

**COST ACTION CA18232 MAT-DYN-NET  
WORKING GROUP 2 WHITE PAPER**

**POLYATOMIC GASES:  
KINETIC MODELLING, COMPACTNESS PROPERTIES  
OF THE LINEARIZED COLLISION OPERATORS**

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1. INTRODUCTION

One of the main focuses of Working Group 2 consists in studying nonlinear phenomena for kinetic-like models. This white paper presents a comprehensive study of modelling of polyatomic gases and mixtures in the collisional kinetic gas theory. The topic was extensively discussed during WG2 meetings and some talks presented the latest advancement in the field. More precisely, three speakers (Andrea Bondesan, Vladimir Djordjić, Damir Madjarević) at the first WG2 meeting organized at Ceptor Andrevlje, Fruška Gora, Serbia, in 2021, presented their work on multi-species and polyatomic Boltzmann equation. The second WG2 meeting, held at the Sorbonne Université campus of Saint-Cyr-l'École, France, in 2022, was primarily devoted to the compactness properties of the linearized polyatomic Boltzmann operators (talks by Niclas Bernhoff, Thomas Borsoni, Marwa Shahine) and related issues (Romina Travaglini, Julien Mathiaud).

In this manuscript, we unify ideas and notations for modelling of polyatomic gases in different settings: (i) resonant collisions, (ii) continuous internal energy with Borgnakke-Larsen procedure, (iii) discrete internal energy. Moreover, we complement the presentation by extending the concepts to gas mixtures composed of monatomic and polyatomic gases, both in continuous and discrete approaches for the internal energy. With this unified notation, we write the Boltzmann equation and the corresponding linearized Boltzmann operator. Then, we briefly present recent results on its compactness property.

This analysis is the basis for a more complete review of compactness results for the linearized Boltzmann operator for polyatomic gases, which will be presented in the form of a review article to be submitted to the Proceedings of the Final MAT-DYN-NET Conference.

2. POLYATOMIC GAS MODELLING

In this section, we describe various models of polyatomic gases existing in the literature. In some cases, we also explain the extension to multispecies gaseous mixtures.

Let us first briefly recall the description of a single monatomic gas. Consider two monatomic molecules of mass  $m$  undergoing an elastic collision process. Denote their pre-collisional velocities  $v, v_*$ , which become  $v', v'_*$  after collision. The microscopic momentum

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and energy are conserved through the process, expressed as follows

$$(1) \quad mv + mv_* = mv' + mv'_*,$$

$$(2) \quad \frac{1}{2}m|v|^2 + \frac{1}{2}m|v_*|^2 = \frac{1}{2}m|v'|^2 + \frac{1}{2}m|v'_*|^2.$$

Introducing a parameter  $\sigma \in \mathbb{S}^2$ , one obtains the collision rules, giving the expression of the post-collisional velocities

$$(3) \quad v' = \frac{1}{2}(v + v_*) + \frac{1}{2}|v - v_*|\sigma, \quad v'_* = \frac{1}{2}(v + v_*) - \frac{1}{2}|v - v_*|\sigma,$$

in terms of pre-collisional ones. For (much) more details on the monatomic case, the reader may refer, for instance, to [27].

At the macroscopic level, the main distinction between monatomic and polyatomic gases can be observed when the specific internal energy of the gas is considered. Let us denote by  $\hat{e}$  its dimensionless form. Namely, for a monatomic gas, it is known that the dimensionless specific heat at constant volume is  $\hat{c}_v = 3/2$  and consequently  $\frac{d\hat{e}}{dT} = 3/2$ . However, for thermally perfect (non-polytropic) gases, the specific heat  $\hat{c}_v$  is a temperature-dependent quantity and, in general, it is only known through its definition  $\hat{c}_v(T) = \frac{d\hat{e}}{dT}$ . Even if  $\hat{c}_v(T)$  is assumed to be constant with respect to the temperature, which corresponds to calorically perfect or polytropic gases, it is experimentally observed that, at room temperature,  $\hat{c}_v > 3/2$  [23, 24]. Hence, such a behavior of polyatomic gases is a consequence of more complex collisions than the ones for monatomic gases, and in particular, (2) has to be reconsidered.

Two approaches to model polyatomic gases have been developed in parallel. They share the same idea: associate an internal energy to a polyatomic molecule and consequently rewrite (2). The main difference lies in the form of the internal energy they use, either a *continuous* or *discrete* one.

The continuous approach introduces a continuous internal energy  $I \geq 0$  as an additional argument of the distribution function, and a nonnegative function  $\varphi$  of  $I$  which becomes a parameter of the model to capture a proper form of the specific internal energy  $\hat{e}$ . First, [13] proposed a power-law form of  $\varphi$ , that is, for any  $I \geq 0$ ,

$$(4) \quad \varphi(I) = I^{\delta/2-1},$$

where  $\delta > 0$  is related to the number of internal degrees of freedom of the molecules. More specifically, for polytropic gases,  $\delta$  is constant and  $\delta = 2\hat{c}_v - 3$  [19]. The model is accurate for diatomic gases (for instance  $\text{N}_2$ ,  $\text{O}_2$ ,  $\text{NO}$ ,  $\text{CO}$ ,  $\text{H}_2$ ) for temperatures close to the room temperature. Later, [18] presented the model without prescribing a specific form of  $\varphi$ . This general form is supposed to allow for a more general macroscopic internal-energy law and eventually capture non-polytropic gases.

With the discrete approach [17, 20, 22], the internal energy can only take a finite number of given values  $\{I^{(1)}, \dots, I^{(N_{\text{int}})}\}$ . Then the parameters  $(\varphi^{(1)}, \dots, \varphi^{(N_{\text{int}})})$  account for the degeneracy of the different energy levels [20]. The degeneracy  $\varphi^{(k)} \in \mathbb{R}_+$  of the internal energy  $I^{(k)}$  corresponds to the number of different states that give rise to the same specific internal energy  $I^{(k)}$ .

**2.1. Borgnakke-Larsen procedure.** Originally presented in [7], this model was the first one studied in the literature when dealing with a continuous internal energy variable in a kinetic setting. It can be found, written in various forms, for instance in [13, 18].

Let us consider two colliding polyatomic molecules of mass  $m$  with respective velocities and internal energies  $(v, I)$  and  $(v_*, I_*)$ , changing to  $(v', I')$  and  $(v'_*, I'_*)$ . The microscopic momentum and total energy are conserved as follows

$$(5) \quad mv + mv_* = mv' + mv'_*,$$

$$(6) \quad \frac{m}{2}|v|^2 + I + \frac{m}{2}|v_*|^2 + I_* = \frac{m}{2}|v'|^2 + I' + \frac{m}{2}|v'_*|^2 + I'_*.$$

In the center-of-mass reference frame, using the relative velocities  $V = v - v_*$ ,  $V' = v' - v'_*$ , the energy conservation can equivalently be rewritten as

$$(7) \quad \frac{m}{4}|V|^2 + I + I_* = \frac{m}{4}|V'|^2 + I' + I'_* =: E,$$

which defines the total energy  $E$  in the center-of-mass frame. The Borgnakke-Larsen procedure splits  $E$  into kinetic and internal energy contributions using a parameter  $R \in [0, 1]$  in the following way

$$(8) \quad RE = \frac{m}{4}|V'|^2, \quad (1 - R)E = I' + I'_*,$$

and then associates those energies to the post-collisional velocities and internal energies with the help of parameters  $\sigma \in \mathbb{S}^2$  and  $r \in [0, 1]$ ,

$$(9) \quad v' = \frac{v + v_*}{2} + \sqrt{\frac{RE}{m}}\sigma, \quad v'_* = \frac{v + v_*}{2} - \sqrt{\frac{RE}{m}}\sigma,$$

$$(10) \quad I' = r(1 - R)E, \quad I'_* = (1 - r)(1 - R)E.$$

The collision kernel  $B \geq 0$  is assumed to satisfy symmetry properties reflecting an interchange of colliding molecules, as well as microreversibility assumptions corresponding to the pre/post-collision change, which means that

$$(11) \quad \begin{aligned} B(v, v_*, I, I_*, r, R, \sigma) &= B(v_*, v, I_*, I, r, R, \sigma), \\ B(v, v_*, I, I_*, r, R, \sigma) &= B\left(v', v'_*, I', I'_*, r', R', \frac{V}{|V|}\right), \end{aligned}$$

with

$$(12) \quad R' = \frac{m|V|^2}{4E}, \quad r' = \frac{I}{I + I_*} = \frac{I}{(1 - R')E}.$$

The associated Boltzmann collision operator can then be defined, for any measurable function  $f$  for which it makes sense and for almost every  $v$  and  $I$ , by

$$(13) \quad \begin{aligned} Q(f, g)(v, I) &= \int_{\mathbb{R}^3 \times \mathbb{R}_+ \times (0, 1)^2 \times \mathbb{S}^2} \left( f' g'_* \frac{\varphi(I)\varphi(I_*)}{\varphi(I')\varphi(I'_*)} - f g_* \right) \\ &\quad \times \frac{\tilde{B}(v, v_*, I, I_*, r, R, \sigma)}{\varphi(I)\varphi(I_*)} (1 - R)\sqrt{R} dv_* dI_* dR dr d\sigma, \end{aligned}$$

with  $\tilde{B}$  satisfying (11), and where we used the standard notations  $f' = f(v', I')$ ,  $g'_* = g(v'_*, I'_*)$ ,  $f = f(v, I)$ ,  $g_* = g(v_*, I_*)$ , the prime quantities  $v'$ ,  $v'_*$ ,  $I'$  and  $I'_*$  being defined by (9)–(10). Results that are of interest for this review use the specific form (4) of the weight factor, namely  $\varphi(I) = I^{\delta/2-1}$ ,  $\delta > 0$ . In this case, one can use another collision kernel defined as

$$B(v, v_*, I, I_*, r, R, \sigma) = \frac{\tilde{B}(v, v_*, I, I_*, r, R, \sigma)}{(II_*)^{\delta/2-1}(r(1-r))^{\delta/2-1}(1-R)^{\delta-2}} = \frac{\tilde{B}(v, v_*, I, I_*, r, R, \sigma)E^{\delta-2}}{\varphi(I)\varphi(I_*)\varphi(I')\varphi(I'_*)},$$

which clearly still satisfies assumption (11). Then the collision operator reads, for almost every  $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$ ,

$$(14) \quad Q(f, g)(v, I) = \int_{\mathbb{R}^3 \times \mathbb{R}_+ \times (0,1)^2 \times \mathbb{S}^2} \left( f' g'_* \left( \frac{I I_*}{I' I'_*} \right)^{\delta/2-1} - f g_* \right) \\ \times B(v, v_*, I, I_*, r, R, \sigma) (r(1-r))^{\delta/2-1} (1-R)^{\delta-1} \sqrt{R} dv_* dI_* dR dr d\sigma.$$

For convenience, we state a part of the  $H$ -theorem that defines the equilibrium state.

**Proposition 1.** *The three following properties are equivalent:*

$$(i) \quad Q(M, M) = 0,$$

$$(ii) \quad \int_{\mathbb{R}^3 \times \mathbb{R}_+} Q(M, M)(v, I) \log(M(v, I) I^{1-\delta/2}) dv dI = 0,$$

(iii) *there exist  $n \geq 0$ ,  $u \in \mathbb{R}^3$  and  $T > 0$  such that, for almost every  $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$ ,*

$$(15) \quad M(v, I) = \frac{n}{(k_B T)^{\delta/2} \Gamma(\delta/2)} \left( \frac{m}{2\pi k_B T} \right)^{3/2} I^{\delta/2-1} \exp \left( -\frac{m|v-u|^2}{2k_B T} - \frac{I}{k_B T} \right),$$

where  $\Gamma$  represents the usual Gamma function.

**2.2. Polyatomic gas with resonant collisions.** A resonant behaviour can be observed, for instance, in the collisions between selectively excited  $\text{CO}_2$  molecules [25]. In that case, the microscopic internal and kinetic energies are separately conserved during the collisional process.

Consider two resonant-colliding polyatomic molecules of mass  $m$  with velocities and internal energies  $(v, I)$  and  $(v_*, I_*)$ , which change into  $(v', I')$  and  $(v'_*, I'_*)$  due to the collision process. In the resonant kinetic model introduced in [11], we have the following microscopic momentum and energy conservations

$$(16) \quad mv + mv_* = mv' + mv'_*,$$

$$(17) \quad \frac{m}{2}|v|^2 + \frac{m}{2}|v_*|^2 = \frac{m}{2}|v'|^2 + \frac{m}{2}|v'_*|^2,$$

$$(18) \quad I + I_* = I' + I'_*.$$

Due to the conservations (16)–(17), which are separate, we inherit the natural monatomic parametrization (3) of the velocities. Then, in [11], the internal energies are parametrized using the same idea as in the Borgnakke-Larsen model recalled in the previous subsection. More precisely, the authors introduce a parameter allowing to distribute the conserved internal energy between the prime internal energies of both molecules. In [9], however, this parameter is not used, and (equivalently) replaced by a direct parametrization through  $I' \in [0, I + I_*]$ , where  $I'_*$  is then chosen as

$$(19) \quad I'_* = I + I_* - I'.$$

Let us describe the model with this last parametrization. We consider a collision kernel  $B \geq 0$  which is required to be symmetric, *i.e.*

$$(20) \quad B(v, v_*, I, I_*, I', \sigma) = B(v_*, v, I_*, I, I'_*, \sigma),$$

and to satisfy a microreversibility property, that is

$$(21) \quad B(v, v_*, I, I_*, I', \sigma) = B \left( v', v'_*, I', I'_*, I, \frac{V}{|V|} \right),$$

where  $V = v - v_*$  denotes again the relative velocity. The associated invariant measure is

$$B(v, v_*, I, I_*, I', \sigma) \mathbf{1}_{[0, I+I_*]}(I') \varphi(I) \varphi(I_*) \varphi(I') \varphi(I + I_* - I') dI' dI_* dI d\sigma dv_* dv,$$

where  $\mathbf{1}_{[0, I+I_*]}$  is the characteristic function of  $[0, I + I_*]$ . Note that (21) is the microreversibility condition written in both [9] and [8], but the measure was inaccurately written in [9] and corrected in [8].

**Remark 1.** *A resonant collision kernel is related to a collision kernel similar to the ones used in Subsection 2.1 in the following way. Consider a collision kernel function  $\hat{B} := \hat{B}(v, v_*, I, I_*, r, R, \sigma)$  satisfying the symmetry/microreversibility conditions (11). Following [8], and keeping the notation  $E$  for the center-of-mass energy, obviously conserved during the collision process, one can build a resonant collision kernel  $B$  from  $\hat{B}$  through*

$$(22) \quad B(v, v_*, I, I_*, I', \sigma) = \hat{B} \left( v, v_*, I, I_*, \frac{I'}{I + I_*}, 1 - \frac{I + I_*}{E}, \sigma \right) E \mathbf{1}_{[0, I+I_*]}(I').$$

Note that the characteristic function can be dropped (it is only added here for the sake of clarity) since  $\hat{B}$  is zero when computed for values of parameters outside  $[0, 1]$ .

This allows to define the Boltzmann collision operator  $Q$  associated to the resonant model. For any measurable function  $f$  for which it makes sense, we can write, for almost every  $(v, I) \in \mathbb{R}^3 \times \mathbb{R}_+$ ,

$$(23) \quad Q(f, g)(v, I) = \int_{\mathbb{R}^3 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2} \left( f' g'_* \frac{\varphi(I) \varphi(I_*)}{\varphi(I') \varphi(I + I_* - I')} - f g_* \right) \\ \times B(v, v_*, I, I_*, I', \sigma) \mathbf{1}_{[0, I+I_*]}(I') \frac{\varphi(I') \varphi(I + I_* - I')}{\Psi_{\text{res}}(I + I_*)} dv_* dI_* dI' d\sigma,$$

where we used again the standard notations  $f' = f(v', I')$ ,  $g'_* = g(v'_*, I'_*)$ ,  $f = f(v, I)$ ,  $g_* = g(v_*, I_*)$ , with the prime quantities  $v'$ ,  $v'_*$  and  $I'_*$  defined by (3) and (19), and, for any  $Z \geq 0$ ,

$$\Psi_{\text{res}}(Z) = \int_0^Z \varphi(I') \varphi(Z - I') dI'.$$

The equilibria are characterized thanks to the following  $H$ -theorem proven in [9].

**Proposition 2.** *The three following properties are equivalent:*

$$(i) \quad Q(M, M) = 0,$$

$$(ii) \quad \int_{\mathbb{R}^3 \times \mathbb{R}_+} Q(M, M)(v, I) \log \left[ \frac{M(v, I)}{\varphi(I)} \right] dv dI = 0,$$

(iii) *there exist  $n \geq 0$ ,  $u \in \mathbb{R}^3$  and  $T_{\text{kin}}, T_{\text{int}} > 0$  such that, for almost every  $v$  and  $I$ ,*

$$(24) \quad M(v, I) = \frac{n}{q(T_{\text{int}})} \left( \frac{m}{2\pi k_B T_{\text{kin}}} \right)^{3/2} \varphi(I) \exp \left( -\frac{m|v - u|^2}{2k_B T_{\text{kin}}} - \frac{I}{k_B T_{\text{int}}} \right),$$

where the internal energy partition function  $q$  is defined, for any  $T > 0$ , by

$$(25) \quad q(T) = \int_{\mathbb{R}_+} \exp \left( -\frac{I}{k_B T} \right) \varphi(I) dI.$$

Note that (24) is a product of two Gibbs distributions, which can also be named a Maxwell distribution similarly to the monatomic case, with two different temperatures  $T_{\text{kin}}$  and  $T_{\text{int}}$ .

**Remark 2.** In [9], the authors provide a framework for  $\varphi$  of the following form: there exist  $\beta_1, \beta_2 \geq 0$ , and  $C, C' > 0$  such that

$$CI^{\beta_1} \leq \varphi(I) \leq C'I^{\beta_1}, \quad I \in (0, 1),$$

and that, for any  $a > 0$ , there exists  $C_a > 0$  such that

$$C_a I^{\beta_2 - a} \leq \varphi(I) \leq C' I^{\beta_2}, \quad I \geq 1.$$

For the sake of upcoming discussions, we rewrite the collision operator (23) and equilibrium distributions (24) by explicitly using (4) for  $\varphi$ . First, one can compute  $\Psi_{\text{res}}(Z) = Z^{\delta-1} \Gamma(\delta/2)^2 / \Gamma(\delta)$ , and thus (23) reads, for almost every  $v$  and  $I$ ,

$$(26) \quad Q(f, g)(v, I) = \frac{\Gamma(\delta)}{\Gamma(\delta/2)^2} \int_{\mathbb{R}^3 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2} \left( f' g'_* \left( \frac{II_*}{I'(I + I_* - I')} \right)^{\delta/2-1} - f g_* \right) \\ \times B(v, v_*, I, I_*, I', \sigma) \mathbf{1}_{[0, I+I_*]}(I') \frac{(I' I'_*)^{\delta/2-1}}{(I + I_*)^{\delta-1}} dv_* dI_* dI' d\sigma.$$

The equilibrium (24) becomes, for almost every  $v$  and  $I$ ,

$$(27) \quad M(v, I) = \frac{n}{\Gamma(\delta/2)} \left( \frac{m}{2\pi} \right)^{3/2} (k_B T_{\text{int}})^{-(\delta+3)/2} I^{\delta/2-1} \exp \left( -\frac{m|v-u|^2}{2k_B T_{\text{kin}}} - \frac{I}{k_B T_{\text{int}}} \right).$$

**2.3. Polyatomic gas with discrete internal energies.** Let us now describe another approach to model the degrees of freedom associated to internal energy for a single polyatomic gas. Instead of considering a continuous internal energy variable, one can introduce  $N_{\text{int}} \geq 2$  different internal energies  $\{I^{(1)}, \dots, I^{(N_{\text{int}})}\} \subset \mathbb{R}_+$ , see for instance [17, 20, 22]. Each collision can then be represented by two pre-collisional pairs and two corresponding post-collisional pairs, respectively indexed by  $(k, \ell)$  and  $(k', \ell')$ , with  $k, \ell, k', \ell' \in \{1, \dots, N_{\text{int}}\}$ . More precisely, consider two colliding molecules of mass  $m$  with velocities and internal energies  $(v, I^{(k)})$  and  $(v_*, I^{(\ell)})$ , changing into  $(v', I^{(k')})$  and  $(v'_*, I^{(\ell')})$ , and define the internal energy gap

$$\Delta I^{(k\ell, k'\ell')} = I^{(k')} + I^{(\ell')} - I^{(k)} - I^{(\ell)}.$$

The microscopic momentum and energy conservations are now written as

$$(28) \quad mv + mv_* = mv' + mv'_*,$$

$$(29) \quad \frac{m}{2}|v|^2 + \frac{m}{2}|v_*|^2 + I^{(k)} + I^{(\ell)} = \frac{m}{2}|v'|^2 + \frac{m}{2}|v'_*|^2 + I^{(k')} + I^{(\ell')}.$$

Equivalently, the conservations can be rewritten, defining the total energy  $E^{(k\ell, k'\ell')}$  in the center-of-mass reference frame, as

$$\frac{m}{4}|V|^2 + I^{(k)} + I^{(\ell)} = \frac{m}{4}|V'|^2 + I^{(k')} + I^{(\ell')} = E^{(k\ell, k'\ell')}.$$

The post-collisional velocities are then given by

$$v' = \frac{v + v_*}{2} + \sqrt{|V|^2 - \frac{4\Delta I^{(k\ell, k'\ell')}}{m}} \frac{\sigma}{2}, \quad v'_* = \frac{v + v_*}{2} - \sqrt{|V|^2 - \frac{4\Delta I^{(k\ell, k'\ell')}}{m}} \frac{\sigma}{2}.$$

The nonnegative collision kernel  $B$  is again assumed to satisfy symmetry and microreversibility relations as follows

$$\begin{aligned} B(v, v_*, I^{(k)}, I^{(\ell)}, I^{(k')}, I^{(\ell')}, \sigma) &= B(v_*, v, I^{(\ell)}, I^{(k)}, I^{(k')}, I^{(\ell')}, \sigma) \\ &= B(v, v_*, I^{(k)}, I^{(\ell)}, I^{(\ell')}, I^{(k')}, -\sigma), \\ B(v, v_*, I^{(k)}, I^{(\ell)}, I^{(k')}, I^{(\ell')}, \sigma) &= B\left(v', v'_*, I^{(k')}, I^{(\ell')}, I^{(k)}, I^{(\ell)}, \frac{V}{|V|}\right), \end{aligned}$$

In this discrete internal energy case, the distribution function is studied under the form  $f = (f^{(1)}, \dots, f^{(N_{\text{int}})})$ , where the component  $f^{(k)} = f^{(k)}(t, x, v)$  is the distribution function for particles with internal energy  $I^{(k)}$ , for any  $k \in \{1, \dots, N_{\text{int}}\}$ . This allows now to define the Boltzmann collision operator associated to the  $k$ -th component of the distribution function, for almost every  $v \in \mathbb{R}^3$ ,

$$(30) \quad Q^{(k)}(f, g)(v) = \sum_{\ell, k', \ell'=1}^{N_{\text{int}}} \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left( f^{(k')}(v') g^{(\ell')}(v'_*) \frac{\varphi^{(k)} \varphi^{(\ell)}}{\varphi^{(k')} \varphi^{(\ell')}} - f^{(k)}(v) g^{(\ell)}(v_*) \right) \\ \times B(v, v_*, I^{(k)}, I^{(\ell)}, I^{(k')}, I^{(\ell')}, \sigma) \varphi^{(k')} \varphi^{(\ell')} \frac{|V'|}{(E^{(k\ell, k'\ell')})^{1/2}} dv_* d\sigma.$$

The equilibrium states are characterized by the following  $H$ -theorem.

**Proposition 3.** *The three following properties are equivalent:*

- (i)  $Q^{(k)}(M, M) = 0$  for any  $k \in \{1, \dots, N_{\text{int}}\}$ ,
- (ii)  $\sum_{k=1}^{N_{\text{int}}} \int_{\mathbb{R}^3} Q^{(k)}(M, M)(v) \log \left[ \frac{M^{(k)}(v)}{\varphi^{(k)}} \right] dv = 0$ ,
- (iii) there exist  $n \geq 0$ ,  $u \in \mathbb{R}^3$  and  $T > 0$  such that, for every  $k \in \{1, \dots, N_{\text{int}}\}$  and almost every  $v$ ,

$$(31) \quad M^{(k)}(v) = \frac{n}{q} \left( \frac{m}{2\pi k_B T} \right)^{3/2} \varphi^{(k)} \exp \left( -\frac{m|v-u|^2}{2k_B T} - \frac{I^{(k)}}{k_B T} \right),$$

with  $q = \sum_{k=1}^{N_{\text{int}}} \varphi^{(k)} \exp \left( -\frac{I^{(k)}}{k_B T} \right)$  being the discrete version of the integral (25).

## 2.4. Polyatomic models for mixtures.

### 2.4.1. Borgnakke-Larsen model for a mixture of monatomic and/or polyatomic gases.

Consider a mixture of  $N \geq 2$  monatomic or polyatomic species. Let us denote by  $\mathcal{M}$  the set of indices corresponding to monatomic gases, and  $\mathcal{P}$  the one corresponding to polyatomic gases, so that  $\mathcal{M} \cup \mathcal{P} = \{1, \dots, N\}$ . For any polyatomic species  $i \in \mathcal{P}$ , the parameter used in (4) is denoted by  $\delta_i > 0$ , which is related to the number of internal degrees of freedom of the molecules. For two colliding molecules of species  $i$  and  $j$ , with respective masses  $m_i$  and  $m_j$ , velocities  $v$  and  $v_*$ , and (if polyatomic) internal energies  $I$  and  $I_*$ , the microscopic momentum and energy conservations are now written as

$$\begin{aligned} m_i v + m_j v_* &= m_i v' + m_j v'_*, \\ \frac{m_i}{2} |v|^2 + \frac{m_j}{2} |v_*|^2 + I \mathbf{1}_{i \in \mathcal{P}} + I_* \mathbf{1}_{j \in \mathcal{P}} &= \frac{m_i}{2} |v'|^2 + \frac{m_j}{2} |v'_*|^2 + I' \mathbf{1}_{i \in \mathcal{P}} + I'_* \mathbf{1}_{j \in \mathcal{P}}, \end{aligned}$$

or equivalently with the energy conservation law in the center-of-mass frame

$$E_{ij} = \frac{\mu_{ij}}{2} |V|^2 + I \mathbf{1}_{i \in \mathcal{P}} + I_* \mathbf{1}_{j \in \mathcal{P}} = \frac{\mu_{ij}}{2} |V'|^2 + I' \mathbf{1}_{i \in \mathcal{P}} + I'_* \mathbf{1}_{j \in \mathcal{P}},$$

where  $\mu_{ij} = \frac{m_i m_j}{m_i + m_j}$  is the reduced mass.

Let us now detail, for each case, the explicit expressions of the collision rules with a Borgnakke-Larsen-like parametrization for polyatomic gases [18], as well as the ones of the corresponding collision operators [2, 1].

**Collision between two monatomic molecules.** In this case, the collision rules can be written with the same parametrization  $\sigma \in \mathbb{S}^2$  as in the single species case, *i.e.*

$$v' = \frac{m_i v + m_j v_*}{m_i + m_j} + \frac{m_j}{m_i + m_j} |V| \sigma, \quad v'_* = \frac{m_i v + m_j v_*}{m_i + m_j} - \frac{m_i}{m_i + m_j} |V| \sigma.$$

The collision kernels  $B_{ij}(v, v_*, \sigma) \geq 0$  are again assumed to satisfy a symmetry and a microreversibility property as follows

$$(32) \quad B_{ij}(v, v_*, \sigma) = B_{ji}(v_*, v, -\sigma) = B_{ij} \left( v', v'_*, \frac{V}{|V|} \right),$$

**Remark 3.** *Due to the indistinguishability of particles of the same species, in a binary intraspecies collision, we do not distinguish which of the two particles has which velocity after the collision (both outcomes are assumed to be equally probable). Therefore, either pre- or post-collisional velocities can be separately interchanged without affecting the collision kernel. Noting that  $\sigma = \frac{v' - v'_*}{|v' - v'_*|}$ , one obtains the symmetry properties*

$$B_{ii}(v, v_*, \sigma) = B_{ii}(v_*, v, \sigma) = B_{ii}(v_*, v, -\sigma) = B_{ii}(v, v_*, -\sigma).$$

Note that the last two equalities are also consequences of the first symmetry and the microreversibility property.

In an interspecies collision, this is not the case anymore. The two particles are now distinguishable and one has to tell apart which particle has which velocity. The interchange of the particle roles, highlighted by the interchange of indices in the collision kernels, implies the interchange of both pre- and post-collisional velocities simultaneously. Therefore, the only symmetry property which remains true is (32).

The Boltzmann collision operator is then written, for almost every  $v$ , as

$$(33) \quad Q_{ij}(f, g)(v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} (f' g'_* - f g_*) B_{ij}(v, v_*, \sigma) dv_* d\sigma.$$

**Collision between two polyatomic molecules.** When at least one polyatomic species is involved, the velocity collision rules become

$$(34) \quad v' = \frac{m_i v + m_j v_*}{m_i + m_j} + \frac{m_j}{m_i + m_j} \sqrt{\frac{2 R E_{ij}}{\mu_{ij}}} \sigma,$$

$$(35) \quad v'_* = \frac{m_i v + m_j v_*}{m_i + m_j} - \frac{m_i}{m_i + m_j} \sqrt{\frac{2 R E_{ij}}{\mu_{ij}}} \sigma.$$

With the usual Borgnakke-Larsen parametrization, the repartition between the two microscopic internal energies provides

$$(36) \quad I' = r(1 - R)E_{ij}, \quad I'_* = (1 - r)(1 - R)E_{ij}.$$

Again, symmetry and microreversibility are required for the collision kernels, *i.e.*

$$B_{ij}(v, v_*, I, I_*, r, R, \sigma) = B_{ji}(v_*, v, I_*, I, 1 - r, R, -\sigma) = B_{ij} \left( v', v'_*, I', I'_*, r', R', \frac{V}{|V|} \right).$$

**Remark 4.** *When  $i \neq j$ , the interchange of the particle roles implies the interchange of both the pre- and post-collisional internal energies, additionally to the interchange of both the pre- and post-collisional velocities as in Remark 3. Thus the symmetry property has to involve both changes  $\sigma$  into  $-\sigma$  and  $r$  into  $1 - r$ .*



The collision operator for two polyatomic molecules of species  $i, j \in \mathcal{P}$  reads, for almost every  $v$  and  $I$ ,

$$(37) \quad Q_{ij}(f, g)(v, I) = \int_{\mathbb{R}^3 \times \mathbb{R}_+ \times (0,1)^2 \times \mathbb{S}^2} \left( f' g'_* \left( \frac{I}{I'} \right)^{\delta_i/2-1} \left( \frac{I_*}{I'_*} \right)^{\delta_j/2-1} - f g_* \right) \\ \times B_{ij}(v, v_*, I, I_*, r, R, \sigma) r^{\delta_i/2-1} (1-r)^{\delta_j/2-1} (1-R)^{\delta_i/2+\delta_j/2-1} \sqrt{R} dv_* dI_* dR dr d\sigma.$$

**Collision between one polyatomic molecule and one monatomic molecule.** In the case of a collision between one polyatomic and one monatomic molecule, the collision rules (34)–(35) still hold. Nevertheless, other expressions are changed, since there is no parameter  $r$  anymore associating the internal energy to each species.

If a polyatomic molecule of species  $i \in \mathcal{P}$  collides with a monatomic molecule of species  $j \in \mathcal{M}$ , we have for the internal energy

$$I' = (1-R)E_{ij},$$

the symmetry and microreversibility assumptions on  $B_{ij}$  are given by

$$(38) \quad B_{ij}(v, v_*, I, R, \sigma) = B_{ji}(v_*, v, I, R, -\sigma) = B_{ij} \left( v', v'_*, I', R', \frac{V}{|V|} \right),$$

and the collision operator is written, for almost every  $v$  and  $I$ , as

$$(39) \quad Q_{ij}(f, g)(v, I) = \int_{\mathbb{R}^3 \times (0,1) \times \mathbb{S}^2} \left( f(v', I') g(v'_*) \left( \frac{I}{I'} \right)^{\delta_i/2-1} - f(v, I) g(v_*) \right) \\ \times B_{ij}(v, v_*, I, R, \sigma) (1-R)^{\delta_i/2-1} \sqrt{R} dv_* dR d\sigma.$$

In the opposite case, when  $i \in \mathcal{M}$  and  $j \in \mathcal{P}$ , the post-collisional internal energy is given by

$$I'_* = (1-R)E_{ij},$$

the assumptions on  $B_{ij}$  are given by

$$(40) \quad B_{ij}(v, v_*, I_*, R, \sigma) = B_{ji}(v_*, v, I_*, R, -\sigma) = B_{ij} \left( v', v'_*, I'_*, R', \frac{V}{|V|} \right),$$

and the collision operator becomes, for almost every  $v$ ,

$$(41) \quad Q_{ij}(f, g)(v) = \int_{\mathbb{R}^3 \times \mathbb{R}_+ \times (0,1) \times \mathbb{S}^2} \left( f(v') g(v'_*) \left( \frac{I_*}{I'_*} \right)^{\delta_j/2-1} - f(v) g(v_*, I_*) \right) \\ \times B_{ij}(v, v_*, I_*, R, \sigma) (1-R)^{\delta_j/2-1} \sqrt{R} dv_* dI_* dR d\sigma.$$

In the previous equalities (33), (37), (39) and (41), both  $f$  and  $g$  are scalar functions related to the species  $i$  and  $j$ . In order to define the  $i$ -th component  $Q_i$  of the vector collision operator, we must emphasize that its argument has to be all the scalar functions related to any species at the same time. In other words, we use the vector forms  $f = (f_1, \dots, f_N)$ ,  $g = (g_1, \dots, g_N)$ , and then write, for any  $i \in \{1, \dots, N\}$ ,

$$(42) \quad Q_i(f, g) = \sum_{j=1}^N Q_{ij}(f_i, g_j).$$

Then, as usual, the equilibria are described thanks to the following  $H$ -theorem.

**Proposition 4.** *The three following properties are equivalent:*

- (1)  $Q_i(M, M) = 0$  for any  $1 \leq i \leq N$ ,  
(2) the following equality holds

$$\sum_{i \in \mathcal{M}} \int_{\mathbb{R}^3} Q_i(M, M)(v) \log M_i(v) dv + \sum_{i \in \mathcal{P}} \int_{\mathbb{R}^3 \times \mathbb{R}_+} Q_i(M, M)(v, I) \log (M_i(v, I) I^{1-\delta_i/2}) dv dI = 0,$$

- (3) there exist  $n = (n_1, \dots, n_N) \in \mathbb{R}_+^N$ ,  $u \in \mathbb{R}^3$  and  $T > 0$  such that, if  $i \in \mathcal{M}$ , for almost every  $v$ ,

$$(43) \quad M_i(v) = n_i \left( \frac{m_i}{2\pi k_B T} \right)^{3/2} \exp \left( -\frac{m_i |v - u|^2}{2k_B T} \right),$$

and if  $i \in \mathcal{P}$ , for almost every  $v$  and  $I$ ,

$$(44) \quad M_i(v, I) = \frac{n_i}{\Gamma(\delta_i/2)} \left( \frac{m_i}{2\pi} \right)^{3/2} (k_B T)^{-(\delta_i+3)/2} I^{\delta_i/2-1} \exp \left( -\frac{m_i |v - u|^2}{2k_B T} - \frac{I}{k_B T} \right).$$

2.4.2. *Mixture of polyatomic gases with discrete internal energies.* We now extend the model described in Section 2.3 to a mixture of  $N$  polyatomic gases [20, 22], with molecular masses  $m_1, \dots, m_N$ , where the polyatomicity of each species  $i \in \{1, \dots, N\}$  is modeled by  $N_{\text{int},i} \geq 1$  different internal energies  $\{I_i^{(1)}, \dots, I_i^{(N_{\text{int},i})}\} \subset \mathbb{R}_+$ .

Observe that if  $N_{\text{int},1} = \dots = N_{\text{int},N} = 1$  (with  $\varphi_1^{(1)} = \dots = \varphi_N^{(1)} = 1$ ), the model reduces to the case of a mixture of monatomic species. We obtain a mixture model of monatomic and polyatomic species as soon as there exist at least one index  $i$  such that  $N_{\text{int},i} = 1$ , with  $\varphi_i^{(k)} = 1$ , meaning that species  $i$  is monatomic, and at least one index  $j$  such that  $N_{\text{int},j} \geq 2$ , meaning that species  $j$  is polyatomic.

Each collision can then be represented by two pre-collisional pairs and two corresponding post-collisional pairs, respectively indexed by  $k, \ell$  and  $k', \ell'$ , with  $k, k' \in \{1, \dots, N_{\text{int},i}\}$ , and  $\ell, \ell' \in \{1, \dots, N_{\text{int},j}\}$ . More precisely, consider two colliding molecules of mass  $m_i$  and  $m_j$  with velocities and internal energies  $(v, I_i^{(k)})$  and  $(v_*, I_j^{(\ell)})$ , changing into  $(v', I_i^{(k')})$  and  $(v'_*, I_j^{(\ell')})$ , and define the internal energy gap

$$(45) \quad \Delta I_{ij}^{(k\ell, k'\ell')} = I_i^{(k')} + I_j^{(\ell')} - I_i^{(k)} - I_j^{(\ell)}.$$

The microscopic momentum and energy conservations are given by

$$(46) \quad m_i v + m_j v_* = m_i v' + m_j v'_*,$$

$$(47) \quad \frac{m_i}{2} |v|^2 + \frac{m_j}{2} |v_*|^2 + I_i^{(k)} + I_j^{(\ell)} = \frac{m_i}{2} |v'|^2 + \frac{m_j}{2} |v'_*|^2 + I_i^{(k')} + I_j^{(\ell')}.$$

Equivalently, the energy conservation can be rewritten in the center-of-mass reference frame, with the total energy

$$E_{ij}^{(k\ell, k'\ell')} = \frac{\mu_{ij}}{2} |V|^2 + I_i^{(k)} + I_j^{(\ell)} = \frac{\mu_{ij}}{2} |V'|^2 + I_i^{(k')} + I_j^{(\ell')}.$$

The post-collisional velocities are then given by

$$v' = \frac{m_i v + m_j v_*}{m_i + m_j} + \sigma \frac{\mu_{ij}}{m_i} \sqrt{|V|^2 - \frac{2}{\mu_{ij}} \Delta I_{ij}^{(k\ell, k'\ell')}}},$$

$$v'_* = \frac{m_i v + m_j v_*}{m_i + m_j} - \sigma \frac{\mu_{ij}}{m_j} \sqrt{|V|^2 - \frac{2}{\mu_{ij}} \Delta I_{ij}^{(k\ell, k'\ell')}}}.$$

The symmetry and microreversibility assumptions on the collision kernels for  $(i, j) \in \{1, \dots, N\}^2$  are

$$\begin{aligned} B_{ij}(v, v_*, I_i^{(k)}, I_j^{(\ell)}, I_i^{(k')}, I_j^{(\ell')}, \sigma) &= B_{ji}(v_*, v, I_j^{(\ell)}, I_i^{(k)}, I_j^{(\ell')}, I_i^{(k')}, -\sigma) \\ &= B_{ij}(v', v'_*, I_i^{(k')}, I_j^{(\ell')}, I_i^{(k)}, I_j^{(\ell)}, \frac{V}{|V|}) \\ B_{ii}(v, v_*, I_i^{(k)}, I_i^{(\ell)}, I_i^{(k')}, I_i^{(\ell')}, \sigma) &= B_{ii}(v_*, v, I_i^{(\ell)}, I_i^{(k)}, I_i^{(k')}, I_i^{(\ell')}, \sigma). \end{aligned}$$

The corresponding collision operator is written, for almost every  $v$ , as

$$(48) \quad Q_{ij}^{(k)}(f, g)(v) = \sum_{k'=1}^{N_{\text{int},i}} \sum_{\ell, \ell'=1}^{N_{\text{int},j}} \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left( f^{(k')}(v') g^{(\ell')}(v'_*) \frac{\varphi_i^{(k)} \varphi_j^{(\ell)}}{\varphi_i^{(k')} \varphi_j^{(\ell')}} - f^{(k)}(v) g^{(\ell)}(v_*) \right) \\ \times B_{ij}(v, v_*, I_i^{(k)}, I_j^{(\ell)}, I_i^{(k')}, I_j^{(\ell')}, \sigma) \varphi_i^{(k')} \varphi_j^{(\ell')} \frac{|V'|}{\left(E_{ij}^{(k\ell, k'\ell')}\right)^{1/2}} dv_* d\sigma,$$

with constant positive degeneracies  $\varphi_i^{(1)}, \dots, \varphi_i^{(N_{\text{int},i})}$  for each species  $i$ . In the previous equality (48),  $f$  is the vector function consisting of the components for all different internal energies of species  $i$ , and  $g$  the one consisting of the components for all different internal energies of species  $j$ . In order to define the  $i$ -th component of the vector collision operator, its argument has to be all these vector functions related to any species at the same time, as in the case of continuous energies (42). Therefore, we use the vector form of all components for different internal energies of all species

$$f = \left( f_1^{(1)}, \dots, f_1^{(N_{\text{int},1})}, f_2^{(1)}, \dots, f_{N-1}^{(N_{\text{int},N-1})}, f_N^{(1)}, \dots, f_N^{(N_{\text{int},N})} \right),$$

and using the same notation for a vector function  $g$ , the  $i$ -th component of the collision operator is given, for any  $i \in \{1, \dots, N\}$ , by

$$Q_i^{(k)}(f, g) = \sum_{j=1}^N Q_{ij}^{(k)}(f_i, g_j).$$

We can then set, for any  $i$ ,

$$(49) \quad Q_i(f, g) = \left( Q_i^{(1)}(f, g), \dots, Q_i^{(N_{\text{int},i})}(f, g) \right),$$

which allows to state a part of the  $H$ -theorem that defines the equilibrium state.

**Proposition 5.** *The three following properties are equivalent:*

- (1)  $Q_i(M, M) = 0$  for any  $i \in \{1, \dots, N\}$ ,
- (2)  $\sum_{i=1}^N \sum_{k=1}^{N_{\text{int},i}} \int_{\mathbb{R}^3} Q_i^{(k)}(M, M)(v) \log \left[ \frac{M_i^{(k)}(v)}{\varphi_i^{(k)}} \right] dv = 0$ ,
- (3) there exist  $n = (n_1, \dots, n_N) \in \mathbb{R}_+^N$ ,  $u \in \mathbb{R}^3$  and  $T > 0$  such that, for any  $i \in \{1, \dots, N\}$  and  $k \in \{1, \dots, N_{\text{int},i}\}$  and almost every  $v$ ,

$$(50) \quad M_i^{(k)}(v) = \frac{n_i}{q_i} \left( \frac{m_i}{2\pi k_B T} \right)^{3/2} \varphi_i^{(k)} \exp \left( -\frac{m_i |v - u|^2}{2k_B T} - \frac{I_i^{(k)}}{k_B T} \right),$$

$$\text{with } q_i = \sum_{k=1}^{N_{\text{int},i}} \varphi_i^{(k)} \exp \left( -\frac{I_i^{(k)}}{k_B T} \right).$$

**2.5. Boltzmann equation and linearized collision operator.** The Boltzmann equation describes the time evolution of a system composed by a large number of particles, described by a distribution function  $f$  defined on the phase space of the system. For the sake of simplicity, we also assume that the system is isolated, so that there is no external force acting on the particles. The time evolution of the distribution function  $f$  is governed by the Boltzmann equation

$$(51) \quad \frac{\partial f}{\partial t} + (v \cdot \nabla_x) f = Q(f, f),$$

where  $f$  denotes

- the scalar function  $f = f(t, x, v, I)$  in the case of a single polyatomic gas with continuous internal energy,
- the vector function  $f = (f^{(1)}, \dots, f^{(N_{\text{int}})})$  in the discrete internal energy case with  $f^{(k)} = f^{(k)}(t, x, v)$ ,
- the vector function  $f = (f_1, \dots, f_N)$ , with  $f_i = f_i(t, x, v)$  if  $i \in \mathcal{M}$ , and  $f_i = f_i(t, x, v, I)$  if  $i \in \mathcal{P}$ , in the case of a mixture with continuous internal energies,
- the vector function  $f = (f_1, \dots, f_N)$ , where each  $f_i$  is given by the vector function  $f_i(t, x, v) = (f_i^{(1)}(t, x, v), \dots, f_i^{(N_{\text{int},i})}(t, x, v))$ , in the discrete internal energy case.

In each case, the collision operator  $Q$  is a quadratic bilinear operator that accounts for the change of velocities and internal energies of particles due to the binary collisions.

- For a single species,  $Q$  is given by (14) in the Borgnakke-Larsen framework, by (23) in the resonant case, and by the vector form  $Q = (Q^{(1)}, \dots, Q^{(N_{\text{int}})})$ , where each  $Q^{(k)}$ ,  $1 \leq k \leq N_{\text{int}}$ , is given by (30) in the discrete internal energy case.
- In the mixture case, when the internal energy variable is continuous,  $Q$  is naturally defined as the vector expression  $Q = (Q_1, \dots, Q_N)$ , where each  $Q_i$  is given by (42).
- In the mixture case, when the internal energy variable is discrete,  $Q$  is again defined as  $Q = (Q_1, \dots, Q_N)$ , where, this time, each  $Q_i$  is given by (49).

In order for us to describe the linearization setting in a unified way, let us rewrite the scalar collision operator in the following way, for almost every  $w = (v, I)$ ,

$$(52) \quad Q(f, g)(w) = \int_D (f' g'_* \Phi - f g_*) A(W) dW,$$

where the integration variable  $W$  is

$$(53) \quad W = \begin{cases} (v_*, I_*, I', \sigma) & \text{for the resonant case,} \\ (v_*, I_*, R, r, \sigma) & \text{for the Borgnakke-Larsen framework,} \end{cases}$$

the integration domain  $D$  is either  $D = \mathbb{R}^3 \times (\mathbb{R}_+)^2 \times \mathbb{S}^2$  or  $D = \mathbb{R}^3 \times (\mathbb{R}_+) \times (0, 1)^2 \times \mathbb{S}^2$ ,  $\Phi = [(II_*) / (I'I'_*)]^{\delta/2-1}$ , which is obviously similar for all continuous internal energy models, and

$$(54) \quad A(W) = \begin{cases} B(v, v_*, I, I_*, I', \sigma) \frac{\varphi(I') \varphi(I+I_*-I')}{\Psi_{\text{res}}(I+I_*)} & \text{(resonant),} \\ B(v, v_*, I, I_*, r, R, \sigma) \\ \quad \times (r(1-r))^{\delta/2-1} (1-R)^{\delta-1} \sqrt{R} & \text{(Borgnakke-Larsen).} \end{cases}$$

In the case of vector quantities, (52) can be extended in a straightforward way. First, in the discrete internal energy case,  $Q^{(k)}$  writes, for almost every  $w$ ,

$$(55) \quad Q^{(k)}(f, g)(w) = \sum_{k', \ell, \ell'=1}^N \int_D \left( f^{(k')} (v') g^{(\ell')} (v'_*) \Phi^{(k\ell, k'\ell')} - f^{(k)} (v) g^{(\ell)} (v_*) \right) A^{(k\ell, k'\ell')} (W) dW,$$

where  $w = v$ ,  $W = (v_*, \sigma)$ ,  $D = \mathbb{R}^3 \times \mathbb{S}^2$ ,  $\Phi^{(k\ell, k'\ell')} = (\varphi^{(k)} \varphi^{(\ell)}) / (\varphi^{(k')} \varphi^{(\ell')})$  and

$$(56) \quad A^{(k\ell, k'\ell')} (W) = B(v, v_*, I^{(k)}, I^{(\ell)}, I^{(k')}, I^{(\ell')}, \sigma) \frac{\varphi^{(k')} \varphi^{(\ell')} |V'|}{(E^{(k\ell, k'\ell')})^{1/2}}.$$

Second, in the mixture case with a continuous internal energy variable,  $Q_i$  writes, for almost every  $w$ ,

$$(57) \quad Q_i(f, g)(w) = \sum_{j=1}^N \int_D \left( f' g'_* \Phi_{ij} - f g_* \right) A_{ij}(W) dW,$$

where  $w = (v, I)$  if  $i \in \mathcal{P}$  and  $w = v$  if  $i \in \mathcal{M}$ ,  $W$  is defined by

$$(58) \quad W = \begin{cases} (v_*, I_*, R, r, \sigma) & \text{if } i, j \in \mathcal{P}, \\ (v_*, R, \sigma) & \text{if } i \in \mathcal{P}, j \in \mathcal{M}, \\ (v_*, I_*, R, \sigma) & \text{if } i \in \mathcal{M}, j \in \mathcal{P}, \\ (v_*, \sigma) & \text{if } i, j \in \mathcal{M}, \end{cases}$$

with the relevant corresponding domain  $D$ ,  $\Phi_{ij}$  is defined by

$$\Phi_{ij} = \begin{cases} \left( \frac{I}{I'} \right)^{\delta_i/2-1} \left( \frac{I_*}{I'_*} \right)^{\delta_j/2-1} & \text{if } i, j \in \mathcal{P}, \\ \left( \frac{I}{I'} \right)^{\delta_i/2-1} & \text{if } i \in \mathcal{P}, j \in \mathcal{M}, \\ \left( \frac{I_*}{I'_*} \right)^{\delta_j/2-1} & \text{if } i \in \mathcal{M}, j \in \mathcal{P}, \\ 1 & \text{if } i, j \in \mathcal{M}, \end{cases}$$

and  $A_{ij}(W)$  by

$$(59) \quad A_{ij}(W) = \begin{cases} B_{ij}(v, v_*, I, I_*, r, R, \sigma) \\ \quad \times r^{\delta_i/2-1} (1-r)^{\delta_j/2-1} (1-R)^{\delta_i/2+\delta_j/2-1} \sqrt{R}, & \text{if } i, j \in \mathcal{P}, \\ B_{ij}(v, v_*, I, R, \sigma) (1-R)^{\delta_i/2-1} \sqrt{R}, & \text{if } i \in \mathcal{P}, j \in \mathcal{M}, \\ B_{ij}(v, v_*, I_*, R, \sigma) (1-R)^{\delta_j/2-1} \sqrt{R}, & \text{if } i \in \mathcal{M}, j \in \mathcal{P}, \\ B_{ij}(v, v_*, \sigma) & \text{if } i, j \in \mathcal{M}. \end{cases}$$

Last, the case of a mixture of polyatomic gases with discrete internal energies is a straightforward extension of (55) and (57) by writing, for almost every  $w$ ,

$$Q_i^{(k)}(f, g)(w) = \sum_{j=1}^N \sum_{k'=1}^{N_{\text{int},i}} \sum_{\ell, \ell'=1}^{N_{\text{int},j}} \int_D \left( f_i^{(k')} (v') g_j^{(\ell')} (v'_*) \Phi_{ij}^{(k\ell, k'\ell')} - f_i^{(k)} (v) g_j^{(\ell)} (v_*) \right) A_{ij}^{(k\ell, k'\ell')} (W) dW,$$

where  $w = v$ ,  $W = (v_*, \sigma)$ ,  $D = \mathbb{R}^3 \times \mathbb{S}^2$ ,  $\Phi_{ij}^{(k\ell, k'\ell')} = (\varphi_i^{(k)} \varphi_j^{(\ell)}) / (\varphi_i^{(k')} \varphi_j^{(\ell')})$  and

$$(60) \quad A_{ij}^{(k\ell, k'\ell')} (W) = B_{ij}(v, v_*, I_i^{(k)}, I_j^{(\ell)}, I_i^{(k')}, I_j^{(\ell')}, \sigma) \frac{\varphi_i^{(k')} \varphi_j^{(\ell')} |V'|}{(E_{ij}^{(k\ell, k'\ell')})^{1/2}}.$$

Further, the associated equilibria for a single species are Maxwellian distributions  $M$  given by (15) in the Borgnakke-Larsen framework, (27) in the resonant case, and (31) when handling discrete internal energy levels. For mixtures, the Maxwellian distributions  $M_i$  are defined in (43)–(44) for the Borgnakke-Larsen model, and (50) in the discrete internal energy case.

The standard perturbative setting for the Boltzmann equation (51), combined with the  $H$ -theorem, leads to considering deviations of Maxwellian distributions under the form

$$(61) \quad f = M + M^{1/2}h.$$

In this case, the linearized Boltzmann operator is defined as

$$(62) \quad \mathcal{L}h = M^{-1/2} [Q(M, M^{1/2}h) + Q(M^{1/2}h, M)].$$

In the case of mixtures, this equation has to be understood in the following sense for any  $1 \leq i \leq N$

$$(63) \quad [\mathcal{L}h]_i = M_i^{-1/2} \sum_{j=1}^N \left[ Q_{ij}(M_i, M_j^{1/2}h_j) + Q_{ij}(M_i^{1/2}h_i, M_j) \right].$$

This linearized Boltzmann operator can be written as  $\mathcal{L} = K - \nu \text{Id}$ , where the collision frequency  $\nu$  is defined with the notations of (52) as

$$\nu(w) = \int_D M_* A(W) dW.$$

The extension to vector quantities, with the notations of (55) or (57), is straightforward.

The operator  $K$  consists of three contributions and is given with the notations of (52) by

$$(64) \quad Kh(w) = M^{1/2} \int_D \left( (M^{-1/2}h)' + (M^{-1/2}h)'_* - (M^{-1/2}h)_* \right) M_* A(W) dW.$$

The extension to discrete internal energies is similar as in (55), whereas the extension to mixtures has to be understood as in (57) and (63).

### 3. COMPACTNESS PROPERTY OF $K$

Recent works have tackled the question of the compactness of the operator  $K$ , defined in (64), for the different polyatomic models presented in Section 2. In these papers, the compactness property is proved under some assumptions on the collision kernels, basically imposing some bounds on their growth.

**Monatomic gases.** Let us briefly recall under which assumption the operator  $K$  is compact for monatomic gases, in the case of hard potential and with Grad's cut-off assumption, since it is the framework of all papers which tackled this question for polyatomic gases. For more references on the monatomic case, see the review paper [12]. For both monatomic single species and mixtures of monatomic gases, compactness of the operator  $K$  has been proved [21, 10] under the assumption  $(H_1)$  stated below.

**Hypothesis 1** ( $H_1$ ). *There exist a constant  $C > 0$  and an exponent  $0 < \zeta < 1$  such that the possible collision kernels  $B$  or  $B_{ij}$ , for any  $1 \leq i, j \leq N$ , satisfy*

$$B(v, v_*, \sigma), B_{ij}(v, v_*, \sigma) \leq C |V| \left( 1 + \frac{1}{|V|^{2-\zeta}} \right).$$

Since monatomic gases are discussed in detail in [12], we do not discuss them here.

For a single polyatomic gas, we described three models: one written within the Borgnakke-Larsen framework, one for resonant collisions, and one with discrete internal energies. In those three cases, the assumptions on  $B$  made by the authors are slightly different. Let us state them below.

**Single polyatomic gas with continuous internal energy.** For the model written with the Borgnakke-Larsen procedure, several contributions appeared recently, obtained under different assumptions.

**Hypothesis 2** ( $H_2$ ). *There exist a constant  $C > 0$  and an exponent  $0 < \zeta < 1$  such that*

$$B(v, v_*, I, I_*, r, R, \sigma) \leq CE \left( 1 + \frac{1}{(|V| |V'|)^{1-\zeta/2}} \right).$$

**Hypothesis 3** ( $H_3$ ). *Let  $\zeta > -1$ . There exist a constant  $C > 0$  and a function  $\Psi(r, R)$ , satisfying the symmetry condition  $\Psi(r, R) = \Psi(1-r, R)$  and the integrability condition*

$$\Psi(r, R)^2 (1-r)^{\delta-3-\zeta} r^{\delta/2-2} R(1-R)^{3\delta/2-3-\zeta} \in L^1((0, 1)^2),$$

*such that*

$$B(v, v_*, I, I_*, r, R, \sigma) \leq C \Psi(r, R) E^{\zeta/2}.$$

In this case, the compactness has been proved in two different contributions.

**Theorem 1** (proved in [4]). *For any  $\delta \geq 2$ , under Hypothesis ( $H_2$ ), the operator  $K$  is compact from  $L^2(\mathbb{R}^3 \times \mathbb{R}_+)$  into itself.*

**Theorem 2** (proved in [16], [26]). *For any  $\zeta > -1$ , for  $\delta$  and  $B$  satisfying Hypothesis ( $H_3$ ), the operator  $K$  is compact from  $L^2(\mathbb{R}^3 \times \mathbb{R}_+)$  into itself.*

Observe that Hypothesis ( $H_3$ ) couples the value of  $\delta$  with the assumption on the collision kernel  $B$ , through the integrability of the function  $\Psi$ . Let us also mention that in the diatomic case ( $\delta = 2$ ), the operator  $K$  was also proved to be compact in [14], but under more restrictive assumptions than Hypothesis ( $H_3$ ) with  $\delta = 2$ .

**Single polyatomic gas with resonant collisions.** In the resonant case, the collision kernel is assumed [8, 9] to be upper-bounded by a tensored form on  $(|V|, \cos \theta)$  on the one hand and on  $(I, I_*, I')$  on the other hand.

**Hypothesis 4** ( $H_4$ ). *There exist two functions  $b_{\text{kin}}$  and  $b_{\text{int}}$  satisfying, for some constant  $C > 0$  and some exponents  $\zeta \in [0, 1)$ ,  $\zeta_1 \in [0, 1/2)$  and  $\zeta_2 \in (-\delta, \delta)$ ,*

$$0 \leq b_{\text{kin}}(|V|, \cos \theta) \leq C [|\sin \theta| (|V|^2 + |V|^{-1}) + |V| + |V|^{-\zeta} + |\sin \theta|^{-\zeta_1}]$$

$$0 \leq b_{\text{int}}(I, I_*) \leq C \frac{(I + I_*)^{\zeta_2/2}}{\Psi_{\text{res}}(I + I_*)},$$

*such that*

$$B(v, v_*, I, I_*, I', \sigma) \leq b_{\text{kin}}(|V|, \cos \theta) b_{\text{int}}(I, I_*) \mathbf{1}_{I' \leq I + I_*},$$

*or any linear combination of such terms.*

Under this assumption, the compactness of  $K$  can be proved.

**Theorem 3** (proved in [9]). *Under Hypothesis ( $H_4$ ), the operator  $K$  is compact from  $L^2(\mathbb{R}^3 \times \mathbb{R}_+)$  into itself.*

**Single polyatomic gas with discrete internal energy.** In the case of discrete internal energies, an analogous result to Theorem 1 has been proved under the following assumption.

**Hypothesis 5** ( $H_5$ ). *There exist a constant  $C > 0$  and  $0 < \zeta < 1$  such that for any  $1 \leq k, k', \ell, \ell' \leq N_{\text{int}}$*

$$B(v, v_*, I^{(k)}, I^{(\ell)}, I^{(k')}, I^{(\ell')}, \sigma) \leq C \left( E^{(k\ell, k'\ell')} \right)^{1/2} \left( 1 + \frac{1}{(|V||V'|)^{1-\zeta/2}} \right).$$

**Theorem 4** (proved in [3]). *Under Hypothesis ( $H_5$ ), the operator  $K$  is compact from  $L^2(\mathbb{R}^3)^{N_{\text{int}}}$  into itself.*

**Mixture of monatomic and polyatomic gases with continuous internal energy.**

When considering a mixture with polyatomic gases, several configurations can occur, if also monatomic gases exist in the mixture. Moreover, as for the case of a single species, different contributions appeared in the literature, using different assumptions. These contributions are natural extensions of the results we mentioned in the previous subsection about the single species case.

**Hypothesis 6** ( $H_6$ ). *There exist a constant  $C > 0$  and  $0 < \zeta < 1$  such that the possible  $B_{ij}$ , for any  $1 \leq i, j \leq N$ , satisfy*

$$\begin{aligned} B_{ij}(v, v_*, I, I_*, r, R, \sigma), B_{ij}(v, v_*, I, R, \sigma), B_{ij}(v, v_*, I_*, R, \sigma), B_{ij}(v, v_*, \sigma) \\ \leq C E_{ij}^{1/2} \left( 1 + \frac{1}{(|V||V'|)^{1-\zeta/2}} \right). \end{aligned}$$

**Hypothesis 7** ( $H_7$ ). *Let  $\zeta_{ij} > -1$ . There exist a constant  $C > 0$  and functions  $\Psi_{ij}(r, R)$  satisfying the symmetry condition  $\Psi_{ij}(r, R) = \Psi_{ij}(1-r, R)$  and the integrability conditions*

$$\begin{aligned} \Psi_{ij}(r, R)^2 (1-r)^{\delta_j/2-2} r^{(\delta_i+\delta_j)/2-3-\zeta_{ij}} R (1-R)^{\delta_i/2+\delta_j-3-\zeta_{ij}} \in L^1((0, 1)^2), \\ \Psi_{ij}(r, R)^2 (1-r)^{\delta_j-3-\zeta_{ij}} r^{\delta_i/2-2} R (1-R)^{\delta_i/2+\delta_j-3-\zeta_{ij}} \in L^1((0, 1)^2), \end{aligned}$$

such that

$$B_{ij}(v, v_*, I, I_*, r, R, \sigma) \leq C \Psi_{ij}(r, R) E_{ij}^{\zeta_{ij}/2}.$$

**Theorem 5** (proved in [5]). *For any  $(\delta_i)_{1 \leq i \leq N}$  with  $\delta_i \geq 2$ , under Hypothesis ( $H_6$ ), the operator  $K$  for a mixture of polyatomic gases involving possibly also monatomic gases is compact from  $L^2(\mathbb{R}^3)^{|\mathcal{M}|} \times L^2(\mathbb{R}^3 \times \mathbb{R}_+)^{|\mathcal{P}|}$  into itself, up to an index reordering.*

**Theorem 6** (proved in [15], [26]). *For any  $(\zeta_{ij})_{1 \leq i, j \leq N}$  with  $\zeta_{ij} > -1$ , for  $(\delta_i)_{1 \leq i \leq N}$  and  $B_{ij}$  satisfying Hypothesis ( $H_7$ ), the operator  $K$  for a mixture of polyatomic gases is compact from  $L^2(\mathbb{R}^3 \times \mathbb{R}_+)^N$  into itself.*

Observe that, as in Hypothesis ( $H_3$ ), ( $H_7$ ) couples the values of  $\delta_i$  and  $\delta_j$  with the assumption on the collision kernel  $B_{ij}$ , through the integrability of the function  $\Psi_{ij}$ .

**Mixture of monatomic and polyatomic gases with discrete internal energy.**

As before, for discrete internal energies, the single species case is also extended to the mixtures of polyatomic gases, with possibly monatomic species. The assumption on the collision kernel is adapted as follows.

**Hypothesis 8** ( $H_8$ ). *There exist a constant  $C > 0$  and  $0 < \zeta < 1$  such that for any  $1 \leq k, k' \leq N_{\text{int}, i}$ ,  $1 \leq \ell, \ell' \leq N_{\text{int}, j}$ ,*

$$B_{ij}(v, v_*, I_i^{(k)}, I_j^{(\ell)}, I_i^{(k')}, I_j^{(\ell')}, \sigma) \leq C \left( E_{ij}^{(k\ell, k'\ell')} \right)^{1/2} \left( 1 + \frac{1}{(|V||V'|)^{1-\zeta/2}} \right).$$



The compactness result follows.

**Theorem 7** (proved in [6]). *Under Hypothesis (H<sub>8</sub>), the operator  $K$  for a mixture of polyatomic gases involving possibly also monatomic gases, is compact from  $L^2(\mathbb{R}^3)^{N_{\text{int}}^{\text{tot}}}$ , where  $N_{\text{int}}^{\text{tot}} = \sum_{i=1}^N N_{\text{int},i}$ , into itself.*

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