Modelling the water and carbon dioxide production rates of Comet 67P/Churyumov–Gerasimenko

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ABSTRACT
The European Space Agency Rosetta/Philae mission to Comet 67P/Churyumov–Gerasimenko in 2014–2016 is the most complete and diverse investigation of a comet carried out thus far. Yet, many physical and chemical properties of the comet remain uncertain or unknown, and cometary activity is still not a well-understood phenomenon. We here attempt to place constraints on the nucleus abundances and sublimation front depths of H2O and CO2 ice, and to reconstruct how the nucleus evolved throughout the perihelion passage. We employ the thermophysical modelling code ‘Numerical Icy Minor Body evolUtion Simulator’, or NIMBUS, to search for conditions under which the observed H2O and CO2 production rates are simultaneously reproduced before and after perihelion. We find that the refractories to water–ice mass ratio of relatively pristine nucleus material is $\mu \approx 1$, that airfall material has $\mu \approx 2$, and that the molar abundance of CO2 relative H2O is near 30 per cent. The dust mantle thickness is typically $\leq 2$ cm. The average CO2 sublimation front depths near aphelion were $\sim 3.8$ m and $\sim 1.9$ m on the northern and southern hemispheres, respectively, but varied substantially with time. We propose that airfall material is subjected to substantial fragmentation and pulverisation due to thermal fatigue during the aphelion passage. Sub–surface compaction of material due to CO2 activity near perihelion seems to have reduced the diffusivity in a measurable way.

Key words: comets: individual: 67P/Churyumov–Gerasimenko – methods: numerical

1 INTRODUCTION

One of the main goals of the European Space Agency Rosetta/Philae mission (Glassmeier et al. 2007) to Comet 67P/Churyumov–Gerasimenko (hereafter, 67P/C–G) is to understand comet activity. Specifically, this goal was formulated as the ‘Study of the development of cometary activity and the processes in the surface layer of the nucleus and inner coma (dust/gas interaction)’ (Schwehm & Schulz 1999). In essence, this problem includes understanding: 1) the composition of the nucleus (i.e., the relative abundances of refractories and different types of volatiles) and how it relates to that of the coma; 2) the location of different volatiles underneath the surface, e.g., the thickness of the dust mantle and depths where super– and hyper–volatiles are being released; 3) the physical parameters that govern the diffusion of heat and mass in the near–surface layer; 4) the mechanisms that govern comet outgassing, including the reasons for perihelion outgassing asymmetries; 5) the mechanisms that govern dust mantle formation, erosion, and the dust coma particle size–frequency distribution; 6) the effect of comet outgassing on the spin properties and orbit of the nucleus.

The purpose of this paper is to contribute to this Rosetta goal by placing novel constraints on the nucleus refractories/water–ice mass ratio, the nucleus molar CO2 abundance relative H2O, the depths of H2O and CO2 sublimation fronts, and the vapour diffusivity (indicative of the size–scale of near–surface macro porosity) in Comet 67P/C–G. To achieve these goals we use the thermophysical model NIMBUS (Numerical Icy Minor Body evolUtion Simulator; Davidsson 2021) to investigate under what conditions the model reproduces the global production rates of H2O and CO2 measured by ROSINA throughout most of the Rosetta mission (Fougere et al. 2016a). Furthermore, we calculate the corresponding forces acting on the nucleus due to outgassing, to investigate the conditions under which the observed net non–gravitational changes during one orbit are being reproduced.

The longer–term goal of this work is to apply the currently developed nucleus outgassing torques to the spin state evolution model developed by Samarasinha & Belton (1995), Samarasinha & Mueller (2002), and Samarasinha et al. (2011), to investigate the conditions under which the measured changes to the spin period, spin axis orientation, and gradual non–gravitational changes to the orbit are being reproduced. This may constrain the moments of inertia of the nucleus, and further our understanding of the interior and the activity of Comet 67P/C–G.

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1 Revised ROSINA production rates were published when most of our work had been completed (Combi et al. 2020; Läuter et al. 2020). However, differences with respect to Fougere et al. (2016a) are small and do not materially affect the result presented in the paper.
Various attempts to estimate the refractories/water–vapour mass ratio in the 67P/C–G coma, as well as the refractories/ices mass ratio of the 67P/C–G nucleus have been reviewed by Choukroun et al. (2020). Unfortunately, they are not yet well–constrained. The lower limits of the refractories/water–vapour mass ratio range 0.01–5 for different methods and authors, while the upper limits range from 1.7 to at least 10 (Rotundi et al. 2015; Fulle et al. 2016b; Biver et al. 2019; Combi et al. 2020; Choukroun et al. 2020). The lower limits on the refractories/ices mass ratio of the nucleus range 0.2–3.1, while the upper limits range from 3 to 99 (Herique et al. 2016; Fulle et al. 2016a, 2017; Blum et al. 2017; Hu et al. 2017; Pätzold et al. 2019; Choukroun et al. 2020). Most of these values rely on: 1) estimates of the coma dust mass obtained by retrieving the dust size–frequency distribution from OSIRIS images and determining the bulk densities of individual particles collected by the GIADA and COSIMA instruments; 2) estimates of the coma vapour mass by ROSINA, VIRTIS, and MIRO; and 3) interpretations in terms of composition of the measured nucleus bulk density, permittivity, total nucleus net mass loss, and integrated water vapour loss. These estimates are complicated by the fact that a disputed amount of material with unknown ice abundance is ejected into the coma, where some of the ice is sublimated, before the solids reunite with the nucleus as airfall material (e. g., Thomas et al. 2015; Keller et al. 2015b, 2017; Davidsson et al. 2021).

The nucleus refractories/water–ice mass ratio was estimated as 9–99 by Hu et al. (2017) and as 19 by Blum et al. (2017), based on nucleus thermophysical modelling that fitted the pre–perihelion water production rate. These models assumed a fixed dust mantle thickness (no erosion and a static water sublimation front). Skorov et al. (2020) demonstrated the importance of considering a variable dust mantle thickness in order to reach the steep observed dependence of water production on heliocentric distance. We here extend these studies by considering thermophysical modelling that includes mantle erosion and a moving sublimation front, leading to a dynamically changing dust mantle thickness, which evolves independently on different latitudes. The coupled heat conduction and gas diffusion processes are calculated more rigorously than in these previous works, and we perform a detailed study of the diffusivity of the nuclear material, needed in order to reproduce the observations. Furthermore, we consider both the pre– and post–perihelion branches, which have significantly different water production rate dependencies on heliocentric distance (Hansen et al. 2016; Fougere et al. 2016a), in order to investigate the cause of this perihelion water production asymmetry. Doing so, our goal is to obtain a more reliable estimate of the nucleus refractories/water–ice mass ratio, by considering a more realistic thermophysical model.

Hoang et al. (2020) applied a thermophysical model with the goal of simultaneously reproducing the H2O, CO2, and CO production rates of Comet 67P/C–G for two short pre–perihelion time intervals (Sep 17 through Oct 13, 2014, and Jan 11 through Feb 5, 2015). They considered different combinations of abundances and initial depths of the sublimation fronts. Their models that best reproduced the H2O production did not perform well for CO2, and vice versa. No conclusion was drawn regarding the depth below the surface where CO2 is located.

Herny et al. (2021) used thermophysical modelling to reproduce the CO2/H2O, CO/H2O, and CO/CO2 abundance ratios observed by ROSINA. Unfortunately, their model produced 5 times more water vapour than observed, therefore they scaled down all modelled production rates by that factor. The overproduction occurred because the modelled southern hemisphere lacked a dust mantle, which led to an extreme erosion of 17 m with both H2O and CO2 exposed at the surface. Herny et al. (2021) acknowledged that neither ice exposure nor level of erosion were consistent with the observed nucleus. Because of the scaling they introduced, the resulting abundances and northern CO2 sublimation front depth must be considered highly uncertain. Therefore, we are not aware of any study of the Rosetta data that convincingly determined the depth of the CO2 sublimation front, or estimated the nucleus CO2 abundance. We here attempt such determinations, by striving to simultaneously fit the measured production rates of both H2O and CO2, considering both the pre– and post–perihelion branches.

In this paper, a novel approach is taken towards dust mantle erosion. We first describe the need for such an approach, before outlining the approach itself. Classically, the removal of dust grains at the upper boundary relied on calculating the net force resulting from nucleus gravity, the centrifugal force from nucleus rotation, and the drag force on grains due to nucleus outgassing (e. g., Shu’man 1972; Fanale & Salvail 1984; Rickman et al. 1990; Espinasse et al. 1993; Orosei et al. 1995). It was assumed that the dust grains would become cohesionless as soon as the surrounding ice sublimated. This approach was questioned by some authors (e. g. Kührt & Keller 1994; Möhlmann 1995), who emphasised the potential role of dust mantle cohesion. Laboratory measurements of the cohesion of dust–mantle analogues (i. e., determining the net effect of inter–grain van der Waals forces) show that uniform but highly porous aggregates of μm–sized silica grains have tensile strengths ~ 10^3 Pa (Güttler et al. 2009), but that hierarchically arranged aggregates of such grains may have effective tensile strengths as low as ~ 1 Pa (Skorov & Blum 2012).

Based on a comparison between the expected mantle tensile strengths and the calculated local peak gas pressure within the mantles, Skorov & Blum (2012) concluded that H2O sublimation is not capable of driving cometary dust activity, and that CO2 sublimation only does so at heliocentric distances r_h < 3 au. Using similar lines of argumentation, Gundlach et al. (2015) concluded that the dust mantle of 67P/C–G necessarily must be very weak, thus strongly hierarchical, consisting of weakly attached ‘pebbles’ in the mm–cm–size range. This has been taken as evidence (e. g., Gundlach et al. 2015; Blum et al. 2017) that comet nuclei formed through the gentle gravitational collapse of pebble swarms (e. g. Nesvorny et al. 2010; Wahlberg Jansson & Johansen 2014), in turn formed by streaming instabilities in the Solar Nebula (e. g., Youdin & Goodman 2005; Johansen et al. 2007). However, for CO–driven activity, Jewitt et al. (2019) demonstrate that the size of pebbles that is needed in order to bring cohesion below the peak gas pressure, is too large for such pebbles to be dragged into the coma, unless the heliocentric distance is r_h > 7 au. This was dubbed the ‘cohesion bottleneck’ by Jewitt et al. (2019). Because strong dust activity is common among comets and Centaurs in the 7–12 au region (Jewitt 2009; Sárneckzy et al. 2016; Kulyk et al. 2018), and sometimes takes place as far out as ~ 25 au (Jewitt et al. 2017; Hui et al. 2018), the existence of a cohesion bottleneck (as currently formulated) does not seem to be empirically supported. Resolving this issue is important, particularly because it has consequences for the debate on comet formation.

Because of the difficulties surrounding the cohesion bottleneck problem, and the orders–of–magnitude uncertainties in the actual strengths of cometary mantles, we here start the development of a novel approach to dust mantle erosion. In this paper, we do not attempt to apply a dust mantle erosion rate based on first principles, because those principles (as evident from the description above) are not well–understood. Instead, we will enforce an erosion rate based on our best understanding of the empirical dust production rate of 67P/C–G, inferred from various types of Rosetta observations. We then adjust the nucleus model parameters (primarily the refractories/water–ice mass...
ratio and the diffusivity) until the model matches the observed H$_2$O and CO$_2$ production rates (and by construction, the dust production rate). By doing so, we build an archive that contains the temperature and the vapour pressures of H$_2$O and CO$_2$ as functions of depth, that arise as natural consequences of energy and mass conservation, at given mantle erosion rates. In a forthcoming publication, this numerical information will be used to ‘reverse-engineer’ the dust erosion process. Specifically, correlations between vapour pressures, temperatures, their amplitudes and frequencies of oscillation, and associated mantle erosion rates will be established for different heliocentric distances, nucleus latitudes, and time of day. By considering various fatigue processes and crack propagation mechanisms, this may allow for a better understanding of dust production, and estimates of the tensile strength of the 67P/C–G mantle. The final goal of that exercise will be to define an algorithm that can be applied in thermophysical models, that calculates the appropriate dust mantle erosion rate based on the instantaneous temperature and vapour pressure profiles with depth, that arise during simulations. This algorithm, that is benchmarked against 67P/C–G, can then be tested for other comets.

This paper is organised as follows. The thermophysical model is briefly recapitulated in Section 2 (for a detailed description, see Davidsson 2021). Section 3 discusses the production rates of water and dust of 67P/C–G. Specifically, Section 3.1 discusses the problem of isolating the contribution from the nucleus itself to the observed water production (the thermophysical model water production rate should be compared to that of the nucleus, and not to the total observed rate that potentially also have contributions from an extended source). Section 3.2 defines the time-dependent mantle erosion rate, based on the inferred empirical dust production, that here is used as input to the thermophysical model, for the reasons described above. Section 4 contains our results and focuses on four topics: 1) the pre–perihelion H$_2$O and CO$_2$ production rates (Section 4.1); 2) the post–perihelion H$_2$O and CO$_2$ production rates (Section 4.2); 3) the resulting erosion of the nucleus, the depths of the H$_2$O and CO$_2$ sublimation fronts, and their temperatures (Section 4.3); 4) the forces on the nucleus due to outgassing and the resulting non–gravitational change of the orbit (section 4.4). These results are discussed in Section 5 and our conclusions are summarised in Section 6.

2 THE THERMOPHYSICAL MODEL

In order to calculate the thermophysical evolution of the nucleus, we use NIMBUS developed by Davidsson (2021). NIMBUS models the nucleus as a 1932 m radius spherical body (surface–area equivalent to the real nucleus; Jorda et al. 2016) consisting of a porous mixture of refractory dust and ices (in the current manuscript only crystalline water ice and CO$_2$ ice are considered). The model body is divided into 18 equal–angle latitudinal slabs, and 100 radial cells per latitude (growing in geometric progression from 4 mm thickness at the surface to 200 m at the core). The model nucleus is given the spin axis orientation (equatorial system $\{\alpha, \delta\} = (69.37^\circ, 64.13^\circ)$) from the shape reconstruction (Jorda et al. 2016), orbital elements from the Minor Planet Center, and NIMBUS calculates local illumination conditions at each latitude for any given orbital position and rotational phase. Nominally, NIMBUS tracks the solid–state and radiative conduction of absorbed solar heat radially and latitudinally. Sub–surface H$_2$O and CO$_2$ ice sublimate and consume energy when sufficiently warm, and the vapours are diffusing radially and latitudinally along local temperature and gas pressure gradients (transporting energy through advection). Longitudinal flows are ignored because the rotation speed of the nuclear surface vastly exceeds the diffusion speed. The vapour either finds its way across the outer nucleus boundary and enters the coma, or recondenses internally if reaching a sufficiently cold region (releasing latent energy).

However, the current application uses an alternative implementation called NIMBUS (with d for ‘dust’). Here, the latitudinal heat and gas diffusion are switched off for technical reasons in order to allow for erosion of dust (and other solids, if present) from the upper surface and shrinking of the nucleus. For the short time scales considered here (one orbit) these flows are negligible. If the uppermost locations of H$_2$O and CO$_2$ ice at a given latitudinal slab (called the ‘sublimation fronts’ of respective species) withdraw underground because the front moves faster than the erosion rate, an ice–free dust mantle is formed along with a CO$_2$–free region that only contains H$_2$O ice and refractories. The gas diffusion rate, and hence the total comet outgassing, is sensitive to the depths of the sublimation fronts and the near–surface temperature and gas pressure gradients. Furthermore, the removal of ice and corresponding increase of the porosity reduces the heat conductivity (all these processes are being modelled). Because all simulations in this paper are using NIMBUS, there is no risk of confusion between the variants, thus the thermophysical model is simply referred to as NIMBUS in the following.

A detailed description of the differential equations for energy and mass conservation that are being solved by NIMBUS, as well as many auxiliary physical functions for heat conduction, heat capacity, saturation pressures, mass flux rates et cetera, are provided by Davidsson (2021) and are not repeated here. We emphasise that the applied conductivity and heat capacity are constantly evolving quantities that are functions of the particular composition, porosity, and temperature that prevail at a given time and location. However, the resulting value of the thermal inertia near the surface is typically $\sim 40$–60 MKS (1 MKS = 1 J m$^{-2}$ K$^{-1}$ s$^{-1/2}$), similar to what has been measured for 67P/C–G (Schloerb et al. 2015; Spohn et al. 2015; Marshall et al. 2018).

By relying on laboratory measurements of most material parameters applied in NIMBUS, the number of free parameters is small. The free parameters to be discussed in the current manuscript are limited to the erosion rate of solids from the surface (see Section 3), the initial depths of the sublimation fronts applied at aphelion, the refractories/water–ice mass ratio $\mu$, the molar CO$_2$ abundance relative to water, and the gas diffusivity that is being parameterised by the length $L$, radius $r_p$, and tortuosity $\xi$ of tubes in the Clausius formula (see equation 46 in Davidsson 2021). Different values may be assigned to the northern and southern hemispheres when needed, as described in Section 4.

The NIMBUS calculations provide internal temperatures and abundances, as well as the nucleus production rates for H$_2$O and CO$_2$ for each latitude slab, at a temporal resolution that corresponds to a dynamical time step (typically varying between a few seconds and a few hundreds of seconds). Saving that amount of data to file for simulations that cover years in the simulated world would create unmanageable data volumes. Therefore, NIMBUS saves selected rotational periods at a given resolution. In this paper, every 12$^{th}$ rotation period was stored (roughly once per week given the $\sim 12$ h rotation period), with a 10$^{th}$ resolution in terms of rotational phase. In order to produce continuous outgassing curves, every stored rotation is copied to the following eleven ones. The errors introduced by this approach are small, but result in a certain level of discontinuity seen in some of the figures.

The escape of gases across the upper surface gives rise to a force acting on the nucleus because of linear momentum conservation. Calculating this reaction force acting on a surface sublimating into vacuum is not trivial. Davidsson & Skorov (2004) used a Monte
Carlo approach to calculate the velocity distribution function of water molecules emerging from a highly porous medium with a near-surface temperature gradient. They used the velocity distribution as a source function to a Direct Simulation Monte Carlo (DSMC) model that calculates the evolution of the velocity distribution function due to molecular collisions within the base of the comet coma (i.e., a numerical solution to the Boltzmann equation containing a non-zero collision integral). This type of calculations are necessary in environments where the gas is far from being in thermodynamic equilibrium (i.e., the velocity distribution function is strongly non-Maxwellian and the hydrodynamic Euler equations for conservation of mass, momentum, and energy do not apply). The model by Davidsson & Skorov (2004) evaluates the force acting on the surface as the sum of momentum transfer during molecular ejection from the nucleus because of sublimation, and inelastic molecule–surface collisions due to coma gas that has been backscattered toward the nucleus within the Knudsen layer. Such a complex treatment is out of scope in the current paper. Also, we cannot directly apply the existing simulations by Davidsson & Skorov (2004) for two reasons: 1) those are only valid when ice is intimately mixed with dust up to and including the surface, while the current NIMBUS simulations result in the formation of ice–free dust mantles; 2) those only considered H₂O ice, while the current work considers both H₂O and CO₂.

Therefore, we apply the classical approach (e.g., Rickman 1989) of defining a force that is proportional to the local outgassing rate \( Z \) (molec m⁻² s⁻¹) and to the mean molecular speed of a Maxwellian gas \( \langle V \rangle \) (regardless of direction of travel), multiplied to a momentum transfer coefficient \( \eta \) that corrects for the fact that the mean molecular velocity along the surface normal does not equal \( \langle V \rangle \).

\[
F = -\eta \sum_i \sum_j Z_i m_j \langle V \rangle_{i,j} s_i n_i.
\]

(1)

Here, the summation is made over all nucleus facets \( i \) having outward surface normals \( n_i \) and areas \( s_i \), and over the two species \( j = 1 \) (H₂O) and \( j = 2 \) (CO₂). The mean molecular speed is given by

\[
\langle V \rangle_{i,j} = \frac{8k_B T_i}{\pi m_j}
\]

(2)

where \( k_B \) is the Boltzmann constant, \( T_i \) is the surface temperature of facet \( i \), and \( m_j \) is the mass of a H₂O \( (j = 1) \) or CO₂ \( (j = 2) \) molecule.

The evaluation of \( \eta \) is a topic of debate, with values typically falling in the range 0.4 ≤ \( \eta \) ≤ 1 (see Rickman 1989; Davidsson & Skorov 2004, and references therein). We nominally ran the simulations with \( \eta = 1 \), but re-normalise in Section 4.4 in order to comply with measured non-gravitational changes of the orbit. Although NIMBUS works with a spherical model nucleus rotating at a fixed 12.4043 h period (Mottola et al. 2014), we apply a mapping procedure that takes into account the actual nucleus shape and spin period changes over time, as described in Section 4.1.

3 NUCLEUS WATER PRODUCTION AND EROSION RATES

The comet nucleus emits water vapour directly from its surface, along with fine dust (≤ 1 mm) that may be considered fully refractory, and larger chunks (1 mm–1 m; e.g. Rotundi et al. 2015; Davidsson et al. 2015; Agarwal et al. 2016) that potentially contain water ice. The latter might constitute an extended (distributed) source of water vapour in the coma, before the majority of these heavy particles reunite with the nucleus as airfall material (e.g. Thomas et al. 2015; Keller et al. 2015b, 2017; Davidsson et al. 2021). The transition size of ~ 1 mm between dust and chunks is determined by the diurnal thermal skin depth: dust grains are isothermal and unable to carry ice, while chunks are thermally heterogeneous. As demonstrated by Davidsson et al. (2021) for a 1 cm chunk, such particles may have a dust mantle, an icy interior, strongly different daytime and nighttime temperatures, and activity lifetimes on the order of days. The empirical information available is the total observed water production \( Q_{H₂O} \) from nucleus and chunks (for symbols used in Section 3, see Table 1). However, the contribution \( Q_{nuc} \) from the nucleus itself needs to be isolated, for direct comparison with water production rates calculated by NIMBUS. Furthermore, in the current application, NIMBUS needs the dust mantle erosion rate \( E \) as input. We here use simple methods to retrieve those rates from available empirical data. We make the following assumptions:

A#1. The dayside area elements on the nucleus and on coma chunks have the same average water production rates \( q_w \), and production rates of fine dust \( q_d \) (both measured in units of kg m⁻² s⁻¹). Thus, chunks are considered ‘miniature comets’.

A#2. The size distribution of chunks is given by a power-law. It can be used to let all chunks be represented by an average radius \( r_c \) (in terms of surface area).

A#3. The ejection rate of chunks into the coma is proportional to the total water production rate \( Q_{H₂O} \) of the comet, i.e., \( n_c \propto Q_{H₂O} \) (chunks s⁻¹). This accounts for a nucleus source of chunks (\( Q_{nuc} \)), but also that large chunks in the dm–m class will produce smaller chunks as well.

A#4. The production rate of fine dust is proportional to that of water vapour, or \( q_d \propto q_w \).

By making these assumptions, the dust production rate takes the same functional form as the water production rate. This can be motivated by considering the brightness of the comet, that is proportional to the amount of fine dust in the coma. Hansen et al. (2016) point out that the coma brightness determined by ground-based telescopes is highly correlated with the water production rate that has been inferred from the ROSINA measurements. A careful reconstruction of both the dust production rate and the water production rate was made by Marschall et al. (2020). They find that the dust–to–gas mass ratio changed over time (i.e., A#4 is not strictly valid). However, during the period 200 days pre–perihelion to 100 days post–perihelion (when most of the gas and dust are being produced), the dust–to–gas mass ratio is still rather stable: Marschall et al. (2020) find that it is 0.5 ± 0.25, except for a brief period around 100 days pre–perihelion when the dust–to–gas mass ratio increased to ~ 1.3. Considering that the production rate changed by orders of magnitude in this period, the fact that their ratio remained quasi–constant to within ±50 per cent for most of the time shows that A#4 is a reasonable approximation.

3.1 The nucleus water production rate

In order to calculate the nucleus water outgassing rate,

\[
Q_{nuc}(t) = 2\pi R_{nuc}^2 q_w(t),
\]

(3)

we need \( q_w(t) \), which is defined by

\[
q_w(t) = \frac{Q_{H₂O}(t)}{A_{tot}(t)}.
\]

(4)

according to A#1, where \( A_{tot} \) is the total sublimating area. \( A_{tot} \) is ultimately constrained by the amount of airfall accumulated during one apparition, as described in the following. If the number of coma chunks at a given moment is \( N_c \) then (according to A#2)

\[
A_{tot}(t) = 2\pi r_c^2 N_c(t) + 2\pi R_{nuc}^2.
\]

(5)
Δ therefore to the sum of contributions from the nucleus and chunks in the coma. When proportionality constant (the flight time from source to airfall target). In order to evaluate the Summary of the functions and parameters used for the dust production model. Note that areas, production rates vapour produced during the apparition), and use the fact that the on the northern hemisphere of the comet, half the nucleus surface, has a layer thickness (here, molec s⁻¹), which should be converted to kg s⁻¹ when applied in equations 4–8 and 17) we fitted the of seasonal airfall deposits $h = 0.87$ m according to Davidsson et al. (2021), and a macro–porosity $\psi = 0.4$ for airfall material, similar to that of gravitationally reaccumulated low–mass rubble–pile asteroids (Abe et al. 2006). This yields $N_c = 1.97 \cdot 10^{11}$. In order to define $Q_{H2O}(t)$ (here, molec s⁻¹), which should be converted to kg s⁻¹ when applied in equations 4–8 and 17) we fitted the following functions to Rosetta/ROSINA measurements by Fougere

### Table 1

| Symbol       | Description                                      | Unit       |
|--------------|--------------------------------------------------|------------|
| $A_c$        | Fraction of nucleus area emitting chunks per nucleus rotation |           |
| $\Lambda_{tot}$ | Total comet surface area                          | m²         |
| $C$          | Correction factor in equation (9)                |            |
| $E$          | Dust mantle erosion rate                          | kg m⁻² s⁻¹ |
| $F(t)$       | Total comet fine dust production rate              |            |
| $G(t)$       | Total nucleus dust to comet $H_2O$ production rate |            |
| $h$          | Thickness of airfall layer deposited per appearance | m         |
| $k_c$        | Proportionality constant in equation 6            | kg⁻¹       |
| $M_{H_2O}$   | Total comet $H_2O$ mass loss per apparition       | kg         |
| $M_{tot}$    | Total comet mass loss per apparition              | kg         |
| $N_c$        | Number of coma chunks                            |            |
| $\tilde{N}_c$ | Number of chunks ejected into coma per apparition |            |
| $n_c$        | Ejection rate of chunks into the coma            | s⁻¹        |
| $q$          | Differential size frequency distribution power–law index |          |
| $q_d(t)$     | Fine dust production flux                         | kg m⁻² s⁻¹ |
| $q_w(t)$     | $H_2O$ production flux                            | kg m⁻² s⁻¹ |
| $Q_{H2O}(t)$ | Total comet $H_2O$ production rate                | kg s⁻¹     |
| $Q_{tot}(t)$ | Total nucleus $H_2O$ production rate              | kg s⁻¹     |
| $r_c$        | Coma chunk radius                                 | m          |
| $R_m$        | Effective nucleus radius                          | m          |
| $\Delta t$  | Dynamical life–time of coma chunks                | s          |
| $\rho_c$     | Airfall layer bulk density                        | kg m⁻³     |
| $\psi$       | Airfall layer macro porosity                      |            |

We assumed (A#3) that

$$n_c(t) = k_c Q_{H2O}(t),$$

therefore $N_c$ is given by

$$N_c(t) = k_c Q_{H2O}(t) \Delta t,$$

where $\Delta t$ is the average dynamical life–time of chunks in the coma (the flight time from source to airfall target). In order to evaluate the proportionality constant $k_c$, we integrate equation (6) over one orbit,

$$N_c = \int_0^P n_c(t) \, dt = k_c \int_0^P Q_{H2O}(t) \, dt = k_c M_{H2O}$$

(8)

(where $P$ is the orbital period, and $M_{H2O}$ is the total amount of water vapour produced during the apparition), and use the fact that the total number of chunks $N_c$ produced during the perihelion passage is related to the thickness of the airfall deposition layer accumulated on the northern hemisphere of the comet,

$$2\pi R_{max}^2 h \rho_c (1 - \psi) = C \left( \frac{4\pi}{3} r_c^3 \rho_c \right) N_c.$$

(9)

The left hand side of equation (9) is the total mass of accumulated airfall material in the northern hemisphere, assuming that it covers half the nucleus surface, has a layer thickness $h$, and that the chunks with bulk density $\rho_c$ assemble in this layer with a macro–porosity of $\psi$. The right hand side of equation (9) has the mass of a single coma chunk within parenthesis, which yields the total mass of coma chunks when multiplied with the total number of chunks $N_c$. The correction factor $C$ is compensating for the fact that $r_c$ and $N_c$ are defined to represent the coma chunks in terms of their surface area, which is not necessarily a good measure of their volume. Note that $\rho_c$ cancel out in equation (9), i.e., the current derivation does not depend on the bulk density of the coma chunks.

We now proceed to evaluate $r_c$ and $C$. For a differential size frequency distribution of chunks on power–law form, $K r^{-q}$, the surface area distribution is $K r^{-q} r^2 = K r^{3-q}$. With lower and upper truncation radii ($r_{\min}$, $r_{\max}$), we define the most typical radius $r_c$ (in terms of surface area) as

$$\int_{r_{\min}}^{r_c} (r')^{2-q} \, dr' = \frac{r_c^{3-q} - r_{\min}^{3-q}}{2},$$

(10)

i.e., the radius for which all smaller chunks collectively have the same surface area as the combined surface area of all larger chunks.

The total surface area of chunks is

$$S_c = 4\pi K \int_{r_{\min}}^{r_{\max}} (r')^{3-q} \, dr' = \frac{4\pi K}{(4-q) q^2}$$

(11)

which means that the number of $r_c$–sized chunks carrying this area is

$$N_c = \frac{S_c}{4\pi r_c^2}$$

(12)

The differential volume distribution is $K r^{-q} r^3 = K r^{3-q}$, which means that the total volume of all chunks is

$$V_c = \frac{4\pi K}{3} \int_{r_{\min}}^{r_{\max}} (r')^{4-q} \, dr' = \frac{4\pi K}{(4-q) r_{\min}^{4-q} r_{\max}^{4-q}}.$$ 

(13)

The correction factor should make sure that the right–hand side of equation (9) equals the correct volume, thus

$$V_c = C \left( \frac{4\pi}{3} r_c^3 \right) N_c.$$ 

(14)

Insertion of equations (11)–(13) into equation (14) yields

$$C = \frac{3-q}{r_c (4-q) r_{\max}^{4-q} r_{\min}^{4-q}}.$$ 

(15)

We now proceed to evaluate equations (3)–(15), for numerical values of independent and dependent parameters, see Table 2. Philae/ROLIS images of airfall material at Agilkia show that the differential size distribution of chunks has $q = 3.8$ at radii $0.02 \leq r \leq 0.5$ m (Mottola et al. 2015). We extend the distribution to $r_{\min} = 0.0081$ m, where it starts to flatten, according to Philae/CIVA images (Poulet et al. 2017). That yields $r_c = 0.0184$ m (equation 10) and $C = 2.34$ (equation 15). When evaluating equation (9) we use $R_m = 1932$ m, for which a sphere has the same surface area as the nucleus of 67P/C–G (Jorda et al. 2016), the average thickness of seasonal airfall deposits $h = 0.87$ m according to Davidsson et al. (2021), and a macro–porosity $\psi = 0.4$ for airfall material, similar to that of gravitationally reaccumulated low–mass rubble–piles asteroids (Abe et al. 2006). This yields $N_c = 1.97 \cdot 10^{11}$. In order to define $Q_{H2O}(t)$ (here, molec s⁻¹), which should be converted to kg s⁻¹ when applied in equations 4–8 and 17) we fitted the following functions to Rosetta/ROSINA measurements by Fougere

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Table 2. Numerical values for independent (input) and dependent (output) constants applied in the evaluation of equations (3)–(15).

| Symbol | Value | Unit |
|--------|-------|------|
| Independent constants | | |
| $h$ | 0.87 | m |
| $M_L$ | $(1.05 \pm 0.34) \cdot 10^{10}$ | kg |
| $q$ | 3.8 | |
| $R_{\text{nuc}}$ | 1932 | m |
| $r_{\text{min}}$ | 0.0081 | m |
| $r_{\text{max}}$ | 1 | m |
| $\Delta t_f$ | 12 | h |
| $\psi$ | 0.4 | |
| Dependent constants | | |
| $C$ | 2.34 | |
| $k_c$ | 38.4 | chunks kg$^{-1}$ |
| $M_{\text{H}_2O}$ | $5.13 \cdot 10^9$ | kg |
| $N_c$ | $1.97 \cdot 10^{11}$ | |
| $r_c$ | 0.0184 | m |

where the first+second and third rows correspond to the pre- and post-perihelion branches, respectively, $r_h = r_h(t)$ is the heliocentric distance of the comet (au), and $q_{\text{orb}} = 1.24$ au is the perihelion distance. The two branches have distinctively different slopes far from perihelion (also see Hansen et al. 2016), and the pre-perihelion exponential term in equation (16) is needed to reproduce a near-perihelion surge in water production and to yield a seamless transition to the post-perihelion branch. Integrating equation (16) yields a total water loss $M_{\text{H}_2O} = 5.13 \cdot 10^9$ kg, which is consistent with other ROSINA–based estimates by Läuter et al. (2020) of $4.0 \pm 0.6 \cdot 10^9$ kg and by Combi et al. (2020) of $4.9 \pm 1.5 \cdot 10^9$ kg, but somewhat higher than $2.4 \pm 0.1 \cdot 10^9$ kg based on Rosetta/MIRO (Biver et al. 2019) and losses ranging (2.3–3.1) $\cdot 10^9$ kg recorded by SWAN/SOHO during three previous apparitions (Bertaux 2015). This yields $k_c = 38.4$ kg$^{-1}$ from equation (8). Applying $\Delta t_f = 12$ h (a typical flight-time of coma chunks; Davidsson et al. 2021), equations (3)–(5) can be evaluated.

Figure 1 (upper panel) shows that $0.92 \leq Q_{\text{nuc}}/Q_{\text{H}_2O} \leq 1$, i.e., the extended source of water contributes at most 8 per cent of the water vapour near perihelion. Because this deviation is substantially smaller than the scatter in the measured water production rate data (see Figs. 5 and 9), we decided to compare NIMBUS water production rates directly with the observed $Q_{\text{H}_2O}$ instead of $Q_{\text{nuc}}$.

3.2 The nucleus dust erosion rate

Equations (8)–(9) provide the constant $k_c$ that allows us to estimate the fraction of the nucleus surface area responsible for chunk ejection during one nucleus rotation period $P_{\text{rot}} = 12.4 \times 3600$ s (Mottola et al. 2014),

$$A_c = \frac{r^2_k q_c P_{\text{rot}}}{2 R^2_{\text{nuc}}}.$$  (17)

With $A_c$ not exceeding ~ 4 per cent at any time (Fig. 1, middle panel), the vast majority of the surface is eroding because it ejects fine (≤ 1 mm) dust. The water production of the nucleus is therefore controlled by the thickening or thinning of the dust mantle resulting from gradual small-scale erosion and water sublimation—front withdrawal. Chunk ejection will be relatively rare and is a local phenomenon. Therefore, we restrict the erosion rate (to be applied in NIMBUS) to $q_d$ itself. We express the total nucleus dust erosion rate $E$ in units of the total water production rate,

$$E = G(t) Q_{\text{H}_2O} = G(t) q_w A_{\text{tot}}(t).$$  (18)

But

$$E = 2\pi R^2_{\text{nuc}} q_d$$  (19)

which means that

$$G(t) = \frac{2\pi R^2_{\text{nuc}} q_d}{q_w A_{\text{tot}}(t)}.$$  (20)

According to A#4,

$$q_d = F q_w,$$  (21)

thus

$$G(t) = \frac{2\pi R^2_{\text{nuc}} F}{A_{\text{tot}}(t)}.$$  (22)

The mass ratio $F$ between (escaping) fine dust and water vapour can be constrained through the total mass loss of the nucleus during the perihelion passage, $M_L = (1.05 \pm 0.34) \cdot 10^{10}$ kg, determined
with Rosetta/RSI (Pätzold et al. 2019). Specifically (equations 4, 8),

\[ M_L = \int_0^P (q_w + q_d) A_{\text{tot}} \, dt = M_{\text{H}_2\text{O}} + FM_{\text{H}_2\text{O}}, \quad (23) \]

or

\[ F = \frac{M_L - M_{\text{H}_2\text{O}}}{M_{\text{H}_2\text{O}}}. \quad (24) \]

Numerically, \( F = 1.05 \), which means that the total amounts of refractories and water vapour lost to space by 67P/C–G was nearly equal. Equation (22) yields \( G(t) \), shown in the lower panel of Fig. 1. With \( 0.96 \leq G(t) \leq 1.05 \), it is clear that the total erosion rate (kg s\(^{-1}\)) of fine dust \( E \) is very similar to the observed total water production rate \( \dot{Q}_{\text{H}_2\text{O}} \), and the differences are smaller than the scatter in water production rate measurements (see Figs. 2 and 3). Therefore, we decided to apply \( \dot{Q}_{\text{H}_2\text{O}} \) itself, for the total dust erosion rate of the nucleus. Specifically, the local erosion rate (kg m\(^{-2}\) s\(^{-1}\)) was set proportional to local illumination conditions (determined by latitude and time of day), such that the total amount of eroded dust per unit time equalled \( \dot{Q}_{\text{H}_2\text{O}} \).

We note that \( h = 0.87 \) m, estimated by Davidsson et al. (2021) through mass transfer calculations, is consistent with the deposition of 1.4 ± 0.8 m in Hapi (Cambianica et al. 2020) and 0.7 ± 0.3 m in Ma’at (Cambianica et al. 2021), based on measurements of boulder shadow lengths and their temporal changes. Marshall et al. (2020) estimated a deposition of 0.14+0.23−0.14 m. Applying \( h = 2.2 \) m (the upper limit according to Cambianica et al. 2020) instead of \( h = 0.87 \) m would increase the peak contribution from the extended source from 8 to 18 per cent. The fraction of the nucleus surface being responsible for chunk ejection would increase from 4 to 11 per cent. The erosion would be a factor 0.86 ≤ \( G(t) \) ≤ 1.05 times the total water production. With a larger number of chunks needed to produce a thicker airfall layer, the nucleus is responsible for a somewhat smaller fraction of the water production. Therefore, the erosion taking place because of the gradual removal of fine dust on ~ 90 per cent of the surface, proceeds at a somewhat lower rate. Given the factor 2–3 dispersion in measured water production rates, a factor 0.82 reduction of the nominal production rate that we try to match (remembering that NIMBUS in principle should reproduce the contribution from the nucleus, not the full measured \( \dot{Q}_{\text{H}_2\text{O}} \), that also includes the extended source) has a negligible impact on our results. A smaller \( h \) value, as suggested by Marshall et al. (2020) would further motivate our decision of using \( G(t) = 1 \).

4 RESULTS

The spin axis orientation of 67P/C–G is such that the northern hemisphere is being illuminated pre–perihelion (see, e. g.: Keller et al. 2017). The comet reaches the inbound equinox at \( r_h = 1.67 \) au when the sub–solar point enters the southern hemisphere. At the \( r_h = 1.24 \) au perihelion, the southern hemisphere is fully active while the northern hemisphere has polar night. When the outbound equinox is reached at \( r_h = 2.6 \) au post–perihelion, the sub–solar point moves into northern latitudes again. It is crucially important to be aware of these changes when interpreting the behaviour of nucleus activity. We discuss the pre–perihelion branch in Section 4.1, the post–perihelion branch in Section 4.2, the overall properties of the solutions in Section 4.3, and the outgassing force properties in Section 4.4.

4.1 The pre–perihelion branch

The goal of the NIMBUS reproduction of the Rosetta/ROSINA H\(_2\)O and CO\(_2\) production rate measurements (Fougerè et al. 2016a) on the pre–perihelion branch is to constrain the physical and chemical properties of (primarily) the northern hemisphere of 67P/C–G under pre–apophelion conditions. We first focus on the water production rate.

A substantial number of short test simulations (i. e., for limited ranges in heliocentric distance) were performed in order to: 1) understand the sensitivity of the solutions to different parameter values in different parts of the orbit; 2) to get a first feel for the relevant parameter ranges; 3) work out a strategy for how to determine the diffusivity and nucleus mass ratio \( \mu \) between refractories and water ice.

One set of tests showed that the influence of \( \mu \) is dominating over that of diffusivity at perihelion. Specifically, going from \( \mu = 4 \) to \( \mu = 1 \) (20 to 50 per cent water ice by mass) led to a 250 per cent increase in water production rate (i. e., the production rate depends linearly on the weight–percentage of water ice). However, increasing the diffusivity by a full three orders of magnitude (from \( \{L, r_p\} = \{10, 1\} \mu m \) to \( \{10, 1\} mm \), using \( \xi = 1 \) just resulted in a 50 per cent increase in water production. The reasons for the weak influence of diffusivity during strong sublimation were outlined by Davidsson et al. (2021). In essence, diffusivity significantly changes the sub–surface temperature and vapour pressure distributions, but in such a way that the resulting outgassing rate remains quasi–constant. Furthermore, these preliminary tests indicated that \( 1 \leq \mu \leq 2 \) seems to provide the best reproduction of the gas production rate of 67P/C–G.

A second set of tests were performed far from perihelion (at \( r_h = 3.5 \) au). They revealed a strong dependence of the water production rate on diffusivity, but a comparably weak one on \( \mu \). A three orders of magnitude increase in diffusivity leads to roughly the same factor of increase in the water production rate. However, the water production rate still scales linearly with the weight percent of the water ice (changing from \( \mu = 2 \) to \( \mu = 1 \), or from 33 per cent to 50 per cent, increases the production rate by a factor 1.5).

It is therefore clear that the diffusivity can be determined by considering an arbitrary (but realistic) \( \mu \)-value, and varying \( \{L, r_p\} \) until the synthetic water production rate matches the observed one at large heliocentric distances. This should not merely be done locally, but for a substantial piece of orbital arc prior to the test point, in order to allow for proper thermal adjustment of the nucleus. With the best–fit diffusivity at hand, it can be applied during local simulations at perihelion, in order to fit the actual \( \mu \)-value. The ultimate test of this combination of diffusivity and water abundance is to perform a full simulation from aphelion to perihelion and demonstrate that the entire empirical water production rate curve is fitted both in terms of shape and magnitude.

In the following, we perform such an analysis, and illustrate the principles just described. We assumed \( \xi = 1 \) and tested \( \{L, r_p\} \) combinations of \( \{10, 1\} \mu m, \{100, 10\} \mu m, \) and \( \{1, 0.1\} mm \) (the second and third have 10 and 100 times higher diffusivity than the first, respectively). Note that the thermophysical solution is insensitive to the individual \( \{L, r_p, \xi\} \) values (any combination of numerical values that yield the same diffusivity are equivalent).

These models were run for \( \mu = 2 \) (an educated guess based on the previous test simulations), from the \( r_h = 5.68 \) au aphelion, to the 3.0 ≤ \( r_h \) ≤ 3.6 au region where the first ROSINA data were acquired (Fougerè et al. 2016a). Figure 2 (left) shows that the best fit to the early ROSINA data was obtained for \( \{L, r_p\} = \{100, 10\} \mu m \) (red solid curve). The dependence of the water production on the
The water production rate calculated from aphelion at 5.68 au to 2.9 au inbound, having a small overlap with the first available Rosetta/ROSINA data. The arbitrary nucleus temperature initial condition is rapidly corrected. At large heliocentric distances, the water production rate is strongly sensitive to the diffusivity (via the tube length $L$, radius $r_p$, and tortuosity $\xi$) but insensitive to the nucleus mass ratio $\mu$ between refractories and water ice. Right: A close–up on the region where data and models overlap. The model with $\{L, r_p\} = \{100, 10\} \mu m$, $\xi = 1$, and $\mu = 2$ provides the best fit. The effect on the water production rate by increasing the water ice mass fraction from 33 per cent ($\mu = 2$) to 50 per cent ($\mu = 1$) is smaller than the scatter in the measured data.

| Refractories/water–ice mass ratio $\mu$ | Model perihelion H$_2$O production rate |
|----------------------------------------|----------------------------------------|
| 2.0                                    | 0.53$Q_{H_2O}$                         |
| 1.5                                    | 0.64$Q_{H_2O}$                         |
| 1.0                                    | 0.89$Q_{H_2O}$                         |
| 0.5                                    | 1.69$Q_{H_2O}$                         |

Table 3. NIMBUS was run for four different nucleus mass ratios between refractories and water ice $\mu$ during one week near perihelion. The resulting model water production rates are expressed with respect to the measured rate $Q_{H_2O} = 1.87 \cdot 10^{28}$ molec s$^{-1}$ according to equation (16).

The challenge for NIMBUS is to properly reproduce this hand–over of prime responsibility for activity from the northern to the southern hemisphere. We decided to apply $\{L, r_p\} = \{100, 10\} \mu m$ for the southern hemisphere of 67P/C–G as well. In a handful of simulations during one week centred on the perihelion passage, we attempted to constrain the refractory/water–ice mass ratio of the southern hemisphere, $\mu_S$. One week (~ 14 nucleus rotations) is sufficient to establish a balance between dust mantle erosion and H$_2$O sublimation–front motion, i.e., reaching a quasi–constant dust mantle thickness, and to establish a diurnal steady–state thermal cycling in the region responsible for water outgassing. The results of these simulations are summarised in Table 3.

As can be seen, a reduction of the refractories/water–ice mass ratio from $\mu = 2$ to 0.5 makes the modelled water production grow from 0.53 to 1.69 times the observed rate $Q_{H_2O}$ (as defined by equation 16).

The best reproduction of the perihelion water production rate is obtained for $\mu = 1$ with $0.89Q_{H_2O}$ (particularly because the nucleus production rate $Q_{H_2O} = \mu_{S_{\text{max}}}$ in reality might be some ~ 8 per cent lower than the total observed water production rate according to Section 3.1). .

In order to test whether this solution ($\mu = 1$ and $\{L, r_p\} = \{100, 10\} \mu m$ on both hemispheres) is capable of reproducing the entire pre–perihelion water production rate branch, we ran a model from aphelion all the way up to perihelion with this parameter set. Figure 3 shows that the model (blue curve) provides a reasonable fit, although the production rate beyond $r_h \approx 2$ au tends to be on the high side. We therefore decided to introduce a hemispherical compositional dichotomy, with $\mu_S = 1$ in the south, but a somewhat larger...
\(\mu_N = 2\) in the north (still using \(\{L, r_p\} = \{100, 10\}\) \(\mu m\) and \(\xi = 1\) everywhere). The resulting red curve in Figure 3 is somewhat more convincing, and we consider this our best solution.

At this point, we turned the attention to the CO\(_2\) production. Observations in Aug–Sep 2014 by ROSINA indicated that the CO\(_2\) production predominantly emanated from the southern hemisphere (Hässig et al. 2015). The CO\(_2\)/H\(_2\)O production rate ratio was an order of magnitude higher in parts of the south compared to most of the north, though that number largely reflects a low southern water production due to the poor illumination conditions. The dominance of CO\(_2\) production in the south (although significant amounts were also produced from the Hapi region in the north) was confirmed by Fougere et al. (2016b) for a longer Aug 2014 to June 2015 time-line. Initially, we therefore only considered models with CO\(_2\) ice on the southern hemisphere (using \(\{L, r_p\} = \{100, 10\}\) \(\mu m\), \(\xi = 1\) and \(\mu_S = 1\), as determined earlier).

In order to assign a molar CO\(_2\) nucleus abundance relative H\(_2\)O, we first assumed that the abundance ratio would be close to that of the coma. The coma column density CO\(_2\)/H\(_2\)O ratio was 2.4 ± 0.6 per cent over Aten/Babi, 3.0 ± 0.7 per cent over Seth/Hapi, and 3.9 ± 1.0 per cent over Imhotep in April 2015, according VIRTIS–M measurements analysed by Migliorini et al. (2016). Fink et al. (2016) analysed VIRTIS–M data from February and April 2015 and obtained column density CO\(_2\)/H\(_2\)O ratios ranging 3.3–8.5 per cent, from which they inferred a production rate CO\(_2\)/H\(_2\)O ratio of 2.2–5.6 per cent. Hansen et al. (2016) used ROSINA data to determine average gas mass losses of 83 per cent for H\(_2\)O and 10 per cent for CO\(_2\), corresponding to CO\(_2\)/H\(_2\)O = 12 per cent by mass, or CO\(_2\)/H\(_2\)O = 4.9 per cent by number. Based on these measurements, we first applied a nucleus CO\(_2\)/H\(_2\)O = 5.5 per cent molar ratio.

Figure 4 (left) shows one model for which CO\(_2\) was present up to the very surface on the southern hemisphere at May 2012 aphelion. If that is the case, the CO\(_2\) sublimation front only has time to withdraw to a depth of at most 0.84 m by the time Rosetta made its first observations in Aug 2014. That results in a CO\(_2\) production rate that is too high. The CO\(_2\) sublimation front must therefore be located deeper at the onset of simulations. Initial tests showed that \(d_{\text{CO}_2} = 0.94\) m in the south resulted in a CO\(_2\) production rate that was about right in August 2014 (Fig. 4, left).

When that model was propagated all the way to perihelion (blue curve in Fig. 4, right) it tended to overshoot the observed production for a large fraction of the inbound orbit. It was therefore clear that the contribution from the southern hemisphere had to be smaller, in order to avoid the overshoot, and that some CO\(_2\) production from the north might be necessary, to still fit the large–distance data. We first increased the initial front depth in the south gradually, to \(d_{\text{CO}_2} = 1.94\) m, which produced a curve that followed the lower part of the data cloud at \(r_h \geq 2\) au reasonably well (red curve in Fig. 4, right).

At this point we also tested the sensitivity of the total CO\(_2\) production rate to the assumed nucleus CO\(_2\)/H\(_2\)O ratio. If a substantial fraction of cometary ices are presolar (as suggested by the presence of S\(_2\) and by the xenon isotope composition; Calmonte et al. 2016; Marty et al. 2017) the cometary CO\(_2\) composition may be close to that of protostars. Massive protostars have molar CO\(_2\) abundances relative H\(_2\)O of 10–23 per cent (Gerakines et al. 1999), while low–mass protostars have 32 ± 2 per cent (Pontoppidan et al. 2008). We here apply 32 per cent.

The dependence on the intrinsic abundance was rather weak at large heliocentric distance (see red and green curves in Fig. 4, right). Even when applying almost a sixfold increase in abundance from 5.5 per cent CO\(_2\) to 32 per cent CO\(_2\) relative to water, the resulting increase of the CO\(_2\) production rate was merely a factor ~ 1.5 at \(r_h \geq 1.7\) au, substantially smaller than the scatter of the data. Observations of the CO\(_2\)/H\(_2\)O production rate ratio at large heliocentric distances therefore does not offer meaningful clues on the nucleus CO\(_2\) abundance. However, because of substantial water–driven erosion near the south pole, the CO\(_2\) fronts were locally brought very close to the surface. Near perihelion (within \(r_h \leq 1.4\) au) the CO\(_2\) sublimation front depths stabilised because their propagation speeds matched that of nucleus erosion. This happened at ~ 0.45 m depth when the abundance was 5.5 per cent, but at ~ 0.15 m for 32 per cent abundance. At this point, the high–abundance model produced at most ~ 5 times more CO\(_2\) vapour than the low–abundance model, somewhat short of the factor 5.8 intrinsic abundance difference. There are two likely contributing factors for this discrepancy: 1) downward diffusion and recondensation of vapour below the front during approach to the Sun has altered the CO\(_2\) abundance of the sublimation front at perihelion with respect to that of the deep interior; 2) there are smaller contributions from mid–southern latitudes that still are approaching steady state.

The low–abundance model provided 2.6 · 10\(^{-26}\) molec s\(^{-1}\) just before perihelion (briefly spiking to 4 · 10\(^{-26}\) molec s\(^{-1}\)), while the high–abundance model produced 1.4 · 10\(^{-27}\) molec s\(^{-1}\). The measured rates (within 0.1 au prior to perihelion) had a range 7.9 · 10\(^{-25}\)–1.3 · 10\(^{-27}\) molec s\(^{-1}\) (average 4.8 · 10\(^{-26}\) molec s\(^{-1}\)) before perihelion. However, the CO\(_2\) production peaked shortly after perihelion, with a range 6.4 · 10\(^{-26}\)–6.0 · 10\(^{-27}\) molec s\(^{-1}\), and an average of 2.1 · 10\(^{-27}\) molec s\(^{-1}\). Because the 5.5 per cent–model would not be able to reach the observed range right after perihelion, we consider the 32 per cent–model more representative of the nucleus behaviour. Note, that it would not be possible to obtain a significantly higher CO\(_2\) production rate at perihelion simply by reducing the initial front depth at aphelion. Such a model would stabilise at a similar ~ 0.45 m steady–state depth near perihelion, and provide similar amounts of CO\(_2\) vapour. We therefore think that a nucleus molar CO\(_2\)/H\(_2\)O abundance ratio of ~ 0.3 is a necessity to explain the observed data.

Although the high–abundance model performed well at perihelion, it still grossly under–estimated the production at larger distances. We therefore introduced CO\(_2\) with \(d_{\text{CO}_2} = 1.94\) m on the northern hemisphere as well (as 32 per cent abundance), but as seen in Fig. 4 (right), the resulting production rate (black curve) was too high.

We therefore tested a number of initial depths \(d_{\text{CO}_2} > 1.94\) m for the aphelion CO\(_2\) sublimation front depths in the north. We did this for a nucleus CO\(_2\) abundance of 11 per cent relative H\(_2\)O by number in the north (roughly half–ways between the two extreme values tested previously, remembering that the production rate of CO\(_2\) does not depend strongly on the absolute abundance at large distances). We always applied 32 per cent in the south. We found, that the combined contribution from the south (with \(d_{\text{CO}_2} = 1.94\) m) and the north (with \(d_{\text{CO}_2} = 3.02 \leq d_{\text{CO}_2} \leq 3.77\) m) matched the full width of the observed CO\(_2\) production in August 2014 (\(r_h \approx 3.6\) au). We propagated a model with \(d_{\text{CO}_2} = 3.77\) m in the north and \(d_{\text{CO}_2} = 1.94\) m in the south to perihelion, as shown in Fig. 5 as solid curves.

This model achieves a decent simultaneous reproduction of the pre–perihelion H\(_2\)O and CO\(_2\) production rate measurements. It is possible that further adjustments of the aphelion CO\(_2\) ice depths latitude–by–latitude would make the CO\(_2\) curve follow the centre of the data cloud more closely. However, because the reason for the nearly one order of magnitude scatter in the measured data is unknown, it is not certain that such a solution provides physically real information about the target. It is also possible that clean CO\(_2\) ice is not the sole contributor of CO\(_2\) vapour – a portion may originate from occluded CO\(_2\) within crystallising amorphous water ice. An
additional source of CO$_2$ might be needed to better match the rather high production rate beyond 2.5 au pre–perihelion. For the time being, we settle for the model in Fig. 5 as an acceptable solution, but we may return to a more thorough investigation in a future publication.

The NIMBUS simulations are performed for a spherical model nucleus. Although it has the same surface area as the real irregular nucleus, it is possible that systematic differences in solar–exposed surface area and shape differences causes production rate deviations. To investigate the severity of this problem, we considered an irreg-

Figure 4. Left: Pre–perihelion CO$_2$ production rates (until August 2014) resulting from having CO$_2$ ice exclusively on the southern hemisphere, but at different initial depths $d_{\text{CO}_2}$. Both models have $\{ L, r_p \} = \{ 100, 10 \}$ km, $\mu_S = 2$ in the north, and CO$_2$ relative to water by number. Right: Pre–perihelion CO$_2$ production rates (up to the August 2015 perihelion for models, but somewhat beyond for measurements to show that the CO$_2$ production peaked post–perihelion) for different initial depths, and intrinsic nucleus CO$_2$ abundances (relative H$_2$O by number). The model shown as a black curve has CO$_2$ on both hemispheres, the others only have CO$_2$ in the south. The vertical line marks the inbound equinox.

Figure 5. NIMBUS models of the pre–perihelion H$_2$O and CO$_2$ production rates for spherical and 67P/C–G-shaped model nuclei. The models have $\{ L, r_p \} = \{ 100, 10 \}$ km, $\mu_S = 2$ in the north, and $\mu_S = 1$ in the south. The initial aphelion CO$_2$ sublimation front depth was $d_{\text{CO}_2} = 3.77$ m in the north (11 per cent CO$_2$) and $d_{\text{CO}_2} = 1.94$ m in the south (32 per cent CO$_2$). The spikes in the CO$_2$ production are formed when frost accumulating at shallow depths in cold conditions are released suddenly during illumination. The vertical line marks the inbound equinox.

ular shape model obtained by degrading the $3.1 \cdot 10^6$ facet SHAP5 version 1.5 shape model (Jorda et al. 2016) to $5 \cdot 10^3$ facets. The irregular model nucleus was advanced in $10^2$ rotational angle increments from 3.6 au pre–perihelion to perihelion. For each facet, the co–declination (angle between the positive spin vector and the facet outward surface normal) and the solar incidence angle were calculated, and the closest available proxy on the spherical model was identified. This procedure accounted for the varying spin rate of the comet, i. e., the solar incidence angle is in–phase with the real nucleus. We used spin periods reported by Keller et al. (2015a) and by H. U. Keller (private communication). Because the facet and the proxy have identical illumination histories (apart from potential temporary shadowing taking place at earlier rotational phases), their instantaneous production rates ought to be similar. We apply those production rates locally, adjusted for the actual facet surface area. However, we then apply the model of Davidson & Rickman (2014) to identify the facets that are shadowed by nucleus topography at any given rotational phase. For shadowed facets we re–set their surface temperatures and water production rates to the lowest values encountered on the nightside for that co–declination. The CO$_2$ production rate is maintained during temporary dayside shadowing, because the CO$_2$ sublimation front is located at a depth that is rather insensitive to diurnal temperature variations. However, the applied speed of CO$_2$ molecules when entering the coma reflects the fact that they need to diffuse through a cold surface region.

The error in the H$_2$O production rate introduced by the mapping technique is small. At shadowing onset, the real H$_2$O production drops gradually, while the mapping leads to an abrupt reduction to night–time production levels. Observations of jets show that it takes ~ 1 h for the water activity to diminish to a level where it no longer can sustain a detectable dust production. Thus, the model temporarily has a deficit corresponding to $1 / \dot{P}_{\text{tot}}$ or roughly 8 per cent of the daily water production. However, when the region exits from shadow, the mapping causes an immediate return to full activity, while the real nucleus re–activates gradually. That creates a temporary over–production for the modelled nucleus that partially or fully compensates for the previous deficit. Because we consider
diurnally-averaged production rates, we expect the calculated rate to be off by $\ll$ 8 per cent because of the mapping (compared to a model that would accurately consider the activity changes during shadowing).

For CO$_2$ the situation is different, because it is located at a depth where diurnal temperature variations are damped out (as mentioned previously, CO$_2$ is continuously active). An error is introduced by the mapping technique because the integrated daily energy absorption is too high when shadows are not accounted for. The severity of this problem can be estimated from the total amount of energy absorbed during an orbit at different locations calculated by Sierks et al. (2015). The frequently shadowed Hapi valley receives $\sim 5.5 \cdot 10^9$ J m$^{-2}$ orbit$^{-1}$, which is $\sim 35$ per cent lower than regions with similar co-declination that are not being shadowed. However, this only affects an estimated 1/5 of the northern hemisphere. The estimated CO$_2$ production is therefore $\lesssim 7$ per cent too high, also considering that all the excess energy does not necessarily go to CO$_2$ production. This is small compared to the factor 2–3 spread in the measured data.

We average the total nucleus production over one nucleus rotation, and plot the production rates in Fig. 5 as dashed–dotted curves. At the resolution of the figure, the two sets of curves are barely distinguishable. The largest differences are found near the May 11, 2015 equinox (at $r_h = 1.67$ au), where the production rate of the irregular model nucleus is somewhat below that of the spherical model. That is because the irregular nucleus has the smallest cross section when viewed from within the equatorial plane of the comet. However, the difference is small in comparison to the scatter of the measurements. Therefore, we do not find that the nucleus shape has a measurable influence on the production rates for 67P/C–G. The same conclusion was drawn by Marshall et al. (2019).

4.2 The post–perihelion branch

During the perihelion passage, most of the northern hemisphere has polar night. Solid material emanating from the south rains down in the north as airfall. Davidsson et al. (2021) estimated the average thickness of the airfall layer added to the north as 0.87 m. They found that cm-sized chunks would retain 44 per cent of its original water ice abundance during a 12 h coma transfer, and that dm-sized chunk would retain 94 per cent of its ice. With the average size of returning coma chunks being $\sim 1$ cm (see Table 2), and the intrinsic water abundance in the southern hemisphere found to be $\mu_S \approx 1$, it is reasonable that the airfall material has $\mu \approx 2$. We therefore take the most successful pre–perihelion model, add a 0.87 m layer on the northern hemisphere, and assume it has $\mu_N = 2$, $\{L, r_p\} = \{100, 10\}$ $\mu$m, $\xi = 1$, and a bulk porosity of 70 per cent (including the previously applied 40 per cent macro porosity plus an assumed micro porosity within chunks). We assigned an initial temperature of $T = 150$ K to the airfall material. It would have had $T \approx 200$ K when exposed to the Sun in the coma (Davidsson et al. 2021) but could have cooled for hours once entering the shadow of the nucleus before landing. The near–surface temperature of the nucleus in polar–night regions is typically 70–100 K at perihelion (Davidsson et al. 2021). The nucleus erosion rate was updated for outbound conditions according to equation 16.

The result of this model is seen in Fig. 6. Interestingly, this model fails to reproduce the data for both species. The water production is well–reproduced within 1.8 au, but then the model drops below the data. By the time the outbound equinox is reached on March 21, 2016 at $r_h = 2.6$ au, the modelled H$_2$O production is an order of magnitude too small. The observed CO$_2$ production rate falls by more than an order of magnitude between perihelion and the outbound equinox, while the modelled curve is less steep. There are a few unusually high CO$_2$ measurements near equinox that almost reach the model curve, but the bulk of the data is clearly lower. The discrepancy is a factor $\sim 3$ near equinox, i.e., less severe than that for water.

To investigate the importance of the added airfall layer (admittedly having uncertain thickness and initial temperature) we also propagated the best pre–perihelion model without any airfall layer. That model had H$_2$O and CO$_2$ production rate curves that were very similar to Fig. 6. This can be understood as follows. First of all, most water originates from the south, which is not affected by airfall. However, the north becomes increasingly exposed with time post–perihelion, yet there was no significant deviation in production rate between the models. The main factor influencing the near–perihelion water production rate is the thickness of the dust mantle. That thickness is determined by the $\mu$–value (determining how rapidly the water sublimation front is withdrawing) and the erosion rate (determining how quickly the surface is ‘catching up’ with the moving water sublimation front). With the imposed erosion rates being identical in the two models, and the $\mu$–value being the same, the two models will only differ because they had different initial temperatures at perihelion (150 K for the airfall model and 70–100 K for the other model) and different types of stratification (no dust mantle assumed for the airfall layer, versus a thin dust mantle established pre–perihelion for the other model). Apparently, these differences were equilibrated so rapidly once the airfall material is exposed to sunlight, that they play no practical role. A thin dust mantle is established so rapidly, and the temperature gradient over the near–surface region reaches a repetitive oscillatory behaviour during nucleus rotation so quickly, that the nucleus behaves similarly with or without airfall, as far as water production is concerned. Regarding CO$_2$, the addition of airfall material quenches the contribution from the north (the CO$_2$ mass flux to the surface is reduced by the fact that the CO$_2$ ice suddenly is 0.87 m deeper below the surface than before). However, the vast majority of the CO$_2$ originates from the south, which is unaffected by airfall. Therefore, the quenching of the northern contribution barely affects the total CO$_2$ production.

We proceed to investigate what parameter changes, if any, that
would lead to reproduction of the data. First, we focus on the water production. Our previous experience was that the near-perihelion production rate is sensitive to the water abundance (i.e., the dust/water–ice mass ratio) but that distant production is more sensitive to diffusivity. We therefore postulate that fresh airfall material is capable of solving the problem. A possible mechanism (e.g., Brownlee et al. 2006). However, straight tubes (tortuosity \( \xi = 1 \)) are not particularly realistic either. Therefore, diffusivity was lowered further by considering curvy tubes, with a length being a factor \( \xi \) larger than the vertical distance travelled by flowing through the tube (this is the very definition of tortuosity). Figure 8 shows that an additional factor 25 reduction of the diffusivity does not lower the production rate further. We conclude that \( \{L, r_p\} = (10, 1) \mu m\) and \( \xi \geq 1 \) is necessary for the \textsc{nimbus} curve to touch the upper part of the main data cloud near equinox.

We consider this solution a reasonable reproduction of the CO\(_2\) production rate post–perihelion. For the southern hemisphere we envision a (quasi–primordial) material with \( \mu_S = 1 \), a top layer with \( \{L, r_p\} = (100, 10) \mu m\) (applied for the water production), and a moving CO\(_2\) sublimation front that transits from a region with \( \{L, r_p\} = (100, 10) \mu m\) and \( \xi = 1 \) to one with \( \{L, r_p\} = (10, 1) \mu m\) and \( \xi = 5 \) around \( r_h = 1.4 \) au. For the northern hemisphere we envision the near–perihelion addition of a 0.87 m airfall layer that has \( \{L, r_p\} = (10, 1) \) cm. For CO\(_2\) we applied the same diffusivity as for the southern hemisphere for technical reasons, but the contribution to the total CO\(_2\) production from the north is small (< 5 per cent) and the exact diffusivity value matters little. Figure 9 shows the post–perihelion H\(_2\)O and CO\(_2\) production rate obtained simultaneously by applying these conditions. Best–fit parameters are summarised in Table 4.

### 4.3 Erosion, front depths, and temperatures

We here summarise some aspects of the best available pre– and post–perihelion simulations in terms of erosion, dust mantle thickness, peak daily surface temperature, depth and temperature of the CO\(_2\) sublimation front, as functions of latitude and time.

Pre–perihelion, the southern hemisphere provides 93.4 per cent of the H\(_2\)O and 90.4 per cent of the CO\(_2\). Post–perihelion, the southern hemisphere provides 64.0 per cent of the H\(_2\)O and 96.8 per cent of the CO\(_2\).

Figure 10 shows the amount of erosion taking place up to, and beyond, the perihelion passage. We emphasise that this erosion results from an enforced dust production rate used as input to \textsc{nimbus}.
The northern hemisphere (covered by a freshly deposited 0.87 m layer of H$_2$O–rich material) has $\{L, r_p\} = (10, 1)$ cm, $\xi = 1$, and $\mu_N = 2$. The northern CO$_2$, here located 4–5 m underground has $\{L, r_p\} = (100, 10)$ µm, $\xi = 1$, and abundance 11 per cent relative to water. The southern hemisphere has $\{L, r_p\} = (100, 10)$ µm and $\xi = 1$ at $r_p < 1.4$ au, but at $r_p > 1.4$ au the CO$_2$ (at 32 per cent abundance) moves into a region with $\{L, r_p\} = (10, 1)$ µm and $\xi = 5$ (hence the sudden drop and slow recovery to higher production rates). In the south, the water with $\mu_S = 1$ still diffuses through a $\{L, r_p\} = (100, 10)$ µm and $\xi = 1$ region near the surface.

Figure 9. NIMBUS model of the post–perihelion H$_2$O and CO$_2$ production rates. The northern hemisphere (covered by a freshly deposited 0.87 m layer of H$_2$O–rich material) has $\{L, r_p\} = (10, 1)$ cm, $\xi = 1$, and $\mu_N = 2$. The northern CO$_2$, here located 4–5 m underground has $\{L, r_p\} = (100, 10)$ µm, $\xi = 1$, and abundance 11 per cent relative to water. The southern hemisphere has $\{L, r_p\} = (100, 10)$ µm and $\xi = 1$ at $r_p < 1.4$ au, but at $r_p > 1.4$ au the CO$_2$ (at 32 per cent abundance) moves into a region with $\{L, r_p\} = (10, 1)$ µm and $\xi = 5$ (hence the sudden drop and slow recovery to higher production rates). In the south, the water with $\mu_S = 1$ still diffuses through a $\{L, r_p\} = (100, 10)$ µm and $\xi = 1$ region near the surface.

Figure 10. The accumulated level of surface erosion resulting from the enforced dust production described in Section 3.2, as function of time near perihelion, for selected latitudes on the northern and southern hemispheres. For reference, $\{0, 50, 100, 150, 200\}$ days from perihelion corresponds to heliocentric distances of $\{1.24, 1.38, 1.71, 2.09, 2.47\}$ au.

The amount of erosion varies substantially with latitude, illustrating the long–term effects of varying illumination conditions at different parts of the nucleus, combined with temporal variations in the total dust production rate. The northern hemisphere has an area–averaged erosion of 0.10 m, being as small as 0.04 m at mid–northern latitudes, and peaking with 0.63 m at the north pole.

Between aphelion and ~ 100 days pre–perihelion, the Sun is circum–polar as seen from latitudes above ~ 50° N (see Fig. 2 in Keller et al. 2015b). The continuous heating at such latitudes causes the larger degree of erosion seen in the far north. The modest level of erosion in the north (< 1 m) is consistent with the lack of observed wide–spread erosion in OSIRIS images (being under the resolution limit), except for small isolated patches where erosion rose above detection level and typically reached ~ 1 m (Hu et al. 2017). Taken at face value, these numbers mean that the airfall layer thickness increases every apparition. The southern hemisphere has an area–averaged erosion of 1.2 m, peaking at the south pole with 6.6 m. This is more substantial, but still below the estimated maximum possible level of erosion, that is ~ 10 m according to Keller et al. (2015b).

We now turn to the output features of the models, which result from combining the enforced dust mantle erosion rate with the usage of the best–fit parameters (found in Secs. 4.1–4.2), applied to the energy and mass conservation equations of NIMBUS, selected for their capability of reproducing the observed H$_2$O and CO$_2$ production rates. Figure 11 (upper left) shows the thickness of the dust mantle. The southern hemisphere, which is facing the Sun near perihelion, is covered by a mantle that typically is 1–2 cm thick. The presence of water ice to within millimetres or centimetres of the surface is supported by the switch–off of jets 1–2 h after rotating into darkness (Shi et al. 2016). Note that such a dust mantle is maintained despite the 1.2 m average erosion mentioned before: water ice cannot, and will not, remain at the surface under these conditions. If the erosion makes the mantle too thin, the nucleus (through the energy and mass conservation equations solved by NIMBUS) will adjust its water production rate until the H$_2$O sublimation front has withdrawn to the depth where the energy consumption due to net sublimation balances the energy supply from above, and losses to the interior. Similar dust mantle thicknesses (i. e., ≤ 2 cm) are seen on the northern hemisphere pre–perihelion. At perihelion, a 0.87 m thick airfall layer is added to the northern hemisphere. Most of the northern hemisphere has polar night, thus the water ice is inactive. As a result, water ice in the airfall material remains on the very surface and there is no dust mantle. However, near the equator the airfall material is illuminated and the water ice is sublimating. The reason for this rapid thickening at latitude 5° N can be understood as follows. The airfall material has channels in the centimetre–decimetre class, thus the diffusivity is very large. Therefore, water vapour can enter the coma rather effortlessly, which means that the water sublimation front moves rapidly. Consequently, the dust mantle thickness grows quickly.

Table 4. Best–fit parameters obtained for Comet 67P/Churyumov–Gerasimenko, before (pre) and after (post) perihelion on the northern (N) and southern (S) hemispheres.

| Quantity          | Pre (N) | Pre (S) | Post (N) | Post (S) |
|-------------------|---------|---------|----------|----------|
| $\mu$            | 2       | 1       | 2        | 1        |
| CO$_2$ abundance  | 11 per cent | 32 per cent | 11 per cent | 32 per cent |
| $L$              | 100 µm  | 100 µm  | 10 cm (H$_2$O) | 100 µm (H$_2$O) |
| $r_p$            | 10 µm   | 10 µm   | 1 cm (H$_2$O)  | 10 µm (H$_2$O)  |
| $\xi$            | 1       | 1       | 1        | 1        |
| CO$_2$ depth     | 3.8 m   | 1.9 m   | –        | –        |
The daily peak surface temperature is seen in the top right panel of Fig. 11. The dust mantle in the south reaches temperatures that are substantially higher (300–340 K) than the characteristic temperature of water sublimation (~ 200 K). Such dust mantle temperatures are typical for comets near perihelion according to in situ measurements (e.g., Soderblom et al. 2002; Groussin et al. 2007). Because of polar–night conditions on the northern hemisphere, the near–perihelion temperatures are below 100 K at the north pole. Note the near–perihelion temperature spike at northern latitudes: that marks the deposition of 150 K airfall originating from the southern hemisphere.

The depth of the CO$_2$ sublimation front is seen in the lower left panel of Fig. 11. The initial depth on the northern hemisphere at aphelion was 3.77 m. At the north pole, the CO$_2$ is brought to within ~ 3 m of the surface, primarily because of a rather substantial water–driven erosion. The effect is seen at near–equatorial regions in the north as well, but less strong. The sudden jump in depth of northern–hemisphere CO$_2$–front depths to 4–5 m at perihelion is because of the addition of the airfall layer. The north pole has a peculiar behaviour post–perihelion: the CO$_2$ sublimation front rapidly reaches the surface. This is because vapour, originating from the original front, diffuses upward to the surface where it condenses because of the extremely low post–perihelion temperature (see the upper right panel of Fig. 11). This CO$_2$ frost formation is prevented at, e.g., 45° N, where the surface temperature is warmer.

On the southern hemisphere, the CO$_2$ sublimation front starts at a depth of 1.94 m at aphelion. There is a net reduction of this depth that is rather modest north of 45° S, because of water–driven erosion. However, at the south pole the erosion is so strong that the CO$_2$ is brought to within decimetres of the surface near perihelion. Note that erosion removes several metres worth of material (Fig. 10), substantially more than the original depth of the CO$_2$ sublimation front. The fact that the CO$_2$ ice does not become exposed means that it finds a balance, a few decimetres below the surface, where the propagation speed of the CO$_2$ sublimation front matches the erosion speed of the mantle. VIRTIS observed exposed CO$_2$ ice in an 80 x 60 m patch in the Anhur region in March 2015 (Filacchione et al. 2016). That is somewhat early (~ 145 days pre–perihelion) and too far from the pole (~ 55° S) to be readily explained by the current simulations. However, the retrieved abundance (< 0.1 per cent CO$_2$ ice, Filacchione et al. 2016) is too low to be consistent with a locally and temporarily exposed CO$_2$ sublimation front. It is
of diffusivity is clearly seen on the southern hemisphere in Fig. 11. The effective and the necessary diffusion velocity. When gradients are set up around the front. When the diffusivity is low, requires that sufficiently strong temperature and saturation pressure the sublimation front, to give room to new vapour. Efficient diffusion the available heat flux provided by solid-state conduction. In order to have net sublimation, pre-existing vapour has to diffuse away from the sublimation front, to give room to new vapour. Efficient diffusion requires that sufficiently strong temperature and saturation pressure gradients are set up around the front. When the diffusivity is low, the front temperature may have to climb high in order to reach the necessary diffusion velocity. When \( L, r_p = (100, 10) \), \( \xi = 1 \), and the CO\(_2\) sublimation front is located meters under the surface, the effective CO\(_2\) sublimation temperature is pushed into the \( 110 \leq T \leq 130 \) K range. Similar temperatures for sub–surface sublimation of CO\(_2\) were obtained by Skorov & Blum (2012). The importance of diffusivity is clearly seen on the southern hemisphere in Fig. 11 (lower right) 50 days post-perihelion \( (r_p \geq 1.4 \) au). At that point, the diffusivity is reduced strongly by setting \( L, r_p = (10, 1) \), \( \xi = 5 \). Additionally, the front is located very closely to the warm surface. In such conditions, the temperature at the CO\(_2\) sublimation front is elevated to 165 K in order to allow for the same mass flux and net energy consumption as before.

4.4 Forces acting on the nucleus

The modelling in Secs. 4.1–4.2 provides local outgassing rates \( Z_{i,j} \) and surface temperatures \( T_i \) necessary to evaluate the resultant non–gravitational force acting on the model nucleus according to equation 1. We remind that the force evaluation applies the mapping from the spherical to the irregular nucleus shape model, including the rudimentary treatment of temporary daytime shadowing, as described in Section 4.1. Also, note that the force evaluation accounts for the changes to the spin period throughout the perihelion passage, so that the nucleus has the appropriate rotational phase at any given moment.

We decompose the force vector into its radial, transverse, and normal components \( \mathbf{F} = \{ F_r, F_t, F_n \} \) (i.e., \( F_r \) is along the unit radius vector \( \hat{r}, F_n \) along the angular momentum unit vector of the orbit \( \hat{h} \), and \( F_t \) along the vector \( \hat{h} \times \hat{r} \)). The force components \( F_r, F_t \), and \( F_n \) are plotted in Fig. 12.

For water, the radial component is strongest, as expected (the highest comet outgassing rate takes place near the sun–solar point, causing a reaction force in the opposite direction, that roughly aligns with the radius vector). Yet, the transverse and normal components reach \( \sim 1/3 \) of the radial component magnitude near perihelion. The irregular nucleus shape, in combination with a latitude–dependent activity level, and thermal lag effects caused by the finite conduction timescale of heat to sub–surface ice deposits, evidently causes some significant deviations from perfectly radial alignment of the force vector. All components have a pronounced perihelion–asymmetry, which is a consequence of a stronger outgassing post–perihelion (see equation 16). The width of the curves shows the level of diurnal variations of the force components. Figure 13 shows this more clearly by exemplifying a close–up of the force components due to water outgassing during a couple of days just prior to the perihelion passage, to illustrate their temporal behaviour on the timescale of a nucleus rotation. We emphasise that these variations are primarily caused by changes to the illuminated nucleus cross–section, and secondarily, due to associated differences in the topography that is being illuminated.

Figure 12 also shows the radial, transverse, and normal force components caused by CO\(_2\) outgassing. They are much smaller than those caused by water, for two reasons. Firstly, the CO\(_2\) outgassing rate is an order of magnitude smaller than that of water (see Figs. 5 and 9). Secondly, the CO\(_2\) sublimation front is located at a depth far below the diurnal skin depth, so that day/night differences in the outgassing rate becomes very small. Consequently, the CO\(_2\) outgassing reaction force has similar strength in all directions within the orbital plane, thus cancellation effects are strong.

The sum of the H\(_2\)O and CO\(_2\) force components can be used to calculate the non–gravitational changes of the orbit caused by the comet outgassing. This allows us to further calibrate our model to ensure it complies with measured data, as well as possible. The change in the orbital period is

\[
\Delta \mathcal{P} = H \frac{6\pi \sqrt{1 - e^2}}{M n^2} \left( \frac{e}{q (1 + e)} \int_0^\rho F_r \, dt + \int_0^{\rho} F_t \, \frac{dt}{r_h} \right),
\]

Figure 12. The radial, transverse, and normal force components due to H\(_2\)O and CO\(_2\) outgassing, as functions of time during 300 days surrounding perihelion (using \( \eta = 0.31 \)). Note that force ranges of the three panels are identical, so that the magnitudes of \( \{ F_r, F_t, F_n \} \) can be readily compared. The width of the curves shows the level of diurnal variation of the force magnitude, primarily due to changing cross–section of the irregular nucleus during rotation. The ‘block–like’ structure of the curves is due to the fact that \( \text{Nimbus OUT} \) is output provided every 12th rotation, and then applied for the following eleven revolutions. However, the calculation properly accounts for changes to the spin period also within such blocks. Small jumps in the production rate take place under certain conditions when H\(_2\)O frost formed in the dust mantle (or CO\(_2\) frost in the H\(_2\)O+dust layer) is released vigorously at sunrise.

\[\text{\cite{Yamamoto}}\]
the change in the longitude of perihelion is
\[
\Delta \sigma = -\Delta \Omega \cos \iota + \frac{\sqrt{q(1+e)}H}{Mk_G \epsilon} \left( \int_0^P F_i \left( 1 - \frac{q(1+e)}{r_h} \right) \sin \nu \, dt \right) + \int_0^P F_i \left( 1 + \frac{r_h}{q(1+e)} \right) \sin \nu \, dt,
\]
and the change in the longitude of the ascending node is
\[
\Delta \Omega = \frac{H}{Mk_G \sqrt{q(1+e)} \sin \iota} \int_0^P F_i r_h \sin(\omega + \nu) \, dt,
\]
see, e.g., Sekanina (1993). In these equations, \( M = 9.982 \cdot 10^{12} \) kg is the 67P/C–G nucleus mass (Pätzold et al. 2016), \( e \) is the eccentricity, \( n \) (day\(^{-1}\)) is the mean motion, \( \nu \) is the true anomaly, \( q \) (au) is the heliocentric distance, \( P = (q/(1-e))^{3/2} \) (yr) is the orbital period (recalculated to days), \( \iota \) is the inclination, \( \omega \) is the argument of perihelion, \( k_G \) is the Gaussian gravitational constant, and \( H = 0.049900175 \) au\(^2\) m\(^{-1}\) day\(^{-2}\) allows for the usage of SI units for \( M \) and \( F \), while remaining quantities have Gaussian units. According to several pre–Rosetta orbit determinations discussed by Davidsson & Gutiérrez (2005) the empirical values for 67P/C–G are \( \Delta P = 20 \pm 4 \) min, \( \Delta \sigma = -1.4 \pm 0.6'' \), and \( \Delta \Omega = 1.0 \pm 1.0'' \). As indicated by the error bars, the \( \Delta P \)–value is the most reliable, while the \( \Delta \sigma \)–value is the least reliable.

We find, that reproduction of the empirical \( \Delta P \) requires that our model force (equation 1) is evaluated for \( \eta = 0.31 \pm 0.06 \). This is somewhat below the typically considered interval (0.4 \( \leq \eta \leq 1 \), see Section 2). We discuss possible reasons and implications of this in Section 5. About 36 per cent of the net change in \( \Delta P \) (or 7.2 min) is established pre–perihelion, whereas the remaining 64 per cent (or 12.8 min) of the change happens post–perihelion. When applying \( \eta = 0.31 \) we also find \( \Delta \sigma = -1.4'' \) and \( \Delta \Omega = 0.58'' \). Both parameters are consistent with the empirical counterparts. We find it reassuring that our force model simultaneously reproduces all three of \( \{ \Delta P, \Delta \sigma, \Delta \Omega \} \) for a low but reasonable momentum transfer coefficient.

If the CO\(_2\) contribution is removed when evaluating equation (25) we find that \( \Delta P \) is reduced by merely 0.3 per cent (much below the empirical \( \pm 20 \) per cent uncertainty). It therefore seems like CO\(_2\) has a completely negligible non–gravitational effect on the orbit, at least for Comet 67P/C–G.

If comet outgassing is symmetric about perihelion, the contribution from the radial force component in equation (25) becomes zero when integrated over time, so that a non–zero \( \Delta P \) is entirely caused by the transverse component (see e.g., Rickman et al. 1991). Because comet 67P/C–G has asymmetric outgassing, it is therefore interesting to understand the relative importance of the radial and transverse force components. Evaluating equation (25) without the transverse force yields \( \Delta P = 6.4 \) min, showing that the radial component is responsible for \( \approx 32 \) per cent of the total change of the orbital period. Pre–perihelion, the radial component strives to reduce \( P \) by 4.1 min. Post–perihelion, the radial component instead increases \( P \) by 10.5 min, resulting in the net change \( \Delta P = 6.4 \) min mentioned above. This directly shows that the asymmetric outgassing removes the complete cancellation effect. The transverse component here systematically aims at increasing \( \Delta P \). Interestingly, the pre–perihelion transverse contribution to the change (+11.2 min) is significantly larger than the post–perihelion one (+2.4 min). A glance at the middle panel of Fig. 12, and at the second integral in equation (25), shows the reason for this behaviour. Pre–perihelion, \( F_i \) is larger and systematically positive, while post–perihelion, \( F_i \) is smaller and briefly goes negative during nucleus rotation.

Figure 14 shows the \textit{Nimbus} total non–gravitational force due to both H\(_2\)O and CO\(_2\) in the equatorial J2000 frame. This forward–modelling ‘first–principles’ force is compared with two different empirical solutions: (1) the force derived by Kramer & Läuter (2019) from piece–wise orbital solutions for 67P/C–G provided by the Rosetta flight dynamics team at ESOC; (2) the force according to the ‘Rotating Jet Model’ (Chesley & Yeomans 2005), used by Farnocchia et al. (2021) to reconstruct the 67P/C–G trajectory from Rosetta tracking data and March 2014 to June 2018 high–precision optical astrometry from the Very Large Telescope, Pan–STARRS1, and the Catalina Sky Survey. We refer to those as K&L and RJM, respec-
tively, in the following. Note that K&L and RJM provide acceleration, here re–calculated to force by multiplying with the nucleus mass $M = 9.982 \cdot 10^{12}$ kg (Pätzold et al. 2016) in order to be directly comparable to NIMBUS results. We first note that the RJM solution implies $\Delta P = 24.9$ min, $\Delta \tau = -1.6''$, and $\Delta \Omega = 2.6''$. The $\Delta P$ value is somewhat higher than, but still consistent with, the pre–Rosetta estimate $\Delta P = 20 \pm 4$ min, which would suggest a slight increase of our momentum transfer coefficient from $\eta = 0.31 \pm 0.06$ to $\eta = 0.39$ (which would shift the changes of the perihelion and ascending node longitudes to $\Delta \tau = -1.8''$ and $\Delta \Omega = 0.73''$). The change in the longitude of perihelion is identical to pre–Rosetta values ($\Delta \tau = -1.4 \pm 0.6''$) within error bars, while the change in the longitude of the ascending node is larger (pre–Rosetta $\Delta \Omega = 1.0 \pm 0.4''$). We used $\eta = 0.39$ when plotting the NIMBUS force in Fig. 14.

We note that the three solutions all differ with respect to each other. The NIMBUS $X$– and $Y$–components are similar to RJM pre–perihelion, while their post–perihelion behaviours follows more closely those of K&L. The NIMBUS $Z$–component falls somewhat short of both RJM and K&L. Preliminary tests indicate that a latitude–dependent $\eta$–value might be sufficient to nudge the NIMBUS curves towards either K&L or RJM. A thorough investigation of the mutual discrepancies between NIMBUS, RJM, and K&L is out of scope in the current paper. We intend to return to this issue when analysing the effect of NIMBUS–derived torques on the spin state.

5 DISCUSSION

We start by discussing the outcome of our investigation of extended sources (Section 3.1) and dust erosion (Section 3.2). According to the ratio between equations (3) and (16) shown in the upper panel of Fig. 1, the nucleus contribution to the total water outgassing is $0.92 \leq Q_{\text{nuc}}/Q_{H_2O} \leq 1$. It means that the extended source of water from ice–rich chunks in the coma is at most 9 per cent at perihelion. Biver et al. (2019) used MIRO observations of the inner 20 km of the coma to search for evidence of an extended water source. According to their analysis, an extended source contributes less than 15 per cent of the water near perihelion. We therefore think that our analysis in Section 3.1 is realistic, and that our decision to compare NIMBUS water production calculations directly with the observed $Q_{H_2O}$ is justified.

The erosion rate of the nucleus $E$ is expressed in units of $Q_{H_2O}$ by the function $G(t)$. In order to evaluate $G(t)$ we needed the total sublimating area $A_{\text{tot}}$ of nucleus and chunks, as well as the mass ratio $F$ between eroding refractories and water vapour, according to equation (22). Because $A_{\text{tot}}$ is directly related to $Q_{\text{nuc}}$ (equations 3–4), its validity follows from the previous discussion of extended sources. We find $F = 1.05$ with our method, suggesting that the escaping mass of refractories is very similar to the escaping mass of water vapour. This can be compared to measured values obtained using different instruments and techniques: $F = 0.64$ (Hansen et al. 2016), $F = 0.72$ (Marshall et al. 2020), $F = 1.06$ (Läuter et al. 2019), $F = 1.14$ (Combi et al. 2020), $F = 1.63$ (Läuter et al. 2020), and $F = 3.4$ (Biver et al. 2019), i.e., a mean and standard deviation of $(F) = 1.4 \pm 1$.

We have not considered neither CO nor amorphous water ice in this paper. With CO trapped in amorphous water ice, the crystallisation process could either produce or consume energy, depending on the CO abundance (e.g., González et al. 2008). Because Hoang et al. (2020) demonstrated that crystallisation and CO release has a negligible effect on the $H_2O$ and $CO_2$ production rates, we do not think our omission of CO and amorphous water ice has biased our analysis.

Next, we discuss the refractories/water–ice mass ratio $\mu$ of the nucleus. The southern hemisphere is essentially airfall–free (El-Maarry et al. 2016), therefore its activity near perihelion is representative of the nucleus itself, as opposed to the airfall material covering the northern hemisphere, that already has been processed in the coma. We find that $\mu_S = 1.0$ for the southern hemisphere yields $0.89Q_{H_2O}$ (Table 3), which formally would allow for an extended source of 11 per cent that provides the remaining vapour. As can be seen from Figs. 5 and 6 (or Fig. 9), this provides a satisfactory fit to the data at $r_s \lesssim 1.8$ au, where the southern contribution dominates. As our best estimate, we therefore propose that the least processed parts of the nucleus has a refractories/water–ice mass ratio close to unity. However, if we had applied an erosion based on another $F$ value in the $(F)$ range, we likely would have obtained $0.4 \leq \mu \leq 2.4$ for the nucleus interior.

The northern hemisphere is expected to have a higher refractories/water–ice mass ratio than the south, because of volatile loss in the airfall material prior to its deposition in the north. Davidson et al. (2021) used NIMBUS simulations of coma chunks to demonstrate that a 1 cm diameter chunk is expected to lose 56 per cent of its water ice, while a 10 cm diameter chunk loses ~ 6 per cent of the ice. If such chunks are representative of the airfall material of the north, we would expect $1.1 \leq \mu_N \lesssim 2.3$. Figure 3 shows that $\mu_N = 2$ provides a good fit to the data, whereas $\mu_N = 1$ is somewhat on the high side, suggesting that some loss indeed has taken place.

We now compare our estimate $\mu_N = 2$ with others in the literature, which also considered the pre–perihelion branch when the northern hemisphere dominated activity. Hu et al. (2017) fitted the water production rate curve with a thermophysical model using $\mu_N = 99$ under a 0.5 cm dust mantle, or alternatively, by using $\mu_N = 9$ under a 1 cm dust mantle. In both cases, the dust mantle was assumed to consist of 1 mm diameter solid particles, i.e., the mantles were 5–10 grain–layers thick. Blum et al. (2017) fitted the water production rate curve with a thermophysical model using $\mu_N = 19$ underneath a single monolayer consisting of 1 cm solid grains. These estimates ($9 \leq \mu_N \lesssim 99$) are drastically different from ours ($\mu_N = 2$), and we now discuss the reason for this discrepancy. Both teams used the thermophysical model developed by Gundlach et al. (2011). This model solves the energy conservation equation with terms for heat conduction and energy consumption due to sub–surface sublimation, but does not consider mass conservation. The magnitude of the sub–surface sublimation rate is given by the Hertz–Knudsen formula $Z(T) = p_{\text{sat}}(T)\sqrt{m_1/2\pi k_B T}$ (e.g. Fanale & Salvail 1984), where $p_{\text{sat}}(T)$ is the saturation pressure, times a constant correction factor $\Psi$ to account for the mantle diffusivity. This approach is roughly equivalent to considering exposed surface ice sublimating into vacuum, which covers an area fraction $\Psi$ of any surface element of the nucleus, while an area fraction $1 - \Psi$ is covered by inert dust. From the work of Keller et al. (2015b) we know that such a model requires $\Psi \approx 0.06$ at perihelion (and even smaller values, $\Psi \approx 0.02$, at larger heliocentric distances). It means that 67P/C–G produces $\leq 6$ per cent of the amount of water that an equal–area ice–only nucleus would do. In the model of Gundlach et al. (2011), the correction factor is evaluated as a function of a single parameter: the ratio between the dust mantle thickness and the diameter of the constituent grains. According to that formula, Hu et al. (2017) applies either $\Psi = 0.42$ or $\Psi = 0.59$, while Blum et al. (2017) applies $\Psi = 0.88$. The fact that the $\mu_N$–value of Blum et al. (2017) is intermediate between the two of Hu et al. (2017), while their $\Psi$–value is not, is a consequence of different thermal inertia applied in the models: 16–50 MKS for
100 \leq T \leq 200 \text{ K in Blum et al. (2017)}, but a fixed 30 MKS in Hu et al. (2017). In all cases, the \Psi–values are significantly higher than the necessary 0.02 \leq \Psi \leq 0.06. This forces Hu et al. (2017) and Blum et al. (2017) to introduce very low area fractions of ice underneath the mantles (of order 1–10 per cent) that correspond to the \mu_N–values mentioned above.

**NIMBUS** instead solves the coupled energy and mass conservation equations, which is the traditional and physically correct way of approaching thermophysical modelling (e.g., Espinasse et al. 1991; Prialanik 1992; Tancredi et al. 1994; Orose et al. 1995; Capria et al. 1996; Enzian et al. 1997; De Sanctis et al. 1999). Accordingly, the mass flux through the mantle sensitively depends on the temperature and vapour pressure gradients throughout the mantle, according to the Clausius formula (equation 46 in Davidsson 2021). This mechanism regulates how much vapour that should be removed from the sublimation front, thereby allowing for net production of more vapour. Such net production dictates the amount of energy consumed by sublimation, and therefore has a very strong effect on the overall temperature and gas pressure profiles. This delicate unbalance between sublimation and recondensation processes is governed by the classical volume mass production rate formula (equation 22 in Davidsson 2021). Here, the sub–surface net mass production rate is proportional to the difference \presat(T) – \p(T) between saturation pressure and the actual local pressure \p(T). Because this difference is small, outgassing becomes strongly quenched. Such quenching is evident when considering the ‘active area fraction’ of comets—they typically only produce a few per cent of the gas they would have been capable of producing if the ice was exposed at the surface (as previously exemplified with 67P/C–G itself). The Gundlach et al. (2011) model assumes that the volume mass production is directly proportional to the Hertz–Knudsen formula \Z(T), which is only applicable to flat icy surfaces facing a vacuum. The production rate is lowered only by the factor \Psi, that is large compared to the difference \presat(T) – \p(T) obtained when properly solving the mass conservation equation. The additional quenching that is needed to fit observed production rates is artificially obtained in the works by Hu et al. (2017) and Blum et al. (2017) by considering extremely low ice abundances.

Additionally, our **NIMBUS** simulations consider continuous erosion of the dust mantle, and the movement of the location of the sublimation front, as the finite reservoir of water ice is gradually being consumed. Instead, Hu et al. (2017) and Blum et al. (2017) consider static models where no erosion takes place and the ice is treated as an infinite reservoir. It is clear, that with erosion ranging 0.04–0.63 m on the northern hemisphere (Fig. 10), the slabs considered by Hu et al. (2017) and Blum et al. (2017) would be eroded and ejected into the coma many times over, giving the coma a refractories/water–vapour mass ratio equivalent to that assumed in their model at depth (i.e., 9 \leq \mu_N \leq 99). This is at odds with even the more dustier estimates of the coma composition (e.g., 4 \pm 2; Rotundi et al. 2015), compared to the F–values mentioned above.

We find that a rather small diffusivity in combination with an ice–rich material underneath the thin and continuously evolving dust mantle on the northern northern hemisphere (\mu_N = 2 corresponds to 33 per cent ice by mass) reproduces the measured data. We consider our calculations a more realistic solution to the physical energy and mass conservation problem under study, and suspect that the extremely ice–poor material found in the studies by Hu et al. (2017) and Blum et al. (2017) is an artefact caused by an oversimplified treatment of gas diffusion in porous media. By extension, this also invalidates the work of Fulle et al. (2019), who critically depends on the \mu_N estimate of Blum et al. (2017) for the northern hemisphere airfall, when drawing the conclusion that the refractories/water–ice mass ratio of the bulk nucleus is \sim 10 times higher than the dust/water–vapour mass ratio of escaping material (taken as 0.7–3.1), i.e., 7 \leq \mu \leq 31.

We find that a molar abundance of \sim 30 per cent \mathrm{CO}_2 relative \mathrm{H}_2\mathrm{O} is necessary to reproduce the high post–perihelion \mathrm{CO}_2 production, and that the \mathrm{CO}_2 sublimation front depths on average were located at 3.8 m depth in the north, and at 1.9 m in the south, at aphelion. Thus far, only Herdy et al. (2021) have published estimates of the nucleus \mathrm{CO}_2 abundance (they find a molar abundance of 7–11 per cent) and front depth (about 1 m in the north at perihelion, where we have 3.4–3.8 m before the airfall, and exposed at the surface in the south, where we have 0.15–1.8 m). Thus, our nucleus \mathrm{CO}_2 abundance is higher, and the front depth is larger, than obtained by Herdy et al. (2021). We attribute this difference to the usage of the ‘Effective Area Fraction’ of 20 per cent that Herdy et al. (2021) introduce to quench their high model water production rate down to the observed one. The same quenching is needed for \mathrm{CO}_2. We believe that their \mathrm{CO}_2 production is too high because their \mathrm{CO}_2 front is too shallow, and that the abundance is biased to a too low value for the same reason.

We now discuss the interpretation of our model fits in Section 4.1–4.2 in terms of the diffusivity of 67P/C–G and how it evolved with time and depth. We first focus on \mathrm{H}_2\mathrm{O} and then \mathrm{CO}_2, in both cases starting at perihelion and marching through the orbit (assuming that the comet behaviour is fairly repetitive from one apparition to the next).

One of the biggest surprises in this work is that the comet activity of both hemispheres is strongly asymmetric, in the sense that significantly different model parameters must be used before and after perihelion (see Fig. 6). We first concentrate on the northern hemisphere, which is asymmetric in terms of the \mathrm{H}_2\mathrm{O} production. Close to perihelion, it is the target of substantial airfall. Because of the polar night conditions, it provides a negligible contribution to the water production rate during the first \sim 100 days after perihelion (\sim 1.7 au). It then gradually receives more illumination, and by the time the comet reaches \sim 2.5 au (\sim 200 days post–perihelion) a substantial fraction of the water activity must be provided by the northern hemisphere. Figure 11 (upper right) shows that most of the northern hemisphere is substantially colder at this time, compared to similar distances pre–perihelion. At mid–northern latitudes the difference is several times 10 K. Despite being colder, it produces a \sim 30 per cent higher total water production rate than at the same heliocentric distance pre–perihelion. The only way for a relatively cold hemisphere to produce large amounts of water vapour, at a distance where the sensitivity to the water ice abundance is low, is if the diffusivity is very high.

We find that we need to use a diffusivity corresponding to \{L, r_p\} = \{10, 1\} cm and \xi = 1 (Fig. 7) on the northern hemisphere, post–perihelion. This means that there must be plenty of cavities, cracks, and channels on centimetre–scale or larger, through which water vapour may flow from depth very freely. This is entirely consistent with the presence of a thick layer of loosely stacked chunks with diameters in the centimetre–decimetre scale. Thanks to the last Rosetta images acquired before landing at end–of–mission (414 days post–perihelion at \r_p = 3.8 au), we have close–up images of airfall material at Sais in the Ma’at region on the northern hemisphere (latitude 35\textdegree N). The best images, with a resolution of 1.4 cm px\textsuperscript{-1} and a chunk–size completion limit at \sim 7 cm shows very coarse debris in the 7–70 cm diameter range (Pajola et al. 2017). Therefore, we think that our post–perihelion diffusivity parameter for the northern hemisphere is realistic.

Assuming a repetitive apparition behaviour, the same type of material is responsible for the northern water activity on the inbound
orbit, that was observed by *Rosetta* early in the mission. For that segment of the orbit, a fundamentally different diffusivity is required, $\{L, \, r_p\} = \{100, \, 10\}$ $\mu$m and $\xi = 1$. If real, the three orders of magnitude drop in diffusivity must be caused by a significant change of the size distribution of near-surface material taking place during the aphelion passage. We postulate that the chunks in a top layer crumbled, fragmented, and pulverised into a fine-grained dust cover, having typical cavities and channels of sub-millimetre size. The mechanism for such fragmentation likely starts with the removal of the water ice that binds the chunks together. Figure 11 (upper left) shows that dust mantle growth is significant in the north during post-aphelion. The generally low temperatures at aphelion may have showsthat dust mantle growth is significant in the north during post-aphelion. The generally low temperatures at aphelion may have caused remaining cohesive material (primarily organics) to become brittle. In combination with a substantial diurnal cycling (typically in the 120–160 K range; Davidson et al. 2021) this may have led to thermal fatigue and fragmentation, analogous to regolith-formation on asteroids (Delbô et al. 2014). We note, however, that the timescales of fragmentation differ drastically: the fragmentation of competent rock taking place on asteroids is slow compared to the fragmentation of a cometary low-cohesion grain assemblage that is sublimating. The process we propose would be more akin to the rapid fragmentation observed in comet comae (e.g. Hadamcik & Lévasseur-Regourd 2003; Ho et al. 2007; Jones et al. 2008; Rosenbush et al. 2017).

*Rosetta* observations support such crumbling of the top part of the airfall layer. The ROLIS camera on the *Philea* lander documented the airfall material at Agilki, also in the Ma’at region at latitude 12° N, (at $r_p = 3.0$ au inbound) with 1 cm px−1 resolution (Mottola et al. 2015). Above a chunk diameter of ~0.26 m, the differential size–frequency distribution power–law slopes are very similar for the two sites: $-4.2^{+0.4}_{-0.8}$ at Sais and $-4.3 \pm 0.5$ at Agilki (Pajola et al. 2017). Whereas the fresher airfall at Sais has a distinct break in the distribution at smaller sizes, being $-1.7 \pm 0.1$ in the 0.07–0.26 m region, the aged airfall at Agilki has a much steeper slope (ranging from $-3.8$ to $-3.4$ for two different sub–units) that is more similar to the one at larger sizes (Pajola et al. 2017). Evidently, smaller chunks are relatively more common at Agilki than at Sais, which we attribute primarily to fragmentation processes near aphelion (although transport of small chunks from Hapi to Agilki during activity switch–on may contribute as well; Pajola et al. 2017).

We now shift to the southern hemisphere, which is asymmetric in terms of the model parameters needed to explain the CO$_2$ production. First note that the CO$_2$ sublimation front depth between latitude 45° S and the south pole starts to decrease rapidly around 100 days ($r_h \approx 1.7$ au) pre–aphelion, according to Fig. 11 (lower left). This is caused by strong water–driven erosion of the surface material. This causes a tenfold increase in the modelled CO$_2$ production rate, from $10^{26}$ molec s$^{-1}$ to $10^{27}$ molec s$^{-1}$ between $r_h = 1.7$ au and perihelion according to Fig. 5. The nucleus CO$_2$ outgassing may briefly have reached $6 \times 10^{27}$ molec s$^{-1}$ just after perihelion (measurements in Fig. 6). The measured and modelled surges suggest that the drastic reduction of the CO$_2$ sublimation front depth is real. As already discussed in Section 4.1 this level of outgassing requires a combination of high intrinsic nucleus CO$_2$ abundance, as well as a shallow CO$_2$ front.

The model that reproduces the high near–perihelion CO$_2$ production rate does not fall off as rapidly as the observations farther from perihelion (Fig. 6). We found that a substantial reduction of the diffusivity, by a factor $\sim 100$–250, realised by setting $\{L, \, r_p\} = \{10, \, 1\}$ $\mu$m and $\xi = 1$–5, was required to reproduce the measurements. We now discuss the possible cause of such a change.

In the current simulations, we find that the CO$_2$ vapour pressure reaches 0.7 kPa pre–aphelion at the south pole, but almost a factor 30 higher post–aphelion (because of the imposed strong reduction of diffusivity). The CO$_2$ pressure peaks at the sublimation front and falls off to nearly zero towards the surface, as well as towards regions somewhat below the front. Such gradients would be capable of ejecting refractories and water ice outwards into the coma, as well as compressing material at depth. A pressure difference of 19.1 kPa is sufficient to compress granular water–ice media to 77 per cent porosity according to laboratory measurements by Lorek et al. (2016). Pure silica dust would compress to 62 per cent porosity according to laboratory measurements by Gütlinger et al. (2009), suggesting that compression could be substantial if the material is weakened by the presence of dust. Such compacted terrain would have lower porosity, smaller pores, having less connectivity, thus lower diffusivity and higher tortuosity than uncompressed comet material.

We therefore propose that the intense sublimation near perihelion compressed the material underneath the CO$_2$ sublimation front. When the front gradually moved into this pre–compressed material post–aphelion, as the CO$_2$ was being consumed, the local diffusivity dropped drastically, and the vapour could not flow as freely. We modelled this as an abrupt change at $r_h = 1.4$ au, but in reality it would have been gradual. This caused a reduction of the CO$_2$ outgassing (with respect to Fig. 6), thus explaining the observed data (Fig. 9). As the CO$_2$ front moved into deeper and colder region, its sublimation rate waned, and further compression ceased (see the CO$_2$ front temperature in Fig. 11, lower right, day 100–200 post–aphelion). At the same time, water activity was still substantial, leading to several meters worth of erosion (Fig. 10). That erosion may have consumed most of the compressed layer in the near–surface region. That could explain why CO$_2$ outgassing from the southern hemisphere on the inbound trajectory, after the aphelion passage, was characterised by a relatively high diffusivity anew ($\{L, \, r_p\} = \{100, \, 10\}$ $\mu$m and $\xi = 1$).

We therefore conclude that the idea of fixed nucleus thermophysical parameters may have to be abandoned. Comet activity changes the physical properties of the surface layer, and is therefore self–regulatory. Although this certainly makes the task of modelling comet activity more challenging, it also provides novel opportunities to better understand comet behaviour. The perihelion asymmetry in the water production of 67P/C–G is apparently caused by the large difference in diffusivity between fresh airfall and ‘regular’ nucleus material (that is more similar to aged and pulverised airfall). Nucleus erosion may locally bring the CO$_2$ sublimation front to a steady–state depth near perihelion, where this depth depends on the absolute CO$_2$ abundance. Strong perihelion asymmetries in the CO$_2$ production rate are prohibited by low post–perihelion diffusivity caused by CO$_2$ activity itself.

We note that the H$_2$O production in this scenario is repetitive. After perihelion, the dust mantle thickness returns to its pre–perihelion values at most latitudes (Fig. 11, upper left). The changes in diffusivity caused by fresh airfall deposition and near–aphelion fragmentation would take place each orbit. The low–diffusivity surface layer formed by fragmentation around aphelion is either removed when approaching the Sun, or simply covered with new airfall, in both cases leading to a high–diffusivity surface coverage on the outbound orbital arc. The resulting similarities in the water production rate from one orbit to the next seems to be consistent with observations over several apparitions (Bertaux 2015). The repetitive water outgassing is also evident from the long–term stability of the non–gravitational force: the Jet Propulsion Laboratory solution 2 K215/10 spans 26 years with low RMS residuals.

2 https://ssd.jpl.nasa.gov/tools/sbdb_lookup.html#?ssstr=67P
Concerning CO$_2$, the situation is not as clear. We predict that the CO$_2$ sublimation front is receding from the surface in the north (due to net airfall deposition) and approaching in the south, i.e., there might be changes in the CO$_2$ production from one apparition to the next. However, because CO$_2$ can only be observed from space, future observations will have to determine whether or not the CO$_2$ production pattern is repetitive.

Finally, we discuss the significance of the momentum transfer coefficient. We found that $\eta = 0.31 \pm 0.06$ or $\eta = 0.39$ provided the best match (for slightly different orbital solutions), while classically applied values typically have ranged $0.4 \leq \eta \leq 1$ (see Rickman 1989; Davidsson & Skorov 2004, and references therein). The classical approach assumes that the sublimating surface is flat, faces the vacuum of space, and consists of pure water ice. The expression for the force (equation 1) uses the mean molecular speed $\langle V \rangle = \langle V(T_{\text{surf}}) \rangle$ of a non-drifting Maxwellian gas as a normalisation factor. Fundamental gas kinetic theory leaves no doubt that the actual mean velocity component along the surface normal differs from $\langle V \rangle$, hence the need for the momentum transfer coefficient. If one only considers molecules travelling away from the surface, there is no doubt that $\eta = 0.5$ (e.g., Huebner & Markiewicz 2000). If one considers the fact that downstream molecules will collide with each other, and that some of those are re-directed towards the surface, there is also an additional contribution to the momentum transfer from backflux molecules that hit the surface. Analytical solutions to the conservation equations for this type of Knudsen layer outflow exist, but they do not have unique solutions (Ytuhus 1977). For reasonable assumptions about the downstream Mach number, one finds $0.53 \leq \eta \leq 0.67$ (Crifo 1987; Rickman 1989).

There are several important differences between NIMBUS and the idealised sublimating surface described above: 1) the sublimating water is not exposed, but is located under a dust mantle; 2) molecules diffusing through the mantle thermalise and may depart with a temperature substantially higher/lower than the water ice sublimation temperature, if the mantle surface is hotter/cooler than the ice below (Skorov & Rickman 1995; Christou et al. 2018); 3) the dust mantle may collimate or de-collimate the flow depending on the sign of the temperature gradient across the mantle (Davidsson & Skorov 2004). With respect to a real comet nucleus there are additional differences: 1) the comet surface is not flat on the size scale of a shape-model facet, but macroscopically rough; 2) water molecules in the Knudsen layer diffuse through heavier and thus slower CO and CO$_2$ vapour, modifying their backflux properties; 3) solid chunks in the coma may disturb the water flow by re-directing or emitting molecules, and they may impact the surface themselves.

We expect surface roughness to have the largest and most systematic effect on the momentum transfer coefficient. As soon as a surface element (large enough to act as a local flat surface in the context of outgassing) is tilted with respect to the regional mean outward surface normal, that will reduce $\eta$ for the region. It is also noteworthy that we evaluate $\langle V \rangle$ for the surface temperature. A hot dust mantle may approach 340 K (Fig. 10, upper left), making $\langle V \rangle$ some $\sim 1.3$ times higher than expected for sublimating water ice ($\sim 200$ K). If water molecules do not thermalise at the surface temperature (e.g., by having their last interaction with the solid medium at some colder depth below the surface) that would lower $\eta$ as well (to compensate for a $\langle V \rangle$ that may be too large). We therefore consider $\eta = 0.31 \pm 0.06$ or $\eta = 0.39$ reasonable estimates of the momentum transfer coefficient. Our force model will be further tested in a forthcoming publication focusing on the spin state evolution due to outgassing torques, and the time-resolved non-gravitational changes of the orbit of Comet 67P/C-G.

6 CONCLUSIONS

We have modelled the outgassing of H$_2$O and CO$_2$ from Comet 67P/C-G using the thermophysical code NIMBUS (Numerical Icy Minor Body evolUtion Simulator) by Davidsson (2021). We have adjusted key model parameters until we simultaneously reproduce the pre-and post-perihelion production rates of both species according to ROSINA measurements (Fougere et al. 2016a). The model uses an enforced dust production rate, which has a functional form similar to the observed brightness of the comet and is scaled to be compatible with the observed total mass loss. The goal of this effort is to place constraints on the H$_2$O and CO$_2$ nucleus abundances, retrieve information about the depths of the H$_2$O and CO$_2$ sublimation fronts and how they may have changed with time and latitude, and estimate the diffusivity of the porous near-surface material, which informs about the size scale of macro porosity. We apply the outgassing model in order to calculate the non-gravitational changes of the orbit, and identify the conditions under which the observed changes are reproduced. The longer-term goal of this work is to apply the outgassing model to investigate the evolution of the nucleus spin state.

Our main conclusions can be summarised as follows:

(i) The contribution of an extended coma source to the total comet water production rate is $\sim 8$ per cent at perihelion.

(ii) The refractories/water–ice mass ratio of relatively pristine material on the southern hemisphere is $M_2 \approx 1$. The airfall material on the northern hemisphere has lost some water ice during transfer through the coma and is better characterised by $M_2 \approx 2$.

(iii) The thickness of the dust mantle is typically $\lesssim 2$ cm, suggesting that water ice is ubiquitous near (but not on) the surface.

(iv) The observed CO$_2$/H$_2$O abundance ratio in the coma (e.g., 2.2–5.6 per cent at 1.8–2.2 au pre–perihelion; Fink et al. 2016) is not necessarily a reliable measure of the corresponding ratio within the nucleus. We find that nucleus models with CO$_2$/H$_2$O = 32 per cent reproduce the data. The coma CO$_2$/H$_2$O is sensitive to the depth of the CO$_2$ sublimation front in addition to the intrinsic nucleus CO$_2$/H$_2$O abundance.

(v) We find that the depth of the CO$_2$ sublimation front on the northern hemisphere was $\sim 3.8$ m on average at aphelion. A combination of CO$_2$ loss, nucleus erosion, and airfall deposition may result in a net increase of the front depth with time. The depth of the CO$_2$ sublimation front on the southern hemisphere was $\sim 1.9$ m on average at aphelion. Locally, the depth may have been reduced to as little as $\sim 0.15$ m near the south pole. The CO$_2$ sublimation front depth vary significantly with time and latitude.

(vi) Fresh airfall material has a high diffusivity, suggesting macro porosity on centimetre scales. Aged airfall material has a three orders of magnitude lower diffusivity, suggesting sub-millimetre macro porosity. We propose that a combination of desiccation, temperature-dependent brittleness, and thermal fatigue causes substantial fragmentation of a surface layer during the aphelion passage.

(vii) The model with the best available reproduction of the H$_2$O and CO$_2$ outgassing, results in a net force acting on the nucleus that reproduces the observed non-gravitational changes of the orbital period, longitude of perihelion, and longitude of the ascending node of 67P/C-G, as long as the momentum transfer efficiency $\eta = 0.31 \pm 0.06$ or $\eta = 0.39$ (depending on orbital solution). We interpret the relatively low $\eta$-value as a consequence of small-scale surface roughness, potentially in combination with incomplete thermalisation of molecules diffusing through the hot dust mantle.
