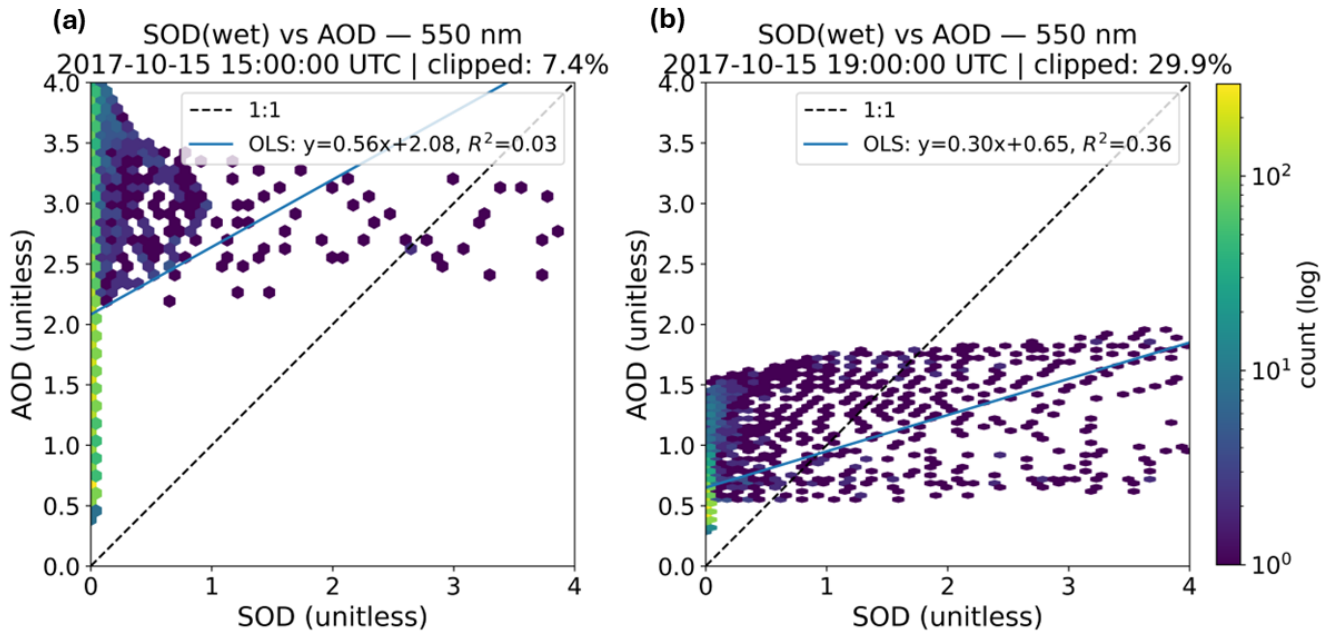


Figure 8: Scatter density plots comparing simulated SOD (wet) and MERRA-2 AOD at 550 nm for 15:00 UTC (panel a) and 19:00 UTC (panel b) on 15 October 2017. The dashed line represents the 1:1 relationship, and the solid line the ordinary least-squares (OLS) regression. Color shading denotes the logarithmic count of grid-point pairs. The clipped percentage indicates the fraction of points excluded from the plot due to exceeding the displayed SOD/AOD range (≥ 4.0).

Table 4 shows that during 13:00–17:00 UTC (fresh), the model exhibits large negative bias to SOD (−2.22 to −0.94), high MAE/RMSE (up to 2.45), and weak linear coupling ($r=0.04$ –0.56; $R^2=0.00$ –0.31), indicating strong background dominance in AOD from MERRA-2 and limited overlap with the simulated plume as seen upper. Skill improves markedly from late afternoon into evening. At 18:00 UTC (fresh), bias is reduced (−0.74), MAE/RMSE attain their lowest values (0.83/0.92), and correlation strengthens ($r=0.66$; $p=0.93$; $R^2=0.44$). Around 19:00–20:00 UTC (mixed), correlations peak ($r=0.70$ –0.72; $p=0.93$ –0.95) with the highest R^2 (0.48–0.52); bias crosses from near zero (−0.06 at 19:00) to slightly positive (+0.37 at 20:00), consistent with a transition from under to mild over-estimation of column optical depth. Later evening hours (21:00–23:00 UTC) maintain elevated correlations ($r=0.57$ –0.68; $p=0.89$ –0.93) but exhibit moderate positive bias (+0.17 to +0.30) and larger errors than at 18:00 UTC. Overall, the best trade-off between amplitude and association occurs at 18:00–20:00 UTC, with 18:00 minimizing error and 19:00–20:00 maximizing explained variance. Table 4 provides a time-resolved evaluation of the statistical relationship between SOD and AOD during the Sertã wildfire period, highlighting the contrasting behaviour of the fresh and mixed phases. During the fresh phase (13:00–19:00 UTC), both dry and wet SOD differ markedly from the MERRA-2 AOD. Across 13:00–17:00 UTC, AOD remains relatively stable (Mean AOD ≈ 0.9 –1.7), whereas SOD increases sharply, especially in the wet configuration, rising from values near zero at 13:00 UTC to about 7 (Mean SOD ≈ 6 –7) by 17:00

UTC. This produces a transition in the bias defined as SOD – AOD from strongly negative (–1.9 to –0.9) to strongly positive (+5 to +6). Correspondingly, MAE and RMSE increase substantially, and correlations remain extremely low ($r \approx 0.02$ – 0.06 , $R^2 \approx 0.00$), indicating that SOD explains virtually none of the spatial variability present in the AOD field. Physically, this reflects limited spatial covariance between the developing, highly localised simulated plume and the smoother regional aerosol structure represented by MERRA-2.

From 19:00 UTC onward, the plume enters the mixed phase (19:00–23:00 UTC), during which SOD intensifies dramatically, reaching Mean SOD values between 35 and 65, while AOD remains nearly constant around 0.8–0.9. This leads to very large positive biases and correspondingly large error metrics. Linear correlations improve modestly (up to $r \approx 0.58$), and R^2 increases to at most 0.34, indicating a partial but still limited recovery of spatial coherence between SOD and AOD. These diagnostics are consistent with progressive plume confinement and accumulation within the regional domain, yielding SOD magnitudes far exceeding the column aerosol load represented in MERRA-2.

Taken together, the hourly statistics confirm that part of the discrepancy between SOD and AOD arises from temporal offsets, plume confinement, and the fundamentally different spatial scales resolved by the model and the reanalysis. These structural differences limit the correspondence between the two datasets throughout the plume evolution.

Table 4: Diagnostic statistics for the Sertão wildfire period, including the mean, bias, mean absolute error (MAE), root-mean-square error (RMSE), Pearson correlation coefficient (r) and Spearman’s rank correlation coefficient (ρ), and coefficient of determination (R^2) of SOD and AOD.

Time (UTC)	Phase	Mean SOD	Mean AOD	Bias (SOD-AOD)	MAE	RMSE	r	ρ	R^2
13:00	Fresh-dry	0.000-00	0.940-94	-0.94-0.94	0.940-	0.980-98	0.03	0.38	0.000-0
					94		0.04	0.38	0
14:00	fresh-dry	0.030-04	1.734-73	-1.71-1.73	1.724-	1.864-85	0.05	0.72	0.000-0
					73		0.12	0.72	2
15:00	fresh-dry	0.310-03	2.242-24	-1.93-2.22	2.362-	3.172-45	0.06	0.84	0.000-0
					22		0.23	0.84	5
16:00	fresh-dry	1.830-07	1.364-36	0.47-1.29	2.774-	10.974-4	0.02	0.84	0.000-2
					29	2	0.45	0.87	0
17:00	fresh-dry	6.370-15	1.294-29	5.08-1.14	6.814-	30.944-2	0.05	0.86	0.000-3
					44	7	0.56	0.90	4
13:00	Fresh-wet	0.000-00	0.940-94	-0.94-0.94	0.940-	0.980-98	0.02	0.38	0.000-0
					94		0.04	0.38	0
14:00	fresh-wet	0.030-04	1.734-73	-1.70-1.73	1.724-	1.864-85	0.05	0.72	0.000-0
					73		0.12	0.72	2
15:00	fresh-wet	0.340-03	2.242-24	-1.90-2.22	2.392-	3.352-45	0.06	0.84	0.000-0
					22		0.23	0.84	5

16:00	fresh- <u>wet</u>	<u>2.100.07</u>	<u>1.364.36</u>	<u>0.734.29</u>	<u>3.024.29</u>	<u>12.674.4</u>	<u>0.02</u>	<u>0.84</u>	<u>0.000.2</u>
							<u>0.45</u>	<u>0.87</u>	<u>0</u>
17:00	fresh- <u>wet</u>	<u>7.420.45</u>	<u>1.294.29</u>	<u>6.134.14</u>	<u>7.834.14</u>	<u>36.514.2</u>	<u>0.05</u>	<u>0.86</u>	<u>0.000.3</u>
							<u>0.56</u>	<u>0.90</u>	<u>4</u>
18:00	fresh- <u>wet</u>	<u>17.760.35</u>	<u>1.094.09</u>	<u>16.670.74</u>	<u>17.82</u>	<u>71.190.9</u>	<u>0.08</u>	<u>0.85</u>	<u>0.010.4</u>
							<u>0.66</u>	<u>0.93</u>	<u>4</u>
19:00	mixed- <u>wet</u>	<u>35.350.83</u>	<u>0.890.89</u>	<u>34.470.06</u>	<u>35.23</u>	<u>115.344.1</u>	<u>0.14</u>	<u>0.83</u>	<u>0.020.4</u>
							<u>0.97</u>	<u>0.70</u>	<u>8</u>
20:00	mixed- <u>wet</u>	<u>51.574.47</u>	<u>0.800.80</u>	<u>50.770.37</u>	<u>51.41</u>	<u>143.192.1</u>	<u>0.32</u>	<u>0.86</u>	<u>0.100.5</u>
							<u>0.72</u>	<u>0.95</u>	<u>2</u>
21:00	mixed- <u>wet</u>	<u>62.624.43</u>	<u>0.830.83</u>	<u>61.790.30</u>	<u>62.41</u>	<u>159.822.1</u>	<u>0.50</u>	<u>0.91</u>	<u>0.250.4</u>
							<u>0.68</u>	<u>0.93</u>	<u>6</u>
22:00	mixed- <u>wet</u>	<u>64.584.03</u>	<u>0.860.86</u>	<u>63.710.47</u>	<u>64.36</u>	<u>159.484.1</u>	<u>0.58</u>	<u>0.93</u>	<u>0.340.3</u>
							<u>0.62</u>	<u>0.94</u>	<u>9</u>
23:00	mixed- <u>wet</u>	<u>58.290.94</u>	<u>0.890.89</u>	<u>57.390.02</u>	<u>58.10</u>	<u>142.474.1</u>	<u>0.58</u>	<u>0.92</u>	<u>0.340.3</u>
							<u>0.57</u>	<u>0.89</u>	<u>2</u>

The statistical diagnostics summarized in Tables S1–S3 described in the Supplementary material, quantify the effects of microphysical perturbations applied in the BASE, CONSERVATIVE, and LOWER ENVELOPE phases on the model–observation agreement during the mixed stage. Across all experiments, background subtraction (TRUE) systematically reduces both bias and error metrics, confirming that a large part of the apparent disagreement arises from regional background aerosols present in MERRA-2 rather than from deficiencies in the simulated plume. After background removal, the mean SOD and AOD become closely aligned (0.55–0.57 vs 0.46–0.57 $\mu\text{g m}^{-3}$ for the ALL mask), and the bias decreases from roughly -0.6 to -0.1 , while MAE and RMSE drop by 30–40 %. The correlation coefficients ($r \sim 0.15$ – 0.17 , $\rho \sim 0.55$ – 0.60) remain moderate, reflecting residual spatial offsets but indicating that SOD captures the large-scale plume variability once the background signal is removed. Supplementary Tables S1–S3 extend the SOD–AOD evaluation by quantifying how the Baseline, Conservative, and Lower Envelope microphysical configurations affect the model–reanalysis agreement during the mixed phase. Across all configurations, the results are highly consistent: mean SOD is one to two orders of magnitude larger than the corresponding MERRA-2 AOD (e.g., $\text{SOD} \approx 18$ – 30 for the ALL mask, increasing to 90 – 200 for the P70–P90 masks, while AOD remains near 1). Consequently, bias values ($\text{SOD} - \text{AOD}$) are strongly positive and increase with the percentile mask (e.g., $+16$ to $+30$ for ALL, rising to $+180$ – 200 for P90). MAE and RMSE follow the same pattern, reaching 80 – 110 for the ALL mask and 250 – 345 for P90. These statistics indicate that the simulated smoke column burden greatly exceeds the column optical depth represented by MERRA-2, regardless of the assumed microphysical configuration. Background subtraction affects only the reanalysis field, reducing AOD by approximately 0.6 (1.17 to 0.57). As a result, bias becomes slightly larger, but MAE and RMSE change only marginally. Correlation coefficients remain extremely weak for the

1670 ALL mask ($r \approx 0.00$ – 0.06 ; $R^2 \approx 0.00$), demonstrating that the discrepancies are not due to a removable background offset but rather reflect fundamental structural mismatches in spatial representativeness between SOD and AOD.

The percentile masks (P70–P90) highlight a systematic deterioration in skill as increasingly high-AOD grid cells are selected. Bias rises to +180–200, RMSE exceeds 300, and correlations become increasingly negative ($r \approx -0.30$ to -0.50), while R^2 remains ≤ 0.24 . This behaviour indicates that the regions of strongest AOD in MERRA-2 correspond to aerosol components

1675 and vertical layers not represented by SOD, including smoothed background mass, coarse-mode contributions, and long-range transported aerosol that the regional plume simulation cannot reproduce. The regression slopes remain near zero ($|\text{slope}| < 0.002$), confirming that variations in SOD magnitude have essentially no explanatory power for the spatial variability of AOD.

Differences across the microphysical perturbations (ABSORBING, WIDE SIGMA, SMALL RG, LARGE RG) are minor, typically altering correlation by ≤ 0.05 and MAE/RMSE by ≤ 2 – 5% . Similarly, the near-identical results across the three

1680 microphysical frameworks (BASE, CONSERVATIVE, LOWER ENVELOPE) demonstrate that reasonable adjustments to κ , $r_{g,dry}$, and σ_g have only a secondary effect on the SOD–AOD comparison. The dominant source of discrepancy therefore lies not in microphysics, but in the excess plume mass and the spatial confinement of the smoke plume in the model domain relative to the broad, regionally smoothed optical depth represented in MERRA-2.

1685 ~~Comparing across microphysical configurations shows that the WIDE SIGMA, SMALL RG, and LARGE RG tests produce changes of less than ± 0.1 in correlation and ± 0.2 in MAE relative to BASE, confirming that realistic perturbations in particle size distribution width or geometric radius have limited impact on the optical diagnostics. Similarly, the ABSORBING variant slightly increases mean SOD (by ~ 0.05 – 0.1) and yields marginally lower bias, consistent with stronger intrinsic absorption compensating for the model’s underestimation of column optical depth. The near-identical metrics between the BASE,~~

1690 ~~CONSERVATIVE, and LOWER ENVELOPE tables further demonstrate the model’s robustness to plausible microphysical adjustments.~~

~~Physically, these results indicate that the residual mismatch between simulated SOD and observed AOD during the mixed phase is dominated by spatial and vertical representativeness errors rather than by uncertainties in particle hygroscopicity or size. Once the uniform background component is removed, the remaining SOD–AOD variability mainly reflects sub-grid~~

1695 ~~plume displacement and MERRA-2’s coarse resolution, not intrinsic optical property biases. This reinforces the interpretation that the BRAMS SFIRE system reproduces the evolving smoke distribution realistically in structure but underestimates its integrated optical depth, an effect only weakly sensitive to the tested microphysical perturbations.~~

~~Several structural and physical factors help explain the partial desynchronization observed between the simulated smoke optical depth (SOD) and the MERRA-2 aerosol optical depth (AOD). The statistical findings can be interpreted in light of~~

1700 several physical and representativeness factors that fundamentally limit the correspondence between SOD and MERRA-2 AOD. Physically, the persistent decoupling between SOD and AOD reflects fundamental representativeness differences between the instantaneous fine-mode SOD fields produced at 2 km resolution and the hourly, 50–70 km column-integrated AOD from MERRA-2. SOD samples near-surface fresh smoke only, whereas AOD includes coarse-mode background aerosols

and vertically extended layers. These structural differences explain the very low covariance and consistently large intercepts. Additional phase shifts arise from temporal mismatch between instantaneous model outputs and the assimilation-centred AOD, as well as plume-scale variability difficult for a coarse reanalysis to reproduce. Taken together, Tables S1–S3 show that BRAMS–SFIRE captures the spatial organisation of the plume but strongly underestimates its integrated optical depth, and that this underestimation is largely insensitive to microphysical perturbations, being instead dominated by representativeness limitations in both the model and the reanalysis.

A primary contributor to this mismatch is the contrast in spatial and temporal resolution between the high-resolution model output and the coarse MERRA-2 reanalysis. The BRAMS–SFIRE runs at 2 km horizontal resolution and produce instantaneous outputs, whereas MERRA-2 provides $\sim 0.5^\circ \times 0.625^\circ$ ($\sim 50 \times 70$ km) hourly means centred near hh:30. This difference implies that sharp smoke gradients and localized peaks captured by the model are heavily smoothed in MERRA-2, both attenuating maximum AOD values and shifting their apparent timing relative to the simulated plume. The resulting smoothing also blends smoke with background aerosols, reducing the spatial contrast between plume and non-plume regions.

Differences in aerosol composition further amplify this representativeness gap between the model and the reanalysis. The SOD evaluated here is derived from fine-mode PM_{2.5} (fresh smoke), while MERRA-2 AOD represents total extinction, integrating coarse-mode dust and sea salt. In regions where coarse-mode aerosols are abundant, total AOD can diverge from, or even anticorrelate with, fine-mode SOD in both space and time. This compositional difference is consistent with elevated regression intercepts, i.e., a background optical load not associated with the fire plume.

Additional discrepancies arise from the way MERRA-2 assimilates observational AOD and represents rapidly evolving wildfire plumes. MERRA-2 assimilates satellite AOD observations (e.g., MODIS, VIIRS), subject to retrieval/sampling constraints; its smoke fields depend on emission inventories and the analysis cycle. Rapid, pyro-convective injections from intense wildfires, characterized by sub-hourly variability and strong vertical transport, are difficult to capture in reanalysis products. This can produce phase shifts in both timing and vertical structure relative to the model, especially during the most active burning period (13–17 UTC).

Humidity-driven growth constitutes another factor influencing the magnitude and spatial alignment of extinction between the model and MERRA-2. The wet SOD uses modelled RH to allow growth in particle size and extinction efficiency. MERRA-2 may employ coarser meteorology and simplified κ parameterizations. Discrepancies in RH and κ directly affect the scattering enhancement and extinction efficiency, contributing to systematic differences in optical depth amplitude. The better agreement obtained under wet conditions supports the physical importance of this process.

Temporal pairing between the model and the reanalysis also introduces structural differences, especially during rapid plume evolution. The comparison pairs instantaneous model fields at H:00 with MERRA-2 hourly means representing roughly [H – 30, H + 30 min]. During periods of rapid-fire intensification or plume advection, this temporal mismatch further smooths and delays AOD peaks relative to modelled SOD maxima, manifesting as the apparent decoupling observed in the early afternoon hours.

Some of the discrepancy may also stem from simplifying assumptions in the optical calculations applied to the BRAMS-SFIRE output. The Mie-based SOD assumes spherical, monodisperse particles with fixed effective radius and density. Under extreme fire conditions, this simplification tends to overrepresent the number of small particles per unit mass, enhancing extinction near the fire front. This effect increases simulated SOD peaks but has a minor influence on broader plume statistics, as confirmed by the microphysical sensitivity tests.

The optical diagnostics ~~made~~ quantified shortwave extinction, whereas wildfires emit intense longwave radiation that alters buoyancy and turbulence, promoting lofting and secondary aerosol formation. Such small-scale feedbacks are not explicitly resolved in MERRA-2, yet they modulate plume height and density and thus the spatial alignment of SOD and assimilated AOD.

3.3 Linking Aerosol Mass, Optical Properties, and Radiative Effects in the Smoke Plume

A broader radiative context is needed to interpret these optical diagnostics, particularly the distinction between shortwave extinction and longwave emission from the fire. The optical analysis presented above primarily concerns shortwave extinction (SOD/AOD). To place these results in context, it is essential to distinguish between the thermal radiation emitted by the fire itself and the attenuation of incoming solar radiation quantified by AOD and SOD. Fires emit thermal infrared radiation due to highly exothermic oxidation reactions involving biomass and oxygen. This thermal radiation is generated locally and contributes to atmospheric heating in the combustion zone. In contrast, AOD and SOD quantify the extinction of solar (shortwave) radiation caused by aerosol scattering and absorption and are therefore associated with changes in the atmospheric radiative balance induced by smoke particles, not with the direct release of energy from combustion.

The thermal radiation emitted by wildfires occurs primarily in the longwave (infrared) spectrum and can be expressed as a radiative flux (W m^{-2}). Although this longwave emission does not directly interact with incoming solar radiation, it significantly alters the local thermodynamic environment, enhancing plume buoyancy, promoting aerosol dispersion, and facilitating the formation of secondary aerosols. These processes indirectly influence the transmission of solar radiation by modifying the spatial and vertical distribution of scattering and absorbing aerosols. Thus, thermal radiation from fire plays a critical role in the radiative energy budget, both through its direct longwave component and through its indirect effects on shortwave radiative transfer via aerosol–radiation interactions.

~~Figure 9 shows the simulated PM2.5, and MERRA 2 BC, and OC mass concentrations at 19:00 UTC on 15 October 2017, corresponding to the mixed phase when the model reanalysis agreement improved. The results reveal a strong spatial coherence between PM2.5 and its carbonaceous components, confirming that smoke particles are predominantly composed of black and organic carbon. As expected for biomass burning emissions, OC concentrations greatly exceed BC, typically by an order of magnitude, indicating that the plume is dominated by smouldering to mixed combustion processes releasing large amounts of semi-volatile organic compounds that rapidly condense into fine-mode particles. These OC/BC ratios are consistent with previous field observations for Mediterranean wildfires.~~

The peak PM_{2.5} and OC concentrations are tightly co-located near the plume core, while BC shows a narrower and more confined distribution near the main fire front. This pattern reflects the combined effect of localized high temperature flaming combustion (source of BC) and broader downwind dispersion of condensable organics (source of OC). The model's 2 km horizontal resolution enables these fine-scale gradients to be resolved, unlike the coarser MERRA-2 ($\sim 50 \times 70$ km, hourly means), which smooths the maxima and blends plume and background air.

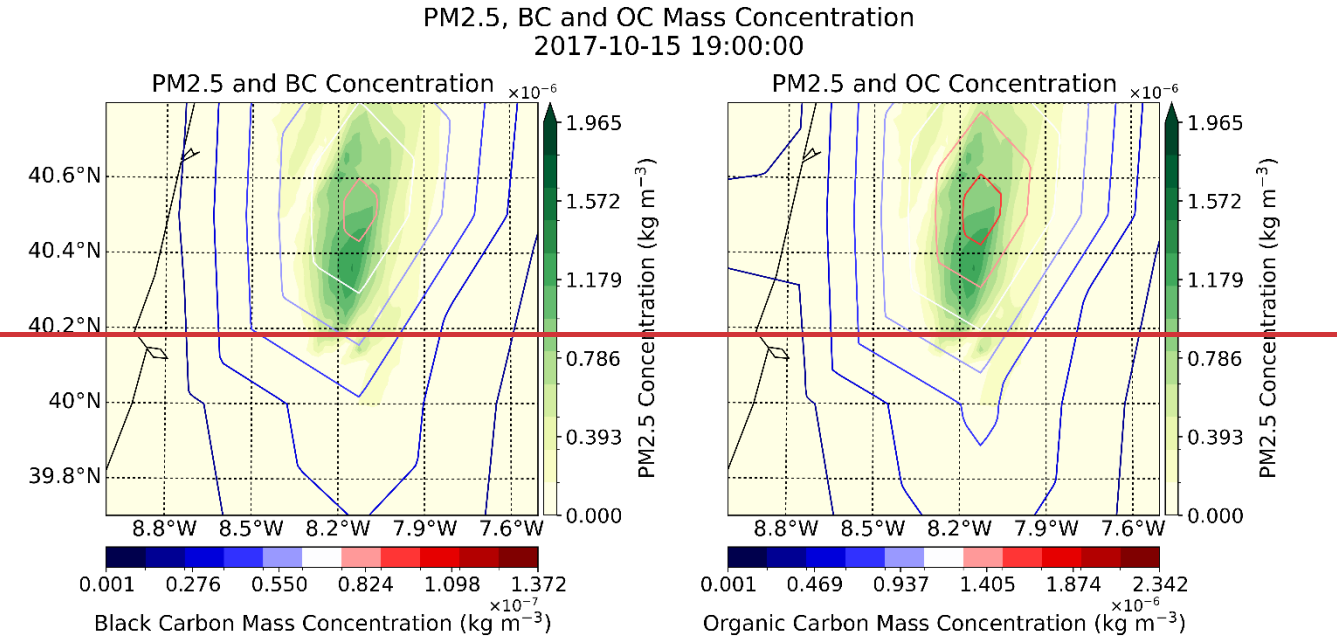
This structural contrast explains both the sharper peaks and stronger spatial gradients in the BRAMS-SFIRE results and the apparent desynchronization between modelled SOD and MERRA-2 AOD discussed earlier. At 19:00 UTC, however, the better spatial overlap between the simulated PM_{2.5}, BC, and OC fields and the reanalysis aerosol load coincides with the improved optical coupling observed at this time. The optical diagnostics presented in Section 3.2 revealed substantial differences between simulated SOD and MERRA-2 AOD, particularly during the early stages of plume development. To understand these discrepancies, it is necessary to examine how the mass distribution and composition of the smoke plume relate to its optical properties and radiative behaviour.

This section therefore shifts the focus from column-integrated optical depth to the underlying aerosol mass fields, PM_{2.5}, black carbon (BC), and organic carbon (OC), and investigates how their spatial structure governs the extinction properties diagnosed in the previous section. Because wildfire smoke is dominated by carbonaceous aerosols with distinct emission pathways and optical roles, analysing their spatial patterns provides essential physical context for interpreting SOD-AOD differences.

While SOD explicitly quantifies shortwave extinction at 550 nm, the radiative environment of the plume is simultaneously influenced by longwave emission from the fire, which enhances buoyancy, contributes to plume rise, and facilitates the formation of secondary aerosols. Although longwave processes do not enter the SOD calculation directly, they modify the thermodynamic structure of the plume and thus affect the dispersion and vertical redistribution of the carbonaceous particles that control shortwave extinction. In this sense, longwave heating indirectly influences the spatial and vertical distribution of scattering and absorbing aerosols.

Figure 9 shows the spatial distribution of column-averaged PM_{2.5} concentration and the corresponding MERRA-2 surface BC and surface OC mass concentrations at 19:00 UTC on 15 October 2017, during the mixed phase when the plume becomes more coherent. The clear spatial coherence between PM_{2.5} and the carbonaceous species is consistent with a dominant carbonaceous contribution to the simulated fine-mode mass associated with biomass burning. As typically observed in wildfire plumes, OC dominates BC by roughly an order of magnitude, consistent with smouldering/mixed-combustion conditions that generate large amounts of semi-volatile organic compounds which rapidly condense into fine-mode particles. BC remains confined to a narrower core associated with flaming combustion, while OC extends farther downwind, forming a broader envelope around the PM_{2.5} plume. This contrast reflects the two-source nature of carbonaceous smoke: BC forms primarily under high-temperature, oxygen-limited flaming conditions, while OC arises from lower-temperature pyrolysis and subsequent condensation processes that disperse more broadly downwind. This structural contrast, narrow BC ridge, broad OC plume, is clearly captured at 2-km model resolution but becomes smoothed at the MERRA-2 grid spacing (~ 50 – 70 km). Such smoothing

dilutes gradients and contributes to the weaker early-phase agreement between SOD and AOD noted in Section 3.2. By 19:00 UTC, however, the plume's organisation improves and the spatial correspondence among PM2.5, BC, and OC becomes more coherent, aligning with the improved SOD–AOD coupling reported for the mixed phase.



PM2.5, BC and OC Mass Concentration
2017-10-15 19:00:00 UTC

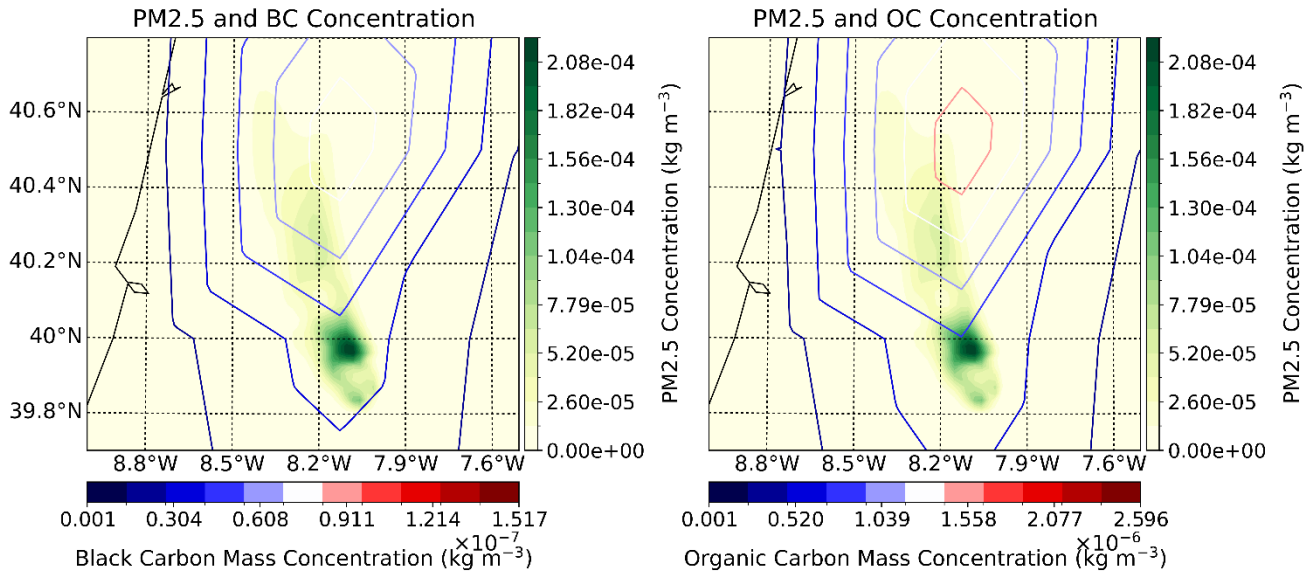
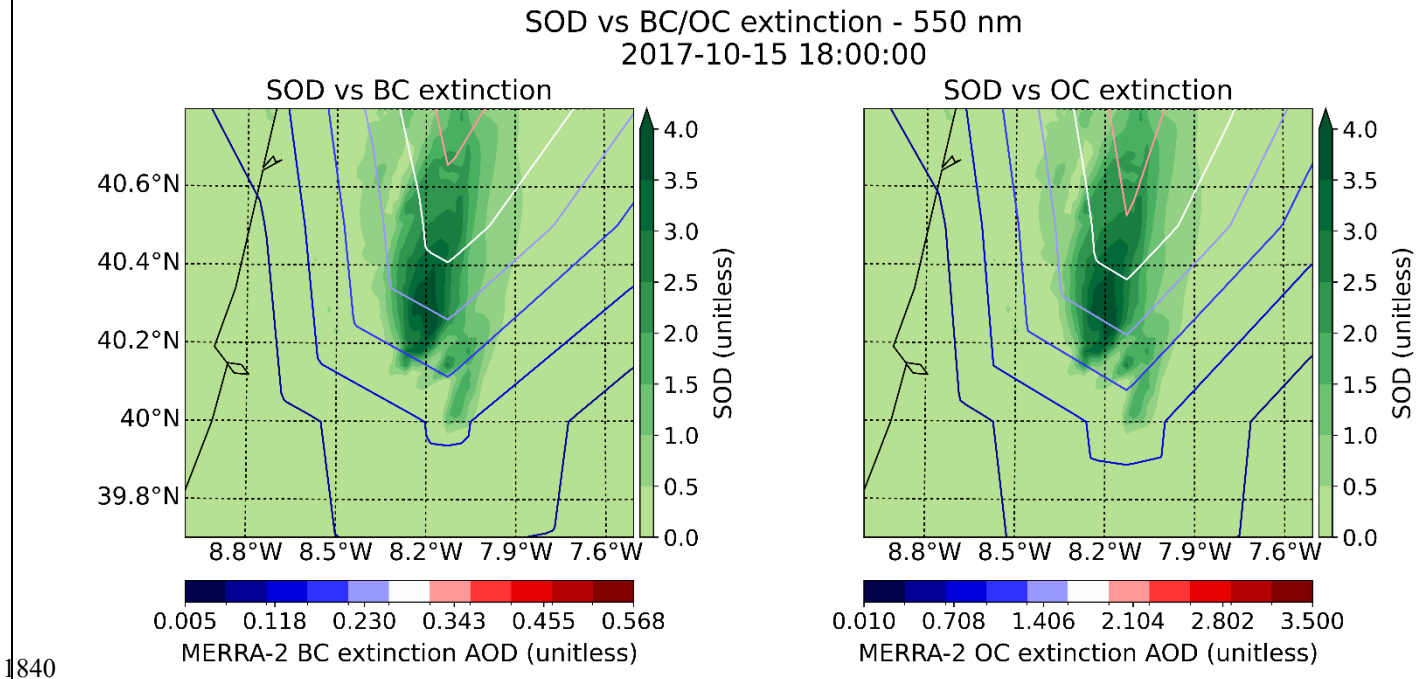


Figure 9: Spatial distribution of column-averaged PM2.5 concentration ($\text{kg}\cdot\text{m}^{-3}$, contours) on MERRA-2 surface BC (left panel) and OC (right panel) mass concentrations ($\text{kg}\cdot\text{m}^{-3}$, colour shading) at 19:00 UTC on 15 October 2017. Figure 9: Spatial distribution of PM2.5 concentrations ($\text{kg}\cdot\text{m}^{-3}$, contours) overlaid on BC (left panel) and OC (right panel) mass concentrations ($\text{kg}\cdot\text{m}^{-3}$, colour shading) at 19:00 UTC on 15 October 2017.

Figure 10 compares the simulated SOD at 550 nm with the MERRA-2 BC and OC extinction AOD during the mixed phase (18:00 UTC, 15 October 2017). As previously shown in Fig. 9, OC dominates the carbonaceous aerosol mass, while BC remains confined to the plume core near the main fire front. This compositional contrast is also evident in the extinction fields: OC extinction exhibits broader and stronger spatial correspondence with the simulated SOD, whereas BC extinction is weaker and more localized.

The 550 nm wavelength, commonly used in satellite retrievals, is particularly sensitive to fine mode aerosol extinction and therefore well suited to represent the optical behaviour of the simulated smoke. The close structural agreement between SOD and OC extinction confirms that organic carbon is the principal contributor to the plume's visible band radiative impact. In contrast, MERRA-2's coarse resolution smooths the sharp gradients resolved by BRAMS-SFIRE, attenuating peak extinction values and introducing slight spatial offsets. To further connect aerosol mass with optical extinction, Figure 10 compares the simulated SOD with the MERRA-2 BC and OC extinction AOD fields at 550 nm for 18:00 UTC. The spatial patterns reaffirm the behaviour already identified in Figure 9: BC extinction remains weak and confined to a narrow region near the fire core, whereas OC extinction extends over a much broader downwind area, mirroring the wider PM2.5 and OC mass envelope characteristic of smouldering and mixed-combustion emissions.

1830 The simulated SOD field shows a much stronger spatial correspondence with OC extinction than with BC, confirming that OC
is the dominant contributor to shortwave extinction at 550 nm in this plume. This is physically expected, as 550 nm is strongly
sensitive to fine-mode scattering aerosols, and OC constitutes the bulk of the fine carbonaceous mass. In contrast, BC, although
strongly absorbing, represents only a small fraction of the total aerosol mass and thus contributes minimally to visible-band
extinction.
1835 Some spatial mismatches remain, primarily due to the coarse horizontal resolution of MERRA-2 (50–70 km), which smooths
gradients that the 2-km BRAMS–SFIRE simulation resolves sharply. This smoothing reduces peak extinction values in the
reanalysis and broadens plume boundaries, producing slight offsets between SOD maxima and the corresponding features in
the MERRA-2 extinction fields.



SOD vs BC/OC extinction - 550 nm
2017-10-15 18:00:00 UTC

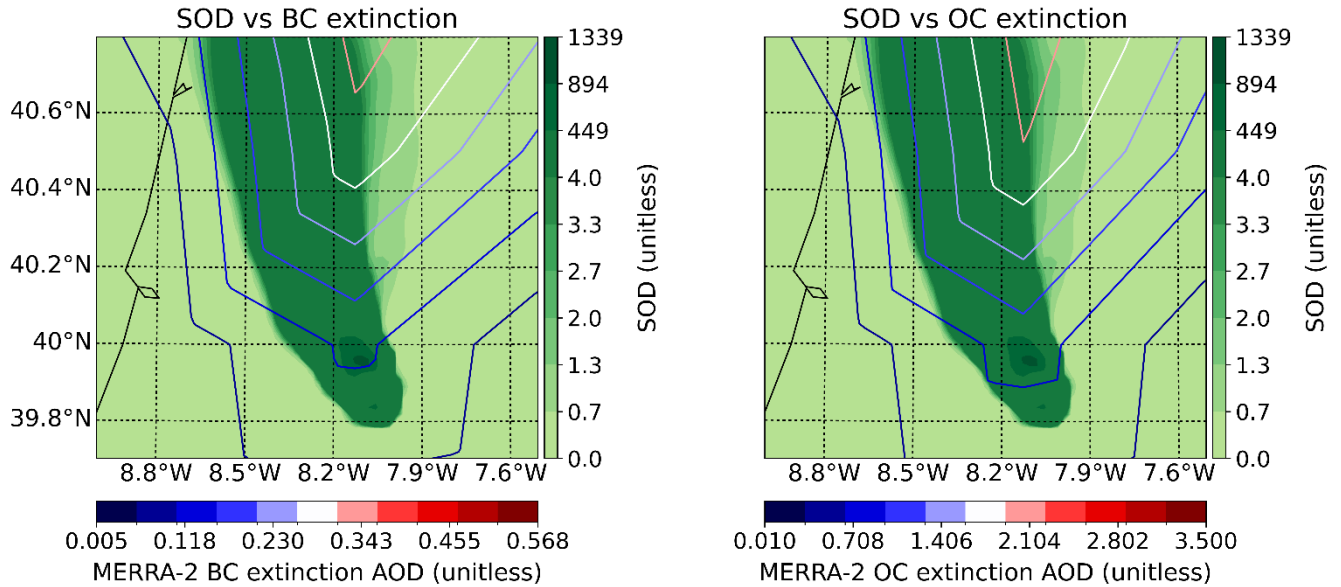


Figure 10: Comparison between simulated SOD (contours) and MERRA-2 extinction AOD at 550 nm for BC (left panel) and OC (right panel), at 18:00 UTC on 15 October 2017.

Figure 11 compares the model diagnosed SOD with the MERRA-2 component extinction AOD at 19:00 UTC during the mixed phase: (a) BC and (b) OC. Only about 3% of the samples lie outside the plotting window (“clipped”), so truncation does not affect the conclusions.

In panel (a) (BC), the ordinary least squares fit line blue has a very small slope (-0.07) and a positive intercept (0.03). The weak slope indicates that variability in SOD is only weakly expressed in the MERRA-2 BC extinction channel at this hour and over this domain. The positive intercept is consistent with a non-zero baseline in BC extinction (e.g., regional background and/or retrieval floor). The hexbin distribution is horizontally elongated relative to the 1:1 line, pointing to weak co-variation that can arise from species partitioning (BC being a minor contributor to total extinction in this case) and from spatial/temporal representativeness differences between the 2-km simulation and the 50-km reanalysis.

In panel (b) (OC), the fit line blue $y=0.44x+0.18$ shows a much stronger sensitivity of OC extinction to SOD: for a unit increase in SOD, OC extinction increases $\sim 6\times$ more than BC. The sizeable intercept (-0.18) suggests a substantial background OC extinction and/or a systematic positive offset of the MERRA-2 OC channel relative to the model baseline. The upward-tilted scatter with hints of saturation at the upper end may reflect a combination of (i) dynamic range limitations in the reanalysis OC product, (ii) sub-grid plume structure in the model that is diluted at reanalysis resolution, and (iii) differences in humidification growth or mixing-state assumptions between our κ -Köhler/Mie optical closure and MERRA-2.

Taken together, the two panels indicate a markedly stronger association between SOD and OC extinction than with BC extinction for this hour, while positive intercepts in both channels point to persistent background extinction. Any additional attribution (e.g., fire phase or cloud contamination) is not inferred here and would require independent diagnostics.

Figure 11 provides a quantitative assessment of how SOD relates to the carbonaceous extinction components of MERRA-2 during the mixed phase (19:00 UTC, 550 nm). Approximately 10 % of the data lie outside the plotting limits, but this level of clipping does not affect the statistical interpretation.

In panel (a), which compares SOD with BC extinction AOD, the ordinary-least-squares (OLS) fit shows a very small slope (≈ 0.06), a small positive intercept (≈ 0.03), and a modest coefficient of determination ($R^2 \approx 0.28$). These values indicate that only a limited fraction of the spatial variability in BC extinction is explained by SOD. This weak coupling is physically consistent with BC representing only a minor fraction of the total carbonaceous mass at this stage and with the coarse $\sim 50\text{--}70$ km MERRA-2 grid smoothing the sharp BC gradients resolved by the 2-km model. The horizontally elongated scatter distribution relative to the 1:1 line further highlights this weak covariance and the strong representativeness differences between the two datasets.

In panel (b), the comparison between SOD and OC extinction AOD yields a substantially stronger statistical relationship. The regression slope (≈ 0.38) is roughly six times larger than for BC, the intercept is higher (≈ 0.16), and the coefficient of determination increases to $R^2 \approx 0.31$. These values reflect the dominant contribution of OC to smoke extinction at 550 nm and the closer correspondence between SOD patterns and the spatial structure of OC in MERRA-2. The slight flattening of the scatter at large SOD values likely results from the coarse resolution of the reanalysis, the limited dynamic range of the OC extinction field, and differences in humidification growth or mixing-state assumptions between the model's κ -Köhler/Mie closure and the GOCART/MERRA-2 framework.

Taken together, these results confirm that OC extinction retains a much clearer imprint of the plume diagnosed by SOD than BC extinction, consistent with OC dominating visible-band extinction in biomass-burning smoke. The positive intercepts in both relationships indicate a persistent background extinction component present even where plume-model covariance is strong. No additional attribution (e.g., combustion phase variability or cloud effects) can be inferred from these diagnostics alone without independent observational constraints.

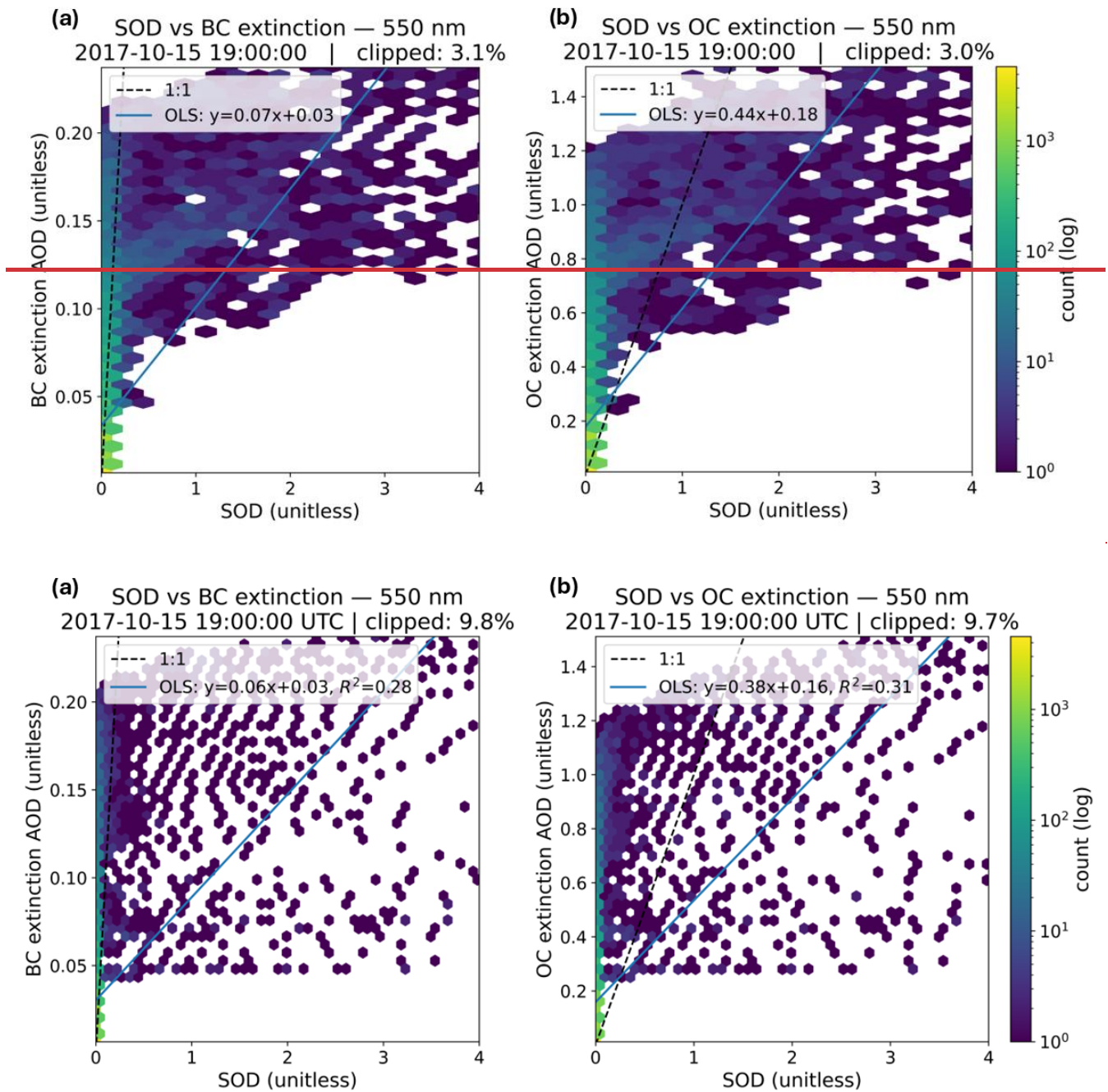


Figure 11: Scatter density plots comparing simulated SOD (wet) with MERRA-2 component extinction AOD for BC (panel a) and OC (panel b) at 550 nm, for 19:00 UTC on 15 October 2017. The dashed line represents the 1:1 relationship, and the solid line the ordinary least-squares (OLS) regression. Colour shading denotes the logarithmic density of grid-point pairs. The clipped percentage indicates the fraction of points excluded from the plot because their SOD or AOD values exceed the displayed range (≥ 4.0).

The statistical evaluation of simulated SOD against MERRA-2 component extinction AODs for black carbon (BC) and organic carbon (OC) is summarized in Table 5. The metrics quantitatively confirm the contrasting behavior already observed in Figs. 10–11, where BC exhibited weak spatial correspondence with SOD, while OC showed a much stronger and more coherent relationship. To extend the analysis beyond the scatter relationships in Figures 10–11, Table 5 provides domain-wide statistical metrics for black carbon (BC) and organic carbon (OC) extinction under all microphysical configurations, quantifying bias, variance explained, and sensitivity to microphysical perturbations. These diagnostics reinforce the contrasting behaviour already identified in the spatial and scatter comparisons: while OC extinction exhibits a coherent and physically interpretable relationship with SOD, BC extinction remains only weakly coupled to the modelled smoke field.

For BC, all three microphysical configurations yield similar statistics, with mean SOD values (0.15–0.17) roughly three times higher than the corresponding MERRA-2 BC extinction (≈ 0.06). The positive bias (0.09–0.12) and moderate RMSE (0.82–0.94) reflect the weak contribution of BC to the total optical depth at 550 nm. Correlation coefficients remain low ($r \approx 0.23$; $\rho \approx 0.75$), and the regression slopes (~ 0.05) indicate that variations in BC extinction explain only a small fraction of the spatial variability in SOD. The small positive intercepts (~ 0.02 –0.06) are consistent with a non-zero background BC extinction, likely representing regional baseline contributions and the limited dynamic range of the coarse-resolution MERRA-2 retrievals. The near-invariance of these metrics across the microphysical setups demonstrates that this weak SOD–BC linkage is structurally robust and largely insensitive to plausible variations in particle-size distribution or hygroscopicity. For BC, all microphysical configurations (Baseline, Conservative, Lower-envelope) produce nearly identical metrics, demonstrating that the SOD–BC relationship is largely insensitive to perturbations in κ , $r_{g,dry}$, or σ_g . Mean SOD values range from 7.6–8.6, overwhelmingly exceeding the corresponding MERRA-2 BC extinction (≈ 0.06), yielding very large positive biases (7.5–8.5) and RMSE values between 52–58. These large errors are expected: BC represents only a minor fraction of carbonaceous aerosol mass in biomass-burning plumes and contributes weakly to visible-band extinction at 550 nm. Correlation coefficients remain low but positive (Pearson $r \approx 0.14$; Spearman $\rho \approx 0.75$), indicating that although BC extinction contains a monotonic spatial ordering relative to SOD, it explains only about 2 % of the SOD variance ($R^2 = 0.02$). The regression slopes for BC (≈ 0.000) confirm that spatial variability in BC extinction barely responds to changes in SOD, while the small intercept (~ 0.058) is consistent with a persistent background BC extinction present in the reanalysis, likely representing non-smoke contributions and the coarse effective resolution of MERRA-2.

In contrast, the OC extinction field exhibits a markedly stronger and more proportional relationship with SOD. Mean OC extinction (~ 0.34) exceeds SOD by a factor of about two, resulting in a systematic negative bias (-0.16 to -0.18) and higher absolute errors (MAE ≈ 0.38 –0.40). However, correlations are slightly higher ($r \approx 0.24$ –0.25; $\rho \approx 0.76$), and the regression slope (~ 0.14) indicates a substantially greater sensitivity of OC extinction to SOD variability compared with BC (by almost a factor of three). The intercepts (~ 0.31 –0.32) point to a persistent OC background or overestimation in MERRA-2, possibly related to climatological secondary organic aerosol loading and the coarse spatiotemporal averaging inherent to the reanalysis. The consistent slope and correlation across the three configurations further support the interpretation that OC dominates the

visible-band extinction signature of the simulated plume. In contrast, the OC extinction field shows a stronger and more physically meaningful connection to SOD. Although mean SOD ($\approx 7.6\text{--}8.6$) still greatly exceeds mean OC extinction (≈ 0.34), the bias is smaller than for BC, and the correlations are modestly higher ($r \approx 0.16$; $\rho \approx 0.75$). The OC regression slopes ($0.001\text{--}0.002$), while still small in absolute terms, are one order of magnitude larger than those obtained for BC, mirroring OC's dominant contribution to carbonaceous aerosol mass and its stronger role in visible-band scattering. The regression intercepts (~ 0.325) indicate a substantial baseline OC extinction in MERRA-2, consistent with the presence of regionally distributed secondary organic aerosols and with the smoothing inherent to the coarse-grid reanalysis. As with BC, the near-identical statistics across the three microphysical experiments reflect that microphysical uncertainties play only a secondary role in controlling the SOD–OC relationship.

The statistics corroborate that OC is the primary optical driver of the modeled smoke at 550 nm, while BC contributes only a minor, localized absorbing component. The weak dependence of both correlations on the assumed microphysical state (σ_g , κ and $r_{g, \text{dry}}$) demonstrates that compositional contrasts, rather than parameter uncertainty, control the observed behaviour. The combined results from the maps (Fig. 10) and scatter analyses (Fig. 11) thus confirm that the radiative impact of the plume is governed mainly by OC-dominated scattering, with BC absorption playing a secondary but spatially concentrated role within the fire core. Overall, the diagnostics confirm that OC dominates the optical signature of the plume at 550 nm, acting as the principal contributor to scattering and thus to the radiative impact of the smoke layer, while BC contributes a much smaller, spatially confined absorbing component. The weak sensitivity of the statistical metrics to the microphysical perturbations further demonstrates that the observed behaviour is governed primarily by species composition and representativeness differences between BRAMS–SFIRE and MERRA-2, rather than by uncertainties in aerosol size distribution or hygroscopic growth.

Table 5: Diagnostic statistics for all the Sertã wildfire period, including the mean, bias, mean absolute error (MAE), root-mean-square error (RMSE), Pearson correlation coefficient (r) and Spearman’s rank correlation coefficient (ρ), and coefficient of determination (R^2), linear-regression slope and intercepts between SOD and BC, OC MERRA-2 extinction AOD.

Carbonaceous aerosols	Phase	Mean SOD	Mean BC/OC	Bias	MAE	RMSE	r	ρ	R^2	slope	intercept
BC	Baseline	<u>7.920.16</u>	<u>0.060.06</u>	<u>7.860.10</u>	<u>7.950.19</u>	<u>53.730.85</u>	<u>0.140.23</u>	<u>0.750.75</u>	<u>0.020.05</u>	<u>0.0000.022</u>	<u>0.0580.056</u>
	Conservative	<u>8.580.17</u>	<u>0.060.06</u>	<u>8.520.12</u>	<u>8.610.20</u>	<u>58.490.94</u>	<u>0.140.23</u>	<u>0.750.75</u>	<u>0.020.05</u>	<u>0.0000.019</u>	<u>0.0580.056</u>
	Lower envelope	<u>7.620.15</u>	<u>0.060.06</u>	<u>7.560.09</u>	<u>7.650.18</u>	<u>52.000.82</u>	<u>0.140.23</u>	<u>0.750.75</u>	<u>0.020.05</u>	<u>0.0000.022</u>	<u>0.0580.056</u>
OC	Baseline	<u>7.920.16</u>	<u>0.340.34</u>	<u>7.58-0.17</u>	<u>8.090.39</u>	<u>53.620.90</u>	<u>0.160.25</u>	<u>0.750.76</u>	<u>0.030.06</u>	<u>0.0010.141</u>	<u>0.3250.314</u>

Conservative	8.580.17	0.340.34	8.24-0.16	8.750.40	58.380.97	0.160.24	0.750.76	0.030.06	0.0010.126	0.3250.315
Lower envelope	7.620.15	0.340.34	7.29-0.18	7.800.38	51.900.87	0.160.25	0.750.76	0.030.06	0.0020.145	0.3250.315

To assess the radiative implications of the simulated aerosol fields, the single scattering albedo (SSA) derived from BRAMS-SFIRE PM2.5 simulations, was compared with MERRA-2 data at 550 nm for 19:00 UTC (Fig. 12). SSA is a fundamental quantity in aerosol-radiation interaction studies, expressing the ratio of scattering to total extinction and thereby indicating the relative dominance of absorbing versus scattering components. Low SSA values denote strongly absorbing aerosols, typically associated with fresh BC-rich smoke, whereas high SSA values are characteristic of more scattering-dominated particles such as sulphates or aged organic aerosols.

At 19:00 UTC, BRAMS-SFIRE simulates relatively high SSA values, ranging mostly between 0.88 and 0.90, with smoother spatial gradients across the plume region. This pattern indicates that the simulated smoke is dominated by moderately scattering aerosols, consistent with partial aging and mixing with less absorbing species during transport. In contrast, MERRA-2 SSA derived from the BC+OC proxy (left panel) exhibits more spatial variability, including localized minima below 0.7 that suggest stronger absorption associated with freshly emitted black carbon-rich particles.

The higher and more homogeneous SSA simulated by BRAMS-SFIRE likely results from rapid dilution and vertical mixing of the plume, as well as from simplifications in the representation of aerosol optical properties and internal mixing states.

When compared with MERRA-2 SSA derived from the total AOD (right panel), the differences between the datasets become more systematic. In this case, MERRA-2 exhibits higher SSA values because the total AOD field includes additional aerosol components, such as sulphates and dust, that are predominantly scattering. Their inclusion enhances the overall scattering fraction in the reanalysis and smooths the horizontal gradients, yielding a more uniform spatial distribution of SSA. In contrast, the simulated field remains slightly lower and more structured, reflecting the localized influence of biomass-burning emissions.

Despite these differences, both datasets consistently delineate the same general plume region, indicating that BRAMS-SFIRE realistically reproduces the spatial extent of smoke-affected areas.

These patterns are further quantified in Fig. 12, which presents scatter density plots comparing simulated and MERRA-2 SSA for BC+OC and total aerosol components. The distributions reveal weak correlations and a narrow dynamic range, with most points concentrated near the upper SSA limit. The regression slopes strongly deviate from the 1:1 line, indicating that the model systematically overestimates SSA relative to MERRA-2, particularly for the BC+OC proxy. This behaviour reflects the combined influence of spatial-resolution differences, the coarse temporal averaging inherent to reanalysis data, and the simplified parameterization of refractive indices and mixing states in the model's radiative module.

Taken together, Figs. 7–12 demonstrate that high-resolution fire-atmosphere models such as BRAMS-SFIRE can realistically reproduce the spatial structure and general radiative characteristics of smoke plumes. However, systematic biases in SSA

1990 magnitude and variability persist, emphasizing the need for further evaluation using temporally and spatially resolved ground-based and satellite observations to refine the model representation of aerosol optical properties and their radiative effects. Beyond extinction behaviour, the single-scattering albedo (SSA) offers a complementary measure of the radiative character of the smoke plume by expressing the relative contributions of scattering and absorption. Accordingly, SSA fields derived from BRAMS-SFIRE were compared with their MERRA-2 counterparts to assess whether the model correctly captures the

1995 scattering-absorption balance within the plume.

Figure 12 contrasts the simulated SSA at 550 nm with two MERRA-2 products at 19:00 UTC: a BC+OC proxy (left panel) and the total-aerosol SSA (right panel). SSA represents the ratio of scattering to total extinction; hence low SSA values correspond to strongly absorbing aerosol (typically BC-rich fresh smoke), while high SSA indicates more scattering-dominated mixtures such as aged organics or background sulphates.

2000 In the BC+OC comparison (Fig. 12, left), BRAMS-SFIRE yields SSA values mostly between 0.88 and 0.90, forming smooth horizontal gradients across the plume. This behaviour is consistent with moderately scattering aerosols and limited absorption. The corresponding MERRA-2 BC+OC proxy, however, exhibits sharper gradients and pockets of markedly lower SSA (<0.82) near the fire core, reflecting stronger BC absorption in the reanalysis than in the model. These contrasts partly arise from MERRA-2's coarse grid (~ 50 – 70 km), which simultaneously smooths plume edges and preserves mesoscale absorption

2005 signatures.

The right panel compares simulated SSA against total MERRA-2 SSA, which includes additional scattering species (sulphates, dust, sea salt). This total-aerosol SSA is higher and more horizontally uniform than the BC+OC proxy, reflecting the dominant contribution of non-carbonaceous scattering aerosols in the reanalysis. Their inclusion brings MERRA-2 SSA closer to the scattering-dominated regime simulated by BRAMS-SFIRE, though spatial differences remain due to the finer plume structure

2010 resolved by the 2-km model.

The discrepancies highlighted in Figure 12 arise from several structural factors: (i) dilution and enhanced mixing in BRAMS-SFIRE, which reduce the local BC mass fraction and therefore increase the SSA (i.e., shift the aerosol population toward more scattering-dominated conditions); (ii) coarse spatial averaging in MERRA-2, which smooths sub-grid gradients but retains regional absorption anomalies; and (iii) fundamentally different mixing-state assumptions. In this study, SSA is computed

2015 offline from PM_{2.5} using a monodisperse, externally mixed Mie scheme, which does not account for absorption enhancement arising from internally mixed BC encapsulated within organic or sulphate material. By contrast, GOCART/MERRA-2 treats fine-mode aerosols as internally mixed, allowing lensing effects that increase BC absorption. Consequently, the SSA estimated from this monodisperse PM_{2.5} aerosol representation tends to overestimate SSA relative to MERRA-2 in the vicinity of the plume core. Because the PM_{2.5}-based optical calculation adopts fixed microphysical parameters within each phase scenario,

2020 the resulting SSA exhibits limited spatial variability, even across regions with strong concentration gradients.

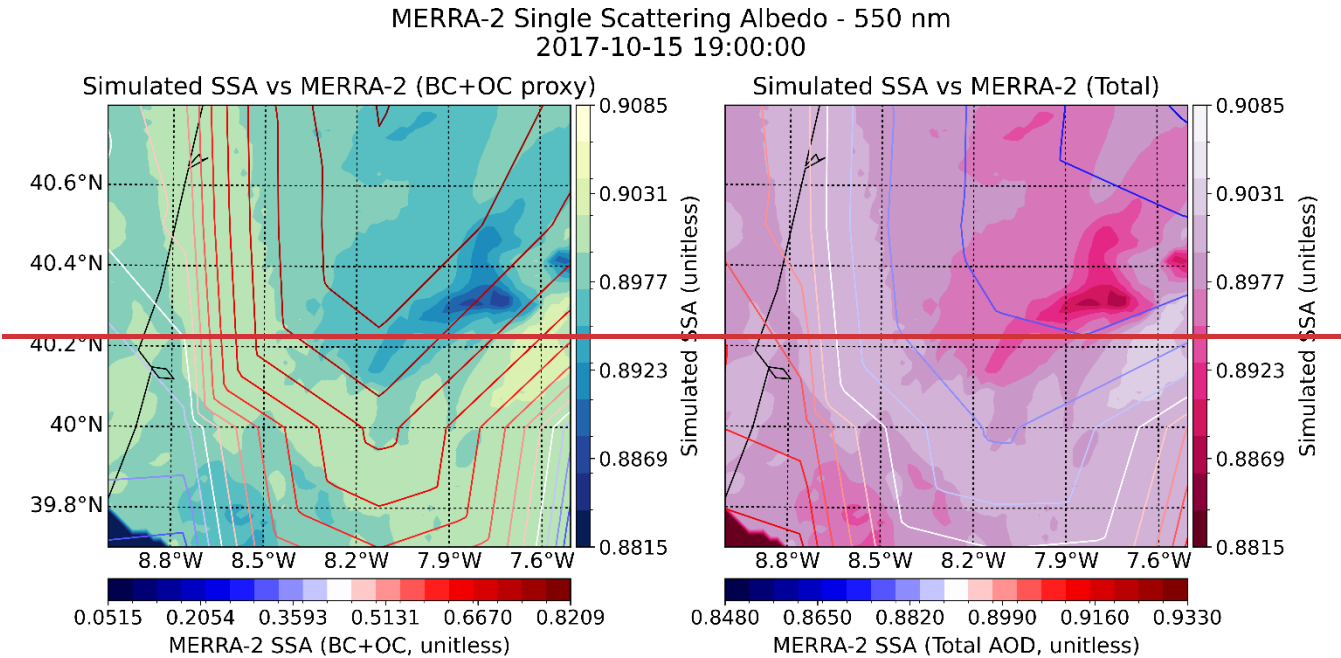
To complement the spatial fields, Figure 13 presents scatter-density comparisons between simulated SSA and MERRA-2 SSA for BC+OC (panel a) and total aerosols (panel b). In both cases, the relationships exhibit weak covariance and low explanatory power ($R^2 < 0.15$). The simulated SSA spans a narrow dynamic range, whereas MERRA-2 displays substantially larger spatial

variability, particularly for the BC+OC proxy. This contrast leads to limited point-wise correspondence between datasets.

Although the total-aerosol comparison shows slightly closer absolute values, correlations remain weak, reflecting structural differences in aerosol representation and mixing-state assumptions.

Taken together, Figures 12–13 indicate that BRAMS–SFIRE captures the plume’s spatial extent and its predominantly scattering-dominated character, consistent with the OC-rich composition shown in Figures 9–11, yet it underrepresents the absorbing component associated with fresh BC. The persistence of SSA biases across all microphysical configurations further demonstrates that these discrepancies are structural, arising from resolution limitations, mixing-state assumptions, and representativeness differences rather than from uncertainties in aerosol microphysics.

2035



MERRA-2 Single Scattering Albedo - 550 nm
2017-10-15 19:00:00 UTC

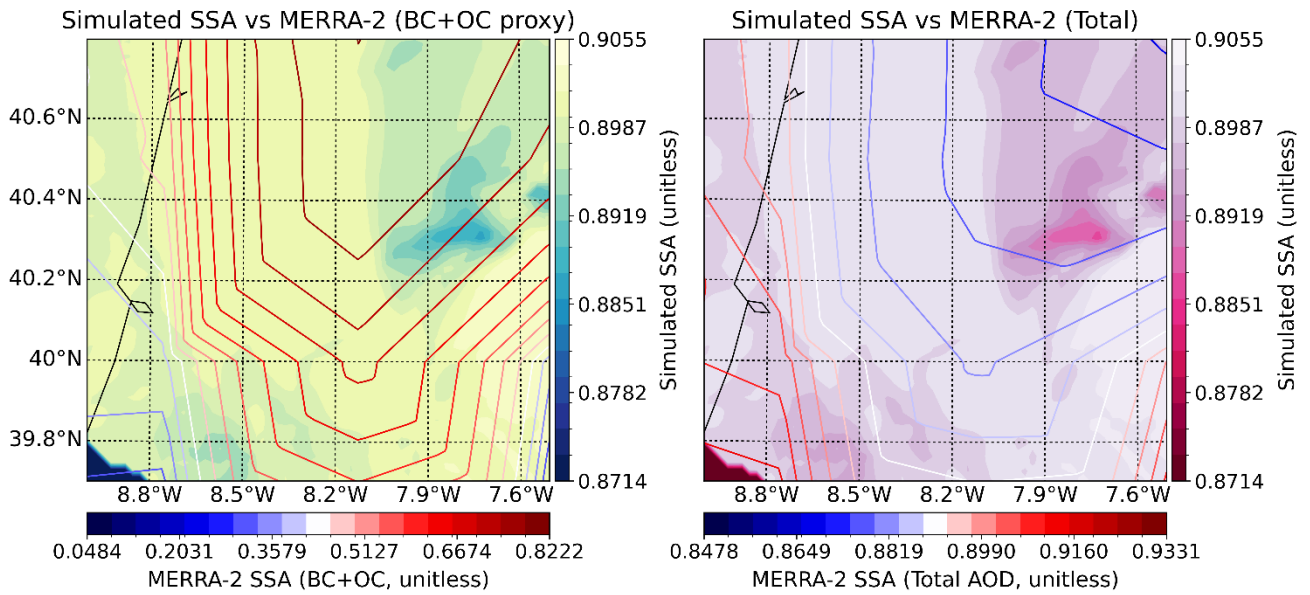


Figure 12: Spatial distribution of SSA at 550 nm derived from BRAMS-SFIRE PM2.5 simulations, overlaid with SSA contours derived from MERRA-2 reanalysis for the wildfire plume on 15 October 2017, at 19:00 UTC. Left panels show MERRA-2 SSA calculated from BC and OC AOD, while right panels represent SSA derived from total AOD (all species).

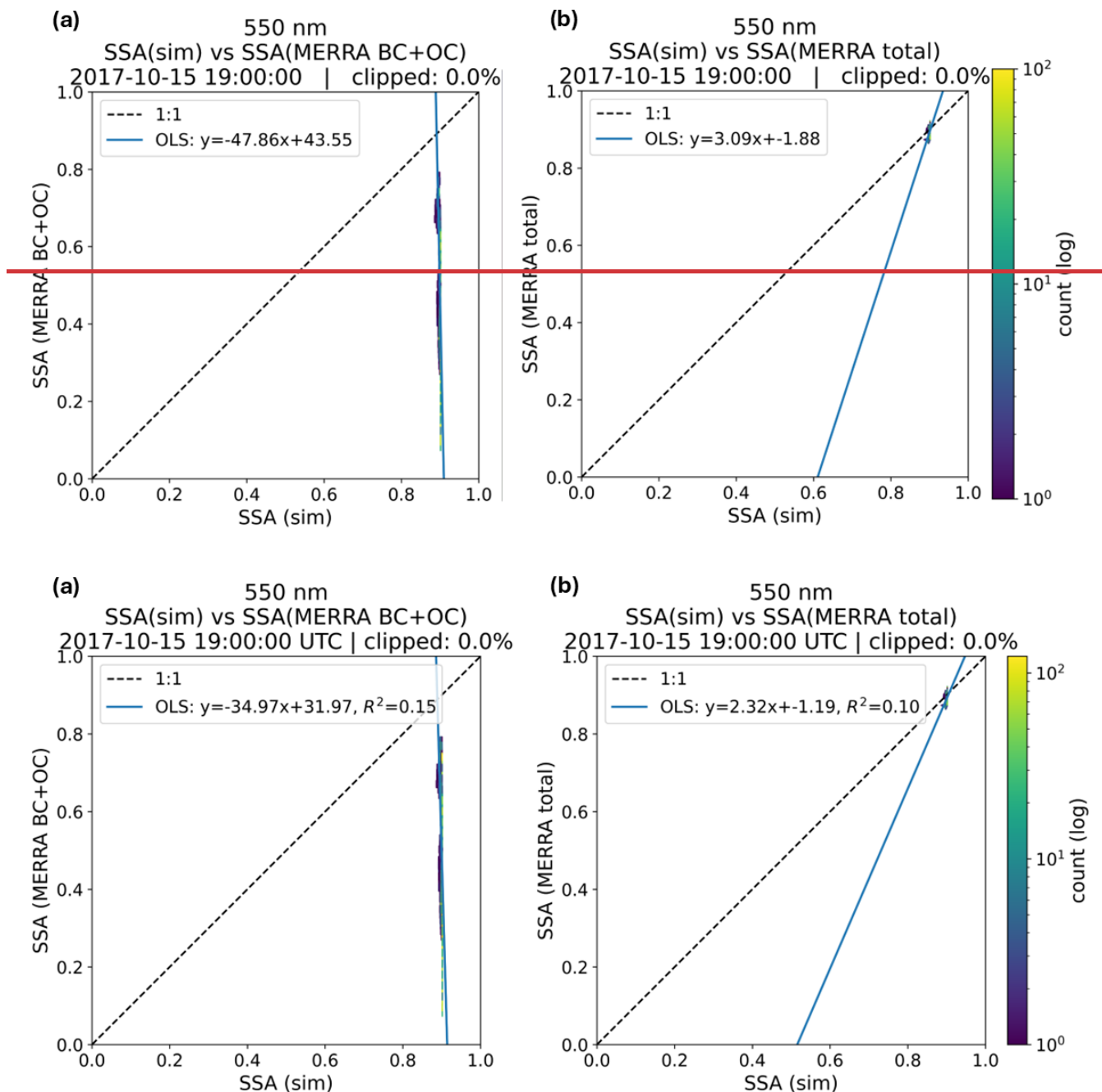


Figure 13: Scatter-density plots comparing single scattering albedo (SSA) derived from BRAMS-SFIRE PM_{2.5} simulations (x-axis) with MERRA-2 SSA proxies at 550 nm for BC+OC (panel a) and total aerosols (panel b) at 19:00 UTC on 15 October 2017. The simulated SSA field is identical in both panels, as it is derived from the same PM_{2.5} distribution and fixed microphysical assumptions; only the MERRA-2 reference field differs (BC+OC proxy versus total aerosol SSA). The dashed line denotes the 1:1

2050 relationship, while the solid line represents the ordinary least-squares (OLS) regression fit. Colour shading indicates the logarithmic
density of grid-point pairs. The clipped percentage denotes the fraction of data excluded for visualisation purposes because their
SOD or AOD values exceed the displayed range (≥ 4.0). Scatter density plots comparing SSA derived from BRAMS-SFIRE PM2.5
simulations with MERRA-2 component AOD at 550 nm for BC + OC (panel a) and for total aerosols (panel b), at 19:00 UTC on 15
2055 October 2017. The dashed line denotes the 1:1 relationship, while the solid line represents the ordinary least-squares (OLS)
regression fit. Colour shading indicates the logarithmic density of grid-point pairs. The clipped percentage refers to the fraction of
data points excluded from the plot because their SOD or AOD values exceed the displayed range (≥ 4.0).

The quantitative evaluation of SSA statistics (Table 6) corroborates the spatial patterns discussed above. When compared
against MERRA-2 SSA derived from the BC + OC extinction AOD, the model exhibits a strong positive bias of -0.36 – -0.37
2060 across all microphysical configurations, indicating a substantial overestimation of the scattering fraction in the simulated
smoke. The mean SSA simulated by BRAMS-SFIRE (~ 0.90) contrasts sharply with the much lower MERRA-2 mean ($\sim$
 0.54), consistent with the visual evidence in Figs. 12 and 14 showing that the model produces optically brighter, less absorbing
plumes. The weak correlations ($r \sim -0.4$ to -0.2) and near zero regression slopes further confirm the limited point-to-point
agreement, reflecting differences in spatial resolution, averaging timescales, and the simplified internal mixing representation
2065 in the model's optical closure. The large positive intercepts (10 – 15) in the regression fits are purely numerical artefacts arising
from the narrow SSA range and should not be interpreted physically.

In contrast, when the comparison is performed against the MERRA-2 total-aerosol SSA (all species combined), the agreement
improves markedly. The bias is nearly eliminated ($\sim +0.01$), and the RMSE drops to -0.02 across all configurations, while the
correlations become weakly positive ($r \sim 0.3$ – 0.5). This improvement is consistent with the inclusion in the MERRA-2 total
2070 SSA of predominantly scattering species such as sulphates and dust, which elevate the overall reanalysis SSA toward the
modelled range. The close mean agreement suggests that, although BRAMS-SFIRE tends to overpredict SSA relative to the
carbonaceous fraction alone, its bulk radiative behavior is broadly consistent with the multi-species aerosol environment
captured by the reanalysis.

Physically, these results imply that the model reproduces the general radiative character of the plume, dominated by moderately
2075 scattering, partially aged smoke, but underrepresents the absorbing component associated with fresh BC. The consistency
across the microphysical configurations (baseline, conservative, and lower-envelope) indicates that these discrepancies are
more structural than parametric, reflecting the inherent limitations of fixed refractive-index assumptions and unresolved sub-
grid-mixing processes.

Table 6 quantifies the SSA behaviour for both the BC+OC and total-aerosol configurations and confirms the spatial patterns
2080 identified in Figures 12–13. When compared against the MERRA-2 BC+OC SSA proxy, the model exhibits a large positive
bias of ~ 0.36 – 0.37 , consistent across the Baseline, Conservative, and Lower-Envelope configurations. This bias reflects a
systematic overestimation of scattering in the simulated plume: the mean model SSA is ~ 0.90 , whereas the BC+OC SSA in

MERRA-2 is only ~0.54 (“Mean simu” and “Mean MERRA-2”). These values corroborate Figure 12, where BRAMS–SFIRE produces a more scattering-dominated (optically brighter, less absorbing) plume than the reanalysis.

The correlations remain weak, Pearson r ranges from -0.42 to 0.24 , and Spearman ρ from -0.30 to 0.29 , indicating little pointwise correspondence between model and reanalysis fields. The OLS slopes are extremely small (≈ 0.06 , -0.18 , -0.17 depending on configuration), and the intercepts span large values (from about -12 to $+15$). These unphysical intercepts arise from the narrow dynamic range of SSA and should not be interpreted in mechanistic terms.

In contrast, the comparison with MERRA-2 total-aerosol SSA yields a markedly better agreement. The bias nearly vanishes ($+0.01$) and both MAE and RMSE reduce to ~ 0.01 – 0.02 . Correlations increase to weak but positive values (Pearson $r \approx 0.35$ – 0.47 , Spearman $\rho \approx 0.32$ – 0.34). This improvement results from the fact that total-aerosol SSA in MERRA-2 includes additional scattering species, notably sulphates, dust, and secondary organics, which raise the reanalysis SSA to values close to those in the model (0.89 – 0.90 , “Mean MERRA-2”). Thus, although BRAMS–SFIRE overestimates SSA relative to carbonaceous-only extinction, its bulk radiative behaviour aligns more closely with the full multi-species aerosol environment represented in MERRA-2.

Overall, these results confirm that the simulated plume is dominated by moderately scattering, OC-rich smoke, while the absorbing BC component is underrepresented relative to the reanalysis. The near-identical SSA statistics across all microphysical experiments show that the discrepancies are structural rather than parametric, arising from simplifications in the optical treatment (e.g., monodisperse, externally mixed particles), the model–reanalysis resolution gap, and differences in mixing-state representation, rather than from uncertainties in κ , $r_{g,dry}$, or σ_g .

Table 6: Diagnostic statistics for all the Sertã wildfire period, including the mean, bias, mean absolute error (MAE), root-mean-square error (RMSE), Pearson correlation coefficient (r) and Spearman’s rank correlation coefficient (ρ), and coefficient of determination (R^2), linear-regression slope and intercepts between SSA derived from PM2.5 simulated by BRAMS–SFIRE and SSA derived from MERRA-2 extinction AODs (BC+OC and total aerosol components)

Carbonaceous aerosols		Phase	Mean simu	Mean MERRA- 2	Bias	MAE	RMSE	r	ρ	R^2	slope	intercept
SSA BC+OC	Baseline		0.900-0.90	0.540-0.54	0.370-0.37	0.370-0.37	0.420-0.42	0.240-0.18	0.290-0.28	0.060-0.03	14.14140-65	-12.21-9.07
	Conservative		0.900-0.90	0.540-0.54	0.370-0.37	0.370-0.37	0.420-0.42	-0.42-0.42	-0.26-0.25	0.180-0.18	-15.63-15.60	14.6314-60
	Lower envelope		0.900-0.90	0.540-0.54	0.360-0.36	0.360-0.36	0.410-0.41	-0.41-0.40	-0.27-0.24	0.170-0.16	-11.17-10.83	10.5510-24
SSA Total	Baseline		0.900-0.90	0.890-0.89	0.010-0.01	0.020-0.02	0.020-0.02	-0.35-0.31	-0.37-0.36	0.120-0.09	-1.88-1.59	2.582-32
	Conservative		0.900-0.90	0.890-0.89	0.010-0.01	0.020-0.02	0.020-0.02	0.470-0.47	0.340-0.33	0.220-0.22	1.571-58	-0.53-0.54

3.43 Temporal Evolution and Distribution of PM2.5 Concentrations simulated

Figure 14 shows histograms of domain wide near surface PM2.5 concentrations ($\mu\text{g m}^{-3}$) at 13:00, 16:00, 19:00, and 22:00 UTC on 15 October 2017. The ordinate is the number of grid cells per bin on a logarithmic scale, with fixed bin edges across panels. Across all time steps, the distributions are strongly right skewed, with a pronounced mode in the lowest bin and a persistent heavy tail reaching $\mathcal{O}(10^4) \mu\text{g m}^{-3}$. The large count in the first bin indicates that most grid cells register very low concentrations (background or weakly impacted air), whereas the long upper tail shows that a comparatively small subset attains very high values. From 13:00 to 19:00 UTC the histograms broaden as counts shift from the lowest bin into intermediate and high bins ($\sim 10^2\text{--}10^4 \mu\text{g m}^{-3}$), evidencing increases in both spread and upper tail occupancy. By 22:00 UTC the tail remains but the highest bins are less populated than at 19:00 UTC, while intermediate bins still retain substantial counts—consistent with partial dilution and aging rather than full clearing. In statistical terms, the fields exhibit pronounced positive skewness and persistent heavy tailed (non-Gaussian) behavior into the evening, alongside an afternoon increase in the fraction of the domain experiencing elevated concentrations.

Figure 14 shows the frequency distributions of domain-wide near-surface PM2.5 concentrations ($\mu\text{g m}^{-3}$) at 13:00, 16:00, 19:00, and 22:00 UTC on 15 October 2017. All panels use identical binning and a logarithmic y-axis to emphasize the occurrence of rare but extremely high concentrations. At every time step, the distributions are highly right-skewed: most grid cells fall within the lowest concentration bins, while a persistent heavy tail extends toward very large PM2.5 values, characteristic of a spatially confined but optically and chemically intense smoke plume.

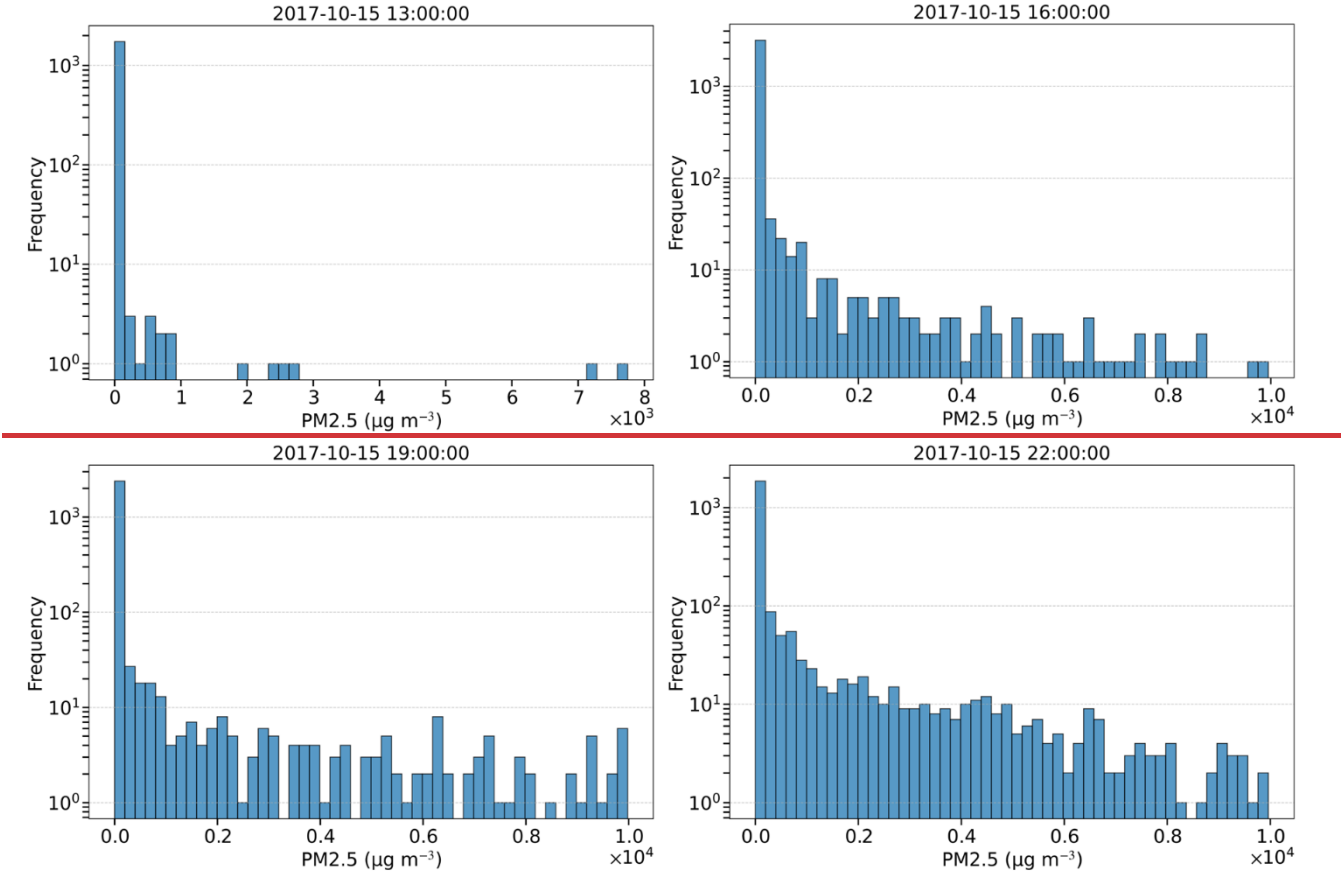
Between 13:00 and 16:00 UTC, the distributions broaden substantially. Although the mode remains anchored in the lowest bin, indicating that the majority of the domain experiences only weak smoke influence, the gradual infilling of intermediate bins and the emergence of a long upper tail reflect the onset of plume intensification and expansion during the early afternoon. By 19:00 UTC, the histogram exhibits its widest dynamic range, with sustained occupancy across intermediate and high concentration classes and peak values approaching $10^7 \mu\text{g m}^{-3}$. This behaviour signals maximum plume loading near the surface, consistent with the period of strongest fire activity and turbulent mixing.

Scientifically, the coexistence of a dominant low concentration mode with a persistent heavy tail indicates a smoke influence that is spatially sparse yet intense where present. The relatively limited footprint and sporadic high values at 13:00 UTC transition, by 16:00–19:00 UTC, to greater occupancy of mid to high bins, which is consistent with plume intensification and lateral spread associated with daytime mixing and peak fire activity. Toward evening (22:00 UTC), reduced surface heating and weaker turbulence are consistent with the partial relaxation of extremes near the surface, while the continued tail suggests that pockets of high PM2.5 persist locally. Operationally, regional exposure is governed by a small fraction of grid cells bearing very high PM2.5, whereas the majority of the area remains lightly affected, implying sharp spatial gradients and transient

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hotspots that evolve through the afternoon and can carry into the evening. By 22:00 UTC, the distribution narrows slightly: the extreme upper tail becomes less populated, suggesting partial dilution and reduced near-surface entrainment following the evening transition. Nevertheless, the heavy tail does not vanish, implying that localized pockets of very high PM_{2.5} persist despite weaker turbulence and declining emissions. Intermediate concentration bins retain notable counts, indicating that the plume continues to influence a non-negligible fraction of the domain even as the intensity of near-surface impacts diminishes. From a physical standpoint, the coexistence of an overwhelmingly low-concentration mode with a pronounced heavy tail underscores the highly intermittent nature of smoke exposure: large portions of the domain remain only weakly affected, while a small number of grid cells experience extreme concentrations that dominate the regional burden. The afternoon broadening of the distributions reflects plume growth, lateral spread, and enhanced turbulent transport, whereas the partial evening contraction corresponds to stabilization and reduced mixing. Such behaviour highlights the operational relevance of intense, spatially localized hotspots, which evolve rapidly through the afternoon and can persist into the evening despite overall decreases in plume activity.



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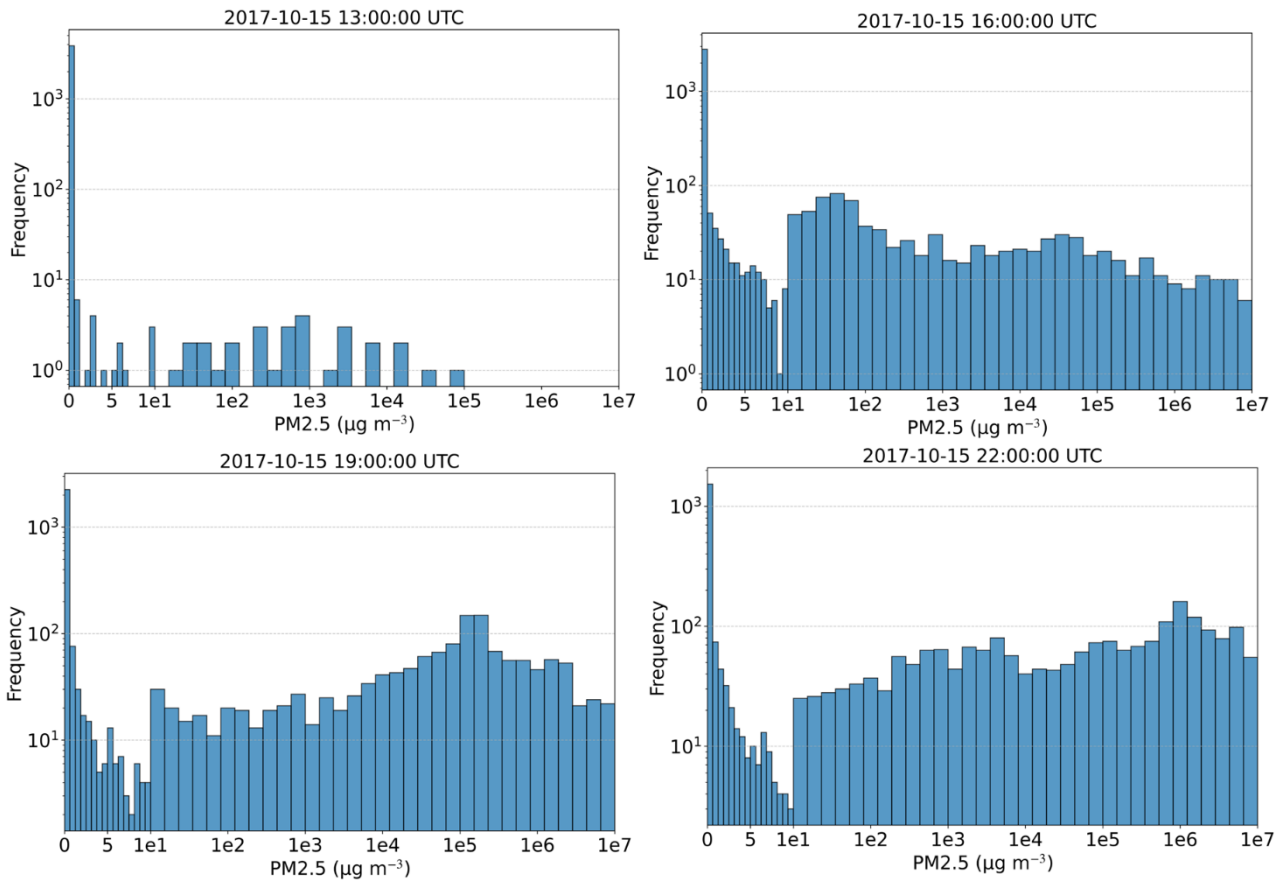


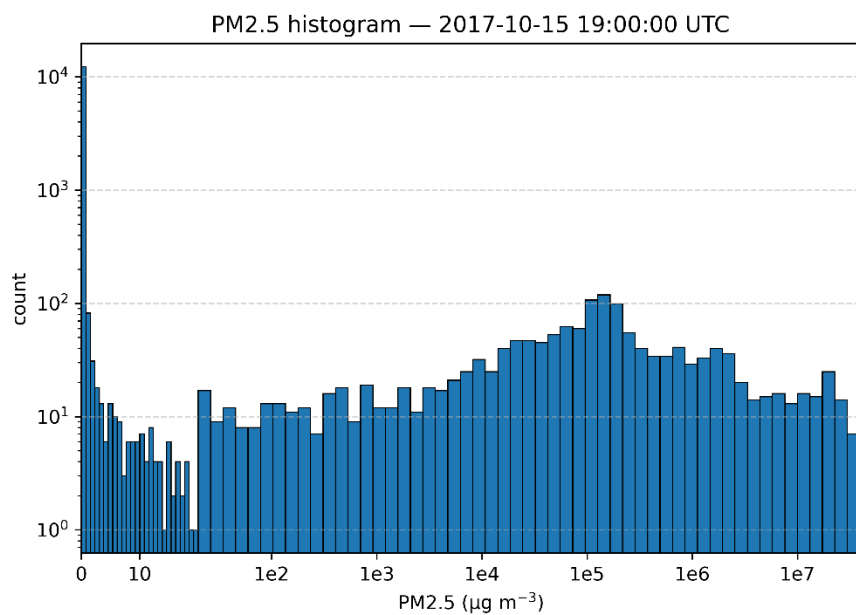
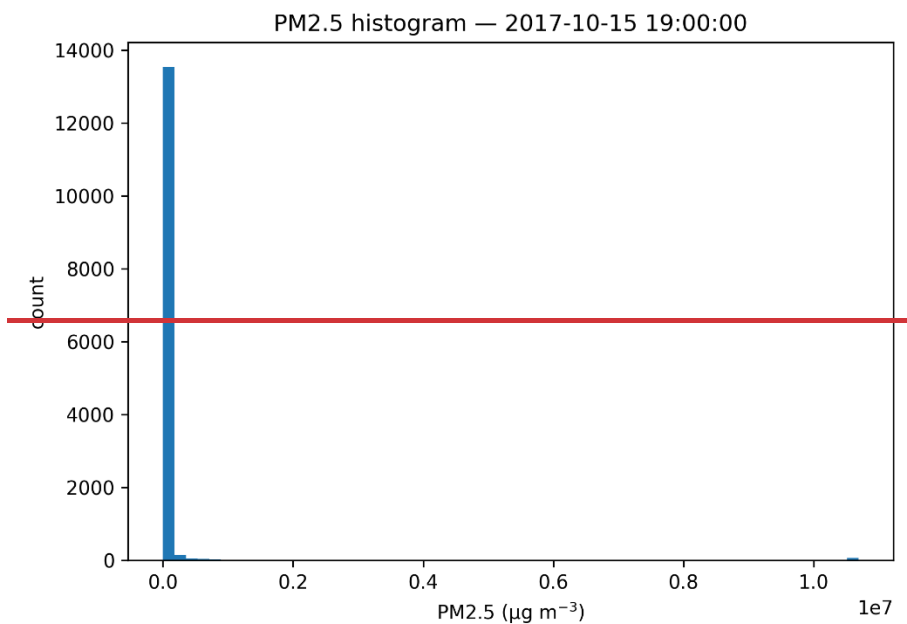
Figure 14: Frequency distribution of PM_{2.5} concentrations ($\mu\text{g}/\text{m}^3$) across the simulation domain on 15 October 2017 at different hours (13:00, 16:00, 19:00 and 22:00 UTC). Each histogram shows the number of grid cells registering PM_{2.5} values within each concentration bin. The vertical axis is plotted on a logarithmic scale to highlight rare but extreme values.

At 19:00 UTC, the histogram in Fig. 15 further emphasizes the strongly right-skewed nature of the PM_{2.5} distribution. After restricting the analysis to values below $10^4 \mu\text{g m}^{-3}$, the majority of grid cells remain below $0.1 \mu\text{g m}^{-3}$, while a small subset occupies the upper bins, forming a sparse heavy tail that approaches the imposed cutoff. The persistence of this tail under a physically motivated cap suggests localized accumulation near the fire core, while the filtering simultaneously suppresses unrealistically large extremes likely attributable to numerical artifacts. This yields a more physically interpretable depiction of the simulated PM_{2.5} field and clarifies that domain-wide exposure at 19:00 UTC is still governed by a small fraction of cells

at the high end. Whereas Figure 14 documents the evolution of PM_{2.5} distributions throughout the day, Figure 15 isolates the histogram corresponding to 19:00 UTC on 15 October 2017, highlighting the structure of the heavy-tailed distribution at the hour of maximum plume loading. Figure 15 shows the domain-wide frequency distribution of simulated PM_{2.5} concentrations at that time. The histogram reveals a pronouncedly right-skewed distribution, with the vast majority of grid cells occupying the lowest concentration bins, while a progressively smaller number populate the intermediate and upper ranges. The logarithmic vertical axis accentuates this structure: although extremely high PM_{2.5} values occur infrequently, they form a distinct heavy tail that extends up to nearly $1 \times 10^7 \mu\text{g m}^{-3}$.

This statistical behavior reflects the intrinsic spatial heterogeneity of the plume. Most of the domain remains only weakly affected by smoke at this hour, whereas a limited set of grid cells, associated with the fire core and the most concentrated portions of the near-surface plume, exhibit exceptionally large PM_{2.5} loadings. These extreme values are physically plausible in the context of intense wildfire activity, where strong pyroconvective injection, limited dilution, and local recirculation can sustain highly elevated concentrations.

The coexistence of a dominant low-concentration mode with a persistent heavy tail indicates a smoke field that is spatially sparse yet extremely intense where present, consistent with the plume morphology seen in the spatial plots. Consequently, domain-wide exposure at 19:00 UTC is governed disproportionately by a small fraction of high-PM_{2.5} cells, underscoring the presence of sharp gradients and localized hotspots that play a central role in the air-quality and radiative impacts of the event.



2180 **Figure 15: Histogram of PM2.5 concentration ($\mu\text{g}/\text{m}^3$) across the simulation domain at 19:00 UTC on 15 October 2017.**

While the model successfully reproduces the spatial organisation and statistical behaviour of the plume, Figures 14–15 show that a very small number of grid cells attain PM2.5 and SOD values far exceeding those reported in observational studies.

Surface and aircraft measurements in intense wildfire environments typically report maximum PM_{2.5} concentrations of 10^3 – 10^4 $\mu\text{g m}^{-3}$ (Gili et al., 2025; Landis et al., 2017), and even the highest shortwave AOD values observed by AERONET, FTIR, or aircraft seldom exceed 10–17.5 (Daniels et al., 2024; Eck et al., 2019; Frausto-Vicencio et al., 2023; Kassianov et al., 2025; Paton-Walsh et al., 2005; Shinozuka and Redemann, 2011). Concentrations in the 10^6 – 10^7 $\mu\text{g m}^{-3}$ range or SOD magnitudes of several thousand therefore have no documented observational analogue.

Such extremes likely arise from the interaction between very sharp emission gradients near the fire front, unresolved sub-grid variability in fuel consumption, and the behaviour of numerical transport schemes under steep concentration contrasts. Large tracer spikes have been documented in models employing Semi-Lagrangian advection, particularly in some global forecasting systems (e.g., ECMWF-type models or other spectral NWP frameworks), where negative-value clipping and subsequent mass-adjustment procedures can generate artificial local extrema (Aranami et al., 2015; Bermejo and Conde, 2002; Sørensen et al., 2013; Zerroukat and Shipway, 2017). However, BRAMS–SFIRE does not use a classical Semi-Lagrangian transport scheme. The atmospheric dynamics are solved in an Eulerian framework derived from the RAMS core, while fire spread is computed using a level-set formulation. In this context, the extreme PM_{2.5} values observed here could arise from the interaction between intense near-source emission gradients, grid-scale representation constraints, including the spatial mapping of vegetation and fuel types, and transport–emission coupling under steep concentration contrasts.

Although these outliers occupy only a very small fraction of the domain and do not significantly affect the large-scale optical diagnostics presented earlier, their presence indicates that further refinement is required in the representation of near-source smoke production and its numerical transport. The underlying causes of these extremes, linked to the parameterisation of fuel consumption, emission intensity, and the FRP formulation, are examined in detail in Section 3.6.

3.5.4 Atmospheric Stability and Thermodynamic Modulation by Aerosol–Radiation Interactions in Wildfire Events

Atmospheric stability is primarily governed by the vertical temperature lapse rate. The behaviour of an air parcel depends on how rapidly it cools adiabatically compared to the ambient temperature profile. If a rising parcel cools more slowly than the environment, it becomes less dense and buoyant, accelerating upward. Conversely, if it becomes denser than the surrounding air, it will descend. When vertical displacements of air parcels are amplified by buoyancy forces, the atmosphere is considered unstable, favouring convection, cloud formation, and potentially severe weather. In contrast, if the parcel is cooler and denser than its environment, vertical motion is suppressed, indicating a stable atmosphere.

Stability is evaluated by comparing the environmental lapse rate with the theoretical adiabatic lapse rates: the Dry Adiabatic Lapse Rate (DALR ≈ 9.8 K km^{−1}) and the Moist Adiabatic Lapse Rate (MALR, typically 4–7 K km^{−1}, depending on humidity). Strongly stable conditions are found during temperature inversions, where temperature increases with altitude. These often occur near the surface at night or under large-scale subsidence, resulting in a subsidence inversion typically between 1–3 km altitude. Such inversions act as barriers to vertical mixing and are crucial for air pollution accumulation.

When moist air parcels rise, they initially follow the DALR until reaching the Lifting Condensation Level (LCL), where condensation begins. The release of latent heat during condensation (an exothermic process) partially offsets adiabatic cooling, increasing the parcel's buoyancy and shifting it to follow the MALR. If sufficient energy is available, the parcel reaches the Level of Free Convection (LFC) and may continue to ascend to the Equilibrium Level (EL), near the tropopause.

The atmospheric layer closest to the surface is the Planetary Boundary Layer (PBL), where turbulence and mixing are most pronounced due to surface heating and friction. The structure and height of the PBL vary diurnally and are strongly influenced by radiative forcing and atmospheric stability. During the daytime, especially in wildfire regions, intense surface heating and smoke-induced turbulence may erode stable layers, promoting deep mixing.

These vertical motions have significant implications for aerosol dispersion. In stable conditions, especially under inversions, particulate matter accumulates near the surface due to suppressed mixing. Under unstable, convective conditions, particles are efficiently mixed and vertically transported.

CAPE quantifies the potential energy that a rising air parcel can convert into kinetic energy if lifted adiabatically. Higher CAPE values suggest stronger updrafts and a greater likelihood of convective development, enhancing vertical mixing and pollutant dispersion. CIN, on the other hand, represents the energy barrier that must be overcome for a parcel to initiate free convection. Large CIN values suppress vertical motion and contribute to the accumulation of pollutants and aerosols near the surface.

The regions impacted by these two energy terms are bounded by two key levels: the LFC and the EL. Below the LFC, the parcel is cooler than its environment, requiring energy input to rise—this energy defines the CIN. Above the LFC, the parcel is positively buoyant, contributing to CAPE. These estimates often assume pseudo-adiabatic processes (no entrainment and removal of condensed water), allowing latent heat release to maintain saturation.

In wildfire scenarios, evaluating CAPE and CIN become particularly relevant for assessing pyroconvection. Wildfires inject substantial heat and moisture into the atmosphere, potentially reducing local CIN (by warming the PBL) and allowing parcels to reach their LFC. When background CAPE is significant, this can trigger the formation of convective clouds (flammagenitus or pyrocumulus), and in extreme cases, deep convective events such as pyroCb (pyrocumulonimbus). Studies have shown that intense fire heat fluxes increase CAPE and reduce CIN, facilitating the vertical transport of smoke and the development of fire-induced storms.

In addition, turbulent fluxes generated by rising air parcels and plume dynamics influence pollutant dispersion. Parcels moving upward often carry higher aerosol concentrations, resulting in well-defined plume cores. This distribution can often be approximated by Gaussian profiles in horizontal cross-sections, in agreement with Fick's law of diffusion, where the diffusion flux is proportional to the gradient in species concentration.

The interaction of aerosol particles with radiation is governed by two fundamental optical processes: scattering and absorption. Scattering occurs when incident electromagnetic radiation is redirected by particles. In the case of Mie scattering, relevant when the particle diameter is comparable to the wavelength of the incident radiation, light penetrates the particle, and the

2250 internal refractive index gradients cause the redirection of light. OC aerosols, being efficient scatterers, predominantly affect shortwave (SW) radiation in the visible spectrum.

Absorption involves the uptake of photon energy by electrons in the atoms or molecules of the aerosol particle. The absorbed energy excites electrons to higher energy levels, and as they relax to their ground states, the energy is primarily dissipated through non-radiative processes, increasing the internal kinetic energy of the particle. This manifests macroscopically as

2255 thermal heating of the particle, i.e., the conversion of radiant energy into thermal energy. BC is a strong absorber in the visible and near-infrared spectra and significantly contributes to atmospheric heating.

While both OC and BC interact with radiation in the UV–visible range (0.3–0.7 μm), the direct radiative effect of aerosols on longwave (LW) radiation is generally weaker than that on shortwave (SW) radiation.

The absorption of SW radiation by BC-rich aerosol layers elevates local temperatures, promoting thermal stability. This may

2260 lead to or enhance thermal inversions, thereby increasing CIN and inhibiting convection and cloud formation. In contrast, OC scattering reduces incoming SW radiation, cools the surface and reducing the vertical temperature gradient. This cooling may decrease CAPE, reducing the buoyant energy available for upward motion.

This thermodynamic modulation by aerosol–radiation interactions is further illustrated in Fig. 16, which presents the differences in shortwave (SW) and longwave (LW) downwelling surface radiative fluxes between simulations with and without

2265 fire at 19:00 and 20:00 UTC on 15 October 2017. In these maps, positive values (light pink in SW and light green in LW panels) correspond to No Fire – Fire > 0 , indicating a reduction in surface irradiance caused by smoke and fire. Conversely, negative LW differences (darker green areas) reflect enhanced downwelling longwave radiation in the presence of fire, largely driven by thermal re-emission from the smoke plume and, to a lesser extent, by cloud or haze formation. At 19:00 UTC (Figs. 16a–b), shortwave fluxes are markedly reduced, locally exceeding -500 W m^{-2} , over the main smoke-affected region, evidencing strong attenuation of solar radiation by dense aerosol layers. Simultaneously, an increase in downwelling LW flux

2270 of up to $+60 \text{ W m}^{-2}$ emerges near the plume core, suggesting an active radiative trapping mechanism: Absorbing components of smoke, particularly BC, take up solar and thermal radiation and re-emit LW energy, enhancing downwelling fluxes beneath the plume. By 20:00 UTC (Figs. 16c–d), the magnitude of the SW deficit remains substantial but becomes spatially more confined, while the LW enhancement persists, closely aligned with areas of maximum column smoke absorption. This pattern

2275 indicates sustained radiative heating within the smoke layer and continued suppression of nocturnal cooling beneath it. These results confirm that smoke acts simultaneously as a solar radiation attenuator and an infrared emitter. The resulting energy imbalance strengthens static stability within the boundary layer and reinforces the “radiative lid” effect, in which reduced SW heating and enhanced LW back radiation stabilize the boundary layer, inhibit vertical mixing, and prolong near-surface smoke persistence.

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This section examines how smoke–radiation interactions modulate atmospheric stability during the wildfire event, linking PM_{2.5} loading, optical properties, and radiative forcing to changes in CAPE, CIN, and boundary-layer structure.

Atmospheric stability is primarily governed by the vertical temperature gradient or lapse rate. The behaviour of an air parcel depends on how rapidly it cools adiabatically compared to the ambient temperature profile. If a rising parcel cools at a rate lower than the environmental lapse rate, it becomes warmer and less dense than its surroundings, gaining positive buoyancy. Conversely, if it becomes denser than the surrounding air, it will descend. When vertical displacements of air parcels are amplified by buoyancy forces, the atmosphere is considered unstable, favouring convection, cloud formation, and potentially severe weather. In contrast, if the parcel is cooler and denser than its environment, vertical motion is suppressed, indicating a stable atmosphere.

Stability is evaluated by comparing the environmental lapse rate with the theoretical adiabatic lapse rates: the Dry Adiabatic Lapse Rate (DALR $\approx 9.8 \text{ K km}^{-1}$) and the Moist Adiabatic Lapse Rate (MALR, typically $4\text{--}7 \text{ K km}^{-1}$, depending on humidity). Strongly stable conditions occur during temperature inversions, where temperature increases with height. Surface-based inversions commonly form at night within the lowest few hundred metres, while subsidence inversions associated with high-pressure systems often appear between $1\text{--}3 \text{ km}$. Such inversions act as barriers to vertical mixing and are crucial for air pollution accumulation.

When moist air parcels rise, they initially follow the DALR until reaching the Lifting Condensation Level (LCL), where condensation begins. The release of latent heat during condensation (an exothermic process) partially offsets adiabatic cooling, increasing the parcel's buoyancy and shifting it to follow the MALR. If sufficient energy is available, the parcel reaches the Level of Free Convection (LFC) and may continue to ascend to the Equilibrium Level (EL), near the tropopause.

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In wildfire scenarios, evaluating CAPE and CIN becomes particularly relevant for assessing pyroconvection. Wildfires inject substantial heat and moisture into the atmosphere, potentially reducing local CIN (by warming the PBL) and allowing parcels to reach their LFC. When background CAPE is significant, this can trigger the formation of convective clouds (flammagenitus or pyrocumulus), and in extreme cases, deep convective events such as pyroCb (pyrocumulonimbus). Studies have shown that intense fire heat fluxes increase CAPE and reduce CIN, facilitating the vertical transport of smoke and the development of fire-induced storms.

In addition, turbulent fluxes generated by rising air parcels and plume dynamics influence pollutant dispersion. Parcels moving upward often carry higher aerosol concentrations, resulting in well-defined plume cores. This distribution can often be approximated by Gaussian profiles in horizontal cross-sections, in agreement with Fick's law of diffusion, where the diffusion flux is proportional to the gradient in species concentration.

The interaction of aerosol particles with radiation is governed by two fundamental optical processes: scattering and absorption. Scattering occurs when incident electromagnetic radiation is redirected by particles. In the case of Mie scattering, relevant when the particle diameter is comparable to the wavelength of the incident radiation, light penetrates the particle, and the internal refractive index gradients cause the redirection of light. OC aerosols act primarily as efficient shortwave scatterers, although certain organic fractions (e.g., brown carbon) can contribute weak absorption in the UV–blue region.

Absorption involves the uptake of photon energy by electrons in the atoms or molecules of the aerosol particle. The absorbed energy excites electrons to higher energy levels, and as they relax to their ground states, the energy is primarily dissipated through non-radiative processes, increasing the internal kinetic energy of the particle. This manifests macroscopically as thermal heating of the particle, i.e., the conversion of radiant energy into thermal energy. BC is a strong absorber in the visible and near-infrared spectra and significantly contributes to atmospheric heating.

While both OC and BC interact with radiation in the UV–visible range (0.3–0.7 μm), for most fine-mode aerosols, LW radiative effects are weaker than SW effects, although dense, absorbing smoke layers can exert measurable LW heating through absorption and thermal re-emission.

The absorption of SW radiation by BC-rich aerosol layers elevates local temperatures, promoting thermal stability. This may lead to or enhance thermal inversions, thereby increasing CIN and inhibiting convection and cloud formation. In contrast, OC scattering reduces incoming SW radiation and cools the surface, reducing the surface–atmosphere temperature contrast and decreasing the lapse rate. This stabilisation of the lower troposphere lowers CAPE and diminishes the buoyant energy available for vertical motion.

To link these thermodynamic mechanisms to the radiative forcing exerted by the plume, Figures 16a–d present the shortwave (SW) and longwave (LW) surface flux perturbations induced by smoke at 16:00 UTC (fresh phase, t1) and 19:00 UTC (mixed phase, t2). In all panels, the fields are expressed as No Fire – Fire, such that positive values denote a reduction in downwelling flux caused by the presence of smoke (i.e., the fire simulation receives less radiative energy at the surface than the no-fire control), while negative values correspond to an increase in downwelling flux in the fire run. This definition allows a direct attribution of radiative effects to smoke processes alone, isolating aerosol scattering, absorption, and thermal re-emission

2350 relative to a clean-air background. Figure 16 therefore provides a physically coherent depiction of how the plume modifies the
surface radiative energy budget during the late-afternoon transition (16:00–19:00 UTC), linking these perturbations to the
aerosol optical characteristics described in Figs. 7–12.

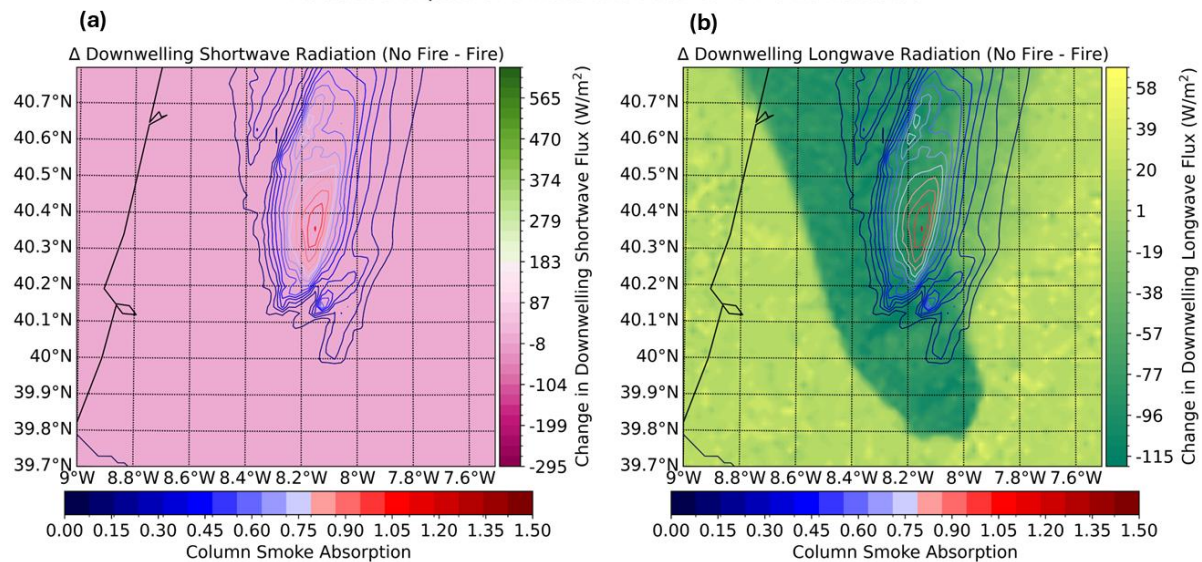
At 16:00 UTC, during the fresh and more concentrated phase of the plume, SW anomalies reach values below -500 W m^{-2}
within the plume core. These large negative differences indicate that the fire simulation receives substantially less solar
2355 radiation at the surface due to strong aerosol extinction. The spatial maxima of SW attenuation are tightly collocated with
regions of enhanced column smoke absorption, highlighting the direct radiative impact of high aerosol loading.

In the longwave band, ΔLW values are predominantly negative (approximately -40 to -60 W m^{-2}) within the same regions,
indicating enhanced downwelling longwave radiation in the fire simulation relative to the no-fire control. This increase in
surface LW flux is consistent with additional atmospheric emissivity associated with the warm, smoke-laden air mass and fire-
2360 induced moisture perturbations.

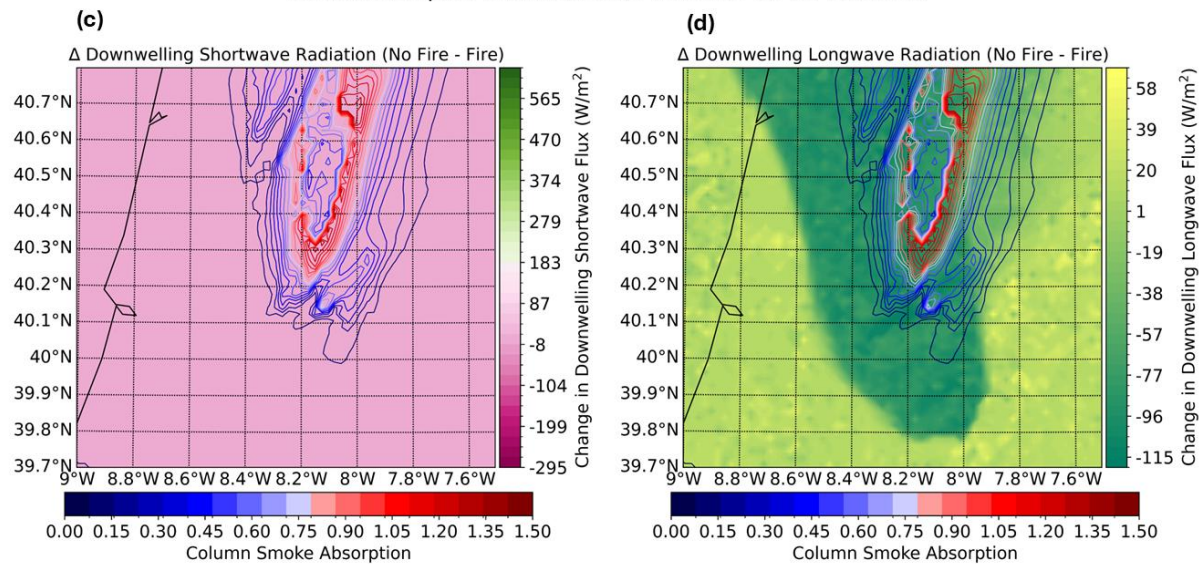
By 19:00 UTC, the smoke plume becomes more diluted, and its column-absorption contours stretch downwind, indicating
transport and dispersion during the transition to the mixed phase. Consistent with this dilution, the shortwave perturbation
remains evident but is weaker and more spatially diffuse, with the strongest SW reductions confined to the regions of highest
column absorption. In the longwave, the perturbation persists and remains closely collocated with the absorption maxima,
2365 indicating enhanced downwelling LW in the fire within the plume core. Together, the SW reduction and LW increase show
that the plume continues to modify the surface radiative budget across both phases, while the spatial structure of the signal
increasingly reflects plume dilution and advection.

Beyond the instantaneous flux perturbations, the reduction in shortwave irradiance within the plume-affected boundary layer
limits surface-driven buoyancy production, while the enhanced longwave emissivity of the smoke layer increases radiative
2370 heating aloft. This differential heating between the surface and the lower troposphere favours the development or strengthening
of a temperature inversion, effectively acting as a radiative lid over the boundary layer. Such radiatively induced modifications
in stability suppress turbulent mixing and promote boundary-layer stabilisation during periods of peak smoke loading,
providing a dynamical pathway through which aerosol optical properties can influence boundary-layer evolution and help
explain the persistence of high near-surface PM_{2.5} concentrations observed in Section 3.4. Because the strength of this
2375 mechanism depends on aerosol absorption characteristics, the SSA biases identified earlier suggest that the model may
underestimate the magnitude of smoke-induced radiative heating within the plume core, implying that the stabilising radiative
lid could be even more pronounced under fully absorbing conditions.

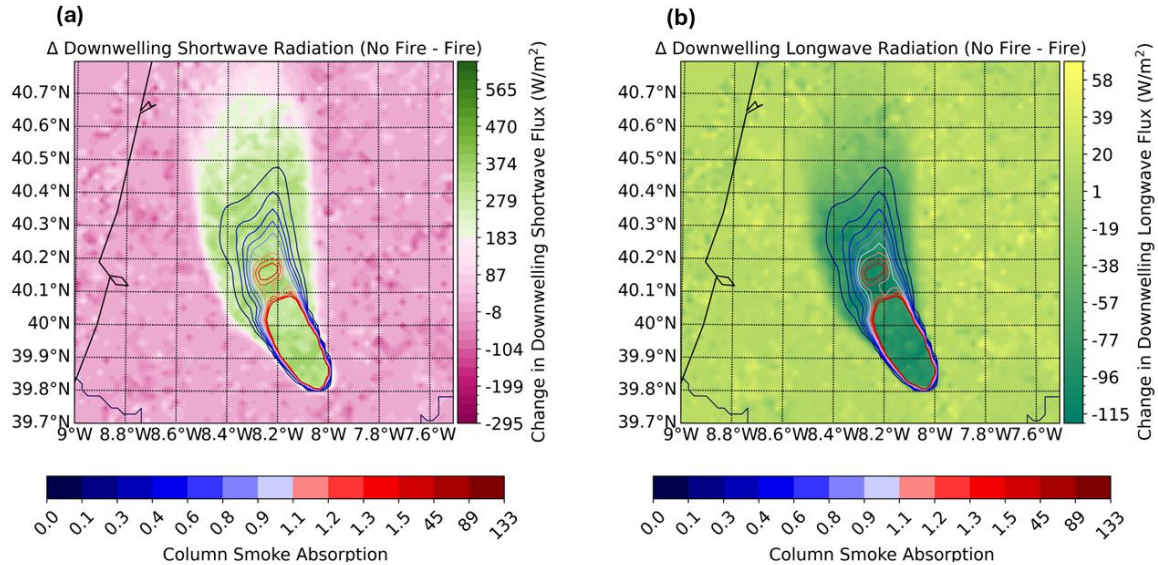
Radiative Impact of Smoke and Fire: 2017-10-15 19:00:00



Radiative Impact of Smoke and Fire: 2017-10-15 20:00:00



Radiative Impact of Smoke and Fire: 2017-10-15 16:00:00 UTC



Radiative Impact of Smoke and Fire: 2017-10-15 19:00:00 UTC

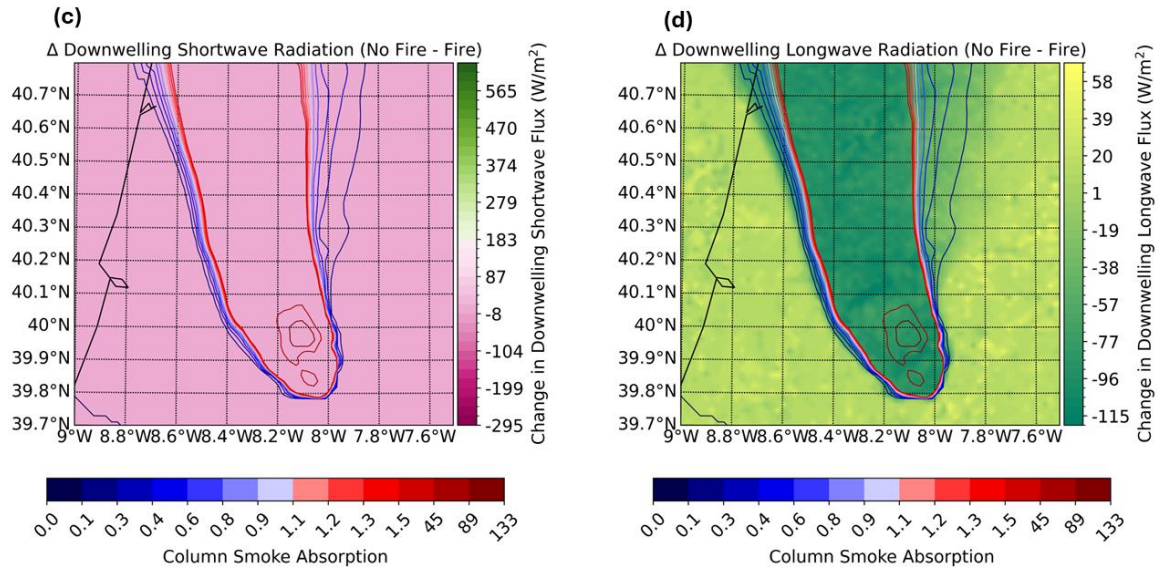


Figure 16: Difference in surface downwelling shortwave (SW) and longwave (LW) radiative fluxes between simulations without fire and with fire (No Fire – Fire) at 16:00 and 19:00 UTC on 15 October 2017. Positive values indicate reduced downwelling radiation in the Fire simulation relative to the no-fire control, while negative values indicate enhanced downwelling radiation at the surface in the Fire case. In the SW panels, negative anomalies reflect strong attenuation of solar radiation within the plume core. In the LW panels, negative anomalies indicate increased atmospheric longwave emission in smoke-affected regions. Coloured contour lines

2385 ~~denote fire-weighted column smoke absorption. Difference in shortwave and longwave surface radiative fluxes between simulations with and without fire, at 19:00, and 20:00 UTC on 15 October 2017. Positive values in the shortwave and longwave flux difference maps (light pink/light green) indicate a reduction in radiation due to the presence of smoke and fire. Negative longwave values (darker green shades) suggest an increase in downward radiation, potentially associated with thermal re-emission from the smoke plume or cloud formation. Coloured contour lines represent fire-weighted smoke absorption, indicating regions where smoke~~
 2390 ~~exerted the strongest radiative influence.~~

Figs. 17–19 show longitudinal cross sections of the smoke extinction (SEC) and absorption (SAC) coefficients at 550 nm simulated by BRAMS-SFIRE under CAPE and CIN conditions along 8.1° W, for 15 October 2017. Colour shading represents the magnitude of the extinction and absorption coefficients, while CAPE and CIN isolines are superimposed: solid black contours denote the fire simulation, and dashed red contours correspond to the no-fire case. The left hand panels (“under CAPE conditions”) depict the same optical fields but without CAPE isolines, as CAPE values were zero throughout the plotted vertical range (–0–1.2 km) and were therefore omitted for clarity.

At 15:00 UTC and 550 nm (Fig. 17), a compact and optically dense smoke layer is confined to the lowest 300–500 m. Extinction and absorption maxima are tightly collocated near 40.0° N, indicating a freshly emitted, BC/OC-rich plume. In the CIN panels, the fire-run isolines (black) appear elevated relative to the no-fire run (red) over the plume core, evidencing a local weakening of the inversion and reduced inhibition consistent with shortwave heating by absorbing smoke.

By 19:00 UTC and 550 nm (Fig. 18), the smoke layer has deepened and become more vertically diffuse, extending intermittently up to ~1 km. Although the plume has partially dispersed, the CIN isolines in the fire-run remain higher than in the no-fire case between 39.9° N and 40.1° N, confirming a persistent thermodynamic perturbation induced by radiative heating. The co-location of enhanced SEC/SAC values with elevated CIN indicates continued warming by aged, lofted smoke. The vertical expansion of the absorbing layer at this stage reflects active turbulent mixing and upward redistribution of radiative energy, which contributes to a more stable layer near the surface and reduced convective coupling above.

At 19:00 UTC and 700 nm (Fig. 19), both SEC and SAC are systematically weaker than at 550 nm, SAC decreases by roughly a factor of 2–3, and SEC by ~30–40 %, yet the vertical meridional structure and the uplift of CIN isolines over the smoke footprint remain clearly discernible. This spectral attenuation is consistent with the reduced optical efficiency at longer wavelengths for mixed BC–OC smoke (including brown carbon) and with progressive chemical ageing and dilution of the aerosol population. At 400 nm, both extinction and absorption coefficients are substantially higher than at 550 nm and 700 nm. Peak SEC values reach approximately $3.3 \times 10^{-2} \text{ m}^{-1}$, compared with $2.3 \times 10^{-2} \text{ m}^{-1}$ at 550 nm, while SAC increases to nearly $6 \times 10^{-3} \text{ m}^{-1}$, about twice that at 550 nm. The enhancement is concentrated within the lowest 500–800 m, coinciding with the core of the smoke layer and the region of elevated CIN in the fire simulation. This spectral behaviour is fully consistent with the optical properties of organic and brown carbon aerosols, which exhibit stronger scattering and absorption in the UV–blue region. The higher coefficients at 400 nm highlight the enhanced radiative sensitivity of shorter wavelengths to OC-dominated

smoke, undersealing the wavelength dependence of aerosol–radiation interactions and their role in modulating heating rates within the lower troposphere.

Meridional cross-sections of extinction (SEC) and absorption (SAC) along 8.1° W (Figs. 17–19) reveal how spectrally dependent radiative heating interacts with lower-tropospheric stability during the evolution of the smoke plume. Colour shading denotes SEC and SAC at the relevant wavelength, while solid black and dashed red isolines represent the Fire and No-Fire CIN and CAPE, respectively. CAPE is absent within the 0–1.2 km layer and is therefore omitted; CIN is shown only where non-zero.

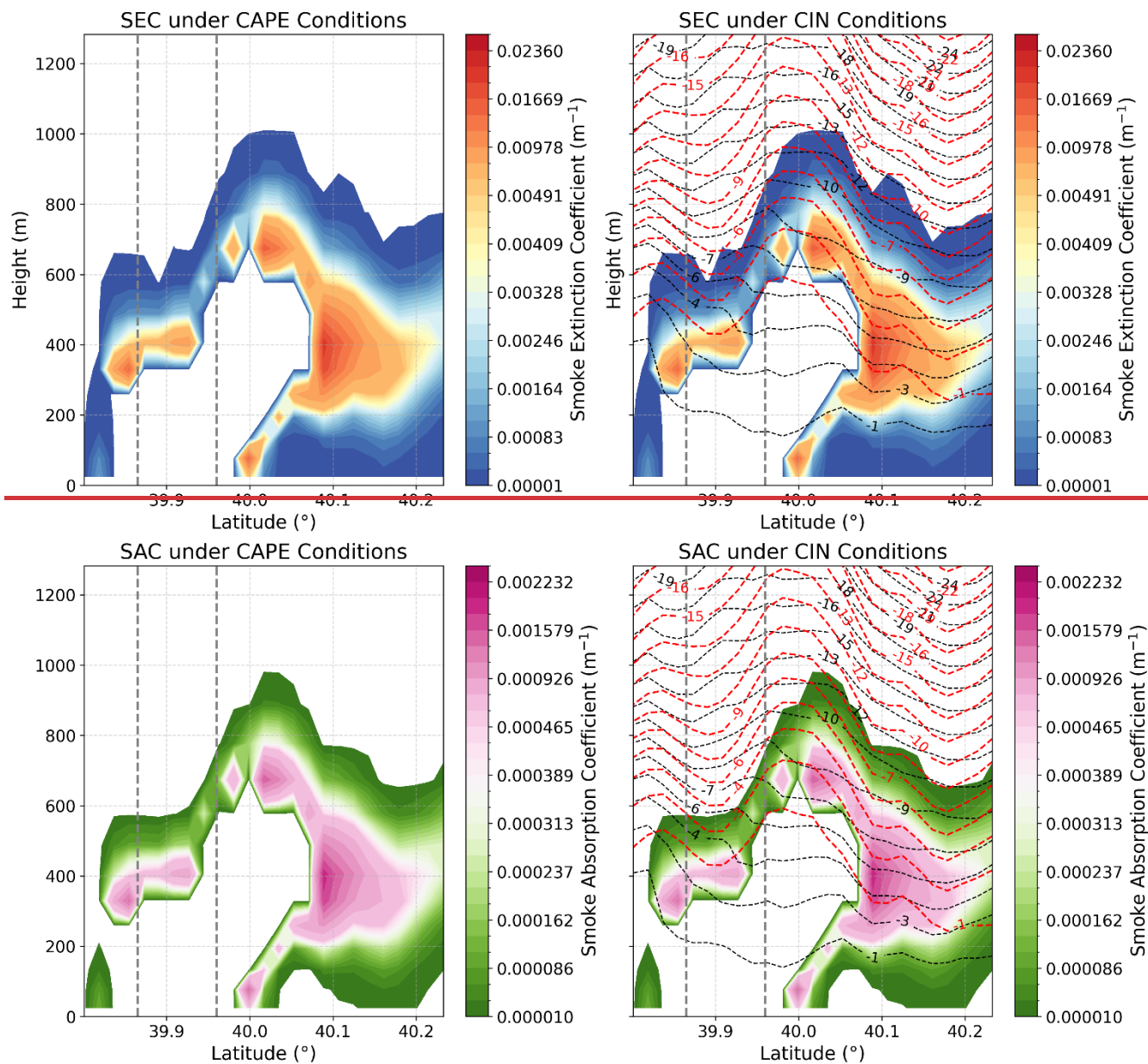
At 15:00 UTC and 550 nm (Fig. 17), extinction and absorption are concentrated within the lowest 300–500 m, forming a compact, optically intense layer centred near 40° N. The near-perfect co-location of SEC and SAC maxima indicates a fresh, BC/OC-rich plume with minimal dilution. CIN isolines in the Fire simulation lie systematically above those of the No-Fire run, evidencing a localized weakening of the low-level inversion. This displacement is consistent with shortwave heating by BC-containing aerosols, which warms the plume and begins to erode static stability, an early manifestation of the radiative-lid mechanism diagnosed from the surface forcing fields in Fig. 16.

By 19:00 UTC (Fig. 18), the plume has deepened and become more vertically diffuse, with SEC and SAC extending intermittently up to ~1 km. CIN perturbations intensify and expand horizontally between 39.9°–40.1° N, demonstrating persistent thermodynamic modification by aged, lofted smoke. The joint action of turbulent mixing and continued radiative heating suppresses surface–atmosphere coupling, favouring the accumulation and persistence of smoke near the surface. The spatial coherence between elevated CIN and enhanced SEC/SAC confirms that smoke-driven warming remains dynamically relevant even after the plume has become partially diluted.

At 700 nm (Fig. 19), extinction and absorption weaken systematically, SAC decreases by a factor of ~2–3 and SEC by 30–40 % relative to 550 nm, yet the plume retains its vertical structure, and CIN isolines continue to be elevated in the Fire simulation. This attenuation reflects the wavelength dependence of mixed BC–OC aerosols: as organic chromophores (brown carbon) become optically less active in the red/near-infrared, BC-driven heating increasingly dominates the radiative response. Conversely, at shorter wavelengths (e.g., 400 nm), SEC and SAC strengthen markedly ($\text{SEC} \approx 3.3 \times 10^{-2} \text{ m}^{-1}$; $\text{SAC} \approx 6 \times 10^{-3} \text{ m}^{-1}$), remaining confined within the lowest 500–800 m, precisely where CIN anomalies are largest. This pronounced shortwave sensitivity, driven by OC and brown carbon absorption, reinforces the mechanism whereby visible/UV heating enhances plume buoyancy relative to its surroundings, modifies lower-tropospheric stability, and prolongs near-surface smoke residence.

Together, Figures 17–19 show that radiative heating by BC and OC governs the vertical thermodynamic imprint of the plume, with 550 nm providing the strongest combined scattering–absorption signal, 700 nm capturing the persistence of BC-induced heating, and 400 nm emphasising the intense shortwave sensitivity of OC-dominated smoke. These spectral responses align with the radiative perturbations diagnosed at the surface (Fig. 16), collectively demonstrating how smoke modifies stability through a vertically structured and wavelength-dependent radiative forcing.

Vertical Profiles - 550 nm Ions: -8.1 — 2017-10-15 15:00:00



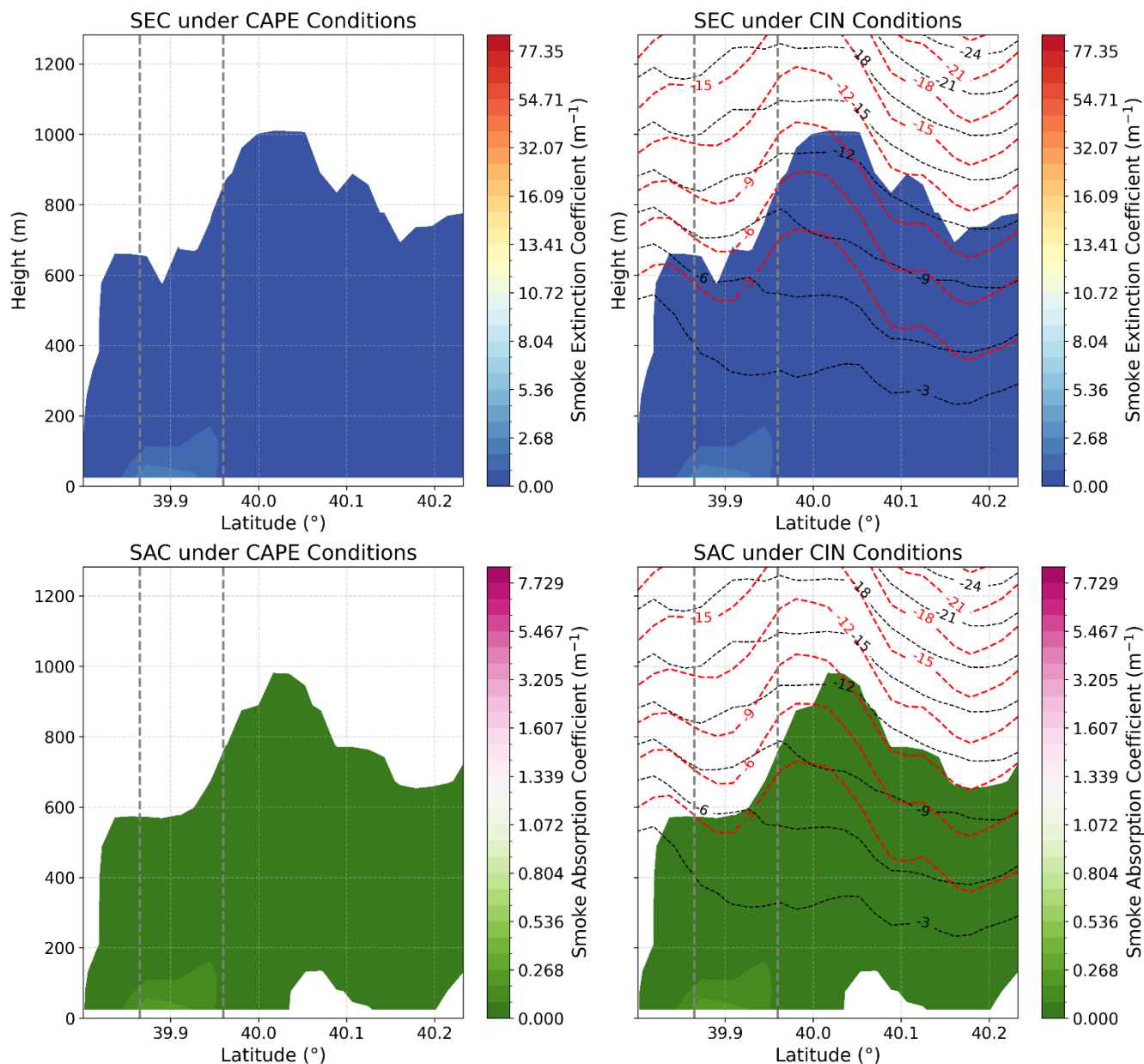
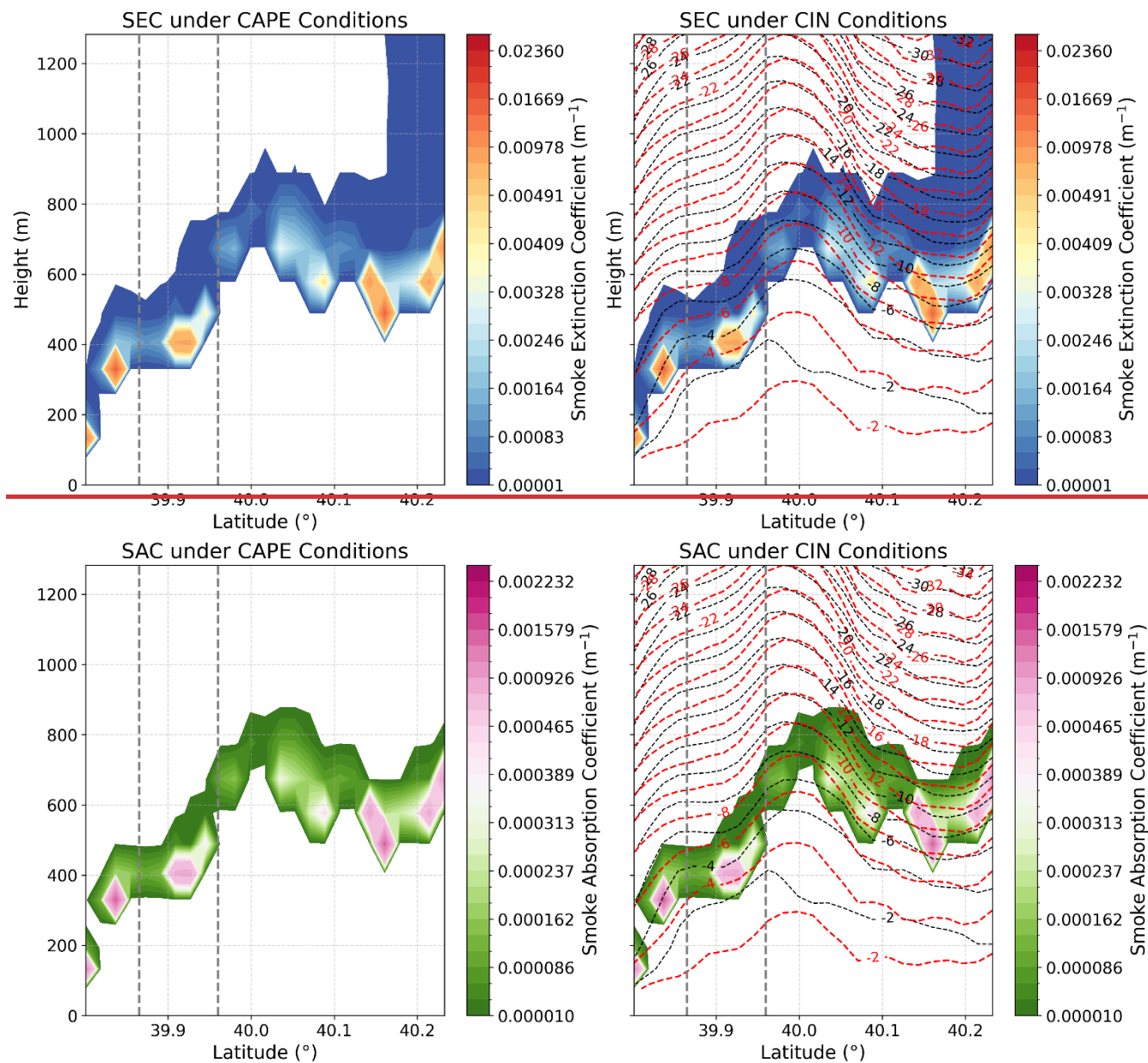


Figure 17: Longitudinal cross-sections of smoke extinction and absorption coefficients at 550 nm along 8.1° W, under CAPE (J kg^{-1}) and CIN (J kg^{-1}) conditions. Dashed black lines indicate the fire simulation, while dashed red lines represent the no-fire scenario, at 15:00 UTC on 15 October 2017. The region enclosed between the two light gray dashed vertical lines represents the observed area affected by the wildfire.



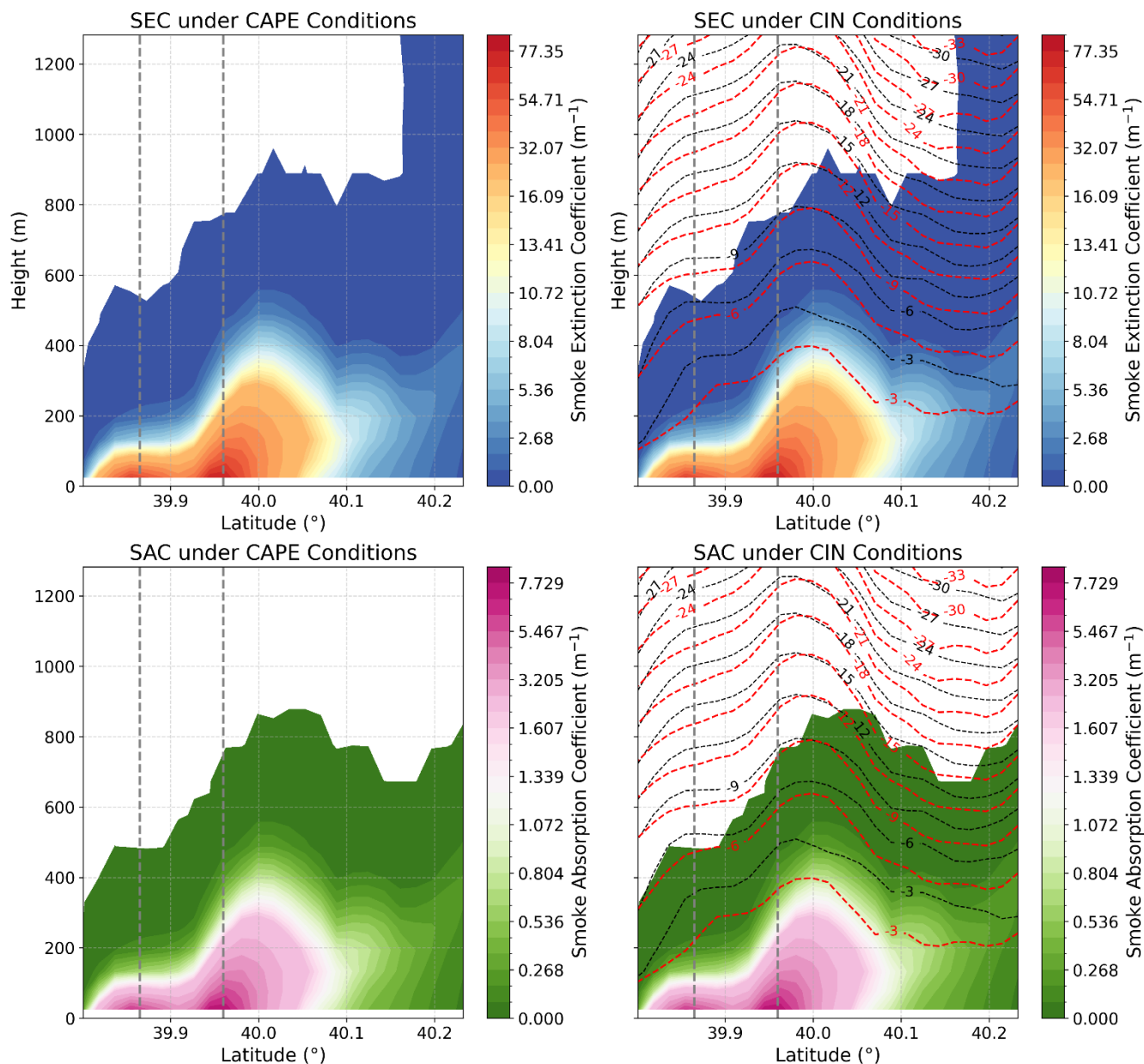
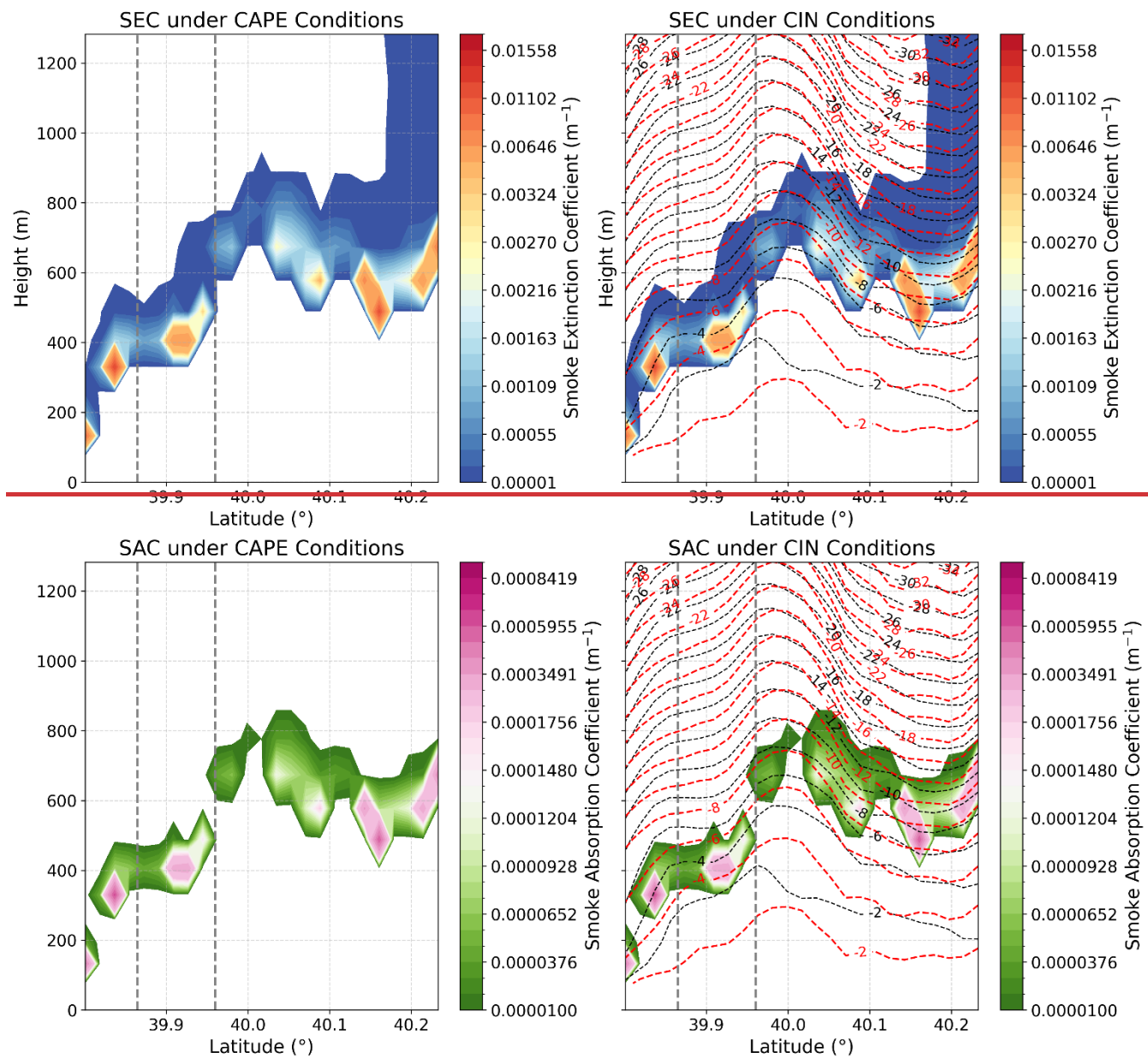


Figure 18: Longitudinal cross-sections of smoke extinction and absorption coefficients at 550 nm and 700 nm along 8.1° W, under CAPE (J kg^{-1}) and CIN (J kg^{-1}) conditions. Dashed black lines indicate the fire simulation, while dashed red lines represent the no-fire scenario, at 19:00 UTC on 15 October 2017. The region enclosed between the two light gray dashed vertical lines represents the observed area affected by the wildfire.



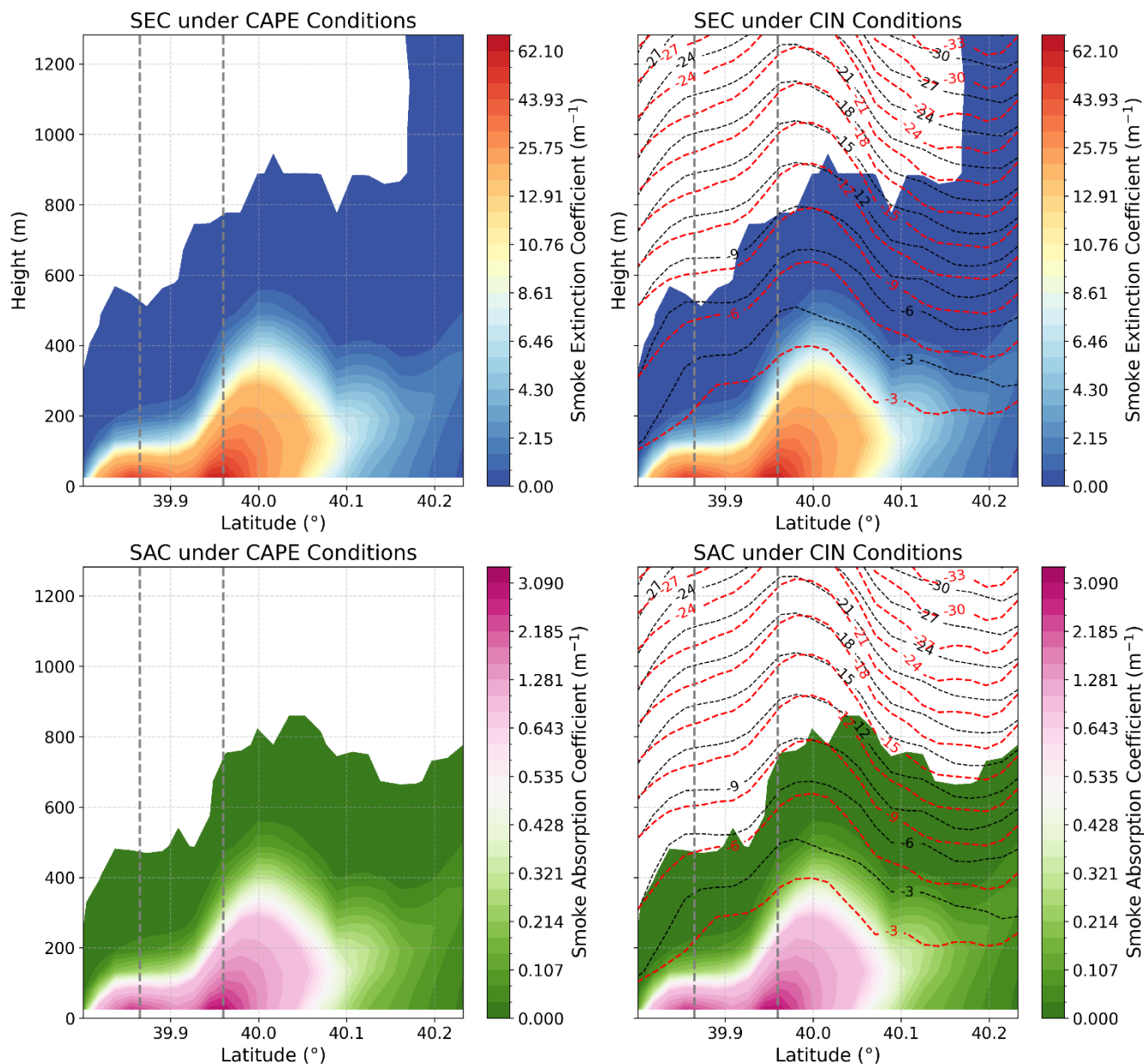


Figure 19: Longitudinal cross-sections of smoke extinction and absorption coefficients at 700 nm along 8.1° W, under CAPE (J kg^{-1}) and CIN (J kg^{-1}) conditions. Dashed black lines indicate the fire simulation, while dashed red lines represent the no-fire scenario, at 19:00 UTC on 15 October 2017. The region enclosed between the two light gray dashed vertical lines represents the observed area affected by the wildfire.

Building upon the previously described vertical redistribution of CAPE and CIN in the presence of smoke, further insights emerge from the detailed analysis of inversion layer dynamics under varying radiative conditions. The combined evaluation of extinction and absorption coefficients with potential temperature and relative humidity fields (Fig. 20–23) demonstrates that smoke-induced radiative perturbations not only modulate static stability but also actively reshape the structure and persistence of inversion layers. The inversion-layer analysis shown in Figs. 20–21 provides a detailed view of how smoke-induced radiative perturbations modify lower-tropospheric stability during the late-afternoon evolution of the plume. When interpreted together with the radiative impacts documented in Fig. 16 and the vertical redistribution of smoke extinction and absorption (Figs. 17–19), these cross-sections reveal that dense smoke layers act as dynamically active radiative agents capable of altering both the height and integrity of low-level inversions.

At 15:00 UTC (Fig. 20), shortly after the onset of peak fire activity, the smoke extinction and absorption coefficients at 550 nm already show clear radiative impacts near the inversion base. Localized heating beneath the inversion results in systematic lifting and partial weakening of the layer compared to the no-fire control, with displacements of roughly 100–150 m. The vertical gradient of potential temperature becomes less pronounced in smoke-affected sectors, indicating early signs of sub-inversion destabilization.

By 19:00 UTC (Fig. 21), these effects intensify: the inversion is further elevated and spatially modulated by concentrated smoke layers. Enhanced absorption coincides with regions of strong extinction near 400–700 m a.g.l., suggesting sustained radiative heating capable of eroding the inversion top and promoting vertical mixing. This restructuring supports the presence of a radiative lid mechanism in which heating beneath the inversion reduces thermal contrast while facilitating upward aerosol transport.

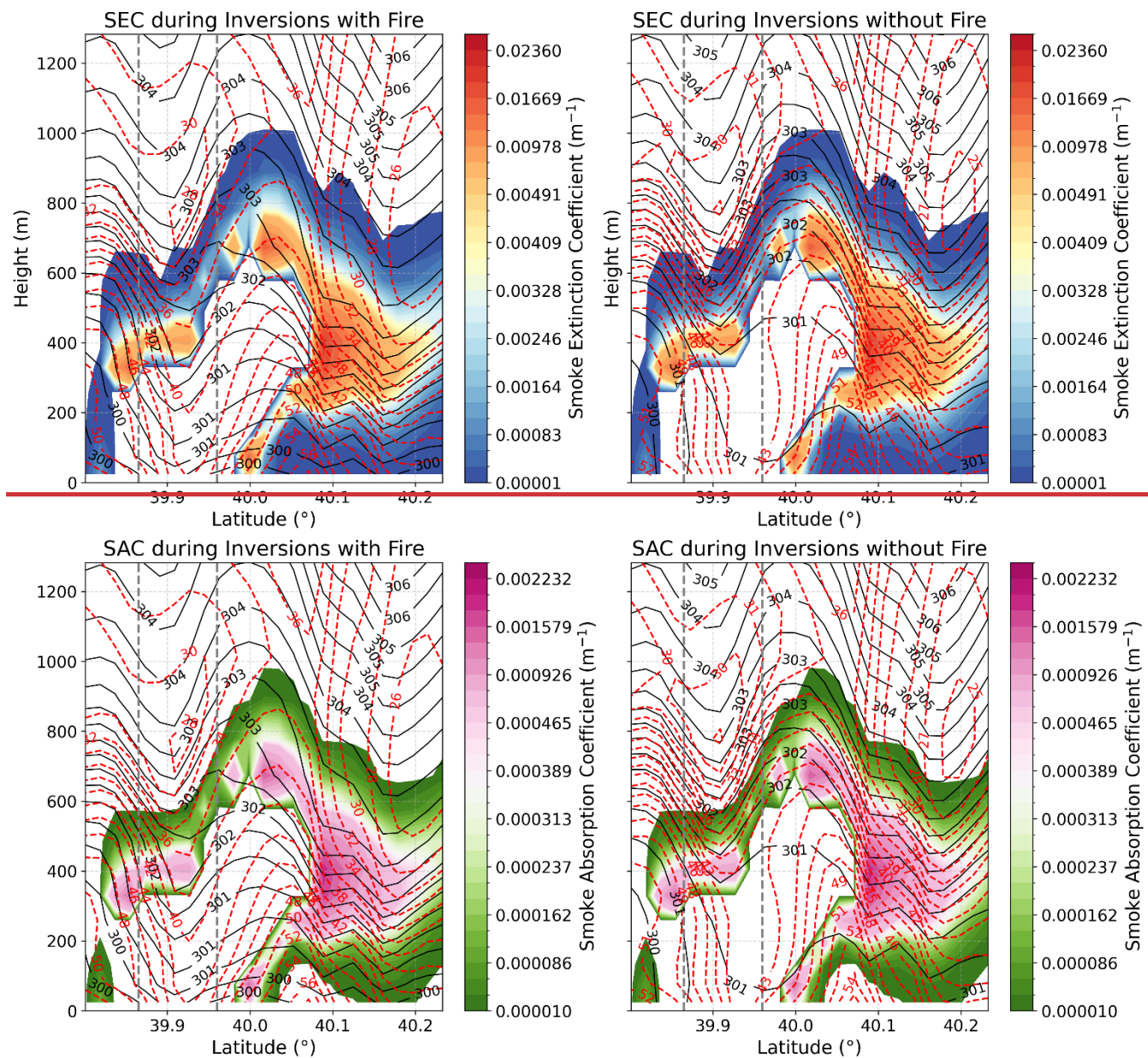
Comparative analysis across wavelengths at 19:00 UTC reinforces the spectral sensitivity of this process. At 400 nm, extinction and absorption maxima are more pronounced and vertically extensive, consistent with the stronger interaction of UV-blue radiation with fine-mode organic carbon aerosols. Conversely, at 700 nm, the response is more subdued, with lower coefficients and smaller vertical displacements, highlighting the reduced efficiency of longer wavelengths in modulating the inversion thermodynamics.

Collectively, these results demonstrate that smoke layers act as dynamically active radiative agents capable of altering inversion height, intensity, and continuity. The interplay between localized absorption-driven heating and weakened thermal gradients enhances entrainment at the plume-inversion interface, contributing to mesoscale thermodynamic adjustments and spatial heterogeneity in boundary layer stability. Such radiative-dynamic coupling underscores the capacity of smoke to modify near-surface stratification and to induce feedbacks on vertical transport processes well beyond the immediate fire area. The inversion-layer analysis shown in Figs. 20–21 provides the dynamical counterpart to the radiative and optical diagnostics discussed in Figs. 16–19. Together, these results reveal how smoke functions not merely as a passive tracer but as an active radiative agent capable of reshaping lower-tropospheric stability during the late-afternoon evolution of the plume.

At 15:00 UTC (Fig. 20), a compact near-surface smoke layer, characterised by strong extinction and absorption at 550 nm, coincides with positive potential-temperature anomalies ($\theta' \approx 1\text{--}1.5\text{ K}$) and reduced relative humidity ($\text{RH}' < 0$) beneath the inversion. These signatures represent the first thermodynamic imprint of radiative heating by the plume: the smoke-induced warming does not physically lift the inversion but erodes it from below, weakening the temperature gradient that sustains its stability. Immediately above the inversion, $\text{RH}' > 0$ indicates moisture redistribution by modified turbulent mixing, consistent with a plume that is already altering the thermodynamic environment rather than simply responding to it. This early behaviour aligns with the shortwave-absorption patterns diagnosed in Fig. 16 and with the vertical concentration of extinction and absorption shown at 550 nm in Fig. 17.

By 19:00 UTC (Fig. 21), the perturbations intensify and extend vertically to 300–600 m, mirroring the deepened SEC/SAC fields documented in Figs. 18–19. The θ' anomalies strengthen along the plume axis, and the accompanying RH' dipole (dry below, moist above) becomes more pronounced. These changes demonstrate that the inversion is becoming thermodynamically weaker and spatially irregular, not through geometric uplift, but through sustained modification of temperature and moisture stratification driven by radiative heating and plume-induced turbulence. This evolution is fully consistent with the radiative-lid mechanism inferred from SW/LW flux perturbations in Fig. 16: strong shortwave attenuation reduces surface heating, while longwave trapping and BC/OC absorption warm the lower troposphere, suppressing boundary-layer deepening and enabling the continued presence of lofted aerosol layers.

The co-location of FIRE–No Fire anomalies with regions of enhanced SEC and SAC further confirms that inversion modification is directly coupled to the plume’s wavelength-dependent radiative forcing. Heating by dense smoke is particularly efficient at short wavelengths (400–550 nm), reinforcing the thermodynamic anomalies at low levels and supporting persistent vertical redistribution of smoke. In this way, the inversion cross-sections provide a dynamical validation of the radiative pathways previously identified, demonstrating how smoke alters both the strength and structure of stability regimes that ultimately govern plume dispersion and residence time.



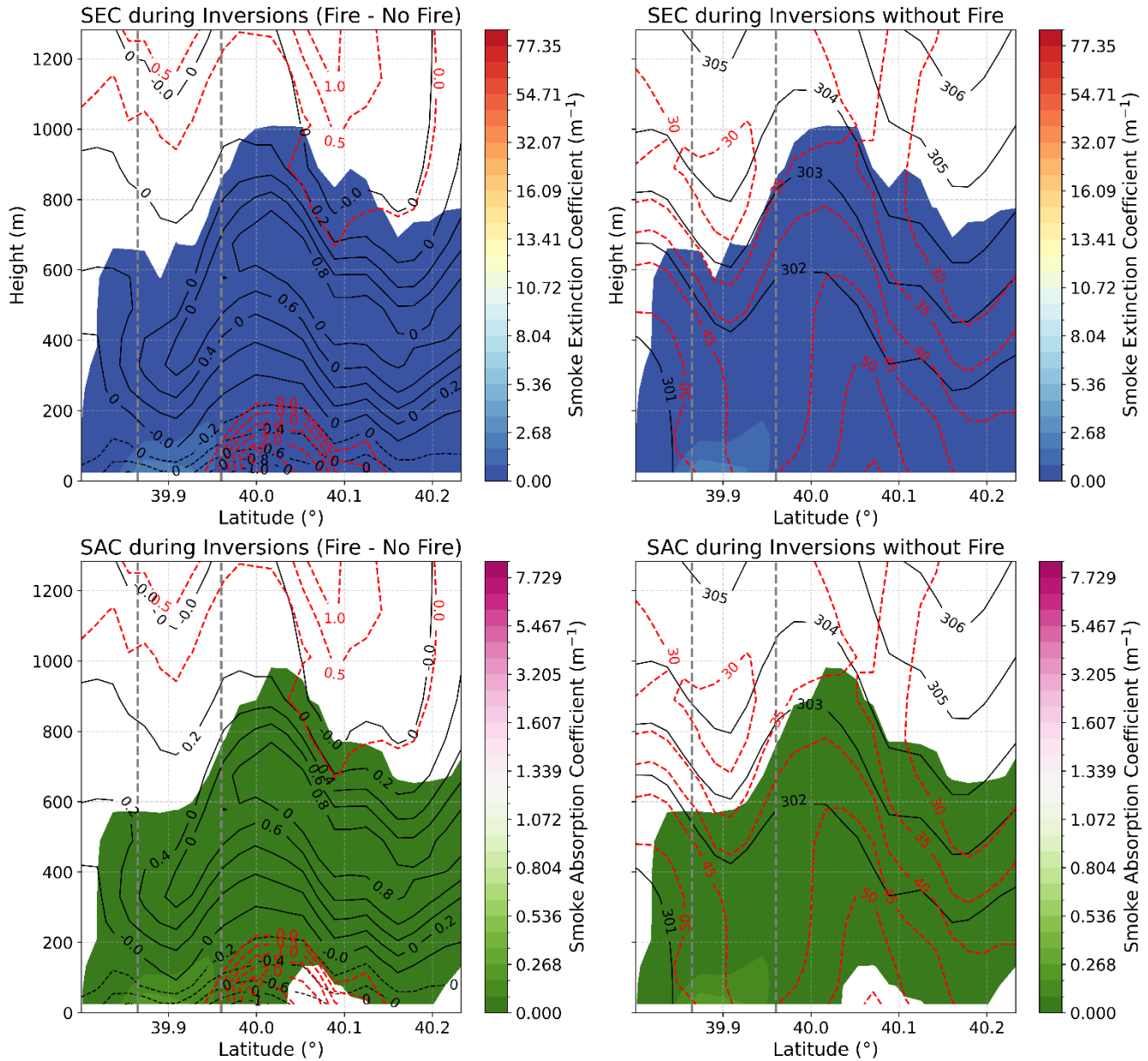
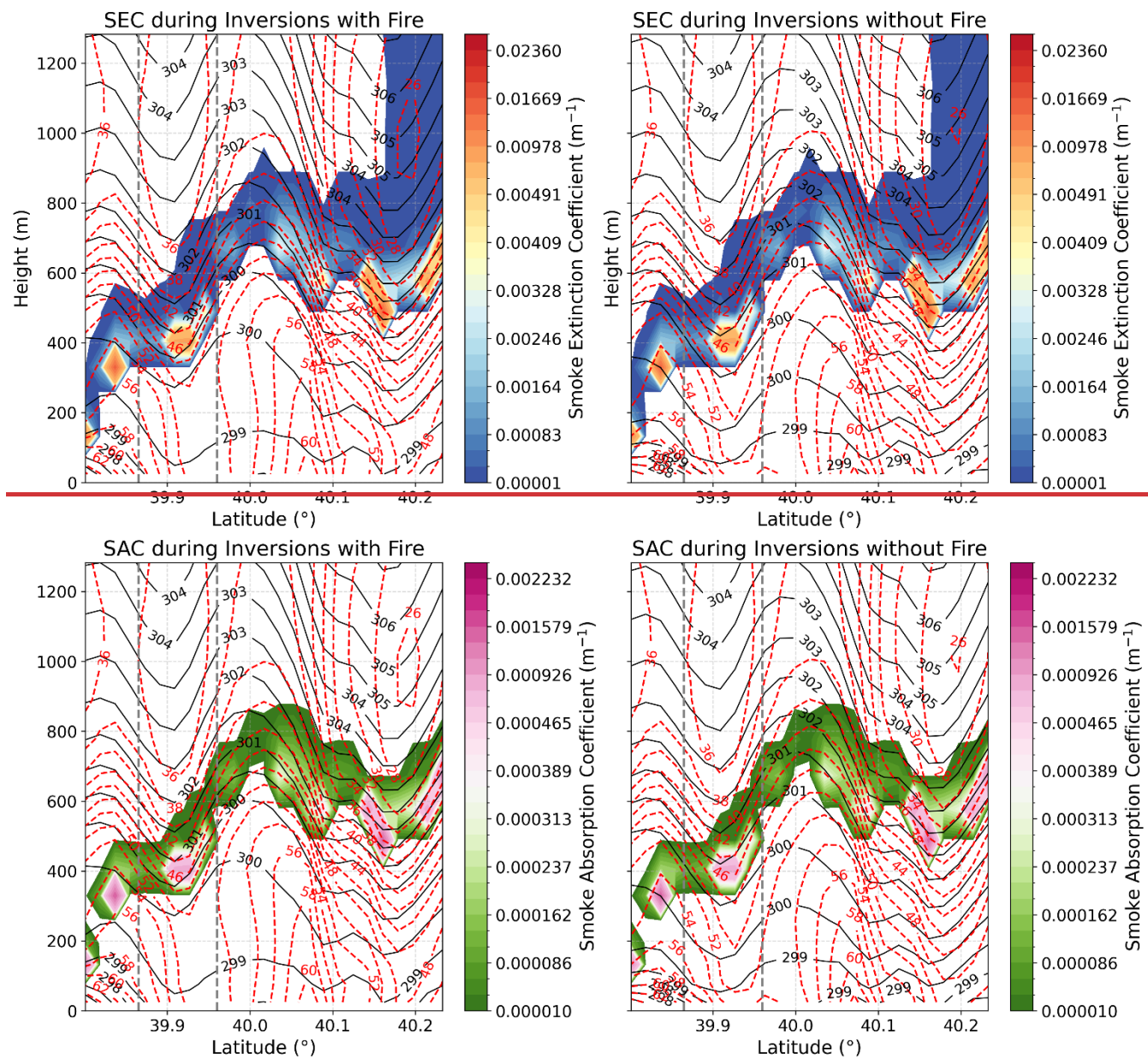


Figure 20: Longitudinal cross-sections of inversion layers overlaid with smoke extinction and absorption coefficients at 550 nm along 8.1° W. Dashed red lines indicate relative humidity (%), and solid black lines represent potential temperature (K). Simulations correspond to 15:00 UTC on 15 October 2017. The region enclosed between the two light gray dashed vertical lines represents the observed area affected by the wildfire.



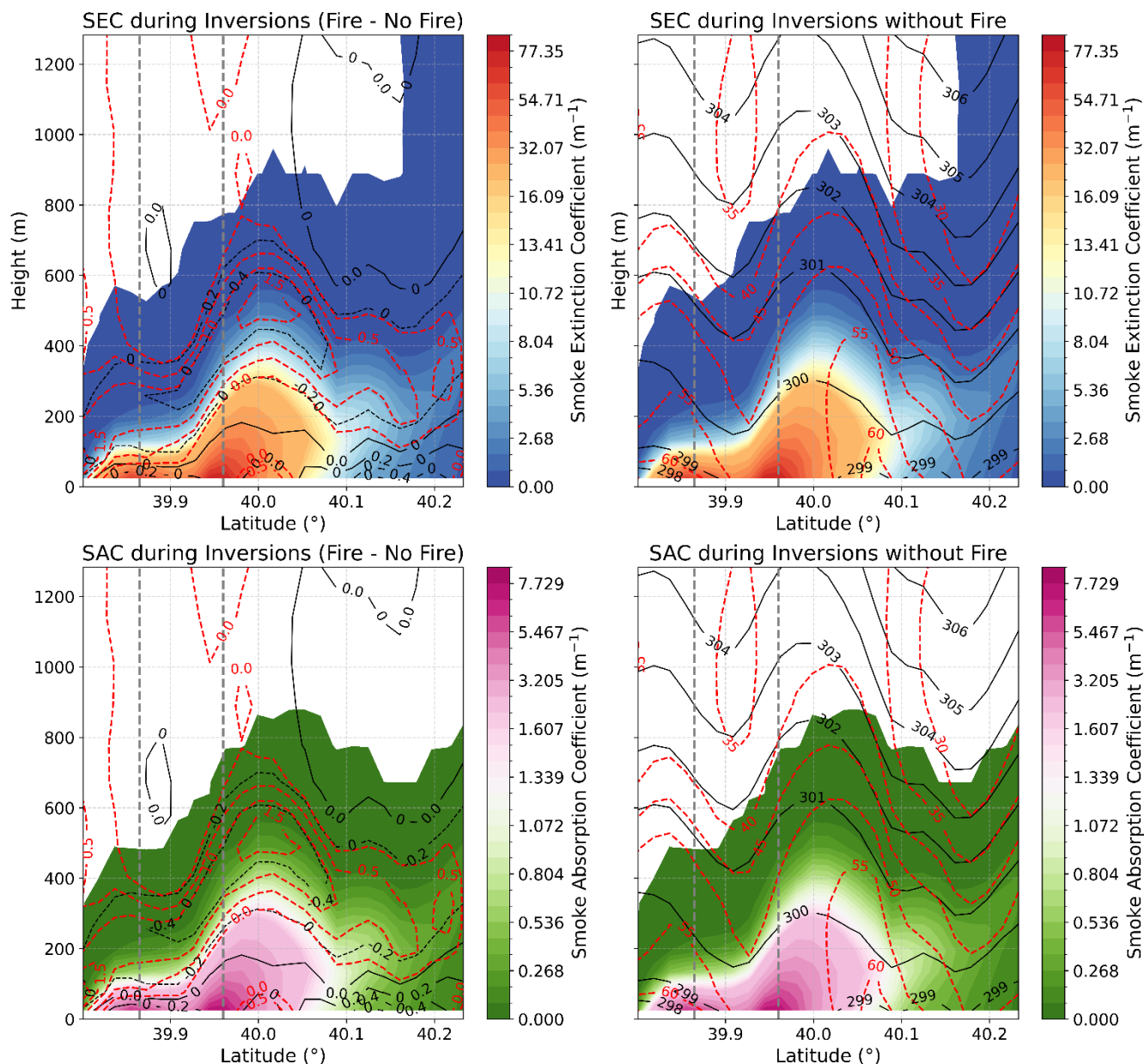


Figure 21: Longitudinal cross-sections of inversion layers overlaid with smoke extinction and absorption coefficients at 550 nm along 8.1° W. Dashed red lines indicate relative humidity (%), and solid black lines represent potential temperature (K). Simulations correspond to 19:00 UTC on 15 October 2017. The region enclosed between the two light gray dashed vertical lines represents the observed area affected by the wildfire.

3.5 Origin and Interpretation of Extreme PM2.5 and SOD Values

Because the BRAMS–SFIRE simulations were performed over a limited regional domain that does not cover all of continental Portugal, a natural concern is that artificial aerosol accumulation might arise through numerical trapping near the downwind boundary. To assess this, we analysed the domain-integrated column PM2.5 north of 40.35° N (Fig. 22). The resulting time series shows no spurious monotonic increase or retention unrelated to plume evolution; instead, column mass increases and declines in phase with the fire activity and plume advection. This confirms that boundary conditions do not dominate the simulated aerosol budget.

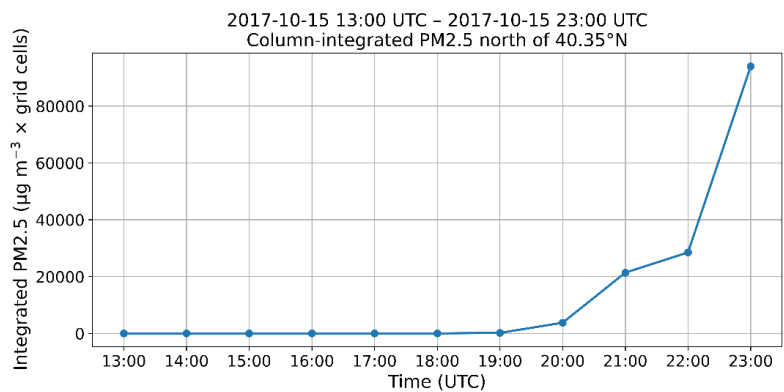


Figure 22: Time series of the domain-integrated column PM2.5 of BRAMS domain north of 40.35° N on 15 October 2017. The values represent the spatial sum of column-integrated PM2.5 over all grid cells located north of the latitude threshold.

To diagnose the physical origin of the sharp local maxima inside the domain, we examined the joint evolution of vertically integrated PM2.5 and surface sensible heat flux at three representative locations along the plume pathway (Source, Midpoint, Endpoint; Fig. 23). In all cases, abrupt increases in PM2.5 coincide with intense pulses of sensible heat flux, a signature of vigorous combustion and rapid vertical injection. These maxima occur in only a few grid cells directly over the active fire front or within the nascent plume core, reflecting steep near-source gradients characteristic of high-intensity crown–surface fire propagation. Such behaviour differs fundamentally from prescribed burns or low-intensity wildfires (Adetona et al., 2016; Miranda et al., 2010), which exhibit broader plume cross-sections and more gradual dilution.

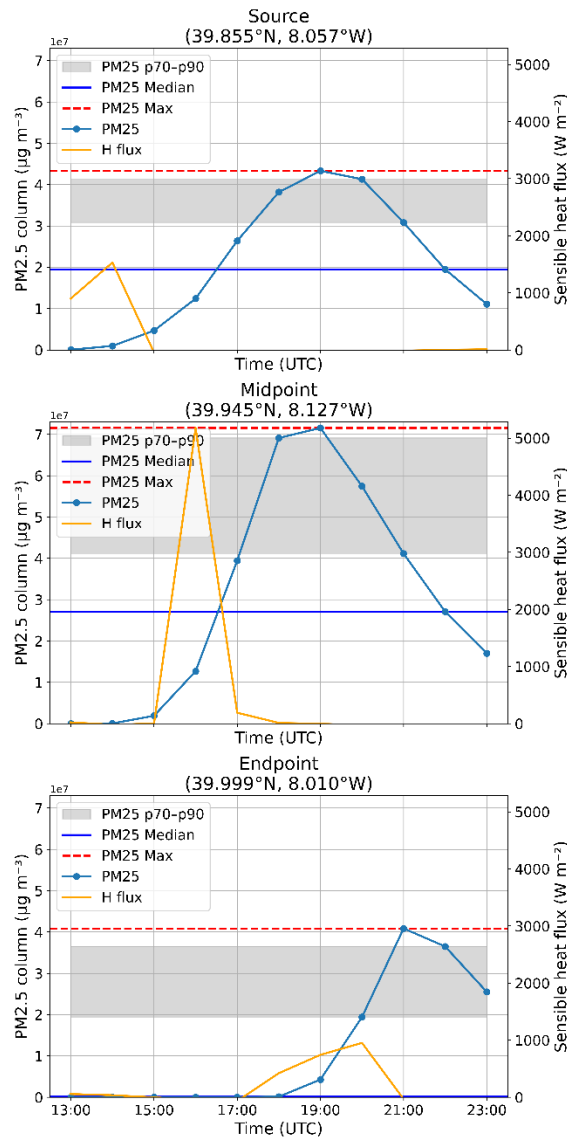


Figure 23: Time series of vertically integrated PM25 concentrations ($\mu\text{g m}^{-3}$) and surface sensible heat flux (W m^{-2}) at three representative grid locations along the plume pathway: Source, Midpoint, and Endpoint. For each location, the shaded band denotes the PM2.5 p70–p90 percentile range, while solid and dashed lines indicate the PM2.5 median and maximum, respectively. The orange curve shows the corresponding sensible heat flux extracted from the same grid cell.

The alignment of the PM2.5 spikes with heat-flux pulses strongly suggests that the extreme concentrations originate from physically plausible, highly localised fire–atmosphere interactions. However, the sensitivity of these peaks to the local sensible heat flux also indicates that uncertainties in fuel load, vegetation composition, and canopy structure can amplify near-source emissions and confine the initial aerosol distribution more strongly than observed. In mixed Mediterranean forest systems,

where fuel heterogeneity is pronounced, misrepresentation of understory and crown biomass can substantially bias the heat release rate and, consequently, the vertical and horizontal gradients of PM_{2.5}. Improved fuel mapping and characterisation would therefore likely reduce the magnitude of these extremes in future simulations.

This interpretation is consistent with the behaviour observed in SOD and extinction fields. Earlier sections showed that SOD exhibits a heavy-tailed distribution and extremely sharp local maxima, some of which exceed values supported by field and remote-sensing observations. These peaks align spatially with the PM_{2.5} spikes identified here, suggesting a shared origin in over-intensified near-source injection rather than in domain-scale numerical artefacts. While numerical transport under very steep concentration gradients can modulate local extremes, the evidence from Figs. 22–23 indicates that the dominant contribution originates upstream, during the emission and injection stage, rather than during plume advection.

This conclusion is consistent with the discrepancies previously noted between BRAMS–SFIRE SOD and MERRA-2 extinction, SSA, and BC/OC partitioning. The strongest disagreements occurred in regions where BRAMS–SFIRE produced exceptionally concentrated plume cores. These differences likely stem not from the radiative or microphysical parametrisations themselves but from the fire source term, which controls the thermal and mass fluxes injected into the atmosphere. In particular, uncertainties in the formulation of the radiative power-to-mass conversion (Subsection 2.1.7) and its dependency on fuel type and combustion phase can introduce biases in the magnitude and vertical placement of smoke emissions. A systematic reassessment of these parameters, together with refined fuel maps for Iberian vegetation types, would help reduce the sharpness of near-source gradients and improve agreement with regional-scale observations.

Finally, consistent with previous observational and modelling studies (Carroll et al., 2025; Huff et al., 2021; Lareau and Clements, 2015; Reid et al., 2005), the extreme values occupy only a negligible fraction of the domain and do not characterise the broader plume. The large-scale structure agrees well with MERRA-2 AOD, indicating that the SOD, extinction, and SSA diagnostics analysed in earlier sections predominantly reflect the regional plume evolution rather than isolated near-source spikes. Taken together, the evidence in Figs. 22–23 demonstrates that the extreme PM_{2.5} and SOD values arise from physically consistent but highly localised fire–atmosphere processes, intensified by uncertainties in fuel representation and emission parametrisation, rather than from numerical accumulation or domain-boundary artefacts.

4 Conclusion

The combined results demonstrate that the BRAMS–SFIRE framework, with explicit smoke–radiation coupling, successfully reproduces the coupled optical and thermodynamic responses of the atmosphere to intense wildfire emissions. The simulations for 15 October 2017 capture both the spectral behaviour and vertical thermodynamic restructuring induced by smoke. Enhanced shortwave absorption at 400–700 nm and localized longwave re-emission generated radiative caps that inhibited nocturnal cooling and displaced Convective Inhibition (CIN) layers upward by 100–200 m. Concurrently, Convective Available Potential Energy (CAPE) increased locally, indicating the onset of radiative–convective feedbacks. The combined

results demonstrate that the BRAMS–SFIRE modelling system, with explicit two-way smoke–radiation coupling, successfully reproduces the key optical, radiative, and thermodynamic responses associated with an intense wildfire event. For the 15 October 2017 episode, the simulations capture both the spectral dependence of smoke extinction and absorption and the resulting restructuring of lower-tropospheric stability. Enhanced shortwave absorption across 400–700 nm, together with localized longwave re-emission, generated radiative caps that inhibited nocturnal cooling and displaced CIN layers upward by approximately 100–200 m. Simultaneously, localized increases in CAPE signal the onset of radiative–convective feedbacks. These features are consistent with the observed diurnal evolution of stability and confirm the central role of smoke-induced heating in modifying boundary-layer dynamics and inversion strength.

These features align with the observed diurnal evolution of stability and corroborate the role of smoke heating in modifying boundary layer dynamics and inversion strength. The comparison between simulated Smoke Optical Depth (SOD) and MERRA 2 Aerosol Optical Depth (AOD) confirms that the apparent amplitude and phase differences mainly reflect the distinct spatiotemporal resolutions and underlying physical quantities of both datasets. The model resolves fine scale and freshly emitted plumes, whereas MERRA 2 provides a smoothed composite representing multiple aerosol sources. Despite these differences, the simulations consistently reproduce the main spatial structure and timing of the observed plume, with the wet configuration yielding the most realistic optical depths, particularly during the mixed phase (18:00–20:00 UTC). The comparison between simulated Smoke Optical Depth (SOD) and MERRA-2 Aerosol Optical Depth (AOD) shows that the apparent amplitude and phase differences primarily reflect the distinct spatial scales, temporal averaging, and compositional assumptions inherent to each dataset. BRAMS–SFIRE resolves fine-scale, freshly emitted plume structures, while MERRA-2 provides a smoothed, multi-species column that integrates regional background aerosols. Despite these inherent differences, the simulations reproduce the main spatial organisation and timing of the observed plume, with the wet microphysical configuration providing the closest match, particularly during the mixed phase (18:00–20:00 UTC), when hygroscopic growth, carbonaceous dominance, and stabilized plume geometry align most favourably.

Diagnostic statistics (Tables S1–S3) show that background subtraction based on upwind AOD systematically improves agreement, reducing biases from -0.7 to -0.05 and increasing correlation coefficients ($r \sim 0.16$ – 0.17 ; $\rho \sim 0.58$). Percentile-based masks (P70–P90) isolate the plume core and confirm that microphysical perturbations, including ABSORBING-like, WIDE SIGMA, and scaled $r_{g,dry}$, produce only modest deviations, reinforcing the robustness of the optical parameterizations. Diagnostic statistics (Tables S1–S3) confirm that upwind-based background subtraction systematically improves agreement, reducing biases and modestly increasing correlation. Percentile masks (P70–P90) isolate the plume core and reveal that microphysical perturbations, including ABSORBING-like, WIDE SIGMA, and scaled $r_{g,dry}$, introduce only small differences in the diagnostics, underscoring the robustness of the implemented optical parameterizations. These results highlight that discrepancies with MERRA-2 arise mainly from representativeness and resolution constraints rather than from deficiencies in the microphysical closure.

At 19:00 UTC, the spatial and spectral consistency between SOD and AOD is maximized. Composition maps and extinction profiles reveal that OC-dominated fine-mode aerosols govern the smoke optical depth at 550 nm, while BC contributes disproportionately to localized heating and inversion strengthening. The combination of hygroscopic growth, carbonaceous fine-mode dominance, and longwave trapping explains why this phase reproduces both the optical and thermodynamic structure of the plume most realistically.

At 19:00 UTC, the model–reanalysis correspondence reaches its maximum: composition fields and extinction profiles confirm that OC-dominated fine-mode aerosols govern optical depth at 550 nm, while BC, though optically less dominant, exerts a disproportionate influence on local heating and inversion modification. The interplay between hygroscopic growth, carbonaceous composition and longwave radiative trapping explains why this period exhibits the most realistic coupling between optical and thermodynamic structure.

Overall, the model reproduces the interlinked optical–radiative–thermodynamic feedback characteristic of large fire plumes: enhanced absorption, inversion reinforcement, CIN displacement, and CAPE modulation. These findings confirm that the implemented microphysical and radiative schemes are physically consistent and that residual discrepancies with MERRA-2 primarily arise from intrinsic resolution and smoothing differences.

The BRAMS–SFIRE coupling thus provides a physically grounded framework for diagnosing wildfire-induced radiative perturbations and their impacts on atmospheric stability. Notably, the inclusion of crown-fire modelling in BRAMS offers enhanced realism in forested and mountainous regions where canopy combustion substantially increases the heat release and aerosol injection heights.

Future work will extend this approach to multi-event climatological analyses and refined aerosol aging processes, further consolidating its potential as a predictive and diagnostic tool for fire–atmosphere interactions under changing climate conditions.

A further conclusion emerging from this study concerns the sensitivity of near-source PM_{2.5} and SOD to uncertainties in fuel characterisation. The additional diagnostics performed here demonstrate that the extreme PM_{2.5} values occur in a very small number of grid cells co-located with peaks in sensible heat flux, indicating that they originate from the intense heat release imposed by the prescribed surface–crown fire regime. While such values are physically plausible for high-intensity crown-fire conditions, their magnitude also suggests that part of the local overestimation likely stems from uncertainties in the specification of vegetation type, fuel load and canopy structure over the burned area. Because these parameters directly control fireline intensity and emission density, improved fuel mapping for Mediterranean mixed-forest understories is expected to reduce the amplitude of these near-source extremes in future simulations. Importantly, these local maxima do not affect the plume-scale optical diagnostics, which remain consistent with MERRA-2 constraints.

Overall, the BRAMS–SFIRE system reproduces the characteristic feedback loop of large fire plumes: enhanced shortwave absorption, inversion reinforcement, CIN displacement, CAPE modulation, and the persistence of near-surface smoke under radiative stabilization. The consistency of these behaviours across multiple configurations demonstrates that the combined

microphysical–radiative schemes are physically sound, and that remaining mismatches with reanalysis datasets stem chiefly from unavoidable scale discrepancies.

Furthermore, the explicit representation of crown-fire processes in BRAMS enhances realism in forested and mountainous terrain, where canopy combustion substantially increases heat release, plume buoyancy and aerosol injection heights. This capability is essential for accurately resolving smoke evolution in Mediterranean-type fire regimes.

Future work will extend this framework to multi-event climatological analyses, improved aerosol-aging representations, refined fuel–vegetation datasets and enhanced observational constraints. These developments will strengthen the model’s capacity to quantify fire-induced radiative perturbations and to diagnose fire–atmosphere interactions under a rapidly changing climate.

Table 1—Symbols and variables used in the text.

Symbol	Definition	Unities
$R_{surface}$	Surface fire spread <u>rate</u>	m s^{-1}
$R_{initialization}$	<u>Equivalent rate of spread used for model initialization</u> ~~Equivalent rate~~	m s^{-1}
R_{active}	<u>Active crown fire spread, set to 40% of the observed 6.1-m windspeed at midflame height</u>	m s^{-1}
R_{10}	<u>Surface fire spread rate for fuel behavior model 10</u>	m s^{-1}
R_{back10}	<u>Backing spread rate for fuel behavior model 10</u>	m s^{-1}
R_{wind10}	<u>Spread rate due to wind factor for fuel behavior model 10</u>	m s^{-1}
$R_{slope10}$	<u>Spread rate due to slope factor for fuel behavior model 10</u>	m s^{-1}
R_{final}	<u>Total fire spread rate</u>	m s^{-1}
$I_{initialization}$	<u>Fireline intensity of the surface fire</u>	W m^{-1}
I_{r10}	<u>Reaction intensity for NFFL fuel behavior model 10</u>	W m^{-1}
I_{final}	<u>Final fire intensity, accounting for the interaction between surface and canopy fuels</u>	W m^{-1}
ϕ	<u>Fire energy flux</u>	W m^{-2}
H	<u>Heat yield of the fuel; mass of fuel consumed in the flaming front</u>	kJ m^{-2}
H_{Low}	<u>Lower heat content of the fue</u>	kJ kg^{-1}
t_r	<u>Residence time for the fuel model</u>	s
σ_{10}	<u>Surface-area-to-volume ratio for fuel behavior model 10</u>	m^{-1}
$w_{surface}$	<u>Initial total mass of surface fuel</u>	kg m^{-2}
FMC	<u>Foliar moisture content</u>	%
FME	<u>Foliar moisture effect</u>	-
FME_0	<u>Reference foliar moisture effect for FMC = 100%</u>	-

<i>CFB</i>	<u>Crown fraction burned</u>	-
<i>P</i>	<u>Radiative power</u>	MW
ϵ	<u>Emissivity</u>	-
σ	<u>Stefan–Boltzmann constant</u>	$\text{W m}^{-2} \text{K}^{-4}$
<i>A</i>	<u>Burnt area</u>	m^2
<i>T</i>	<u>Temperature</u>	K
<i>Q_s</i>	<u>Sensible heat flux</u>	W m^{-2}
<i>c</i>	<u>Specific heat capacity of dry wood</u>	$\text{J kg}^{-1} \text{K}^{-1}$
<i>m</i>	<u>Mass of burned material</u>	kg

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Code availability

The version of the BRAMS model used to produce the results presented in this paper is available under the Creative Commons Attribution 4.0 International License on <https://zenodo.org/records/15830137> (CPTEC/INPE, 2025), along with compilation and simulation instructions.

2695 Author contribution

ICM and LFR developed the coupling within the BRAMS model. ICM also designed the presented experiments, performed the validation, produced the figures and analysis, and wrote the original manuscript. KML and SRF guided the conceptualisation of the coupling implementation in BRAMS. MFF supported the development by correcting conceptual coding errors and assisting with model compilation. RB, VFO, and SC created supporting files for the simulations. In addition, SC contributed to the manuscript review. AIM reviewed the manuscript and supervised the conceptualisation of the model's application.

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Competing interests

The authors declare that they have no conflicts of interest associated with this publication and that no financial support has influenced the outcomes of this work.

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