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ON THE USE OF RECURRENT NEURAL NETWORKS FOR FAST AND ACCURATE NON-UNIFORM GAS RADIATION MODELING

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25 **ABSTRACT** This paper focuses on the construction of a fast though accurate gas
26 radiation model based on a Recurrent Neural Network (RNN) formulation. The model is
27 founded on recent works in which a solution to a non-uniform technique proposed by
28 Godson in the 50s was derived explicitly. The method uses a non-linear transformation
29 of a set of physical / geometrical paths, directly related to a non-uniform path which is
30 first discretized into uniform sub-layers, into a sequence of equivalent absorption
31 lengths. This process, studied thoroughly within the frame of the development of the ℓ -
32 distribution approach, can be naturally handled using an algorithm that takes the form
33 of an RNN model. The method is assessed against LBL calculations in non-uniform high
34 temperature gaseous media and found to provide more accurate results than a CKD
35 (Correlated K-Distribution) model with 16 gray gases. This paper is the first to suggest
36 an RNN to treat radiative transfer in non-uniform gaseous media. Moreover, all the
37 weights involved in the RNN have a clear physical meaning so that the structure of the
38 RNN can be readily interpreted, avoiding the black box disadvantage of most brute force
39 machine learning strategies.

40

41 **Keywords:** gas radiation, Godson, ℓ -distribution, Propagative Form, Recurrent Neural
42 Network.

43

44 **1. INTRODUCTION**

45 There have been several attempts in the recent literature to apply methods based on
46 Machine Learning, including artificial neural networks, to radiative transfer and gas
47 radiation modeling. For instance, refs. [1,2], that are not strictly restricted to gaseous
48 media as considered in the present work, are two examples of application of machine
49 learning techniques to solve the RTE. More related to gas radiation, in ref. [3], a machine
50 learning strategy is used to replace look-up tables in the Full Spectrum Correlated-k
51 (FSCk) method. Applying neural networks instead of look-up tables was shown to
52 reduce significantly the overall computational cost of the FSCk method (both in terms of
53 memory requirements and computation time) without modifying the quality of the FSCk
54 model itself. More recently, in ref. [4], a feedforward neural network strategy is
55 described to model directly gas path transmissivities in atmospheric applications. Errors
56 of a few percent of the full transmission scale, *i.e.* [0,1], were obtained in this work over
57 non-uniform atmospheric paths.

58 The present work is an extension of a recent paper [5] in which a reformulation of the ℓ -
59 distribution approach in terms of neural network was mentioned but not derived in full
60 details. The aim of the present paper is to describe this formulation. The modeling
61 strategy is based on previous works in which explicit functional forms were derived for
62 the solution of Godson's implicit equation [6]. This solution is shown here to be naturally
63 written in a Recurrent Neural Network form (RNN) involving Exponential Linear Units
64 (ELU) as activation functions. The present method is, to the best of the authors'
65 knowledge, the first to consider RNNs to model non-uniform gas path transmissivities.
66 Compared to existing machine learning strategies, that apply brute force neural network
67 methods, the present formulation provides an RNN whose coefficients are fully based on
68 physical modeling. The interpretability of all coefficients appearing in the RNN model is
69 thus possible, as compared with other methods for which neural networks mostly act as
70 black boxes. The modeling strategy is applied here in the context of high temperatures
71 but it can be extended to atmospheric paths with minor modifications. It bridges an old
72 idea (from the 50s) with modern algorithmic developments in probably one of its
73 optimal ways.

74 Almost 70 years ago, in 1953 [6], Warren L. Godson introduced three methods to extend
75 uniform gas radiation models from uniform (ref. [6] was limited to Elsasser's model) to

76 non-uniform configurations. Among these methods, one of them led to the widely used
77 Curtis-Godson (CG) approximation, fully derived in 1955 within the frame of the
78 statistical narrow band model for Lorentz lines [7]. The great success of the CG
79 approximation has almost obliterated the potential of the two other methods proposed
80 in [6], even if one of them was shown from the early beginning to be superior to CG.
81 Deficiencies of the CG approximation in cases of highly non-uniform configurations were
82 observed and studied in the 70s, leading to the Lindquist-Simmons (LS) approximation
83 [8]. This method suggests a new starting point for the treatment of non-uniformities
84 based on the derivative of the transmission function with respect to the gas path length.
85 The LS method usually provides a more accurate and physical treatment of non-uniform
86 paths than CG [9], but introduces some asymmetries in the non-uniform model. A
87 compendium of existing versions of the CG and LS approximations can be found in
88 [9,10].

89 Godson's method was reintroduced in the 70s by Weinreb and Neuendorffer [11], but
90 instead of the Elsasser's model used in [6], a polynomial approximation of
91 transmissivities was applied. Several direct applications of Godson's method to
92 atmospheric configurations can be found, under the names Pseudo Mass Approximation
93 (PMA) or Emissivity Growth Approximation (EGA) in refs. [12-14]. In the high
94 temperature literature, Modest [15] uses a technique similar to Godson's method within
95 the frame of k -distribution models and calls it the Scaled- k method. No reference to
96 Godson's work is made in ref. [15]. All these works (PMA, EGA, Scaled- k) have two
97 elements in common. The first one is that Godson's method is found to be very accurate
98 when assessed against LBL calculations. When such results are available, Godson's
99 method is also found to be as accurate (in most cases more accurate) than the widely
100 used CKD method. The second one is that no one of them have attempted to justify
101 physically the reasons that could explain the accuracy of this non-uniform method.

102 The development of the ℓ -distribution approach [16] has led recently to the concept of
103 quasi-scaled spectra. This assumption, which is a physical/statistical model of
104 relationship between spectra in distinct thermophysical states, was introduced in ref.
105 [17]. It allows understanding most of the properties of Godson's method. Among them, it
106 provides an explanation of the asymmetry of Godson's method in strongly non-uniform
107 configurations, a property noticed from the early beginning, but almost absent from all

108 the papers cited previously [12-15]. This problem of asymmetry is studied in depths in
109 refs. [5,17].

110 The three techniques (Godson's, Scaled- k and ℓ -distribution methods) share similarities
111 but are fundamentally different. For instance, the Scaled- k method requires the
112 definition of a reference state of the gas whereas Godson's and ℓ -distribution methods do
113 not. The Scaled- k and Godson's methods rely on iterative techniques to find a solution of
114 the model's implicit equation (see Eq. (7) later in the paper), whereas in ℓ -distribution a
115 semi-analytical solution of the same equation is used. Consequently, the approach used
116 in ℓ -distribution allows treating non-uniform paths very efficiently, compared to the two
117 other iterative methods. In the Scaled- k and Godson's methods, the implicit equation
118 used to define an effective scaling factor is introduced without reference to any physical
119 model. In ℓ -distribution, on the other hand, the implicit equation is founded on the
120 assumption of quasi-scaling of gas spectra in distinct thermophysical states as noticed
121 previously. Additional details on how the quasi-scaling property connects with Godson's
122 method are provided later in this paper.

123 The ℓ -distribution method was up to now mostly studied in its Archimedean copula
124 version. The main advantage of such a formalism is to help understanding and
125 controlling the properties of the non-uniform model and its impact on the calculation of
126 transmissivities of non-uniform paths using known results from copula theory. Its main
127 disadvantage is to make the model probably hard to understand at first sight for possible
128 users not familiar with the concept of copula and/or gas radiation modeling.
129 Nevertheless, recently, we have shown [5] that the copula formulation of the ℓ -
130 distribution approach can be equivalently written in a propagative form, in which only
131 relationships between equivalent absorption lengths are used. The possibility to
132 reformulate the method in a neural network version was also suggested in the same
133 reference. The same mathematical results as used in the copula version of the model can
134 be applied in the propagative formulation, as they are rigorously equivalent. However,
135 the propagative version is probably simpler to understand. This propagative form,
136 including its recurrent neural network formulation, is the main focus of the present
137 work.

138 The paper is structured as follows. In the second section, the main assumptions used to
139 treat non-uniform paths in the ℓ -distribution approach are detailed. This allows
140 obtaining a definition of effective scaling factors (that is to say scaling coefficients that
141 depend on the gas path length) that coincides with Godson's method. The third section is
142 devoted to an approximation of the quantities used in the ℓ -distribution method using
143 simple relationships. The resulting uniform method, that involves a three coefficients
144 transmission model, is described and assessed against LBL calculations. The same
145 uniform cases as used in ref. [18] are treated to illustrate the quality of the
146 parameterization. The fourth section is devoted to a reformulation of the key elements
147 of Section 3 in terms of recurrent neural networks. As will be shown, the propagative
148 version of the ℓ -distribution approach can be naturally written in a neural form using
149 Exponential Linear Units (ELU) as activation functions without losing its physical
150 interpretation. This reformulation, which is the main result of the present work,
151 provides a proof of the relevance of application of RNN structures for non-uniform gas
152 radiation modeling.

153 This work, even if it is mostly restricted to a simplified though very accurate model and
154 not to real LBL datasets, is the first to suggest an RNN as a non-uniform gas model. It
155 bridges physics and statistical/machine learning points of view in probably one of its
156 optimal ways.

2. FROM SCALED / QUASI-SCALED SPECTRA TO GODSON'S METHOD

The concept of scaled spectra is among the most important ones in non-uniform gas radiation modeling. Even Correlated k -distribution (Ck / CKD) methods rely on this assumption, although the scaling coefficient is not in this case a constant for all values of the absorption coefficient, but depends on it directly. Scaling assumes a linear relationship between gas spectra in distinct thermophysical states, a property that is obviously verified at LBL scale for single wavenumbers.

The hypothesis of scaled spectra assumes the existence of a constant coefficient, written from now on U , such that the spectral absorption coefficients of the gas in two thermophysical states (subscripts 1 and 2) are related by the linear relationship:

$$\kappa_{\nu,2} = U \cdot \kappa_{\nu,1} \quad (1)$$

When gas spectra are scaled, one has for any gas path length L :

$$\tau_2^{\Delta\nu}(L) = \frac{1}{\Delta\nu} \cdot \int_{\Delta\nu} \exp(-\kappa_{\nu,2} L) d\nu = \frac{1}{\Delta\nu} \cdot \int_{\Delta\nu} \exp(-U \cdot \kappa_{\nu,1} L) d\nu = \tau_1^{\Delta\nu}(U \cdot L) \quad (2)$$

The band averaged transmissivity of a non-uniform path in the gas (length L_1 in state 1 and L_2 in state 2) is then:

$$\tau_{12}^{\Delta\nu}(L_1, L_2) = \frac{1}{\Delta\nu} \cdot \int_{\Delta\nu} \exp(-\kappa_{\nu,1} L_1 - \kappa_{\nu,2} L_2) d\nu = \tau_1^{\Delta\nu}(L_1 + U \cdot L_2) \quad (3)$$

A similar relationship can be obtained if one considers n scaled spectra.

For the analysis of more general situations for which gas spectra are not truly scaled, a slight reformulation of the scaled model is required. It is provided below.

As band averaged transmissivities are strictly decreasing functions of pathlengths over absorbing bands that do not contain transparency regions of the gas, they are invertible. This means that one can define, for any transmission function, its inverse ℓ . This is the main principle of the ℓ -distribution approach. Using this inverse ℓ , one can rewrite Eq. (3) in two equivalent forms:

- Archimedean copula c_{11} version [5,19,20]:

182 $\tau_{12}^{\Delta\nu}(L_1, L_2) = C_{11} [\tau_1^{\Delta\nu}(L_1), \tau_2^{\Delta\nu}(L_2)]$ where: $C_{11}(X, Y) = \frac{1}{\Delta\nu} \cdot \int_{\Delta\nu} \exp[-\kappa_{\nu,1} \ell_1(X) - \kappa_{\nu,1} \ell_1(Y)] d\nu$
 183 (4)

184 - Propagative version [5]:

185 $\tau_{12}^{\Delta\nu}(L_1, L_2) = \tau_1^{\Delta\nu}(L_{12})$ where: $L_{12} = L_1 + U \cdot L_2 = \ell_1 \circ \tau_1^{\Delta\nu}(L_1) + \ell_1 \circ \tau_2^{\Delta\nu}(L_2)$ (5)

186 In Eq. (5), the symbol “o” represents the functional composition, *i.e.*, given two functions
 187 f and g one has $f \circ g(x) = f[g(x)]$. In the case of truly scaled gas spectra, all three
 188 formulations provided by Eqs. (3-5) are rigorously equivalent. These relationships can
 189 be readily extended to any n layer non-uniform path and remain exact as soon as all gas
 190 spectra encountered along the non-uniform path are rigorously scaled.

191 In practice, gas spectra are not perfectly scaled. However, in the case of small gradients
 192 of temperature or pressure, it was shown in ref. [17] that real gas spectra can be
 193 considered as quasi-scaled, *i.e.*, given two distinct spectra, it is reasonable to assume that
 194 the two transmission functions can be connected to each other by:

195 $\tau_2^{\Delta\nu}(L) = \int_0^{+\infty} \tau_1^{\Delta\nu}(u \cdot L) dF(u) = \int_0^1 \tau_1^{\Delta\nu}[u(\xi) \cdot L] d\xi, F[u(\xi)] = \xi, \xi \in [0,1]$ (6)

196 in which a non-constant positive scaling coefficient u is introduced. In Eq. (6), F is the
 197 distribution function of the variable u .

198 In quasi-scaling, we thus assume that the two spectra can be related to each other by a
 199 spectral scaling function which is statistically independent from at least one of the two
 200 spectra. Obviously, if the density of the distribution function F of variable u is a Dirac,
 201 this relationship provides the scaled model.

202 Defining explicitly the variable u is complicated in a general frame unless gas spectra
 203 follow rigorously the quasi-scaled property, which is rare (almost as rare as truly
 204 correlated gas spectra). However, application of the mean value theorem to Eq. (6)
 205 shows that for any gas path length L , there exists a particular value of the variable ξ , for
 206 which the corresponding scaling coefficient, that will be from now on written $u(L)$, is
 207 such that:

208
$$\tau_2^{\Delta v}(L) = \int_0^1 \tau_1^{\Delta v}[u(\xi) \cdot L] d\xi = \tau_1^{\Delta v}[u(L) \cdot L] \quad (7)$$

209 The mean value theorem thus replaces the problem of specification of the distribution
 210 function of scaling coefficients, F , by an implicit equation that only involves as input data
 211 the uniform transmissivities. As these transmissivities are usually known (but their
 212 functional form depends on the uniform model selected), the application of the quasi-
 213 scaling assumption is always possible. This property of Godson's method was already
 214 emphasized in ref. [11]. It should be noticed that the implicit formulation of the quasi-
 215 scaling approximation is also similar to the definition of the strictly increasing function
 216 that relates the spectra in Ck / CKD method: in both cases, the explicit link between the
 217 spectra does not need to be fully specified, only its existence is assumed and its effect is
 218 formulated through an implicit relationship.

219 The implicit equation set by Eq. (7) can be solved easily using the formalism introduced
 220 recently in the ℓ -distribution approach and briefly reminded in the next section.

221

3. FROM GODSON'S METHOD TO L-DISTRIBUTION

It is out of the scope of the present paper to fully redevelop the set of equations related to the ℓ -distribution approach. Interested readers can find a comprehensive description of the technique in ref. [16]. We only remind here some of the most important results (Section 3.1) and show how, based on this general theory, one can propose simple though accurate estimate of narrow band transmissivities of high temperature gaseous paths (section 3.2). The simplified model, that involves three parameters, is first described in uniform cases and its extension to non-uniform paths is then detailed in Section 4. Several test cases in uniform scenarios are provided that illustrate the accuracy of the method when assessed against LBL calculations.

3.1. TABULATION OF UNIFORM LBL TRANSMISSIVITIES IN THE L-DISTRIBUTION METHOD

The ℓ -distribution approach can be introduced as follows. Most LBL data are provided in terms of absorption coefficients. At high spectral resolution, LBL sets contain a large number of spectral values. In many applications: 1/ there is no real interest for high resolution data as only spectral averages (from narrow bands up to the full spectrum) gas radiative properties are needed. This is the case for heat transfer applications but also for radiative imaging studies in which the band width is fixed by the imaging device, and 2/ over spectral intervals, the integral form of the radiative transfer equation involves spectrally averaged transmissivities (weighted by the Planck function in the case of wide bands or over the full spectrum). Calculating these non-uniform transmissivities using LBL data requires a two-step process: 1/ (path integral) for each wavenumber inside the band, evaluate the sum of all contributions (sum of $\kappa_{v,i} L_i$) encountered along the path and, 2 / (spectral averaging) evaluate the non-uniform transmissivity by averaging all these spectral contributions.

Based on these observations, a real gain in terms of computational cost could be expected if one could tabulate directly LBL transmissivities since one part of the process (calculation of band averaged transmissivities from high resolution LBL data) required to solve the RTE would be avoided. In other words, if LBL transmissivities could be precalculated in advance, an important reduction of the computational cost could be

252 anticipated. This is the main idea behind the uniform model used in the ℓ -distribution
 253 method.

254 In order to tabulate LBL data in transmission form, we first generate an approximate
 255 model (formally the same as the SNB model for Lorentz lines using the Malkmus'
 256 distribution of linestrengths [9] and the second order k -moment model [21]) called in
 257 refs. [5,16] the "germ" model. Its coefficients are given by the set of equations (no optical
 258 filter is considered here – more general formula involving such an optical filter are
 259 provided in ref. [5]):

$$260 \quad k_p = \frac{1}{\Delta \nu} \cdot \int_{\Delta \nu} \kappa_\nu d\nu \quad (8-a)$$

$$261 \quad k_R^{-1} = \frac{1}{\Delta \nu} \cdot \int_{\Delta \nu} \frac{d\nu}{\kappa_\nu} \quad (8-b)$$

$$262 \quad \beta = \frac{\pi}{k_p/k_R - 1} \quad (8-c)$$

263 Eqs. (8-a) and (8-b) are the definitions of the Planck and Rosseland mean absorption
 264 coefficients of the gas over the spectral band $\Delta \nu$ respectively. Eq. (8-c) is a parameter
 265 that measures the overlapping between spectral lines. Indeed, it coincides exactly with
 266 the overlapping parameter of the SNB model for Lorentz lines with Malkmus'
 267 distribution of linestrengths if the real gas spectrum follows rigorously the assumptions
 268 of this SNB model [9].

269 As can be seen from the definitions (8.a-c), all the parameters involved in the "germ"
 270 model can be evaluated as simple integrals over the absorption coefficients taken from a
 271 LBL dataset.

272 Then, one can notice that the germ model (all quantities related to the "germ" model are,
 273 as in ref. [5], represented by an index "0") is invertible and its inverse is analytical. The
 274 direct model and its inverse are given respectively as:

$$275 \quad \tau_0^{\Delta \nu} (L) = \exp \left[- \frac{\beta}{\pi} \cdot \left(\sqrt{1 + \frac{2\pi k_p L}{\beta}} - 1 \right) \right] \quad (9-a)$$

276
$$\Lambda_0^{\Delta\nu}(X) = \frac{\beta}{2\pi k_p} \cdot \left[\left(1 - \frac{\pi}{\beta} \ln X \right)^2 - 1 \right] \quad (9-b)$$

277 By definition, the inverse $\Lambda_0^{\Delta\nu}$ is such that:

278
$$\Lambda_0^{\Delta\nu} [\tau_0^{\Delta\nu}(L)] = L \quad (10)$$

279 The LBL transmissivity in the gas is defined as:

280
$$\tau^{\Delta\nu}(L) = \frac{1}{\Delta\nu} \cdot \int_{\Delta\nu} \exp(-\kappa_\nu L) d\nu \quad (11)$$

281 Using Eq. (10), we can rewrite this equation as:

282
$$\tau^{\Delta\nu}(L) = Gr [\tau_0^{\Delta\nu}(L)] \quad (12)$$

283 where, for any X in $[0,1]$:

284
$$Gr(X) = \frac{1}{\Delta\nu} \cdot \int_{\Delta\nu} \exp[-\kappa_\nu \Lambda_0^{\Delta\nu}(X)] d\nu \quad (13)$$

285 The Gr function, named the mapping function: 1/ establishes a direct relationship
 286 between the values of the germ model and the exact LBL values, 2/ maps the unit
 287 interval into itself and is strictly increasing (and thus invertible). This function can be
 288 tabulated easily (it suffices to discretize the unit interval into N subintervals and apply
 289 the definition of the Gr function Eq. (13) to generate a look-up table of Gr values). This
 290 direct tabulation method was applied in refs. [5,16,22].

291 **3.2. SIMPLIFIED L-DISTRIBUTION MODEL**

292 The main drawback of the ℓ -distribution method is its memory cost if high resolution Gr
 293 look-up tables are used (typically, 1000 values of X inside $[0,1]$ are used, ensuring an
 294 accuracy on the calculation of transmissivities much lower than 10^{-3} in uniform
 295 calculations [16]). The size of the databases used in the “standard” high temperature
 296 version, already applied in ref. [22], is given in table 1. These databases contain model
 297 parameters for 28 gas temperatures (from 300 K up to 3000 K by 100 K step) for CO_2 ,
 298 CO and H_2O . For H_2O , 9 values of molar fractions (0., 0.05, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0)
 299 are used. Only atmospheric pressure is considered here.

Molecule	CO ₂	CO	H ₂ O
Number of molar fractions	1	1	9
Number of temperatures	28	28	28
Number of spectral bands	449	194	998
Size of the look-up table (Mb)	393.4	170.0	7869.1

301 Table 1. "Standard" parameters used in the building of ℓ -distribution databases (each Gr
302 function uses 1000 values inside $[0,1]$) and the same number is used for the inverse of
303 Gr which is also tabulated – the number of molar fractions and temperatures is fixed by
304 the LBL database provided in ref. [23]. Only atmospheric pressure is considered here.

305

306 In order to reduce the memory cost of the technique, we propose in the following a
307 simple though accurate method to approximate the mapping functions (and their
308 inverse) required in the model.

309 Based on the visualization of mapping functions (see for instance the figures provided in
310 refs. [5,16]), we propose to approximate the mapping functions by simple one parameter
311 power functions, i.e.:

$$312 \quad Gr(X) = X^\lambda \quad (14)$$

313 In this case, their inverses remain simple:

$$314 \quad Gr^{-1}(X) = X^{1/\lambda} \quad (15)$$

315 Consequently, using this simple model, one can condense 2000 values for the Gr function
316 and its inverse, each based on look-up tables containing 1000 single values for each of
317 these functions, into a single coefficient λ . Parameters λ are obtained in this work as
318 solutions of the non-linear least square problem (that only involves one single variable,

319 so that any numerical method can be used to perform this minimization – in the present
 320 work, the bisection method was used to solve Eq. (16)):

$$321 \quad \lambda = \lambda_0 \text{ such that } \frac{\partial}{\partial \lambda_0} \left\{ \int_0^1 [X^{\lambda_0} - Gr(X)]^2 dX \right\} = 0 \quad (16)$$

322 This minimization problem is solved for all states in the initial model database. The size
 323 of the simplified model database after this treatment for the same molecules, set of
 324 temperatures and species concentrations used in Table 1 are given in Table 2. In the
 325 same table, the size of the CKD model for 16 gray gases is also provided for comparison.

326

Molecule	CO ₂	CO	H ₂ O
Simplified ℓ -distribution	0.6 Mb	0.3 Mb	12.3 Mb
CKD (16 gray gases)	5.3 Mb	1.81 Mb	81.1 Mb

327 Table 2. Size of the look-up tables for CKD and simplified ℓ -distribution models - the
 328 same sets of thermophysical states and spectral bands as used in table 1 are considered.

329

330 Once the coefficients λ are estimated, uniform gas path transmissivities can be evaluated
 331 as:

$$332 \quad \tau^{\Delta\nu}(L) = \exp \left[- \frac{\lambda \beta}{\pi} \cdot \left(\sqrt{1 + \frac{2\pi k_p L}{\beta}} - 1 \right) \right] \quad (17)$$

333 that follows directly from Eqs. (9-a, and 14). Their inverse is then:

$$334 \quad \ell(X) = \frac{\beta}{2\pi k_p} \cdot \left[\left(1 - \frac{\pi}{\lambda \beta} \ln X \right)^2 - 1 \right] \quad (18)$$

335 For two states (subscripts 1 and 2), the two previous relationships provide function
 336 $\ell_1 \circ \tau_2^{\Delta\nu}(L)$ as required in the propagative scheme of Eq. (5) as:

$$337 \quad \ell_1 \circ \tau_2^{\Delta\nu}(L) = s^2 \cdot \frac{k_{p,2} \beta_2}{k_{p,1} \beta_1} \cdot L + s \cdot \frac{k_{p,2}}{k_{p,1}} \cdot \left(1 - s \cdot \frac{\beta_2}{\beta_1} \right) \cdot \frac{\beta_2}{\pi k_{p,2}} \cdot \left(\sqrt{1 + \frac{2\pi k_{p,2} L}{\beta_2}} - 1 \right) \quad (19)$$

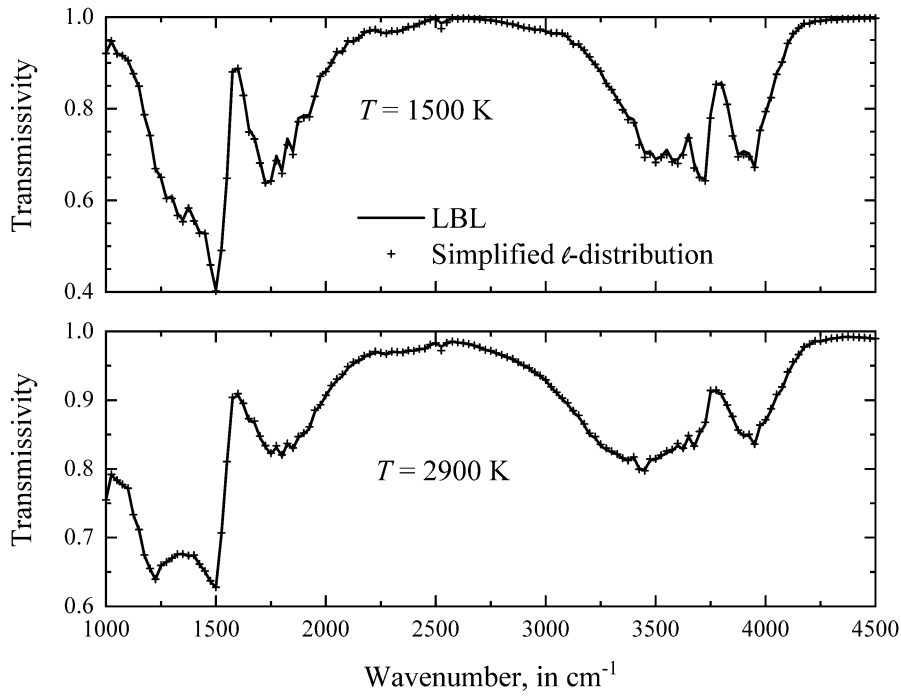
338 where:

$$339 \quad s = \frac{\lambda_2 \beta_2}{\lambda_1 \beta_1} \quad (20)$$

340 This relationship generalizes Eq. (50) of ref. [5], that corresponds to the particular case

$$341 \quad s=1. \text{ It provides the solution to Eq. (7) as } u(L) = \frac{\ell_1 \circ \tau_2^{\Delta\nu}(L)}{L}.$$

342 The set of equations (18-20) defines what will be called from now on the simplified ℓ -
343 distribution method. Examples of application of the transmissivity model set by Eq. (17)
344 in the case of uniform situations are provided in Figures 1 to 4. They are equivalent to
345 Figures 1-3 and 10 of ref. [18]. In each figure, the model is assessed against LBL
346 calculations averaged over 25 cm^{-1} , which is the width of the narrow bands used to
347 generate the simplified ℓ -distribution model parameters used in Eq. (17). The
348 comparisons between LBL and simplified ℓ -distribution results show an excellent
349 agreement, with errors lower than 1% over most parts of the spectrum. The highest
350 errors (they attain 2 percent) are observed in the band head of CO_2 near 2400 cm^{-1} in
351 the case of figure 4. These errors are due to the rather complicated behavior of the
352 mapping function Gr at this spectral location than does not allow a proper adjustment
353 using a single exponent λ to provide more accurate results. On the same cases, the use of
354 the full ℓ -distribution database provides absolute differences between LBL and the model
355 of the order of 10^{-6} . This is the same order of magnitude as already observed in Figure 3
356 of ref. [16], and the results for this model are not provided again here. This high quality
357 of the uniform ℓ -distribution model is fully related to its construction, which was shown
358 to be a tabulation of LBL data in transmission form. The main source of errors is related
359 to the interpolation of the look-up tables of the Gr functions, which is small when 1000
360 values are used over $[0,1]$ as done in the present work. The simplified version developed
361 here is noticeably less accurate, but the gain in terms of memory space is significant (see
362 tables 1 and 2) and the order of magnitude of accuracy (of the order of 1%) appears
363 sufficient for most radiative transfer calculations in high temperature gases. This level of
364 accuracy in uniform cases is comparable with the SNB model described in ref. [18].
365 Notice that most of the equations provided here to treat non-uniform paths, which is the
366 main focus of the paper, can be readily extended to the SNB model of [18], due to their
367 strong formal similarities.



368

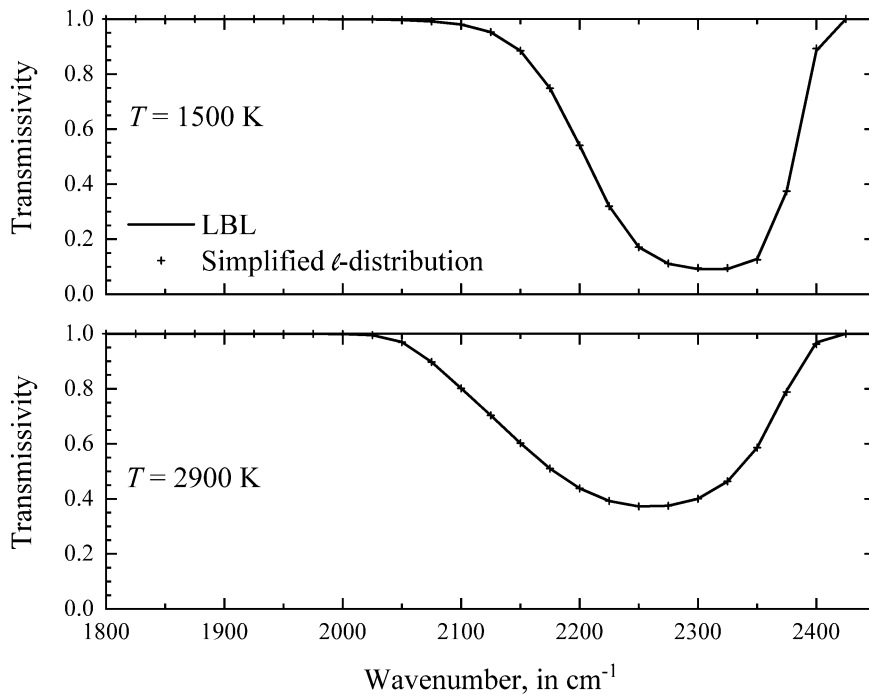
369 **Figure 1.** Transmissivities of H₂O-N₂ mixtures at 1500 K (top) and 2900 K (bottom)–

370

$x_{H_2O} = 0.1$ - length $L=10$ cm - total pressure $P=1$ atm

371

372

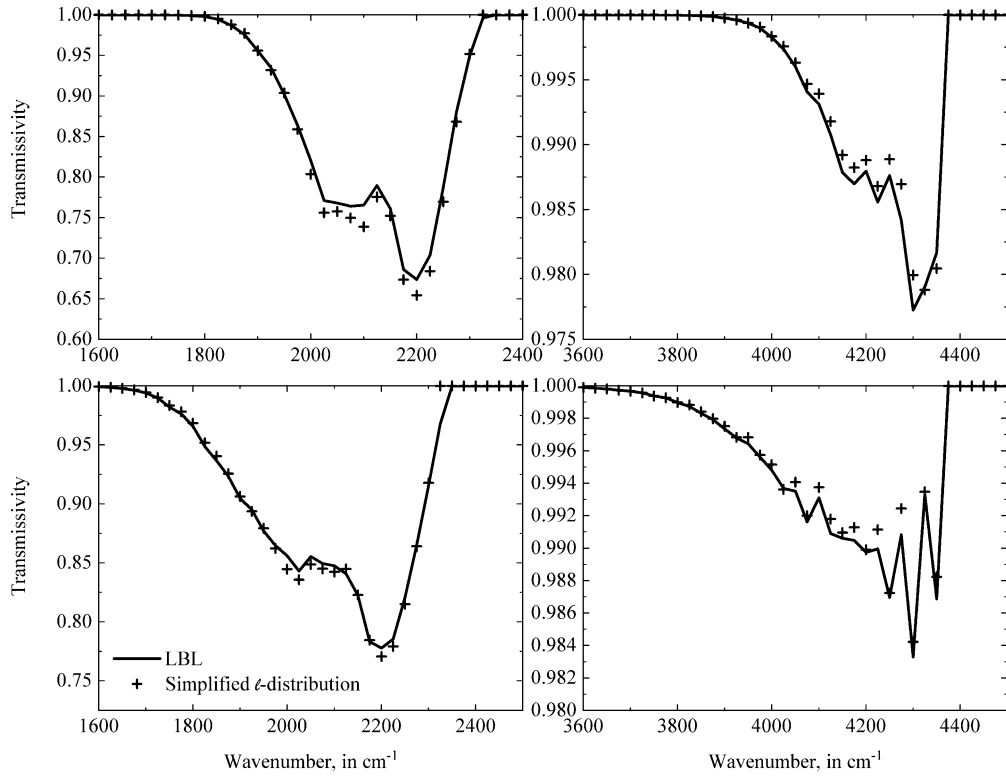


373

374 **Figure 2.** Transmissivities of CO₂-N₂ mixtures at 1500 K (top) and 2900 K (bottom) –

375

$x_{CO_2} = 0.1$ - length $L=10$ cm - total pressure $P=1$ atm



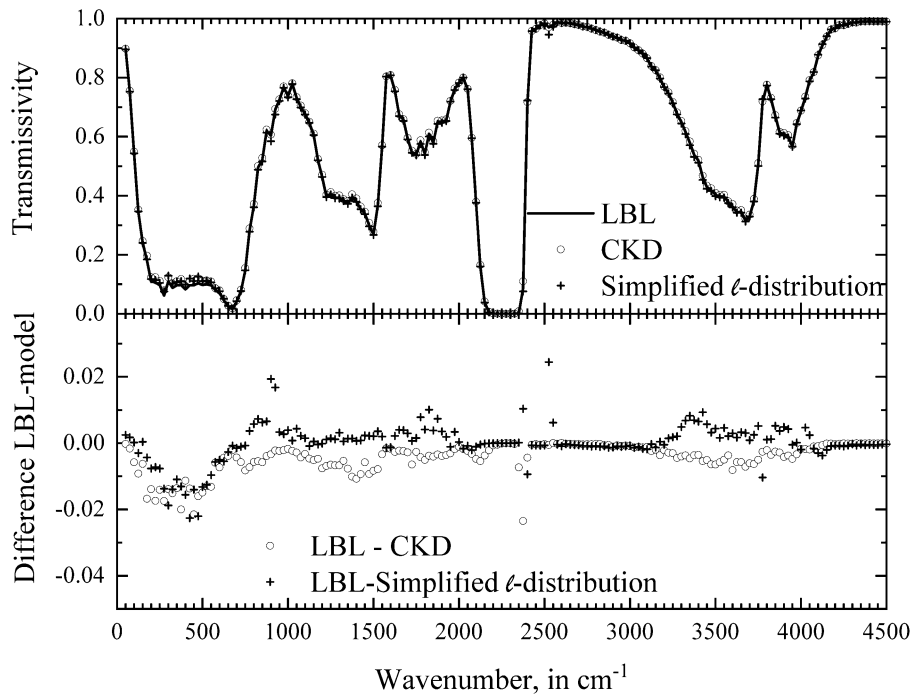
376

377 **Figure 3.** Transmissivity of CO-N₂ mixtures at 1500 K (top) and 2900 K (bottom) –

378

$x_{CO_2} = 0.01$ - length $L=1000$ cm – total pressure $P=1$ atm

379



380

381 **Figure 4.** Transmissivity of a H₂O-CO₂-N₂ mixture with $x_{H_2O}=0.2$ and $x_{CO_2}=0.1$ at 2000 K

382

– length $L=100$ cm – total pressure $P=1$ atm (top) – Absolute difference / LBL (bottom)

4. FROM L-DISTRIBUTION TO RECURRENT NEURAL NETWORKS

Methods based on neural networks have received recently an increasing interest from various fields of applied physics and engineering, including the modeling of fluid flows, signal processing, etc. As noticed in ref. [4], their applications to radiative transfer problems remain in comparison very limited. Some of them were reminded in the introduction.

The aim of artificial neural networks is to mimic the processes involved in the human brain to learn information and to perform various tasks using computers (prediction, classification, recognition, etc). Most usual neural networks appertain to one of the two following main categories [24]:

- Static neural networks: the most usual type of static networks used is called feedforward. This kind of model mostly evaluates non-linear functions of its inputs.
- Dynamic neural networks: recurrent neural networks are classical examples of this kind of methods. In this case, the model is driven by non-linear time (in our case space, as will be shown later) dependent recurrent equations. Recurrent neural networks are founded on unit cells (of the same form as feedforward networks) for which some of the outputs (called state outputs) are fed back to its inputs after applying some time delay.

A cell (or neuron) is a non-linear bounded function of its inputs. It performs two main elementary operations: 1/ it first takes its inputs and evaluate a weighted sum of these variables, including a possible bias (constant) and 2/ the result of this linear model is then modified by an activation function to introduce non-linearities. There exist various types of activation functions: sigmoidal as used in ref. [4], hyperbolic tangent, rectified linear units (ReLUs, $\text{ReLU}(x)=\text{Max}[0,x]$) as applied in ref. [3], etc. Very often, at the exit of the activation function, a second stage of the same couple of processes (linear model fed into another activation function) is used, leading to the concept of hidden layer. Hidden layers perform intermediate computations that have an important role on the quality of the whole model, but do not produce values that have a direct interest for the modeler for which only the final outputs are of importance. Once the structure (number of weights and of hidden layers) is selected and all activation functions are specified, the training of the network mostly consists of estimating the set of weights that provides the

415 best approximation of a given training set by the neural network. Identification of the
416 weights is made by application of optimization methods (more or less sophisticated least
417 square fitting process). Once the weights are known, the neural network is usually
418 assessed against a test set, that differs from the training dataset.

419 Based on this general framework, our aim is to show that the propagative scheme
420 introduced in the previous sections can be rather naturally reformulated using an
421 algorithm that is formally equivalent to a recurrent neural network. This type of
422 structure has not been apparently considered up to now for generating fast transmission
423 methods of gas radiation. However, RNN structures are usually good candidates to treat
424 dynamical systems [25] and time series [26]. It is then not surprising to find the same
425 form to be well adapted to sequences of path lengths, as encountered in the propagative
426 scheme of Eq. (5). Here, we only focus on the simplified transmission model described in
427 Section 3. This choice allows some simplifications and an analytical treatment which is
428 sufficient for the purpose of the present work. Our objective is to explain why the
429 selection of an RNN model for non-uniform gas radiation modeling is relevant, but not to
430 propose a general formulation of non-uniform gas path models as RNNs. Extensions of
431 the present developments to real LBL data are however discussed later in this section.

432 In section 4.1., we first present the concept of Exponential Linear Unit (ELU) introduced
433 in ref. [27]. Among other, we explain why this choice of activation function inside an
434 RNN structure is pertinent for non-uniform gas radiation modeling. In section 4.2., we
435 show how the propagative scheme of Eq. (5) can be rewritten in terms of ELUs and
436 discuss the corresponding algorithm. Its relationship to RNN is emphasized. Several test
437 cases in non-uniform high temperature configurations are used to compare the “direct”
438 ℓ -distribution method based on the uniform model of Section 3 together with the non-
439 uniform treatment based on the RNN version of Eq. (19), derived in Section 4.2, against
440 reference LBL calculations and a CKD model with 16 gray gases absorption coefficients.
441 Multi-layer configurations involving mixtures of CO₂-H₂O-CO-N₂ at high temperature are
442 considered for this purpose and results are detailed in Section 4.3. Finally, Section 4.4
443 provides a discussion of the present modeling strategy and explains how, based on
444 previous works, it can be extended to real LBL datasets instead of the simplified model
445 used here.

446

447

448 **4.1. THE EXPONENTIAL LINEAR UNIT (ELU)**

449 Activation functions are key components of artificial neural networks. For non-uniform
450 gas radiation modeling, Exponential Linear Units (ELUs) have interesting properties.
451 They are detailed here.

452 Exponential Linear Units were introduced recently [27] to be used as activation function
453 in Neural Networks. Their application was found to speed up learning in deep neural
454 networks and improve their classification accuracies. This activation function was
455 shown in ref. [27] to outperform other activation functions on different vision datasets.

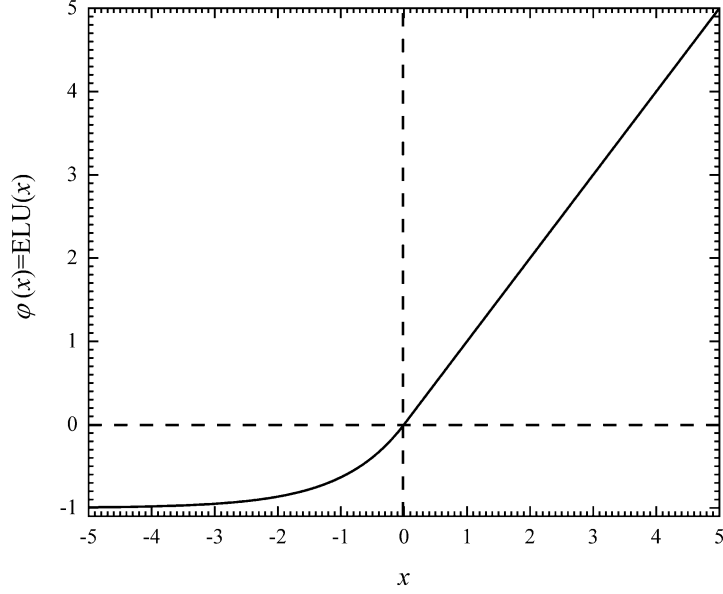
456 These units are similar to rectified linear units (ReLUs), initially introduced within the
457 frame of Boltzmann machines [28]. Compared to ReLUs that are non-negative and thus
458 have a mean activation larger than zero, ELU have a negative component, which
459 decreases the so-called bias shift effect that consists of introducing some possibly
460 artificial bias shift in the next units along the network. A bias shift is a constant that is
461 added to the linear model (weighted average of the inputs) before to enter the activation
462 function.

463 The Exponential Linear Unit with coefficient $\alpha > 0$ is defined as:

$$464 \quad \varphi_{\alpha}(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha (\exp(x) - 1) & \text{if } x \leq 0 \end{cases} \quad (21)$$

465 In order to abridge the notations, we will use from now on the notation $\varphi(x) = \varphi_1(x)$.

466 Properties of ELU (derivative, etc) useful for the design of neural networks are provided
467 in ref. [27]. The function $\varphi(x) = \varphi_1(x)$ is depicted in Figure 5. As can be seen, for
468 negative values of the variable x , the ELU activation function converges slowly toward a
469 negative value.



470

471

Figure 5. The Exponential Linear Unit (ELU)

472

473 The use of ELUs to model gas radiative properties is rather natural, if one notices that
 474 the emissivity of a gas path of length L in the gas is (here in Full Spectrum form):

475
$$\varepsilon(L) = \frac{\pi}{\sigma T^4} \int_0^{+\infty} [1 - \exp(-\kappa_\nu L)] I_{b\nu}(T) d\nu = -\frac{\pi}{\sigma T^4} \int_0^{+\infty} \varphi(-\kappa_\nu L) I_{b\nu}(T) d\nu \quad (22)$$

476 Many existing methods founded on gas path emissivities, including k -distribution and
 477 WSGG models for instance, can thus be considered technically as particular types of
 478 Neural Networks (of the projection pursuit form [29]) involving ELUs. As will be shown
 479 in the next section, the same ELUs can be used to treat path non-uniformities. For this
 480 purpose, we will show how formula Eq. (19) can be rewritten in terms of a two layer
 481 neural network based on ELUs. The resulting propagative scheme of Sections 2-3 will
 482 then be proved to be mathematically equivalent to an RNN constructed with the help of
 483 ELU activation functions.

484 **4.2. REFORMULATION OF THE L-DISTRIBUTION PROPAGATIVE SCHEME AS**
 485 **A RECURRENT NEURAL NETWORK.**

486 Conceptually, the propagative scheme used in the ℓ -distribution approach converts a
 487 sequence of geometrical gas path lengths $\{L_1, L_2, \dots, L_n\}$ into another sequence of

488 equivalent absorption lengths $\{L_{1..n}, L_{2..n}, \dots, L_{nn}\}$. These equivalent absorption lengths
 489 are defined by the recurrence relationships [5], as a generalization of Eq. (5) that is
 490 limited to two layers:

$$491 \quad \begin{cases} L_{nn} = L_n \\ L_{i..n} = L_i + \ell_i \circ \tau_{i+1}^{\Delta v}(L_{i+1..n}) \end{cases} \quad (23)$$

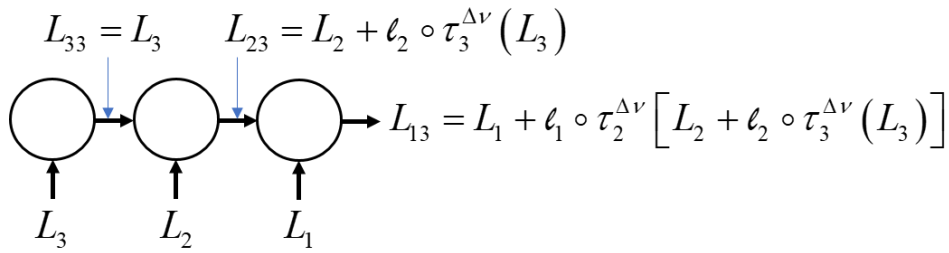
492 As soon as the equivalent absorption path length $L_{1..n}$ is calculated, the transmissivity of
 493 the path $L_1 + L_2 + \dots + L_n$ is then:

$$494 \quad \tau_{1..n}^{\Delta v}(L_1, \dots, L_n) = \tau_1^{\Delta v}(L_{1..n}) \quad (24)$$

495 Any model can be used to calculate $\tau_i^{\Delta v}$. In the present work the uniform model of Eq.
 496 (17) is applied.

497 The propagative scheme can be written in the same form as an RNN, as depicted in
 498 Figure 6 for 3 layers (the general case is a direct generalization of this scheme). This
 499 requires each cell (circle) in the graph to evaluate a function of the form of
 500 $L_i + \ell_i \circ \tau_{i+1}^{\Delta v}(L_{i+1..n})$. Obviously, this necessitates that $L_{n+1..n} = 0$, *i.e.*, the left input on the cell
 501 of the left (this input is not depicted in the figure) is 0.

502



503

504 **Figure 6.** Architecture of a RNN equivalent to the propagative scheme – each cell (circle)
 505 calculates a function of the form $L_{i..n} = L_i + \ell_i \circ \tau_{i+1}^{\Delta v}(L_{i+1..n})$.

506

507 In order to provide a direct reformulation of the propagative scheme of Figure 6 as an
 508 RNN written in terms of ELUs, we first notice that, using the same notations as in Eq.
 509 (19):

510
$$\left(1 + \frac{2\pi k_{p,2}L}{\beta_2}\right)^{-1/2} = \frac{1}{\sqrt{\pi}} \cdot \int_0^{+\infty} y^{-1/2} \exp(-y) \cdot e^{-y \cdot \frac{2\pi k_{p,2}L}{\beta_2}} dy \quad (25)$$

511 If one then uses a Gauss-Legendre quadrature at order N over $[0,1]$, and write
 512 x_j , $j = 1, \dots, N$ and ω_j , $j = 1, \dots, N$ its nodes and weights respectively, it is easy to check
 513 that:

514
$$\left(1 + \frac{2\pi k_{p,2}L}{\beta_2}\right)^{-1/2} \approx \sum_{j=1}^N \omega_j \cdot \exp\left(-u_j \cdot \frac{2\pi k_{p,2}L}{\beta_2}\right) \quad (26)$$

515 where coefficients u_j , $j = 1, \dots, N$ are solutions of:

516
$$P(1/2; u_j) = x_j, \quad j = 1, \dots, N \quad (27)$$

517 in which:

518
$$P(a; u) = \frac{1}{\Gamma(a)} \int_0^u t^{a-1} \exp(-t) dt \quad (28)$$

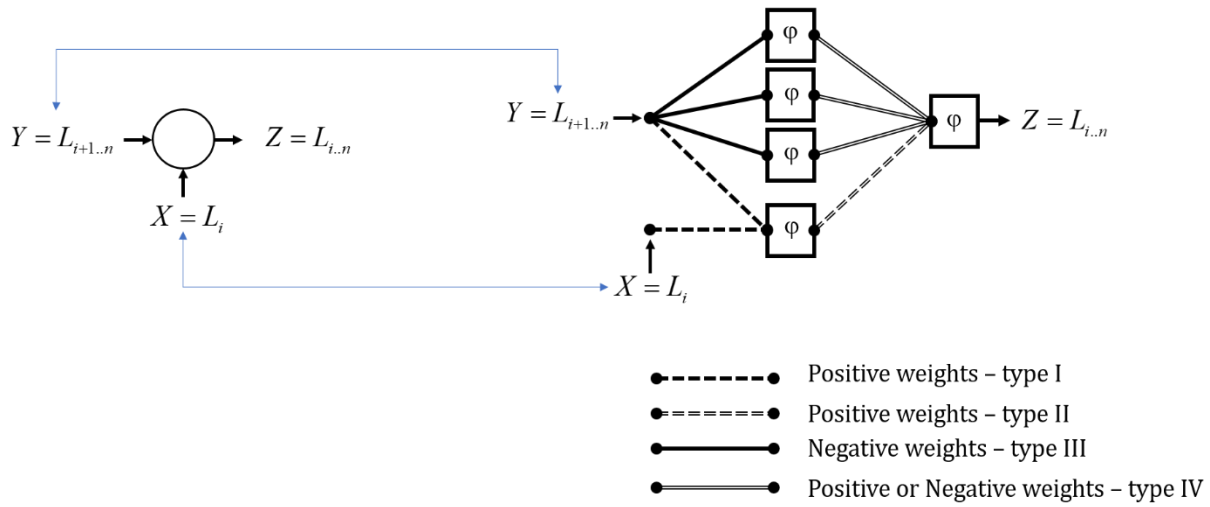
519 is the incomplete Gamma function [30]. In the present work, this function was evaluated
 520 with routines provided in ref. [31] and solutions of Eq. (27) were obtained using the
 521 bisection method.

522 Eq. (26) can then be integrated with respect to the gas path length between 0 and L to
 523 yield:

524
$$\sqrt{1 + \frac{2\pi k_{p,2}L}{\beta_2}} - 1 \approx -\frac{1}{2} \cdot \sum_{j=1}^N \frac{\omega_j}{u_j} \cdot \varphi\left(-u_j \cdot \frac{2\pi k_{p,2}L}{\beta_2}\right) \quad (29)$$

525 This quantity corresponds to the last term at the RHS of Eq. (19). Based on this last
 526 relationship together with Eq. (19), we can eventually formalize the process in each of
 527 the cells of figure 6 in terms of ELUs. This is depicted in figure 7.

528 The specification of the weights that appear in the RNN model of Eq. (29) and figure 7
 529 mostly consists of the evaluation of the quantities u_j , $j = 1, \dots, N$. This means that solving
 530 Eq. (27) is equivalent to a learning stage as it provides all the weights required in the
 531 model. Additional details on this learning stage and on its extension to the case of real
 532 LBL data instead of the simplified model used here are provided later in section 4.4.



534

535 **Figure 7.** Details on the cells (circles) involved in Figure 6 for $N=3$

536

537 As shown in figure 7 (where the quadrature order N is 3, which explains the number of
 538 squares at the top of figure 7. In the case of a general quadrature order N , the total
 539 number of squares in figure 7 would be $N+2$), 4 types of weights are used (they follow
 540 directly from Eqs. (19,20,26)):

541 - type I weights are of the form: $\left\{ 1, s_i^2 \frac{k_{p,i+1} \beta_{i+1}}{k_{p,i} \beta_i} \right\}$. This branch combines its two inputs L_i

542 and $L_{i+1..n}$ to calculate $L_i + s_i^2 \cdot \frac{k_{p,i+1} \beta_{i+1}}{k_{p,i} \beta_i} \cdot L_{i+1..n}$ (related to the first term at the RHS of Eq.

543 (19)).

544 - type III weights are of the form: $-u_j \cdot \frac{2\pi k_{p,i+1}}{\beta_{i+1}}$. At the exit of the three squares on the top

545 of figure 7, we thus have $\varphi \left(-u_j \cdot \frac{2\pi k_{p,i+1} L_{i+1..n}}{\beta_{i+1}} \right) = \exp \left(-u_j \cdot \frac{2\pi k_{p,i+1} L_{i+1..n}}{\beta_{i+1}} \right) - 1$

546 - type IV weights are of the form $-s_i \cdot \frac{k_{p,i+1}}{k_{p,i}} \cdot \left(1 - s_i \cdot \frac{\beta_{i+1}}{\beta_i} \right) \cdot \frac{\beta_{i+1}}{2\pi k_{p,i+1}} \cdot \frac{\omega_j}{u_j}$. These weights can

547 be positive or negative, depending on the sign of the quantities inside the brackets. In
 548 case of strong gradients of temperatures and species concentrations, it was shown in ref.

549 [17] that negative weights should be preferred, requiring possibly a reorganization of
550 the treatment of the layers along the path as explained in ref. [5]. In the test cases
551 considered here and detailed in the next section, only small gradients of temperature
552 and species concentrations are considered between successive layers and this possible
553 problem of asymmetries is not further discussed.

554 - type II weight is 1.

555 Based on these relationships, one can readily check that at the output of each cell, each
556 of which being equivalent to a feedforward neural network whose state output [24] is
557 $z = L_{i,n}$, we receive exactly the same quantity as calculated through Eq. (19). This proves
558 the equivalence between the iterative scheme of Eq. (5) and the graphical algorithm set
559 by figures 6 and 7. Obviously, the use of this algorithm in the case of the simplified
560 transmission model of section 3 is questionable, as an analytical solution, provided by
561 Eq. (19), exists. But its application to more general gas path transmissivities based on
562 LBL calculations instead of the simplified model of Section 3.2 is possible, as studied in
563 ref. [17]. This extension is discussed later, in section 4.4. Examples of application in non-
564 uniform configurations for various choices of the order of the quadrature N are provided
565 in the next section. They illustrate the relevance of the proposed methodology and
566 validate the applicability of the formulation in terms of recurrent neural network in
567 radiative transfer applications.

568 **4.3. APPLICATION IN NON-UNIFORM CONFIGURATIONS**

569 Test cases of the simplified ℓ -distribution model in uniform configurations were already
570 provided in section 3, and shown to yield excellent accuracy when assessed against LBL
571 calculations. In the present section, we evaluate the same model both against reference
572 LBL calculations and a CKD model with 16 gray gases based on a Gauss-Legendre
573 quadrature. For the CKD model, the double (in cases of mixtures of CO₂, H₂O and N₂) and
574 triple (in cases of mixtures of CO₂, CO, H₂O and N₂) integration methods were used to
575 treat mixtures of absorbing species. Here, we only focus on the accuracy of the non-
576 uniform model so that the use of these schemes to handle mixtures in the CKD method is
577 acceptable. However, in order to provide details on the calculation costs and make a fair
578 comparison of the methods in terms of CPU time, a specific version of the CKD model
579 was also written to allow application of the uncorrelated assumption of transmissivities

580 [9] to treat mixtures of absorbing species. This CKD model is only used for this CPU time
 581 analysis as it provides exactly the same results as the method described earlier, but was
 582 restricted to binary mixtures of absorbing species (instead of three for the CKD model
 583 described earlier). Results are provided in Table 3 in the case C1 (non-isothermal
 584 mixture of CO₂ and H₂O) detailed below, with 200 uniform sub-layers along a non-
 585 uniform path. The CPU times corresponds to 10⁵ single narrow band (including both CO₂
 586 and H₂O absorption) calculations. The simplified ℓ -distribution model is thus about 2.5
 587 time more efficient than the CKD model with 16 gray gases.

Model	CPU time
CKD with 16 gray gases	25 s
ℓ -distribution	15 s
Simplified ℓ -distribution	11 s

588 Table 3. CPU time comparisons for 10⁵ single narrow band calculations (200 uniform
 589 sub-paths per non-uniform ray).

590

591 As profiles of temperatures and species concentrations are considered in the following
 592 cases, a few words about the interpolation technique used in the simplified ℓ -distribution
 593 method are needed. This model depends on 3 coefficients, as shown in Eq. (17). The first
 594 two coefficients are mean (Planck and Rosseland) absorption coefficients of the gas.
 595 These coefficients are interpolated to any state not included in the database linearly
 596 with respect to the temperature in the CO and CO₂ cases, bi-linearly with respect to
 597 temperature and H₂O molar fraction in the case of water vapor. The same linear and bi-
 598 linear schemes were used for λ . This very simple method will be shown to provide
 599 accurate results in the test cases considered in this study.

600 The first two non-uniform cases (C1 and C2) were taken from ref. [22] (C1) and ref. [32]
 601 (C2) respectively. Case C3 was proposed recently by Wang in ref. [33]. Based on this
 602 configuration, two total path lengths (C3: 10 cm and C4: 100 cm) are considered. In all
 603 cases, non-uniform paths are divided into 200 uniform sub-paths and the same
 604 discretization is used for all gas radiation methods. Radiative intensities are evaluated at
 605 the location $l=L$. Concerning the simplified ℓ -distribution model, its two formulations are
 606 evaluated: the first one will be referred to as its direct formulation, based on Eq. (19) to

607 treat non-uniformities; the second one will be called RNN and is based on the
 608 formulation described in section 4.2. Various orders of quadrature N (see Eqs. (26-29)),
 609 from 4 (results for a quadrature order of 1 are of poor quality, reason why they are not
 610 provided here) up to 256 are used for the comparisons between the direct model and its
 611 RNN reformulation. Line of sight (0D) calculations are performed.

612 4.3.1. Case C1

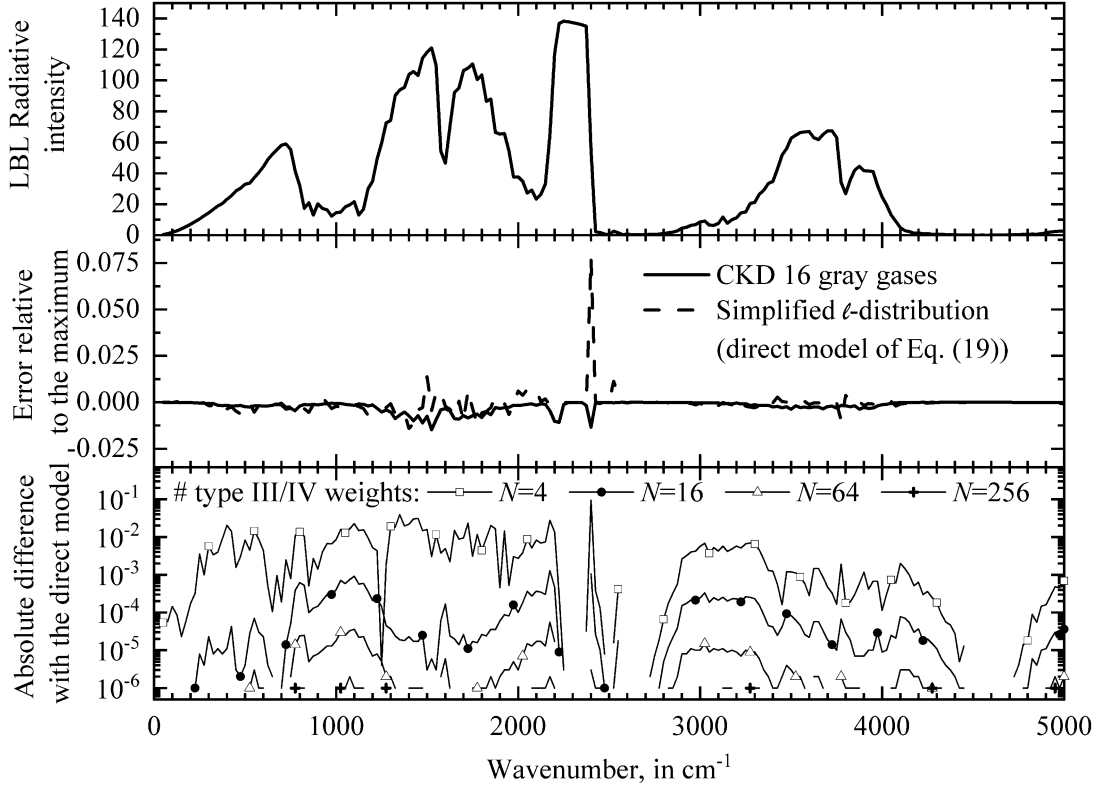
613 In case C1, the profiles of temperature and species concentrations are given as:

$$\begin{cases} T(l) = 700 \text{ K} - 300 \text{ K} \times \cos\left(\frac{\pi l}{L}\right) \\ x_{H_2O}(l) = 0.2 - 0.15 \times \cos\left(\frac{\pi l}{L}\right) \\ x_{CO_2}(l) = \frac{2}{3} x_{H_2O}(l) \end{cases} \quad (30)$$

614

615 where the total distance of the path is $L=300$ cm.

616 Results are depicted in Figure 8. All subsequent figures (from 8 to 11) use the same
 617 structure. On the top, radiative intensities in $W/m^2/sr$ calculated LBL and averaged over
 618 narrow bands (25 cm^{-1}) are provided. In the middle, the difference between the LBL
 619 intensity and its approximate model value (either based on CKD or simplified ℓ -
 620 distribution) divided by the maximum value of narrow band averaged LBL intensity is
 621 given. This choice was made to avoid possible divisions by small values in almost
 622 transparent zones. At the bottom, differences (absolute value of the difference between
 623 band averaged intensities, in log-scale) between the direct non-uniform model and its
 624 RNN approximation for various orders of the quadrature N are given.



625

626

Figure 8. Intercomparison of radiative intensities in Case C1.

627

From Figure 8, one can notice that the overall quality of the simplified ℓ -distribution

628

method is comparable with the CKD model. Only at 2400 cm^{-1} , in the band head of CO_2 ,

629

errors are above 2%, for the same reasons as in the cases of section 3.2. In terms of total

630

intensity, the LBL model provides 6925 $\text{W}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}$, 6870 $\text{W}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}$ (0.8 % / LBL) for

631

CKD and 6910 $\text{W}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}$ (0.2 % / LBL) for the direct simplified ℓ -distribution model. For

632

$N=16$, the difference between the direct model and its RNN version is lower than 0.02

633

$\text{W}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}$ for the calculation of the total intensity.

634

4.3.2. Case C2

635

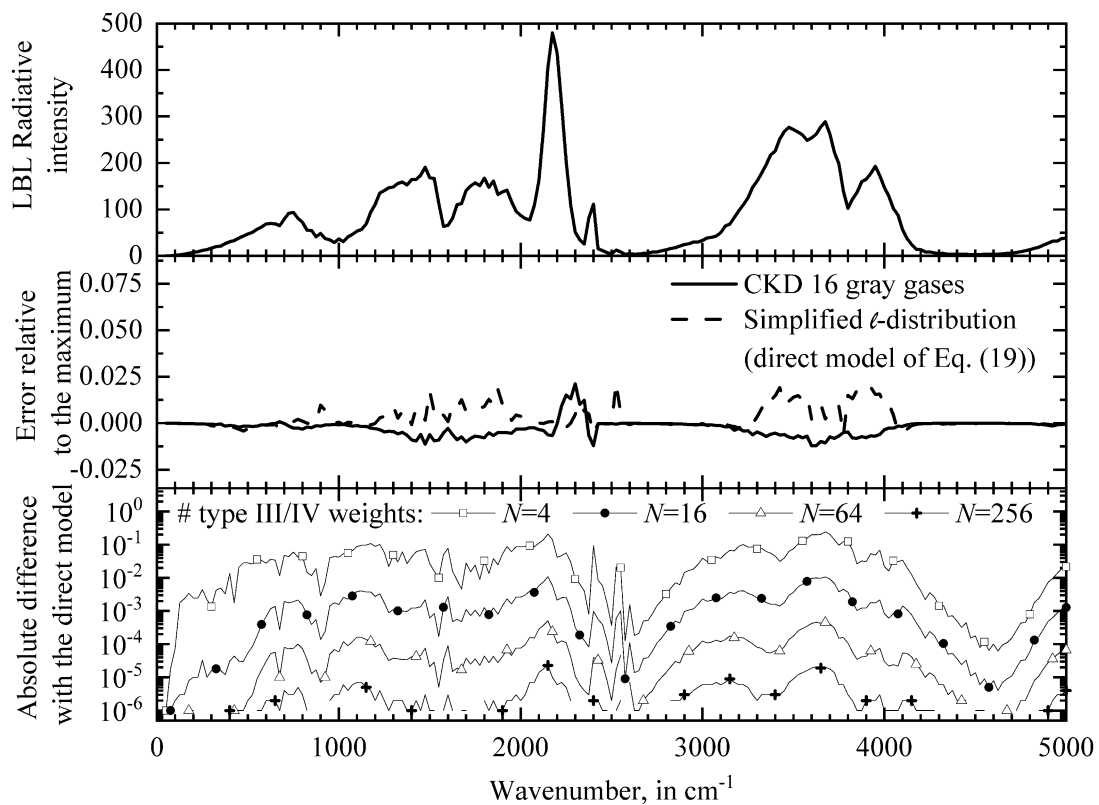
The profiles of temperature and species concentrations used in case C2 are given as:

636

$$\left\{ \begin{array}{l} T(l) = 400 \text{ K} + 1400 \text{ K} \times \left[\sin\left(\frac{\pi l}{L}\right) \right]^2 \\ x_{\text{H}_2\text{O}}(l) = 0.4 \times \left[\sin\left(\frac{\pi l}{L}\right) \right]^2 \\ x_{\text{CO}_2}(l) = \frac{1}{2} x_{\text{H}_2\text{O}}(l) \end{array} \right. \quad (31)$$

637 where the total distance of the path is $L=100$ cm.

638 Results are depicted in figure 9. The same conclusions as in case C1 can be made. A
639 quadrature order of $N=4$ provides large errors and the choice $N=16$ yields small though
640 noticeable differences when compared with the direct model. There errors remain
641 minor, especially when averaged over the full spectrum. Indeed, in terms of total
642 radiative intensities, LBL calculation provides $18919 \text{ W.m}^{-2}.\text{sr}^{-1}$, CKD $19667 \text{ W.m}^{-2}.\text{sr}^{-1}$ (4
643 % / LBL) the direct simplified ℓ -distribution model $19184 \text{ W.m}^{-2}.\text{sr}^{-1}$ (1.4 % / LBL). The
644 difference with its RNN version with $N=16$ is lower than $0.4 \text{ W.m}^{-2}.\text{sr}^{-1}$ when summed
645 over the full spectrum. It is below $0.001 \text{ W.m}^{-2}.\text{sr}^{-1}$ when the quadrature order $N=256$ is
646 used.



647

648 **Figure 9.** Intercomparison of radiative intensities in Case C2.

649 4.3.3. Cases C3 and C4

650 Case C3 uses the following profiles of temperature and species concentrations:

$$651 \quad T(l) = \begin{cases} 1500.0 \sin\left(\frac{5\pi}{3} \frac{l}{L} + \frac{\pi}{4}\right), & 0 \leq l \leq 0.3 \\ 6798.76 \exp\left(-7.3 \frac{l}{L}\right), & 0.03 \leq l \leq L \end{cases} \quad (32-a)$$

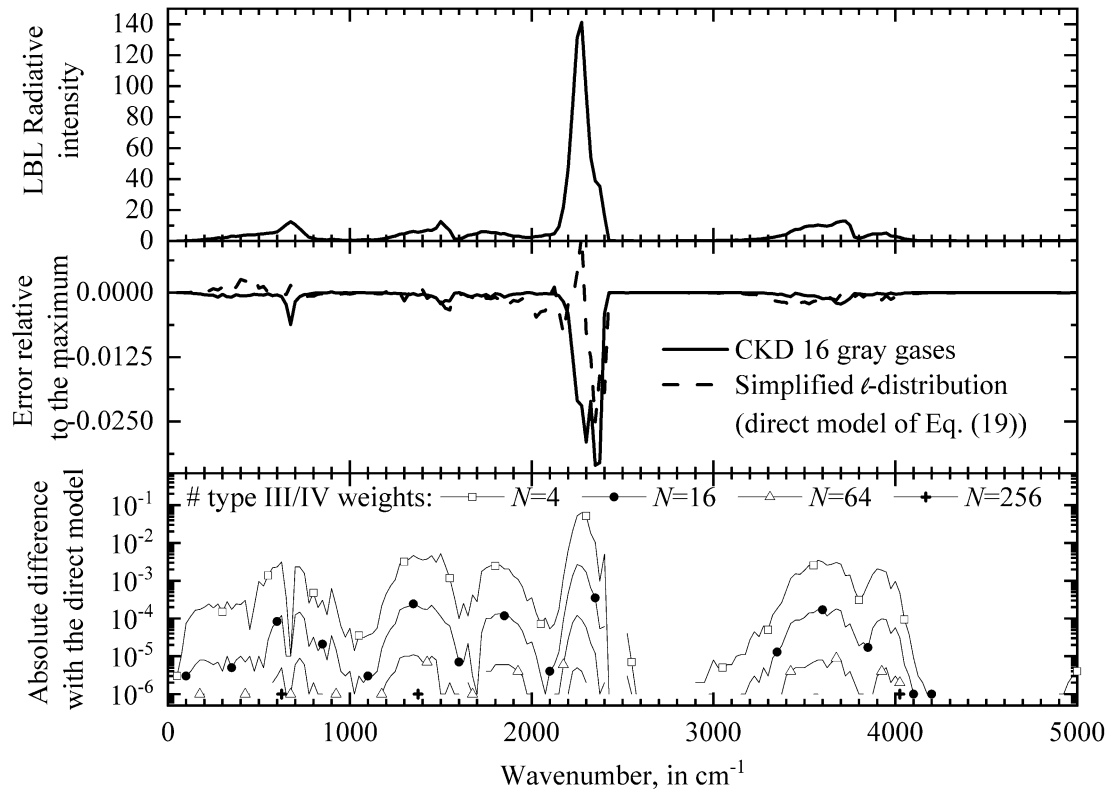
$$652 \quad x_{H_2O}(l) = \begin{cases} 0.1 \sin\left(2\pi \frac{l}{L} + \frac{\pi}{4}\right), & 0 \leq l \leq 0.025 \\ 0.34 \exp\left(-6.28 \frac{l}{L}\right), & 0.025 \leq l \leq L \end{cases} \quad (32-b)$$

$$653 \quad x_{CO_2}(l) = \begin{cases} 0.1 \sin\left(\frac{10\pi}{7} \frac{l}{L} + \frac{\pi}{4}\right), & 0 \leq l \leq 0.035 \\ 0.34 \exp\left(-4.49 \frac{l}{L}\right), & 0.035 \leq l \leq L \end{cases} \quad (32-c)$$

$$654 \quad x_{CO}(l) = \begin{cases} 0.02 \sin\left(\frac{10\pi}{3} \frac{l}{L} + \frac{\pi}{4}\right), & 0 \leq l \leq 0.015 \\ 0.068 \exp\left(-10.47 \frac{l}{L}\right), & 0.015 \leq l \leq L \end{cases} \quad (32-d)$$

655 where the total gas path length is first (case C3) $L = 10$ cm, which complies with the
 656 value used in ref. [33]. Compared to the previous cases that were restricted to mixtures
 657 of two absorbing molecules, 3 absorbing species are considered here (CO_2 , H_2O and CO).
 658 Predictions for this case are shown in Fig. 10.

659 In terms of total radiative intensities, LBL calculation provides $1202 \text{ W.m}^{-2}.\text{sr}^{-1}$, CKD
 660 $1167 \text{ W.m}^{-2}.\text{sr}^{-1}$ (2.9 % / LBL), the direct simplified ℓ -distribution model $1179 \text{ W.m}^{-2}.\text{sr}^{-1}$
 661 (1.9 % / LBL). The difference with its RNN version with $N=16$ is lower than $0.01 \text{ W.m}^{-2}.\text{sr}^{-1}$
 662 $^2.\text{sr}^{-1}$ for the calculation of the total intensity. It is below $0.00001 \text{ W.m}^{-2}.\text{sr}^{-1}$ when $N=256$
 663 is used.



664

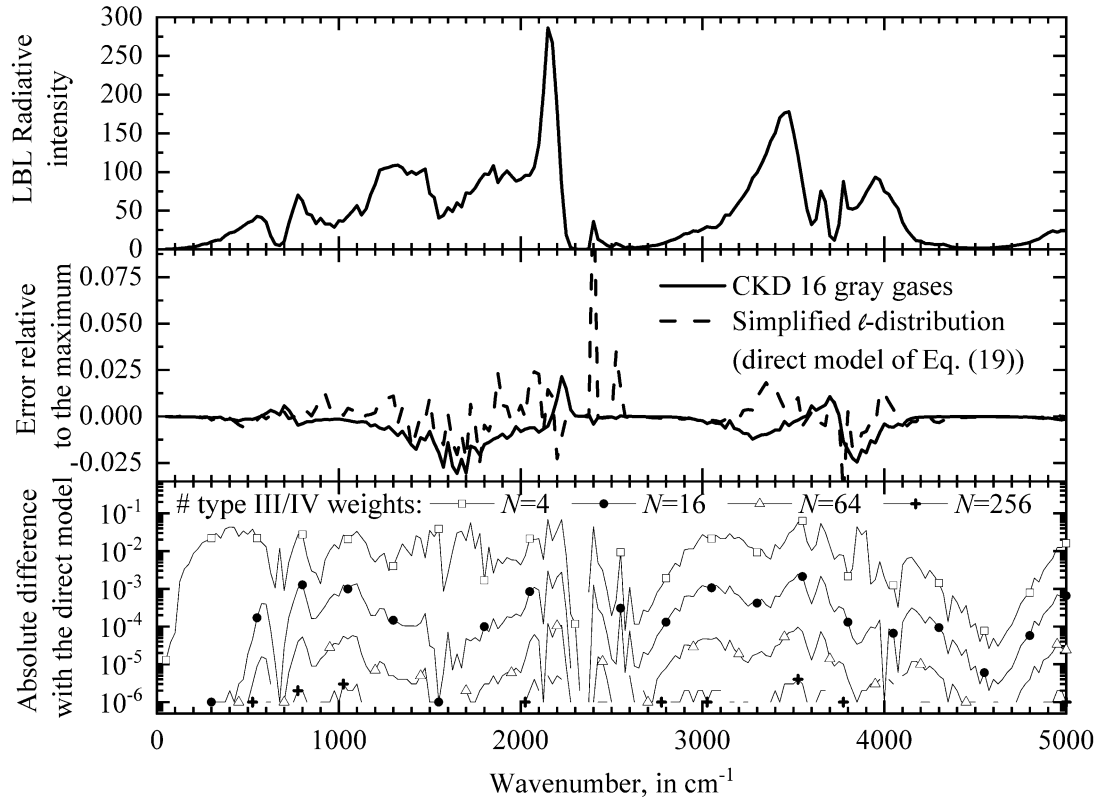
665

Figure 10. Intercomparison of radiative intensities in Case C3.

666 Case C4 is exactly the same as case C3 but the total length of the path is 100 cm. Results
 667 are plotted in Figure 11.

668 In terms of total radiative intensities, LBL calculation provides $10261 \text{ W.m}^{-2}.\text{sr}^{-1}$, the CKD
 669 model $10002 \text{ W.m}^{-2}.\text{sr}^{-1}$ (2.5 % / LBL), the direct simplified ℓ -distribution model 10337
 670 $\text{W.m}^{-2}.\text{sr}^{-1}$ (0.7 % / LBL). The difference between the direct model and its RNN version
 671 with $N=16$ is lower than $0.08 \text{ W.m}^{-2}.\text{sr}^{-1}$. It is below $0.0002 \text{ W.m}^{-2}.\text{sr}^{-1}$ for the calculation
 672 of the total intensity when $N=256$ is used.

673



674
675

676

Figure 11. Intercomparison of radiative intensities in Case C4.

677

678 4.3.4. General comments on the non-uniform test cases

679 The set of test cases considered to evaluate both the direct and RNN versions of the
 680 propagative scheme set by Eq. (5) are limited but cover in fact a wide range of possible
 681 configurations. Indeed, these cases both involve optically thin and thick limits, wide
 682 ranges of values of mean absorption coefficients k_p and overlapping parameters β .
 683 These cases are thus sufficient to validate the RNN version of the propagative scheme
 684 proposed in this paper, which is the main focus of the present work.

685 With a quadrature order equal to $N=4$, large errors are observed (empty squares in
 686 figures 8 to 11). For values of N equal or higher than 16 (plain circles in figures 8 to 11),
 687 the RNN models almost coincide exactly with the one based on a direct application of the
 688 analytical formula Eq. (19). The same value of quadrature order $N=16$ was used in ref.
 689 [17] to treat real LBL data instead of the uniform model of Eq. (17). High temperature
 690 spectra were also considered in this work. This means that other quadrature orders may

691 be needed for atmospheric applications. The treatment of cases C1-4 however provides a
692 proof of the actual possibility to treat non-uniform paths using the RNN structure
693 depicted in Figures 6 and 7.

694 Moreover, the simplified ℓ -distribution model described in this paper has an accuracy
695 which is similar to (and in all the considered cases higher than) the widely used CKD
696 model for the calculation of full spectrum intensities. Considering its small memory cost
697 and its high computational efficiency (the direct model is fully based on Eqs. (17,19),
698 that only involve simple and analytical formulas), this method can be considered as a
699 good candidate for radiative transfer applications in high temperature gaseous media.
700 Its RNN version can be confidently used too, as it provides with a quadrature order of 16
701 almost the same accuracy as the direct method. Notice however that the RNN version is
702 more computationally demanding than Eq. (19). A ratio of about 4 in terms of
703 computational time was observed when the RNN version with $N=16$ is used instead of
704 the direct model.

705 **4.4. DISCUSSION**

706 As noticed earlier in this paper, using the “neural” version depicted in Figures 6-7 to
707 evaluate equivalent absorption lengths has probably little interest in the case of the
708 uniform transmissivity model proposed in Section 3, since for this model these
709 equivalent absorption lengths are analytical. They are indeed provided by Eq. (19).
710 However, the present developments pave the way for further fast transmissivity model
711 developments based on Recurrent Neural Networks, a structure that has not be
712 considered yet to the best of the authors’ knowledge. This point is discussed in this
713 section.

714 The training of NN models is subject to known issues [29]. The choice of the starting
715 values (how to initialize the weights?), overfitting (how to select the optimal number of
716 weights?), and the choice of the structure of the network (how to select the number of
717 hidden units and of layers?) are critical in the definition of the model. Choosing these
718 parameters is difficult in a general frame. Indeed, as NN are most often black box
719 models, it is almost impossible to specify all these quantities in advance. There are
720 several tricks to circumvent these problems but, most of the time, trial and errors

721 techniques are used to select the best combination of parameters (structure, number of
722 weights and initialization) [3].

723 Based on the present work, all these three issues can be solved if one uses the recurrent
724 structure described in this paper.

725 Concerning the structure of the network, it is fixed by the scheme depicted in figure 6.
726 There is no reason to add any additional layer in the method. The choice of the activation
727 function (ELU) is also rather natural. The same kind of formulation in terms of ELUs was
728 used in ref. [17] in the case of real gas spectra. This property extends to any problem for
729 which the Archimedean copula c_{11} that appears in Eq. (4) is of the Levy Subordinated
730 type [34,35]. Direct models of Archimedean copula (not necessarily Levy Subordinated)
731 based on neural networks can be found in ref. [36] but the method is more focused on
732 copula models than the method described here.

733 Concerning the optimal number of weights, it is mostly related to the choice of the
734 number N related to the Gauss-Legendre quadrature used in Eq. (27). In ref. [17], a
735 Gauss-Legendre quadrature at order 16 was selected (the corresponding formulation of
736 ref. [17] is reminded later in this section). As shown in section 4.3, this order of
737 quadrature was found to provide accurate results here too. Notice however, that both
738 the present work and ref. [17] are dedicated to high temperature configurations. This
739 means that adaptation of this quadrature order N may be needed for applications in the
740 atmosphere. A detailed analysis of this specific point in cases of atmospheric paths is
741 kept as future work.

742 Concerning the learning stage and the initialization of the weights, additional details are
743 described in this paragraph. It was shown in ref. [17], that if: 1/ the absorption
744 spectrum in state 1 is gray i.e., $\kappa_{\nu,1} = k_{P,1}$, and 2/ the non-constant scaling coefficient
745 between spectra in states 1 and 2 is bounded and takes values inside a small interval, i.e.,

746 $u(\xi) \in [u_{\min}, u_{\max}]$, $\frac{u_{\max} - u_{\min}}{u_{\min}} \ll 1$, solutions of Eq. (7) take the form:

$$747 \quad \ell_1 \circ \tau_2^{\Delta\nu}(L) = u_{\min} L + \frac{1}{k_{P,1}} \cdot \int_0^{u_{\max} - u_{\min}} [1 - \exp(-k_{P,1} \cdot \nu \cdot L)] dF(\nu) \quad (33)$$

748 where $v = u - u_{\min}$ and $F(v)$ is the distribution function of variable v over the spectral
 749 interval Δv . Eq. (33) can be rewritten as:

$$750 \quad \ell_1 \circ \tau_2^{\Delta v}(L) = u_{\min} L + \frac{\bar{v}}{k_{p,1}} \cdot \int_0^{u_{\max} - u_{\min}} \left[\frac{1 - \exp(-k_{p,1} \cdot v \cdot L)}{v} \right] dF^*(v) \quad (34)$$

751 where $\bar{v} = \int_0^{u_{\max} - u_{\min}} v dF(v)$ is the mean value of v and $F^*(v) = \frac{1}{\bar{v}} \int_0^v v' dF(v')$. Noticing that
 752 as v is positive by definition, $F^*(v)$ is a probability distribution function (its inverse will
 753 be from now on written v^*), one can rewrite Eq. (34) as:

$$754 \quad \ell_1 \circ \tau_2^{\Delta v}(L) = u_{\min} L + \frac{\bar{v}}{k_{p,1}} \cdot \int_0^1 \left[\frac{1 - \exp(-k_{p,1} \cdot v^*(\xi) \cdot L)}{v^*(\xi)} \right] d\xi \quad (35)$$

755 Using the same Gauss-Legendre quadrature as in section 4.2 to estimate the integral
 756 over $[0,1]$, Eq. (35) can be approximated by:

$$757 \quad \ell_1 \circ \tau_2^{\Delta v}(L) \approx u_{\min} L - \frac{\bar{v}}{k_{p,1}} \cdot \sum_{j=1}^N \frac{\omega_j}{v^*(x_j)} \cdot \varphi \left[-k_{p,1} \cdot v^*(x_j) \cdot L \right] \quad (36)$$

758 that takes exactly the same functional form as used in 4.2.

759 Moreover, in the same reference [17], it was verified in real LBL cases that this
 760 formulation can be extended to non-gray cases by simply replacing the mean absorption
 761 coefficient $k_{p,1}$ of Eqs. (33-36) by some moment of the absorption coefficient written μ_s .

762 The general solution of Eq. (7) thus takes the form, similar to Eq. (35):

$$763 \quad \ell_1 \circ \tau_2^{\Delta v}(L) = u_{\min} L + \frac{\bar{v}}{\mu_s} \cdot \int_0^1 \left[\frac{1 - \exp(-\mu_s \cdot v^*(\xi) \cdot L)}{v^*(\xi)} \right] d\xi \quad (37)$$

764 that one can approximate, using again a Gauss-Legendre quadrature at order N , as:

$$765 \quad \ell_1 \circ \tau_2^{\Delta v}(L) \approx u_{\min} L - \frac{\bar{v}}{\mu_s} \cdot \sum_{j=1}^N \frac{\omega_j}{v^*(x_j)} \cdot \varphi \left[-\mu_s \cdot v^*(x_j) \cdot L \right] \quad (38)$$

766 Eqs. (37,38) provide the solution of Eq. (7) in the case of real LBL data. Eq. (38) takes
 767 exactly the same form as the one considered in 4.2. A table of correspondence between
 768 the quantities that appear in Eqs. (19,29) and Eq. (38) is provided in table 4.

769

770

771

Eq. (19,29)	Eq. (38)	Physical meaning
$\frac{2\pi k_{p,2}}{\beta_2}$	μ_s	Mean (moment) absorption coefficient
$s^2 \cdot \frac{k_{p,2} \beta_2}{k_{p,1} \beta_1}$	u_{\min}	Minimum value of scaling coefficient – corresponds to the asymptotic limit of the scaling function at large lengths L .
$s \cdot \frac{k_{p,2}}{k_{p,1}}$	\bar{u}	Mean value of scaling coefficient – corresponds to the asymptotic limit of the scaling function at small lengths L .
$s \cdot \frac{k_{p,2}}{k_{p,1}} \cdot \left(1 - s \cdot \frac{\beta_2}{\beta_1} \right)$	$\bar{v} = \bar{u} - u_{\min}$	Mean value of coefficient v
u_j	$v^*(x_j)$	Characterize the variations of scaling coefficients inside $[u_{\min}, u_{\max}]$

772 Table 4. Relationship between the quantities that appears in Eqs. (19,29) and Eq. (38)

773

774 This means that in the general case, the same algorithm as used in section 4.2 can be
 775 used. In practice, as detailed in ref. [17], several of the quantities that appear in Eq. (38)
 776 need to be adjusted on the LBL transmission curves because if the quasi-scaling
 777 approximation is close to the real behavior of gas spectra, it is not exact. This
 778 minimization process is equivalent to a training or learning stage in the machine
 779 learning terminology. The quantities that are adjusted on the LBL transmission curves,
 780 or equivalently learned from the LBL transmission curves, are essentially the
 781 parameters $v^*(x_j)$, $j = 1, \dots, N$ as soon as the coefficient μ_s is chosen (notice that the

782 exact specification of this coefficient μ_s is not compulsory as it always appears in
 783 formula (38) as the product $\mu_s \cdot v^*(x_j)$ and coefficients $v^*(x_j)$, $j = 1, \dots, N$ are adjusted –
 784 this property arises from the change of distribution from F to F^* between Eq. (33) and
 785 Eq. (34)). From table 4, one can see that the training of coefficients $v^*(x_j)$, $j = 1, \dots, N$ in
 786 the LBL case is equivalent to the choice of coefficients u_j , $j = 1, \dots, N$ in the simplified ℓ -
 787 distribution model. The specification of these coefficients as solutions of Eq. (27) is thus
 788 the same as some training stage. No explicit learning step appears in the simplified ℓ -
 789 distribution approach because an explicit solution can be found but this learning stage is
 790 required when the methodology is applied to real LBL datasets. Combining the results
 791 described in the present paper with those of ref. [17] (or equivalently Eqs. (37,38)) thus
 792 provides all the elements required to generate an RNN model of non-uniform path
 793 transmissivities. This RNN model then has the interesting property that all its weights
 794 have a clear physical meaning, as detailed in table 4, avoiding the black box disadvantage
 795 of this category of methods. The parameters of the simplified ℓ -distribution model, or the
 796 same steps as described in ref. [17], can be used to initialize the optimization of the
 797 parameters of Eq. (38) on real LBL datasets.

798 Furthermore, both feedforward and recurrent neural networks are so-called universal
 799 approximators [25]. Accordingly, in theory, both of them are likely to estimate any non-
 800 uniform path transmissivity. However, the RNN architecture has some advantages
 801 compared to feedforward models. They are briefly discussed here. The iterative process
 802 proposed in this work can be readily adapted to any dimension (number of sub-paths
 803 encountered along a non-uniform path) which makes it appropriate for the treatment of
 804 general radiative transfer problems for which many such uniform sub-paths may be
 805 encountered along a ray. This iterative structure thus appears to be well suited to
 806 radiative transfer calculations, in comparison with any other feedforward networks as
 807 considered in ref. [4]. Indeed, in actual radiative transfer problems, the dimension of the
 808 input space (number of sub-paths along a ray) can quickly become difficult to handle if a
 809 large number of such inputs is treated. This would require the specification of many
 810 weights in feedforward NN models. In practice, large numbers of weights complicate the
 811 training of the model and reduce its computational efficiency compared to a LBL
 812 calculation. The propagative scheme introduced here does not suffer from this limitation

813 since only transitions between successive layers are modeled, *i.e.*, even in the case of a
814 high number of sub-paths, what is modeled remains in dimension 2, as shown in figures
815 6 and 7.

816 Eventually, if the model presented in this work has some advantages compared to other
817 methods for non-uniform path radiative transfer calculations, it also has some
818 limitations. In fact, it can be noticed that the present method provides a gas radiation
819 model formulated in terms of transmissivities. This type of formulation, whose main
820 interest is to produce a fast model as no spectral or pseudo-spectral loop is required, has
821 an impact on the possible choices of RTE solvers. Indeed, the present developments are
822 limited to ray-tracing RTE solvers, which includes Monte Carlo methods but also quasi-
823 Monte Carlo (qMC, [37]) techniques, *i.e.*, numerical methods based on the integral form
824 of the RTE. The present model cannot be used with the Discrete Ordinate Method, for
825 instance, as it uses the differential form of the RTE. However, the present modeling
826 strategy can be applied for coupled calculations to treat engineering problems, in the
827 same way the CKD model is used in refs. [38,39]. Compared to a combination of qMC and
828 CKD, the use of the present model has one dimension less than CKD (no sampling or loop
829 over gray gases) which can be beneficial to reduce the cost of a qMC calculation.
830 Application of the simplified ℓ -distribution method together with a net exchange
831 formulation is also as straightforward as it is for the SNB models [40]. Notice that one
832 part of the justification of the copula formalism is founded on this idea of net exchange,
833 as detailed in ref. [5], illustrating the strong theoretical connection between the present
834 method and net exchange RTE solvers. In these contexts (ray tracing RTE solver and/or
835 net exchange formulation), as shown in the paper, the “direct” simplified ℓ -distribution
836 model can be used confidently. Furthermore, as pointed out several times in the paper,
837 the “neural” version has little interest in the case of the simplified ℓ -distribution model
838 but the present paper provides a proof of concept. The “neural” version may find
839 application in problems for which only a finite set of transitions between layers (*i.e.*
840 distinct states of the gas) needs to be considered in which case, the LBL formulation
841 described two paragraphs above can be used instead of the simplified model of section
842 3.2. Indeed, the quantities that are trained in the RNN version are related to transitions
843 between successive layers so that the number of parameters to identify is directly
844 proportional to the amount of distinct states encountered in the problem. This kind of

845 configuration is relatively rare in high temperature configurations, for which the “direct”
846 simplified ℓ -distribution model can be used, but rather usual in atmospheric sciences
847 (multi-layer atmospheres). Application of the present developments in their recurrent
848 neural network version for radiative transfer studies in the atmosphere, mostly as a
849 continuation of ref. [5] and in which LBL datasets will be used instead of the simplified ℓ -
850 distribution model considered in the present paper, is scheduled as future work.

851

852 **5. CONCLUSION**

853 The main objective of the work was to show that recurrent neural network models are
854 relevant candidates for modeling non-uniform gas path transmissivities. Relationships
855 between a method proposed by Godson in the 50s and RNNs, two a priori strongly
856 distinct ideas, follow from a mathematical analysis and a reformulation of Godson's
857 implicit equation. This reformulation involves the inverse of the transmission function. It
858 provides an analytical method for the treatment of non-uniform paths. Most results
859 provided here follow directly from recent results obtained within the frame of the
860 development of the ℓ -distribution approach.

861 A simplified version of the ℓ -distribution method was introduced. The main advantage of
862 this simplified model is that it allows a fully analytical derivation of all model
863 parameters. Compared with the full database (that requires a few gigabytes), the size of
864 the simplified ℓ -distribution model is lower than 14 megabytes. This method was found
865 to be accurate both in uniform and non-uniform scenarios. Its accuracy of a few percent
866 is sufficient for most radiative heat transfer calculations in high temperature gases.

867 Based on simple analytical developments, it was then shown that the propagative
868 scheme associated with the ℓ -distribution method can be written in an RNN form.
869 Indeed, this propagative scheme consists of a transformation of a series of optical paths
870 into equivalent absorption lengths. The structure of the problem is well suited to RNN
871 models, more usually encountered in the modeling of dynamical systems or the
872 treatment of time series. The RNN formulation, that uses Exponential Linear Units
873 (ELUs) as activation functions, was compared with the analytical solution and found to
874 provide highly accurate estimates of non-uniform path transmissivities. All the weights
875 involved in the RNN formulation have a clear physical meaning. This allows a high level
876 of control and interpretability of the RNN model, a property which is usually hard to
877 ensure with methods purely based on machine learning. The only quantities involved in
878 the RNN model that are not directly related to the uniform model (the set of u_j) are
879 obtained here as solutions of an implicit equation instead of a minimization process.
880 This possibility is related to the choice of the simplified model for the calculation of
881 transmissivities that allows a simplified treatment of the training of the model, but the
882 process is equivalent to a learning stage. Extension of the method to real LBL

883 transmissivities instead of the simplified model was discussed. Future works will be
884 devoted to its application for atmospheric calculations.

885

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889

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