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A Monte Carlo study of photoelectron extraction efficiency from CsI photocathodes into Xe-CH₄ and Ne-CH₄ mixtures

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Abstract. The extraction efficiency f for the photoelectrons emitted from a CsI photocathode into gaseous Xe-CH₄ and Ne-CH₄ mixtures is investigated by Monte Carlo simulation. The results are compared with earlier calculations in Ar-CH₄ mixtures and in the pure gases Xe, Ar, Ne and CH₄. The calculations examine the dependence of f on the density-reduced electric field E/N in the 0.1-40 Td range, on the incident photon energy E_{ph} in the 6.8-9.8 eV (183-127 nm) VUV range and on the mixture composition. Results calculated for irradiation of the photocathode with a Hg(Ar) lamp are compared with experimental measurements for this lamp. To test the electron scattering cross-sections used in the simulations, electron drift parameters in Xe, Ne and their mixtures with CH₄ are also presented and compared with available experimental data.

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1. Introduction

Cesium iodide photocathodes have been extensively used as UV converters in many applications, due to their high quantum efficiency, allied to good stability, resistance to ageing and easy production. In particular, they are frequently used in gas photosensor devices such as gas photomultipliers (GPMs), gas electronmultipliers (GEMS), and other micro pattern gas devices, to detect the primary or/and secondary scintillation produced in radiation detectors [1-6]. However, the transmission of the photoelectrons may be significantly reduced due to backscattering of the photoelectrons in the gas, thus reducing the effective quantum efficiency of the photocathode, an effect which is especially important when the rate of elastic scattering is high, as in the noble gases. In the field of gaseous radiation detectors, and the emission of photoelectrons from CsI in particular, the effect has been investigated experimentally and by

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Monte Carlo simulation, see [7-15] and references therein, where the dependence on gas and mixture composition, reduced applied electric field E/N (E is the field strength and N the number density) and incident photon energy E_{ph} was analyzed. In the broader field of swarm physics [16], which is fundamental to gas discharge and plasma physics, electron back-diffusion has been investigated for more than half a century, together with reflection effects and induced secondary emission [17-26]. In [24-26] Monte Carlo simulation was used to examine electron back-diffusion to an emitting frontier (cathode) in argon and nitrogen, showing in particular, as we also verified in [14], that transmission is very sensitive to the electron initial energy ε_0 and energy distribution profile, increasing in general with decreasing ε_0 , with full transmission for $\varepsilon_0 = 0$.

In previous work [13, 14] we have used Monte Carlo simulation to investigate the extraction efficiency f of photoelectrons emitted from a CsI photocathode into Xe, Ar, Ne and their mixtures, and in CH₄ and Ar-CH₄ mixtures, where f is the fraction of the number of photoelectrons transmitted in the gas compared to vacuum. Due essentially to the electron energy cooling effect related to vibrational excitation of the CH₄ molecules, which has a threshold at low electron impact energy, the addition of CH₄ to noble gases efficiently increases electron transmission and drift velocity. We note that f has been also referred to as *transmission efficiency*, *collection efficiency* or *escape factor* in the literature, but in the present work we adopt the more common designation *extraction efficiency*.

In the present work we extend the investigation to Xe-CH₄ and Ne-CH₄ mixtures, and compare the results for f with those previously obtained in Ar-CH₄ mixtures and in pure Ne, Ar, Xe and CH₄. The Monte Carlo results are presented in Section 3.2 for reduced electric fields in the range $E/N = 0.1$ to 40 Td (1 Td (Townsend) = 10^{-17} V cm²) when the CsI photocathode is irradiated by monochromatic VUV photons with E_{ph} in the 6.7 to 9.8 eV (185-127 nm) range. The 6.7 eV photons belong to the VUV peak of the spectral distribution of a Hg(Ar) lamp, allowing us to compare with the available experimental data for f obtained with this lamp. In addition, electron drift parameters in the pure gases Xe and Ne and their mixtures with CH₄ were calculated and are compared with experimental data from the literature in Section 3.1.

2. Monte Carlo simulation

Detailed descriptions of the simulation model used in the calculations can be found in [13-15], but a summary will be given here.

The photoelectrons are emitted from the CsI photocathode surface ($z=0$) into the gas at 1 atmosphere with initial energies ε_0 chosen either from the distributions measured in [27] when a reflective CsI photocathode was irradiated by monochromatic photons with sixteen E_{ph} values from 6.8 to 9.8 eV, or else from the specific ε_0 distribution measured in [28] when CsI was irradiated with $E_{\text{ph}}=6.7$ eV photons from the Hg(Ar) lamp. The mean values of these ε_0 distributions range from 0.2 to 2 eV. The photoelectron emission angle into the gas is sampled in $[0, \pi/2]$ from a distribution modulated by the so called *escape cone* in the solid for the given ε_0 , as required by momentum conservation when electrons cross the barrier from CsI to gas or vacuum [13, 29]. The simulation follows the drift of the individual photoelectrons in the gas under the influence of an applied uniform electric field perpendicular to the surface of the photocathode along successive free paths taking into account elastic and inelastic collisions with the gas atoms and molecules. The null-collision method [30-32] is used to reproduce the electron free paths between collisions. As in [14], all collisions with CH₄ are assumed to be isotropic, but anisotropy of elastic scattering is accounted for by using the elastic momentum transfer cross-section [33]. To be consistent, a similar formalism is adopted for the elastic collisions with Xe or Ne. The electron history ends either when it hits the photocathode, and it is counted as recaptured, or when return to the photocathode becomes energetically forbidden

(essentially when all the energy ε_0 has been lost in collisions), and it is counted as transmitted. The extraction efficiency f which is the probability that a photoelectron will reach the anode is obtained as $f=m/m_0$, where m is the number of electrons transmitted when at least $m_0=10^6$ photoelectrons are injected into the gas giving a statistical uncertainty below 1%. Note that $f=1$ in vacuum for any ε_0 , while in the gas $f=1$ for the limit $\varepsilon_0=0$. Reflection of backscattered electrons by the photocathode surface may occur [23-26], but reflection coefficients from CsI are not known and the calculations do not account for the effect.

The histories of recaptured photoelectrons often end shortly after emission into the gas, well before electrons reach equilibrium with the field (for instance, in 90Xe-10CH₄ at $E/N=1$ Td and $E_{\text{ph}}=8$ eV, our simulations indicate that recapture occurs after ~ 20 collisions and ~ 40 ps on average). For the calculations of the electron drift parameters, though, a sample of 5×10^4 electrons with initial energies $\varepsilon_0=0$ is followed in the gas allowing a long enough drift time to guarantee that the parameters reach equilibrium values [15] (~ 5 times the relaxation time, which is ~ 4 ns in the case of 90Xe-10CH₄ at $E/N=1$ Td).

The cross-sections used in the simulation for the scattering of the electrons by Xe, Ar and Ne atoms and by CH₄ molecules are represented in figure 1.

In Xe, the elastic momentum transfer cross-section is based on [34-36] below ~ 2 eV and [37, 38] above ~ 2 eV, the integral and partial cross-sections for excitation are obtained from [38] and [39], respectively, and the total ionization cross-section is from [40].

In Ne, we take the cross-section for elastic momentum transfer from [41] below 20 eV and [37] above 20 eV, and the inelastic scattering cross-sections are based on [42, 43] for integral excitation, on [39] for partial excitation and on [40, 44] for ionization.

In Ar and CH₄, the scattering cross-sections have been described in [14]; in CH₄ they are mostly based on the compilation found in [45].

The present study is focused on the extraction at low E_{ph} and ε_0 of photoelectrons from CsI into Xe-CH₄ and Ne-CH₄ gas mixtures when a low drift field (usually below multiplication threshold) is applied in the gas, but the calculations are extended somewhat, up to 40 Td for the extraction efficiency f and 100 Td for the drift parameters, neglecting eventual space charge effects.

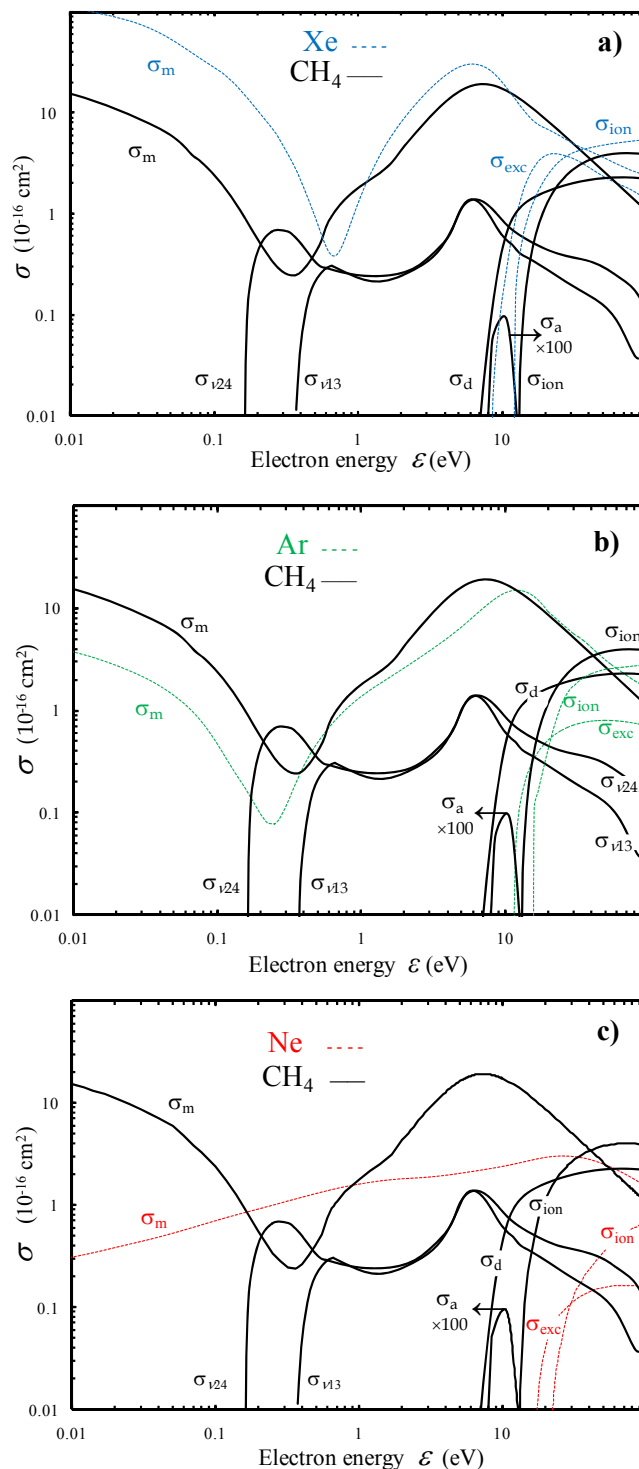


Figure 1. Electron scattering cross-sections a) in Xe and CH₄, b) in Ar and CH₄ and c) in Ne and CH₄: σ_m – elastic momentum transfer; σ_v – vibrational excitation, σ_a – electron attachment; σ_{exc} – electronic excitation; σ_d – neutral dissociation; σ_{ion} – ionization.

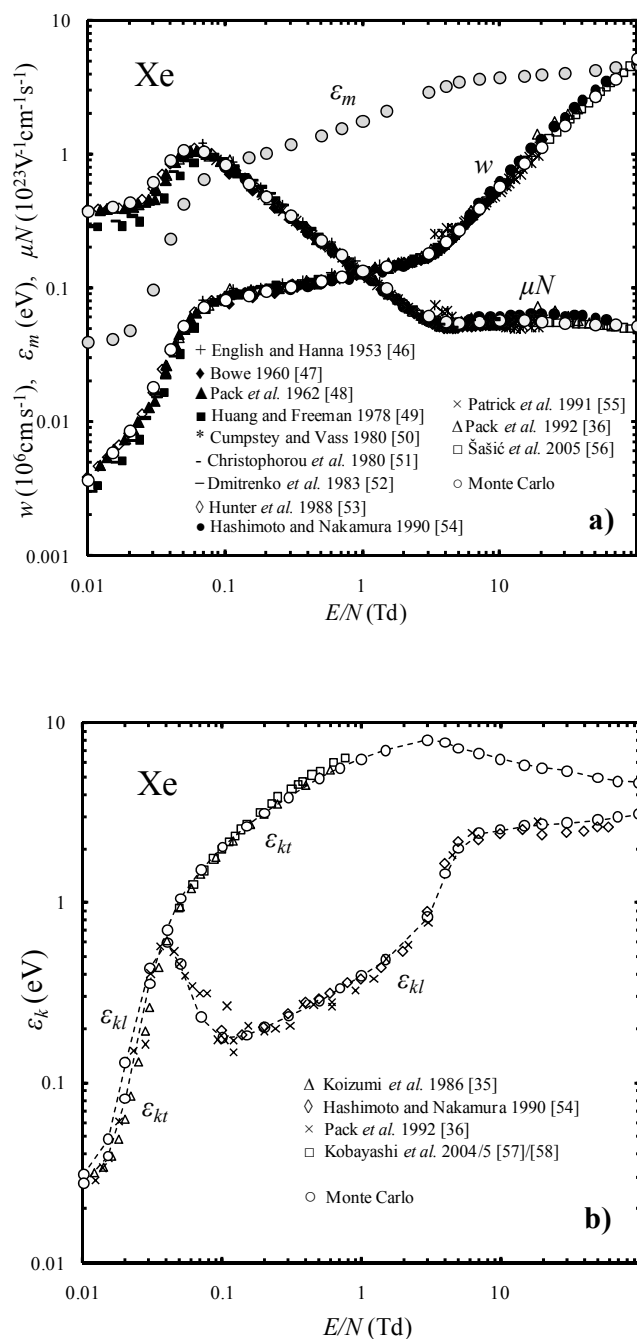


Figure 2. Monte Carlo results in Xe together with experimental data from the literature for a) electron mean energy ε_m , drift velocity w and reduced mobility μN and b) characteristic energies ε_{kl} and ε_{kt} as a function of the reduced electric field E/N . The dashed curves in b) are included to guide the eye.

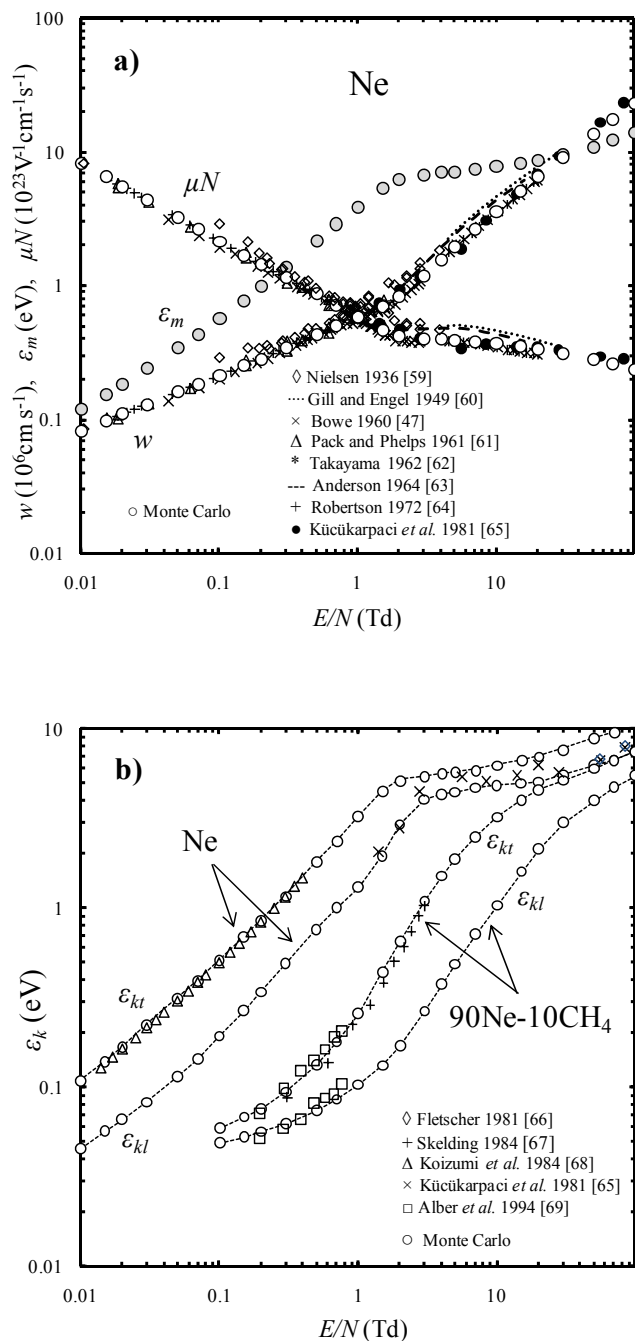


Figure 3. Monte Carlo results together with experimental data for a) electron mean energy ϵ_m , drift velocity w and reduced mobility μN in Ne, and b) characteristic energies ϵ_{kl} and ϵ_{kt} in Ne and in the 90%Ne-10%CH₄ mixture, as a function of the reduced electric field E/N . The dashed curves in b) are included to guide the eye.

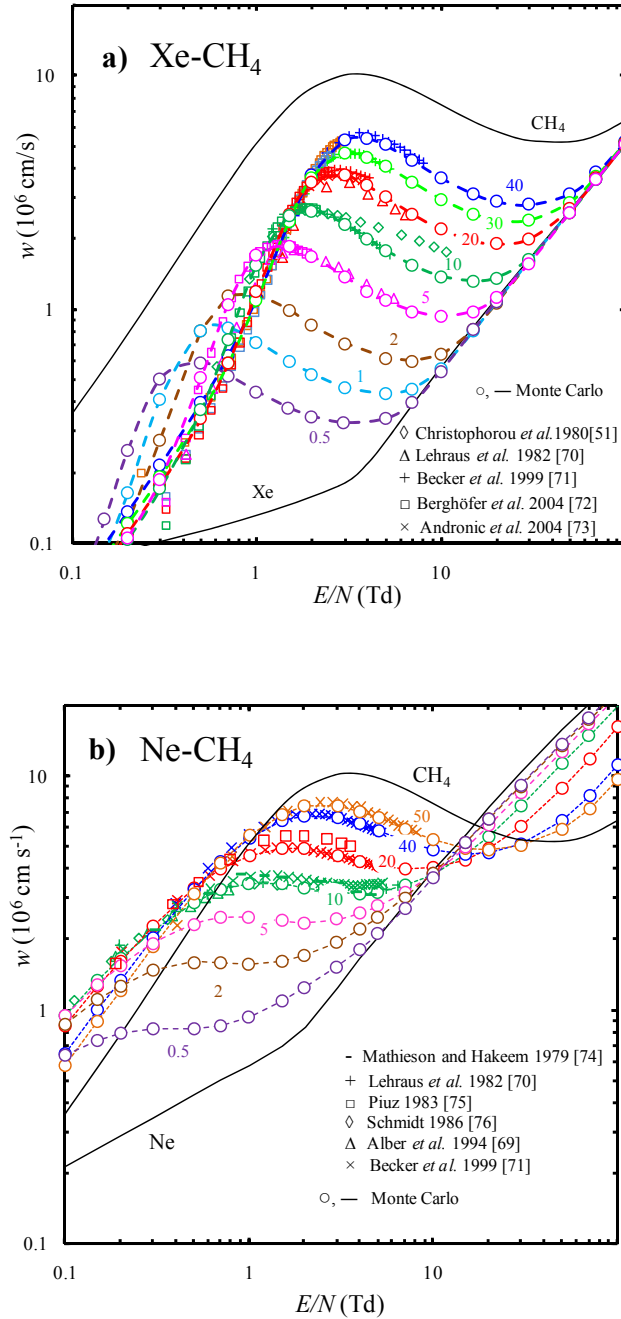


Figure 4. Monte Carlo and experimental drift velocities w as a function of reduced electric field E/N in a) Xe-CH₄ mixtures and b) Ne-CH₄ mixtures with the indicated CH₄ concentrations (%). The Monte Carlo w curves for Xe, Ne and CH₄ are also included for reference. The dashed curves are included to guide the eye.

3. Results and discussion

3.1. Electron drift parameters in Xe, Ne, and Xe-CH₄ and Ne-CH₄ mixtures

The electron scattering cross-sections used in the Monte Carlo simulation were tested by comparing the calculated drift parameters with experimental measurements. These parameters include electron mean energies ε_m , drift velocities w , reduced mobilities $\mu N = N w/E$, and characteristic energies $\varepsilon_{kl} = eD_l/\mu$ and $\varepsilon_{kt} = eD_t/\mu$, where D_l and D_t are the longitudinal and transversal diffusion coefficients. The calculations for Xe are shown together with the available experimental data in figure 2. Figure 3 shows similar results for Ne, while figure 4 has the results for the drift velocities in mixtures of Xe and Ne with CH₄. Good agreement is achieved in general. For example, in figures 2a and 3a the Monte Carlo w values in Xe and in Ne agree within 2% on average with the data from [36, 53, 56] and [62, 64, 65], respectively. Similar good agreement was found in the case of CH₄ discussed in a previous paper [14]. Although the cross-sections used in the present work may not guarantee the completeness established by the so called swarm method as usually required in gas discharge and plasma physics [77-81], figures 2 to 4 show that in the low E/N range relevant for the present work (drift fields $E/N \sim < 20$ Td near the photocathode), our calculations give sufficiently accurate drift parameters. In particular, they reproduce well known characteristic effects very sensitive to cross-sections, namely the anisotropy of diffusion when electrons drift under an electric field [36, 82-85], and negative differential conductivity [81, 86-90]. The NDC effect - a decrease of drift velocity with increasing E/N - may be observed for instance in some mixtures of noble gases with molecular additives (e.g. CH₄), due to the energy cooling of the electrons when large cross-sections for vibrational excitation emerge in the region of the Ramsauer-Townsend minima of the elastic cross-sections (see figure 1). This effect is also at the origin of the general increase in photoelectron extraction efficiency when CH₄ is added to noble gases, as shown in [14] for Ar-CH₄ and in the present work for Xe-CH₄ and Ne-CH₄ mixtures. As pointed out above and as it can be inferred from [24, 25], electron cooling is a key factor to improve the transmission of electrons emitted from a cathode into gas media.

3.2. Photoelectron extraction efficiency in Xe-CH₄ and Ne-CH₄ mixtures

3.2.1. Irradiation of CsI with monochromatic VUV photons. In this section we present the Monte Carlo results for the extraction efficiency f in Xe-CH₄ and Ne-CH₄ mixtures when the CsI photocathode is irradiated with monochromatic photons with energies E_{ph} in the 6.8 eV to 9.8 eV range. The applied electric field E/N varies from 0.1 Td to 40 Td.

The results are compared with our earlier data in Xe, Ar, Ne, CH₄, and Ar-CH₄ mixtures from [13, 14] in figures 5 and 6, one surface for each gas as labelled. The data for the pure gases are represented in figure 5a as functions of E/N and E_{ph} , while the results in Xe-CH₄, Ar-CH₄ and Ne-CH₄ mixtures are shown in figure 5b where we have taken as an example 10% CH₄ content. Results for mixtures are also shown in figure 6 as a function of E/N and CH₄ concentration η , for incident photon energies 6.8 and 9.8 eV.

In figures 5 and 6, we observe in general that f increases as we go from Xe to Ar to Ne to CH₄ or from Xe-CH₄ to Ar-CH₄ to Ne-CH₄. Note that f is higher in each mixture than in the corresponding pure rare gas. We also observe that f increases with E/N and CH₄ concentration, and f decreases with E_{ph} . However, exceptions may occur within specific regions, as observed in figures 5 and 6 (see also figures 7, 8 and 9), namely, f may increase with E_{ph} (until it reaches a maximum, as for Xe-CH₄ mixtures at low E/N and E_{ph} in figure 5b), or f may decrease with η (after rising to a maximum, as in Ar-CH₄ at low E/N and E_{ph} and in Ne-CH₄ at high E/N and E_{ph} ,

as shown respectively on figure 6a for 6.8 eV and figure 6b for 9.8 eV), or f in Ar-CH₄ may rise above f in Ne-CH₄ (for low E/N and E_{ph} , see figure 6a for 6.8 eV).

We note moreover that f increases more rapidly with E/N in CH₄ and reaches considerably higher values than in the rare gases. In addition, f increases very rapidly with the CH₄ concentration η in the mixtures when η is small and is thus very sensitive to the value of η .

The behaviour of the photoelectron extraction efficiency f in pure Xe, Ar, Ne, CH₄, and in Ar-CH₄ mixtures has been extensively discussed before for E_{ph} and E/N ranges similar to the present work [13, 14]. In general, transmission is favoured by longer penetrations λ (lower elastic scattering cross-sections) of the first free path of the photoelectrons into the gas (measured perpendicular to the photocathode), and by low photoelectron emission energy ε_0 or by a swift drop of photoelectron energy in inelastic collisions, the cooling effect we mentioned before. Similar considerations hold for the present results and may be outlined as follows.

As we go from Xe to Ar to Ne in the noble gases, f increases in general because λ and the energy losses in elastic collisions increase in that order. We note that the range of ε_0 is low, and if a photoelectron survives as far as the inelastic thresholds in Xe, Ar or Ne (8.3 eV, 11.6 eV and 16.6 eV respectively), just one inelastic collision may lower the electron energy to values ε lower than ε_0 where recapture becomes energetically forbidden. However, inelastic collisions with the noble gas atoms are infrequent for the range of E_{ph} and E/N investigated and do not contribute significantly to transmission [13, 14]. On the contrary, in CH₄ or in mixtures with CH₄ the inelastic threshold becomes much lower (0.16 eV), corresponding to vibrational excitation of the CH₄ molecules. This process competes efficiently with elastic scattering (see figure 1) and plays a decisive role in increasing photoelectron transmission: energy losses by vibrational excitation may be of the order of ε_0 , and a few vibrational collisions at an early stage can efficiently reduce electron energy and the chances of a return to the photocathode.

On the other hand, the parameter f decreases in general with the incident photon energy E_{ph} in the range investigated. This happens because photoelectrons are emitted into the gas with increasing energies ε_0 as we move to higher E_{ph} . For higher ε_0 , chances of recapture become higher by a combination of effects: firstly, because photoelectron penetration lengths λ become shorter as the scattering cross-sections σ_m rise with ε_0 (particularly after the Ramsauer minima in Ar and Xe), secondly, because larger energy losses are required to reduce the electron energy to a value that guarantees transmission.

We also note that the observed increase of f with applied electric field E/N is essentially related with increased electron guiding towards the anode as the strength of the electric field increases.

Departures of the extraction efficiency f curves from these general trends are related to the fact that a combination of effects is involved and scattering cross-sections are complex functions of electron energy. In particular, in the mixtures the overlap of the cross-sections of the two components and the effective cross-section vary a great deal from one situation to another.

For a better understanding of these effects, some selected examples of the calculated f curves at varying E/N and E_{ph} are shown along figures 7, 8 and 9, together with the corresponding inelastic ratios γ_v and penetrations λ , where $\gamma_v = n_v/n_t$ is the ratio between the number n_v of vibrational collisions with CH₄ molecules and the total number n_t of collisions in the gas, and λ is the mean distance travelled by a photoelectron in the first free path in the gas, measured perpendicular to the photocathode surface. Among the different cases, one can determine the role played by vibrational excitation collisions and by the initial penetration length of the photoelectrons into the gas as discussed above, by checking the connection between the behaviour of the plotted f curves and the curves for λ and the vibrational ratio γ_v .

3.2.2. Irradiation of CsI with a Hg(Ar) lamp. In this section, we present the Monte Carlo results obtained for the extraction efficiency f when the photocathode is irradiated with a Hg(Ar) lamp, allowing for a comparison with our experimental data from [11] and [12] where this lamp has been used. In the calculations, initial energies ε_0 of the photoelectrons are sampled from the energy distribution measured by [28] when a CsI photocathode was irradiated with photons from the VUV peak of this lamp.

The Monte Carlo results obtained in Xe, Ne, CH₄, Xe-CH₄ and Ne-CH₄ are shown in figure 10 together with the experimental measurements where we see that the measurements are consistent with the Monte Carlo predictions. The deviations from the calculated data observed at progressively lower fields at lower η values and in pure Xe or Ne are due to the effect of positive feedback from Xe or Ne self-scintillation [13], not included in the present calculated curves.

The remaining discrepancies between the Monte Carlo results and the measurements are attributed to several factors. Firstly, f is very sensitive to the photoelectron energy ε_0 and to the ε_0 distribution profile, as was shown in [14] and in [24-26], but due to different surface conditions [23] and temperature (thermionic emission [26]) on the photocathode, the photoelectron emission spectra in the measurements is not expected to exactly match the ε_0 -distribution used in the simulations (the distribution measured in [28] for the lamp). Secondly, electron reflection at the photocathode surface [23-26] (not included in the simulations) will also play a role: for instance, if a reflection coefficient of 15% is assumed, the Monte Carlo f curves in Ne-CH₄ (figure 10b) become close to the experimental data. Uncertainty in the mixture composition is an additional factor: at low E/N , f is very sensitive to even very small concentrations of CH₄, and is expected to be equally sensitive to impurity traces contaminating the mixtures. This can explain why the discrepancies between Monte Carlo and measurements in Xe-CH₄ (figure 10a) appear larger than in Ne-CH₄ (figure 10b). Finally we note that the ε_0 distribution used in the calculations of f was measured for 185 ± 0.5 nm photons from the lamp VUV peak [28] while in our f measurements the photons from the entire peak, albeit narrow ($fwhm$ 5nm), will reach the photocathode.

4. Conclusions

Backscattering of the photoelectrons emitted from a photocathode into gas medium may significantly reduce the photoelectron transmission, especially in noble gases, but the addition of a molecular gas like CH₄ significantly reduces the effect. In the present work, a Monte Carlo study of the extraction efficiency f for photoelectrons emitted from a CsI photocathode into Xe-CH₄ and Ne-CH₄ mixtures is presented. The behaviour of the results is discussed in terms of the electron scattering in the gas, analyzing the dependence of f on the mixture composition, density-reduced electric field E/N [0.1-40 Td range], and incident photon energy E_{ph} [6.7-9.8 eV (185-127 nm) range]. The calculated results are compared with earlier data in Ar-CH₄ mixtures and in the pure gases Xe, Ar, Ne and CH₄. A good agreement is found with the available experimental measurements for f when the CsI photocathode is irradiated with a Hg(Ar) lamp.

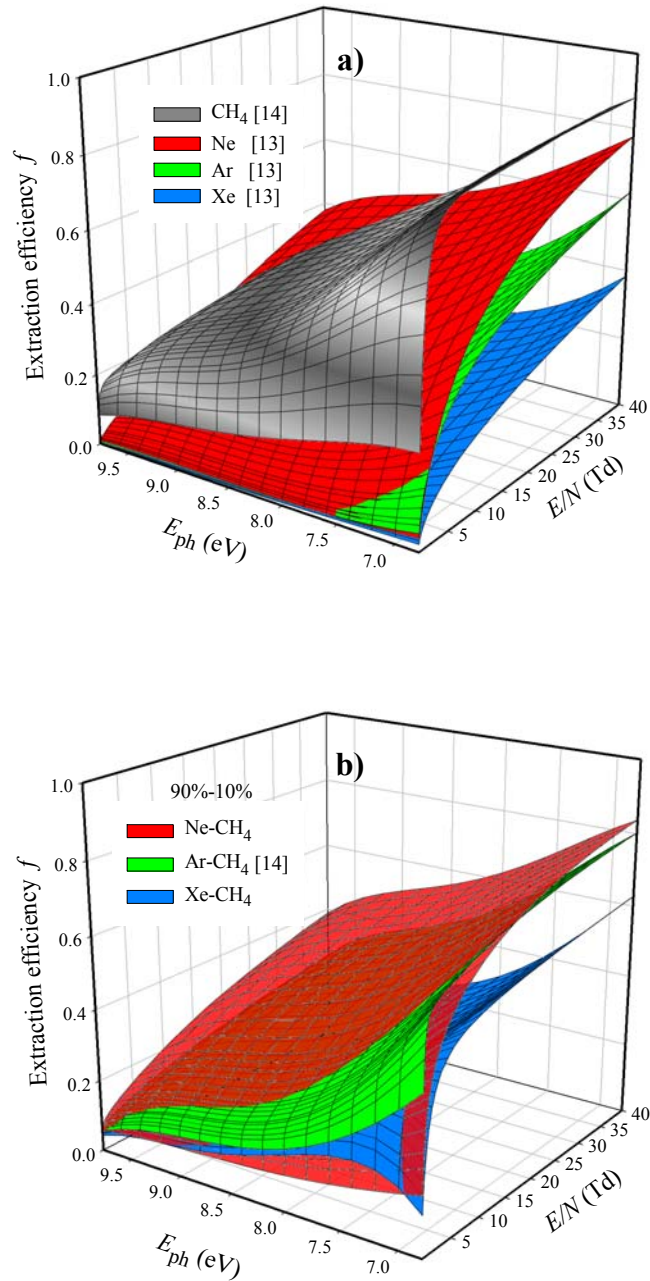


Figure 5. Monte Carlo results for the extraction efficiency f as a function of reduced electric field E/N and incident photon energy E_{ph} for photoelectrons emitted from a CsI photocathode into a) pure gases Xe, Ar, Ne and CH₄, and b) the 90%-10% Xe-CH₄, Ar-CH₄ and Ne-CH₄ mixtures.

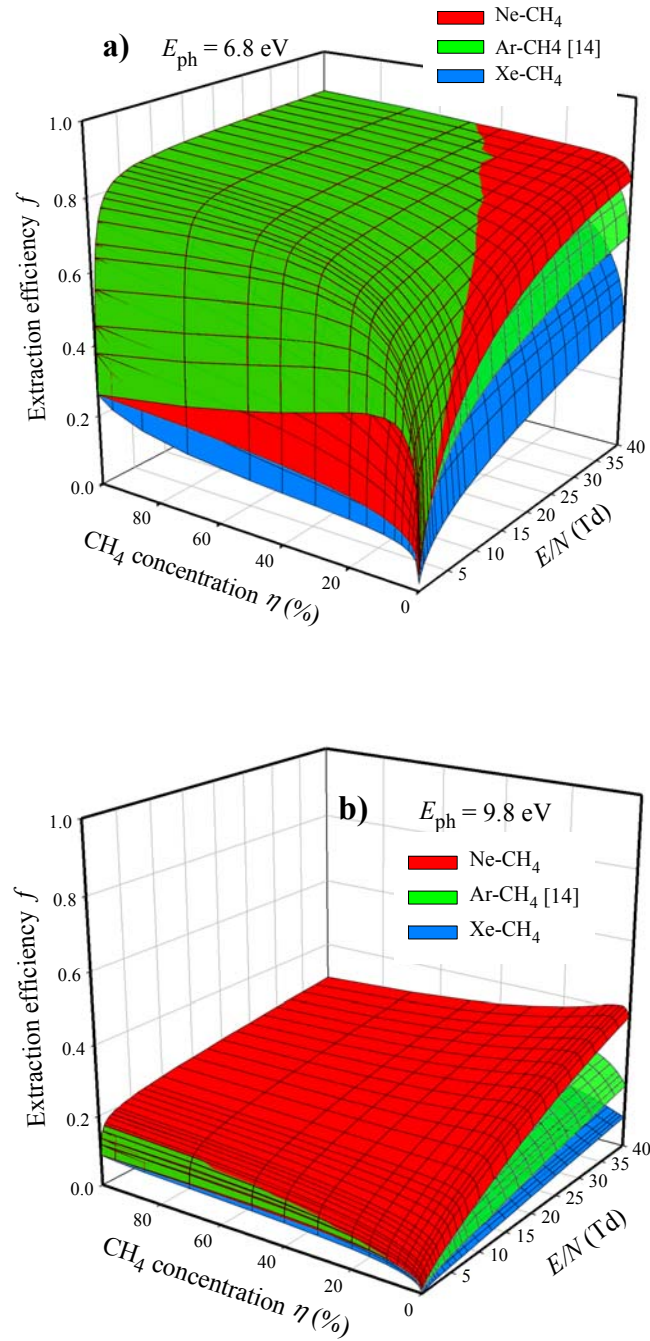


Figure 6. Monte Carlo results for the extraction efficiency f of photoelectrons emitted from a CsI photocathode into Xe-CH₄, Ar-CH₄ and Ne-CH₄ mixtures as a function of reduced electric field E/N and CH₄ concentration η for incident photon energies a) $E_{\text{ph}} = 6.8$ eV and b) $E_{\text{ph}} = 9.8$ eV.

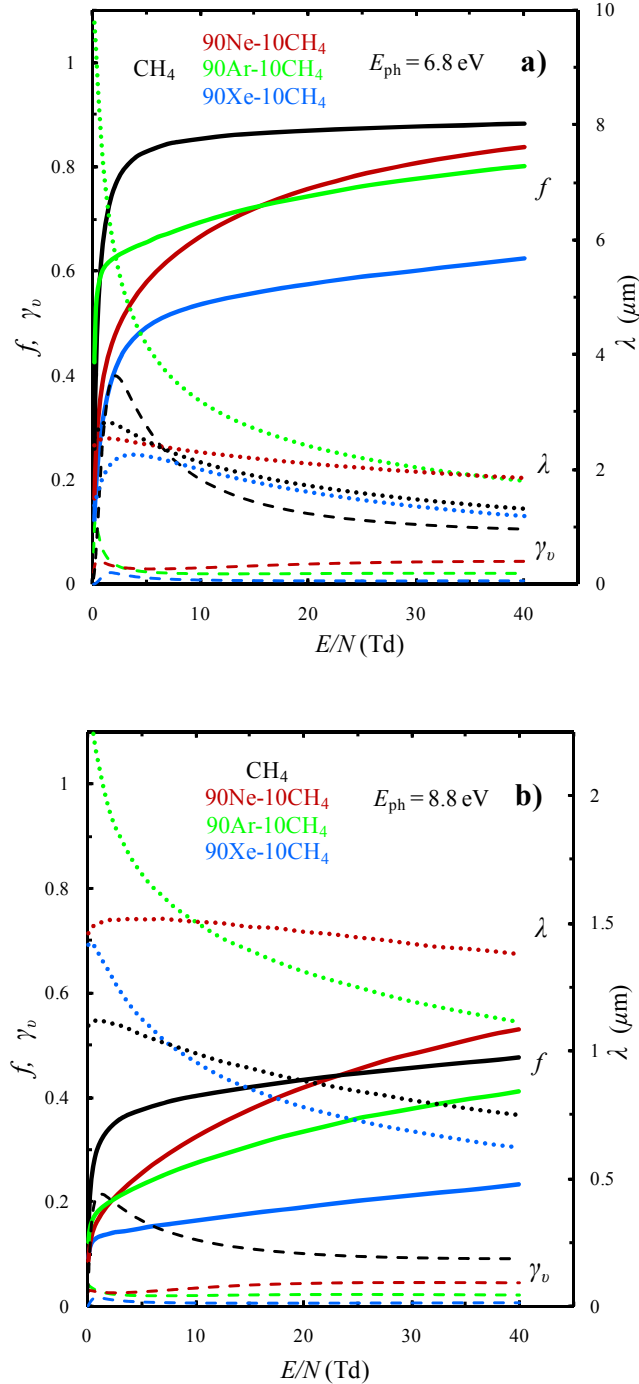


Figure 7. Monte Carlo extraction efficiency f (—) for photoelectrons emitted from CsI into CH₄ and into the 90%-10% Ne-CH₄, Ar-CH₄, Xe-CH₄ mixtures together with the corresponding photoelectron penetration λ (•••) and vibrational excitation ratio $\gamma_v = n_v/n_t$ (---), as a function of the applied electric field E/N for incident photon energies a) $E_{\text{ph}} = 6.8$ eV and b) $E_{\text{ph}} = 8.8$ eV.

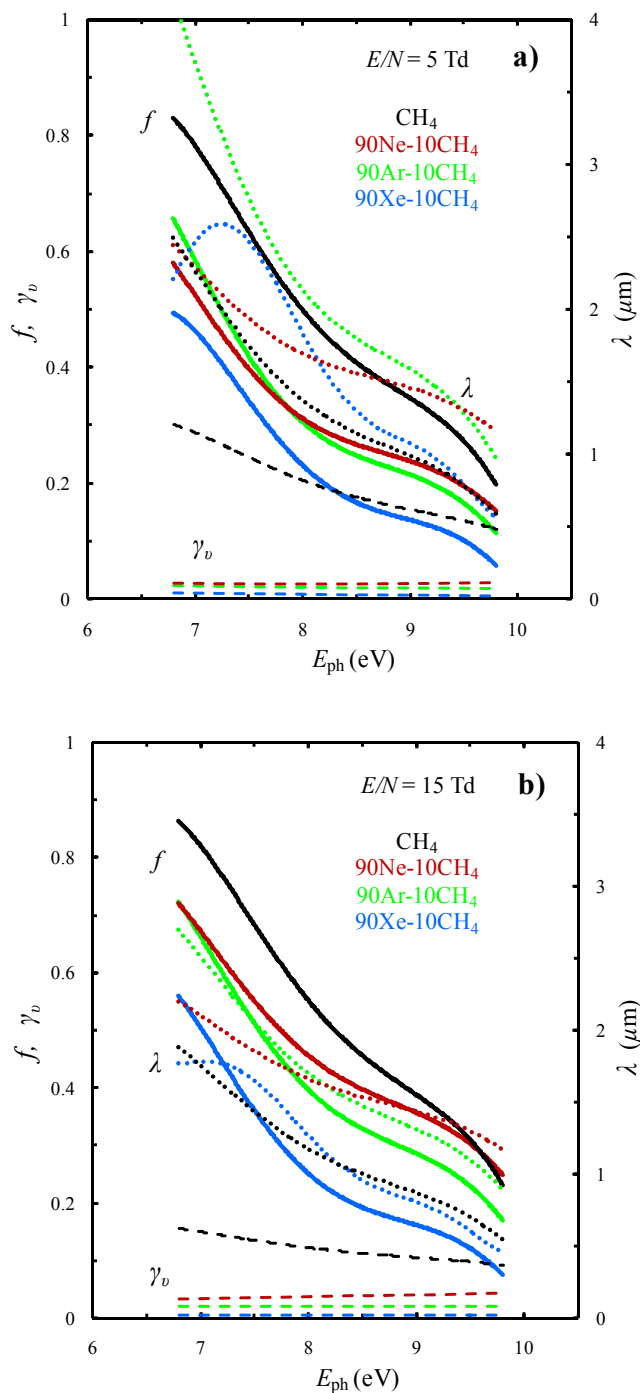


Figure 8. Monte Carlo extraction efficiency f (—) for photoelectrons emitted from CsI into CH₄ and into the 90%-10% Ne-CH₄, Ar-CH₄, Xe-CH₄ mixtures together with the corresponding photoelectron penetration λ (•••) and vibrational excitation ratio $\gamma_v = n_v/n_t$ (---), as a function of incident photon energies E_{ph} for the applied electric fields a) $E/N = 5$ Td and b) $E/N = 15$ Td.

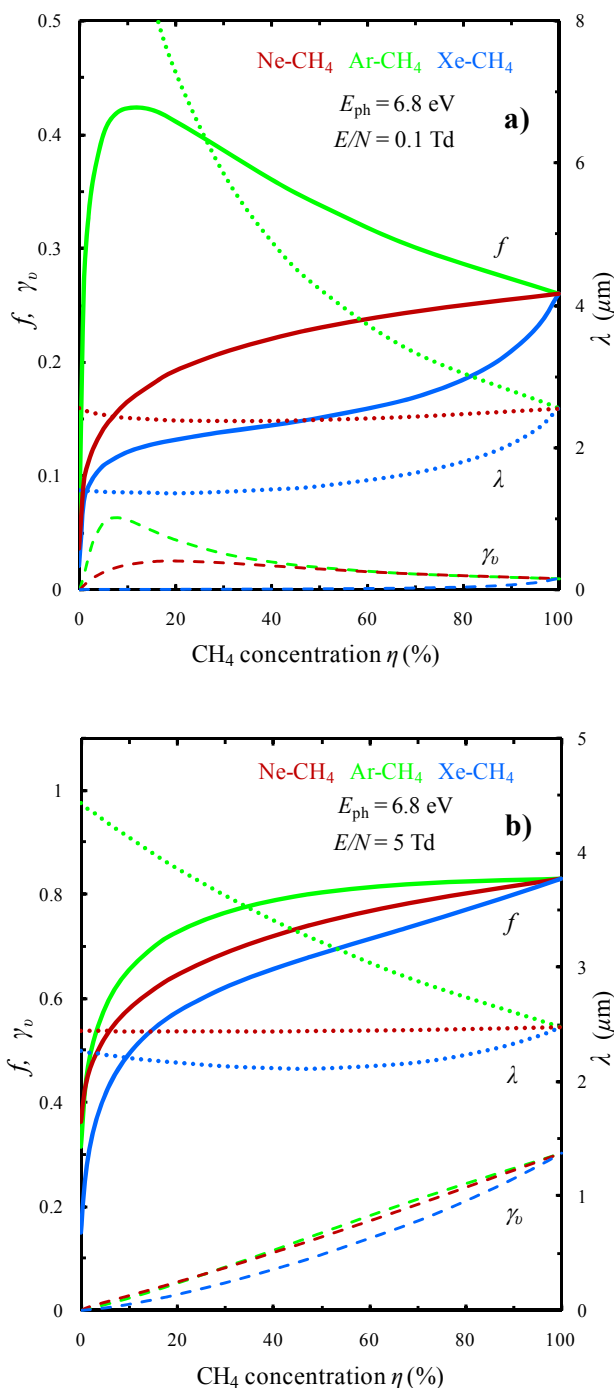


Figure 9. Monte Carlo extraction efficiency f (—) for photoelectrons emitted from CsI into Ne-CH₄, Ar-CH₄ and Xe-CH₄ mixtures together with the corresponding photoelectron penetration λ (•••) and vibrational excitation ratio $\gamma_v = n_v/n_t$ (---), as a function of CH₄ concentration η for incident photon energy $E_{\text{ph}} = 6.8$ eV and applied electric fields a) $E/N = 0.1$ Td and b) $E/N = 5$ Td.

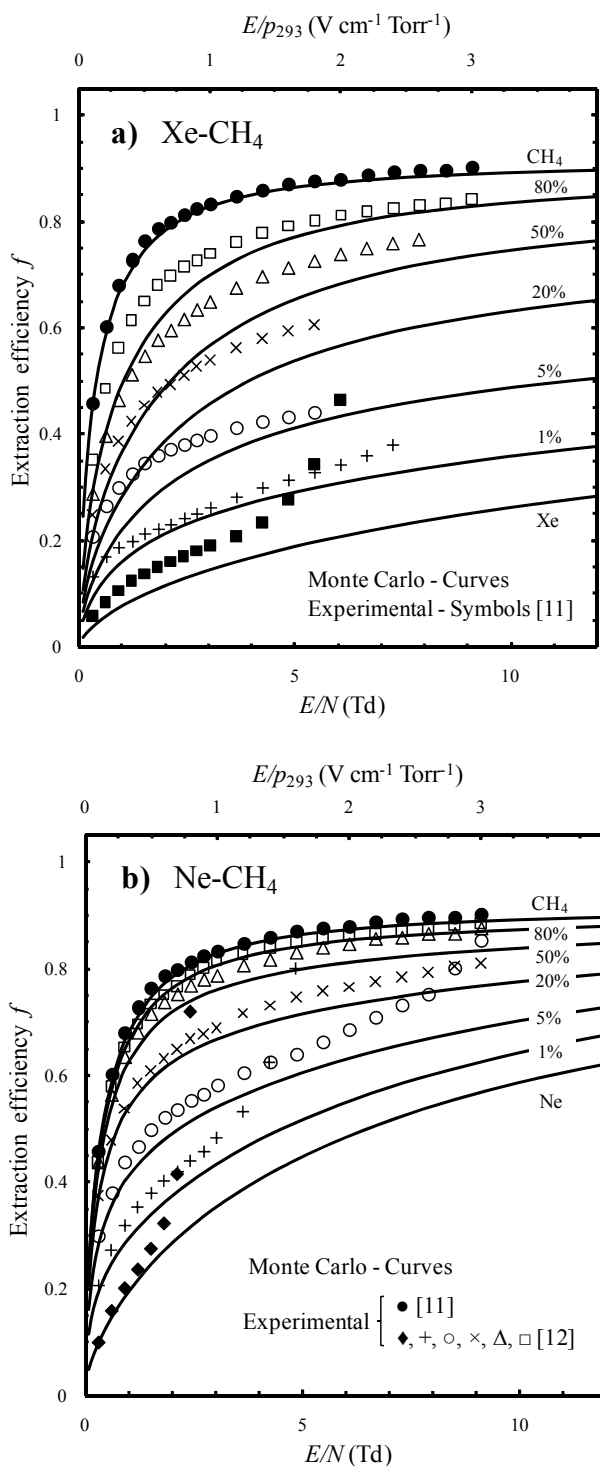


Figure 10. Monte Carlo and measured extraction efficiency f as a function of E/N for the photoelectrons emitted from CsI into a) Xe-CH₄ and b) Ne-CH₄ mixtures with the indicated CH₄ concentrations η (%) when the CsI photocathode is irradiated with a Hg(Ar) lamp. The effect of positive feedback from Xe or Ne self scintillation (not included in the Monte Carlo calculations) is visible on the experimental results in Xe, Ne and in the mixtures with lower η .

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