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The Influence of Heavy Cosmic Rays in Energy Deposition in Molecular Clouds Employing the GEANT4 Code and Voyager I Data

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Abstract

Galactic and extragalactic cosmic rays fully illuminate and trigger several physical and physicochemical changes in molecular clouds (MCs), including gas and grain heating, molecular destruction and formation, and molecular and atomic desorption (sputtering) from dust/ices to gas phase. Besides the major component in cosmic ray inventory (in flux) being electrons, protons, and alphas, particles with larger atomic numbers have a higher rate of energy delivery (due to richer cosmic ray showers) than the lighter particles, and this may add extra energy input into MCs. To understand this issue, we perform complementary calculations to the previous work on MCs, now adding the heavy ions ($12 \leqslant Z \leqslant 29$) in the cosmic ray incoming inventory. Once more, the calculations were performed employing the Monte Carlo toolkit GEANT4 code (considering nuclear and hadron physics). We observe that most projectiles in the heavy ion group have lower deposited energies (roughly 10 times less) than iron with the exception of magnesium ($Z = 12$) and silicon ($Z = 14$) which are about double. Cobalt presents the lowest deposited energies with respect to iron (only 0.5%). The total energy deposition in the current model was only roughly 10% higher (outer layers) and virtually the same at the center of the cloud when compared with the previous model (with only protons + alphas + electrons sources). The results show that energy deposition by heavy ions is small compared with the values from light particles, and also suggest a very low temperature enhancement due to heavy ions within the MC, being the protons the dominant agent in the energy delivery and also in the cloud's heating.

Unified Astronomy Thesaurus concepts: Cosmic rays (329)

1. Introduction

In a molecular cloud (MC), one of the denser and colder regions of the interstellar medium (ISM), the presence of galactic and extragalactic cosmic rays (CRs) plays an important role in the molecular processing as well as in physical chemical processes (e.g., Goldsmith & Langer 1978; Galli & Padovani 2015). The penetrating CR within such media allow, besides molecular destruction and formation, induced gas and grain heating and molecular desorption (sputtering and thermal desorption) from dust/ices to the gas phase (e.g., Dalgarno 2006; Padovani et al. 2009; Pilling et al. 2011).

The interactions between CRs with space environments such as MCs and protoplanetary disks by employing Monte Carlo simulations have been performed in the literature by several groups (e.g., Wood et al. 2004; Herbst & Cuppen 2005; Boettcher et al. 2013; Vaupre 2015; Cui et al. 2016; Kataoka & Sato 2017; Vandenbroucke & Wood 2018; Pazianotto et al. 2021 and references therein). Over the years, these works have been clarifying the effect, mostly of the lighter particles in the energy processing of such interstellar environments. For example, Pazianotto et al. (2021) have shown that the abundant light particles of the cosmic ray inventory (electrons, protons, and alphas) deposited around 260–360 MeV g^{-1} s^{-1} in the major part of an MC (radii >100 from the center of the cloud), the proton being the dominant source. Among the results, the authors also observed that secondary electrons are the second-most important component for energy deposition in almost all layers of the MC and can deliver an energy rate of ∼130 MeV g^{-1} s^{-1} in the outer region of the MC. The effects of lighter CR in the temperature of the cloud have shown the existence of a small enhancement at the distance of 1–2 × 10^4 au from the center, and also a rapid temperature decrease (roughly 7 K) between the outer layer and the second-most outer layer, and that at a distance of 5 × 10^4 au (Av > 10) the gas temperature of MC is below 15 K.

Curiously, despite several experimental studies employing heavy ions (particles with atomic numbers between $12 \leqslant Z \leqslant 29$; see also Pilling et al. 2011) being performed (e.g., Seperuelo Duarte et al. 2009; Pilling et al. 2010a, 2010b; Bergantini et al. 2014), the effects of such particles in cold astrophysical regions are poorly investigated computationally. Usually, the experimental studies, which employ ion accelerator facilities, pointed out that heavy ions besides their lower flux, compared with the lighter particles, should not be neglected (e.g., Andrade et al. 2013, Portugal et al. 2014). For example, as discussed by Pilling et al. (2011), at lower projectile energies (∼100 MeV u^{-1}), particles within the heavy ions group have similar electronic and nuclear stopping power and induce similar effects during collision with matter.

As shown by the measurements performed by Voyager outside the solar system (Cummings et al. 2016), as well as several measurements made in Earth orbit (e.g., Aguilar et al. 2015, 2020, 2021), the cosmic rays also have heavier components. The advances of particle physics experiments in space make it possible to study primordial particles created at the beginning of the universe. They are among the objectives of these experiments, to perform accurate measurements on the energy properties of the constituents of CR, as the spectra and the deposited energy, for example. The experimental efforts, combined with the theoretical models, can help to understand the origin and propagation features of CR.

In an attempt to understand the amount of energy delivered by heavy ions into MC, we perform a new set of calculations

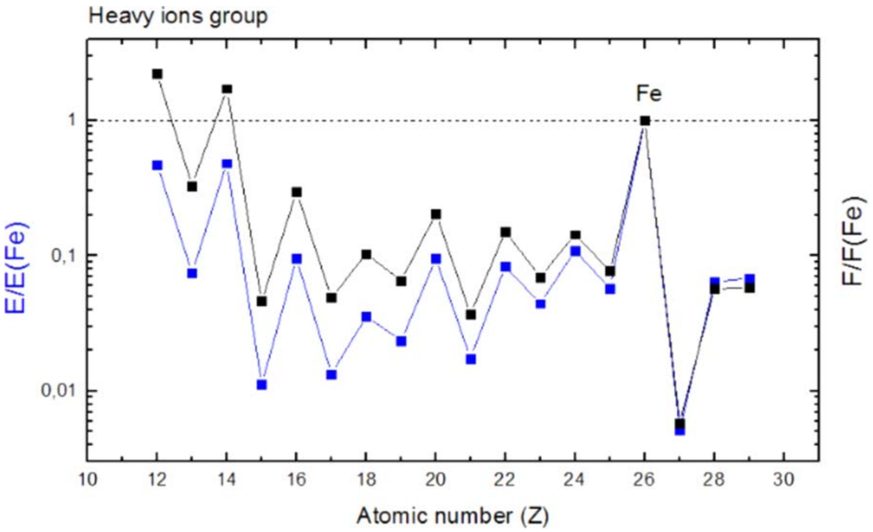

Figure 1. Comparison between deposited energy rate and the integrated flux of the ions within the heavy ions group with respect to the iron. Simulations were performed considering more than 99.99% of the molecular cloud's volume and mass (up to the 9th innermost layer). The integrated flux was taken from Cummings et al. (2016).

applying the same methodology described by Pazianotto et al. (2021) but now considering the presence of heavy ions. This work computes for the first time the simultaneous energy deliverer by light (electrons, protons, and alphas) and heavy ions considering nuclear cascade reactions (hadron and nuclear physics) and CR shower processes within the MC. To quantify the effects of the heavy ions group in the molecular cloud, we first investigate the similarities and the differences in the energy deposition and integrated flux during a comparison between the Fe ions with other members of the heavy ions group. The Fe spectrum of cosmic rays, as for the other particles within the heavy ion group, has been well characterized by the Voyager I measurements (Cummings et al. 2016) and also at the International Space Station, whose observations were reported by Aguilar et al. (2021).

A brief description of the methodology employed in this work is given in Section 2 and the results and discussion in Section 3 with comparisons to the previous work (same calculations but without heavy ions). Section 4 lists the main conclusions of this manuscript.

2. Methodology

In this work we have used the Monte Carlo toolkit Geant4 (Agostinelli et al. 2003; Allison et al. 2006) to perform simulations of the iron nucleus transport throughout the MC. The geometry and composition of the MC and also the incidence and analysis methodology can be found in Pazianotto et al. (2021). The parameterization to simulate the hadronic interactions was performed with QGSP_INCLXX_HP reference physics list. This physics list is the same employed in the previous simulations about the effects of cosmic ray protons, alphas, and electrons on MC, carried out by Pazianotto et al. (2021). Once more, the simulation was performed considering the spherical molecular cloud with 5400 solar masses with a radius around 1×10^6 au, with a density higher in the center, and divided into 13 concentric shells with parameters and energy deposition in each shell described by its average quantities within the shell. The other parameters considered for the simulated object are the density profile law of $1/r^{1.2}$ and average number density of 2×10^2 cm^{-3} containing mostly H atoms (with also C atoms as a minor component to represent dust grains) and with the canonical dust to gas ratio of 1/100 (more details in Pazianotto et al. 2021).

In the current manuscript we expand the previous simulation to include the effects of the heavy ions group. The employed cosmic ray fluxes were taken from the measurements of Voyager I in the ISM published by Cummings et al. (2016). We observe that for energies below $\sim 1 \times 10^4$ MeV the integrated flux of cosmic rays is dominated by lighter particles. For energies above $\sim 10^5$ MeV the integrated flux of all nuclei components is comparable. For comparison purposes, the primary fluence rates (integrated from $\sim 10^{-1}$ to 10^6 MeV) that we have obtained for the simulations are 1.26 protons cm^{-2} s^{-1} sr^{-1}, 0.09 alphas cm^{-2} s^{-1} sr^{-1}, 1.19 electrons cm^{-2} s^{-1} sr^{-1}, and 1.81×10^{-4} irons cm^{-2} s^{-1} sr^{-1}. All simulations were performed in order to obtain the uncertainty below 10%.

3. Results and Discussion

As discussed previously, to quantify the effects of the heavy ion group in the molecular cloud, we first investigate the similarities and differences in the deposited energy rate and in the integrated flux between the Fe ions and the other members of the heavy ions group. The results of these simulations are presented in Figure 1. For the calculation of the energy deposition ratio (presented in blue), we consider the effect up to the 9th inner layer within the cloud (which corresponds to more than 99.99% of cloud volume and mass). We observe in this figure that, within the heavy ions group only atoms with Z equal to 12 and 14 present values of deposited energy ratio similar (half) to the iron. The other components presented values much lower when compared with iron. Similar behavior was also observed in the case of integrated flux (presented in black). Within the group, the most different values with respect to iron were found for cobalt ($Z = 27$) and Phosphorus ($Z = 15$). These individual differences were taken into consideration in the calculation of the total energy delivered by the heavy ion group.

A comparison showing the total energy deposition by Fe ions, protons, electrons, and alpha particles considering all with the same integrated flux (e.g., 1.26 particles cm^{-2} s^{-1} sr^{-1}) was

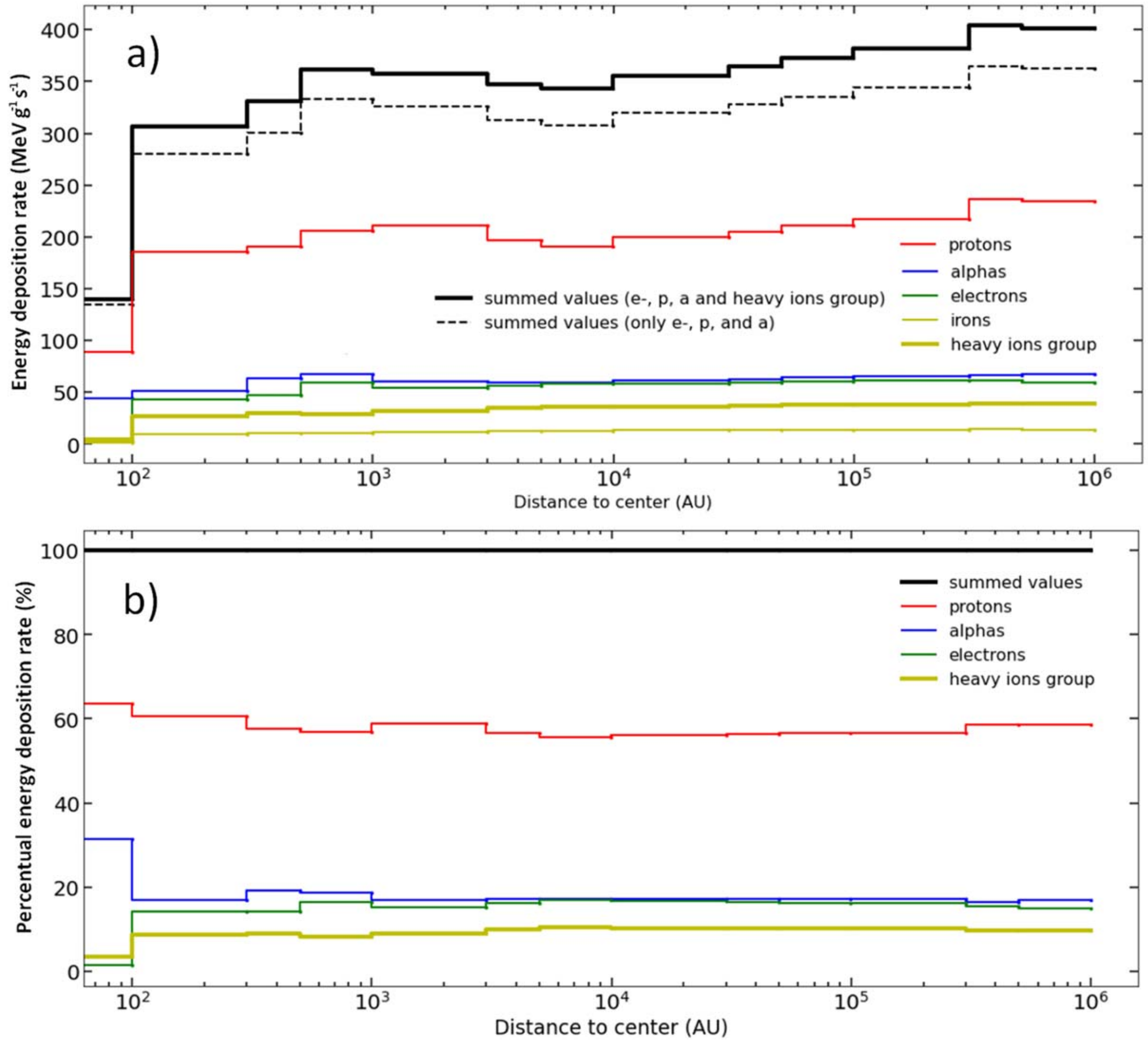

Figure 2. Energy deposition rate for each primary source (and also considering heavy ions group) in the MCs. Panel a shows the units of MeV g^{-1} s^{-1}. Dashed lines show the summed values considered only (electrons + protons + alphas) from the previous simulation (Pazianotto et al. 2021). Panel b presents the energy deposition rate in percentage (protons + alphas + electrons + heavy ions sources). See details in the text.

also performed. The results indicated that in this specific situation (with the same flux), Fe ions were by far the most important species (~100 times more than alphas and ~500 times more than protons) in energy delivery. This comparison also shows that alpha particles deposit five times more energy than protons and that electrons are the less important particles in the energy deposition.

The simulation result with the energy deposition rate for the considered CRs within the molecular cloud in each layer is presented in Figure 2. Figure 2(a) presents the energy deposited rate, in units of MeV g^{-1} s^{-1}, for the primary sources of protons, alphas, electrons, and iron as well as the heavy iron group considered as a whole (considering the energy and flux distribution shown in Figure 2). The solid black line shows summed values obtained in the current simulation (electrons + protons + alphas + heavy ions sources). The dashed line shows the summed values from our previous publication (electrons + protons + alphas; Pazianotto et al. 2021). The energy deposition rate for the Fe source is given by the light yellow curve, and for the heavy ions group by the bold yellow curve. We observe that the current simulation, considering heavy ions in the cosmic ray components, induces an enhancement of about 2% (inner layer) to 10% (outer layers). This points out that the major components in the energy delivered inside MCs are indeed protons (major), alphas, and electrons.

Figure 2(b) shows the energy deposition rate in percentage for the current simulation (electrons + protons + alphas + heavy ions group). Here we clearly observe that protons correspond to roughly 60% of the energy delivered by cosmic rays into the molecular cloud. The alphas and electrons are responsible for about 18 % of energy depostion rate each, for distances larger than 100 au from the center of the cloud. In general, the heavy ions contribute to energy deposition rate below 10%. In the very deep core (>100 au) protons are still the dominant component being responsible for about 63% of the incoming energy, followed by alphas (with roughly 30%). In the central part, the energy deposition due to heavy ions, despite its low value, is higher than the electrons, the less important component there.

Considering that energy deposition rate in the current model is only about 2% (inner layer) to 10% (outer layers) higher than the value calculated in the previous simulation without considering the heavy ion group (Pazianotto et al. 2021), we suggest that the temperature enhancement within the cloud due to cosmic rays is mainly ruled by protons (major) + alphas + electrons, and not by the heavy ion component of CR inventory. The temperature profile of the MC considering the heavy ions group ($12 \leqslant Z \leqslant 29$) and also the medium-mass ions group ($3 \leqslant Z \leqslant 11$), as well the description of the energy delivered by each particle produced during the nuclear cascade, will be the subject of future manuscripts.

4. Conclusion

In this work we perform a new set of calculations on the effects of cosmic ray energy input on MC, now adding the influence of heavy ions ($12 \leqslant Z \leqslant 29$). The simulations of the energy released by CR-induced particles in a typical MC with 5400 $M_\odot$ (containing major H with a low amount of C atoms to simulate the dust component), size of ∼4.8 pc, density lay of $r^{-1.2}$, and an average number density around 300 cm^{-3}. The simulations were carried out employing the Monte Carlo code GEANT4 which takes into account nuclear physics and cascade particle processes. This work computes, for the first time, the simultaneous energy delivery by lighter (electrons, protons, and alphas) and heavier particles considering nuclear cascade reactions (hadron and nuclear physics) and CR shower processes within the MC.

From the investigation of the individual effects of different ions within the heavy ion group, we observe that most ions within this group have lower deposited energies (roughly 10 times less) than iron with the exception of magnesium ($Z = 12$) and silicon ($Z = 14$) which were about double. Cobalt presents the lowest deposited energies with respect to iron (only 0.5%). The total energy deposition by heavy ions in the current model was only roughly 10% higher (outer layers) and virtually the same at the center of the cloud when compared with the previous model with only the protons + alphas + electrons sources (Pazianotto et al. 2021). This suggests a very low temperature enhancement due to heavy ions within the MC, protons being the dominant agent in the energy delivery and also in the cloud's heating. This issue will be investigated in detail in further research.

We hope the current calculation helps to clarify the profile of the energy deposition due to the different particles (lighter and heavier) of CR inventory, as well as put better constraints on the radio observations and chemical networks models of MCs.

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Data Availability

The data underlying this article will be shared upon reasonable request to the corresponding author.

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References

Agostinelli, S., Allison, J., Amako, K., et al. 2003, NIMPA, 506, 250
Aguilar, M., Aisa, D., Alpat, B., et al. 2015, PhRvL, 114, 171103
Aguilar, M., Cavasonza, L. A., Ambrosi, G., et al. 2020, PhRvL, 124, 211102
Aguilar, M., Cavasonza, L. A., Allen, M. S., et al. 2021, PhRvL, 126, 041104
Allison, J., Amako, K., Apostolakis, J., et al. 2006, ITNS, 53, 270
Andrade, D. P. P., de Barros, A. L. F., Pilling, S., et al. 2013, MNRAS, 430, 787
Bergantini, A., Pilling, S., Rotarhd, H., et al. 2014, MNRAS, 437, 2720
Boettcher, E., Zweibel, E. G., Yoast-Hull, T. M., & Gallagher, J. S. III 2013, ApJ, 779, 12
Cui, Y., Puhlhofer, G., & Santangelo, A. 2016, A&A, 591, A6
Cummings, A. C., Stone, E. C., Heikkila, B. C., et al. 2016, ApJ, 831, 18
Dalgarno, A. 2006, PNAS, 103, 12269
Galli, D., & Padovani, M. 2015, Cosmic Rays and the InterStellar Medium Conf. (CRISM), 221 *(Montpellier, France, 24–27 June 2014)* 030
Goldsmith, P. F., & Langer, W. D. 1978, ApJ, 222, 881
Herbst, E., & Cuppen, H. M. 2005, PNAS, 103, 12257
Kataoka, R., & Sato, T. 2017, Geoscience Frontiers, 8, 247
Padovani, M., Galli, D., & Glassgold, A. E. 2009, A&A, 501, 619
Pazianotto, M. T., Pilling, S., Quesada Molina, J. M., Federico, C. A., et al. 2021, ApJ, 911, 129
Pilling, S., Seperuelo Duarte, E., da Silveira, E. F., et al. 2010a, A&A, 509, A87
Pilling, S., Seperuelo Duarte, E., Domaracka, A., et al. 2010b, 523, A77
Pilling, S., Seperuelo Duarte, E., Alicja, D., et al. 2011, PCCP, 13, 15755
Portugal, W., Pilling, S., Boduch, P., et al. 2014, MNRAS, 441, 3209
Seperuelo Duarte, E., Boduch, P., Rothard, H., et al. 2009, A&A, 502, 599
Vandenbroucke, B., & Wood, K. 2018, A&C, 23, 40
Vaupre, S. 2015, PhD thesis, Université Grenoble Alpes entitled Cosmic-ray ionization of dense molecular clouds. Astrophysics [astro-ph]. English. NNT: 2015GREAY049ff. tel-01273899f These dirigee par Cecilia Ceccarelli et codirigee par Pierre Hily-Blant https://tel.archivesouvertes.fr/tel-01273899/document
Wood, K., Mathis, J. S., & Ercolano, B. 2004, MNRAS, 348, 1337