ON BGK APPROXIMATION
FOR REACTIVE AND NON–REACTIVE FLOWS

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ABSTRACT

In the framework of recently introduced consistent BGK approximations of the Boltzmann equations for both reactive and non–reactive gas mixtures, the problem of an appropriate choice of the relaxation times, which represent the crucial parameters of the model, is addressed. In this first approach, BGK results are tested versus the only exact analytical solutions available in the literature for mixtures, namely the BKW modes for space-homogeneous inert Maxwellian molecules. Results indicate, as expected, that using the actual average collision times in the BGK equations produces a too fast dissipation (entropy production) with respect to the Boltzmann description, and that the best fit in that trend is obtained if such times are amplified by a suitable factor, roughly of order 2 in the cases run.

Keywords. Kinetic theory, gas mixtures, BGK model, BKW modes.

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1. INTRODUCTION

In addition to its own intrinsic interest, a kinetic investigation of rarefied gas mixtures, with or without chemical reactions, is an essential step in order to achieve a rigorous derivation and justification for the most common macroscopic descriptions used in the hydrodynamic regime [1, 2]. On the other hand, it is immediately clear that nonlinear collision integrals of Boltzmann type are quite cumbersome to handle, especially in the chemical frame [3], and simpler approximate models would be convenient for practical applications. Relaxation time approximations of the type proposed by Bhatnagar, Gross, and Krook [4] and by Welander [5] (usually denoted as BGK models) lend themselves as obvious candidates in this respect. Such synthetic models of classical gas dynamics prescribe relaxation towards a local equilibrium with a strength determined by a suitable characteristic time, and have been extended rather recently in the literature [6, 7] in order to deal with a bimolecular chemical reaction

\[ A^1 + A^2 \rightleftharpoons A^3 + A^4. \] (1)

In particular, the latter paper follows the consistent BGK strategy proposed in [8] for inert mixture, which avoids the well known drawbacks which arise for a multi-species gas [9]. The idea is resorting to a single BGK collision term for each species \( s \) \((s = 1, 2, 3, 4)\), describing both mechanical (elastic) and chemical encounters, and drifting the distribution function \( f^s \) towards a suitable local Maxwellian \( \mathcal{M}_s \), whose macroscopic parameters are not the actual fields, moments of \( f^s \) (number density \( n^s \), drift velocity \( \mathbf{u}^s \), temperature \( T^s \)), but some other fictitious fields \( n_s, u_s, T_s \), constructed “ad hoc” in order to recover the exact exchange rates for mass, momentum and energy, as given by the whole Boltzmann-like collision operator for Maxwellian molecules [10]. It has been shown in [7] that such BGK model is a consistent approximation of the Boltzmann kinetic description, which reproduces in particular the correct macroscopic conservation equations and the correct collision equilibria,
as Maxwellians at a common mass velocity and temperature, and with num-
ber densities related by the well known mass action law. Furthermore, the
hydrodynamic limit for small collision times of the chemical BGK equations
has been worked out in [11] via an asymptotic Chapman-Enskog expansion,
and compared to the pertinent corresponding limits of Boltzmann and BGK
equations for reactive and non-reactive gas mixtures.

The present paper is aimed at proceeding further along the lines proposed
in [7, 11] by investigating some questions that were left there as open prob-
lems. In particular, we shall focus on the proper choice of the relaxation times
to be used in the model. In both inert and reactive cases it has been shown
[7, 8] that keeping the overall collision frequency parameters large enough pre-
vents physical inconsistencies, and lower bounds have been given to guarantee
positivity of temperature fields as well as, in the reactive case, positivity of
the density fields. On the other hand, too large values of such relaxation pa-
rameters would enhance artificially the relaxation speed due to the collision
mechanism, in a model which by construction drives very fast all distribution
functions towards a Maxwellian shape. In the preliminary space-homogeneous
computations performed in [7, 11], collision frequencies were chosen in order
to reproduce the average number of collisions (both mechanical and chemical)
undergone by each species in the mixture, which can be analytically estimated
for Maxwellian molecules when the mechanical process is faster than the chem-
ical one. This option fulfils all consistency constraints mentioned above. Also,
it turns out that varying relaxation parameters with respect to those reference
values does not affect appreciably the results, except for an initial layer. The
reason is that evolution of the main macroscopic observables is exactly repro-
duced by the model, irrespective of such parameters, and this is the fact that
essentially determines the overall evolution in the bulk time region. As a pre-
liminary step towards an optimization of the macroscopic collision frequencies
to be adopted, we shall check here whether the application of a multiplica-
tive factor to the evaluated count of collisions leads to an improvement of the
BGK results, and we shall look for the optimal factor in this sense. As a test for the correctness of the relaxation process it seems appropriate to resort to the time evolution of the proper $H$-functional [7, 8], which can be numerically computed following a solution. Of course, all of that requires the availability of exact solutions for the distribution functions or of accurate numerical results at the kinetic level, including the initial layer, to be used for comparison with BGK results. A systematic investigation on this matter is scheduled as future work. For now, we shall confine ourselves to comparisons with the so-called BKW-modes, which are (to our knowledge) the only available analytical solutions valid for a gas mixture [13]. They apply to space-homogeneous gas mixtures of non-reactive Maxwellian molecules, and represent the extension to a multi-component gas of the famous exact solutions to the Boltzmann equation devised by Bobylev [14], and independently by Krook an Wu [15]. The present test will then be necessarily restricted to the non-reactive case. However, as far as we know, comparisons of this kind, even for the inert model proposed in [8], are lacking in the literature. In addition, it would be obviously desirable to get a first concrete, though rough, estimate of the (presumable) reduction that must be applied to collisionality in the BGK model in order to achieve the best approximation also of the correct Boltzmann dissipation rate.

The article is organized as follows. After presenting in Section 2 the main features of the considered BGK model, Section 3 is devoted to a detailed description of the family of BKW exact solutions holding for a general $N$-component gas mixture, emphasizing their construction and their main features. Finally, Section 4 presents a discussion on the results of the extensive numerical calculations that have been performed for varying parameters. For different values, over wide ranges, of collision frequencies, masses, and initial conditions the optimal reduction factor is computed by a least square test on the time evolution of the entropy functional, as provided by running our model BGK equations, versus the same functional, as resulting from the exact BKW solution. Some numerical results are finally plotted for illustrative purposes.
2. BGK EQUATIONS

We point out here the main features of the relaxation time approximation introduced in [8] for an inert mixture and extended in [7] to the chemical reaction model worked out in [3, 16]. Kinetic equations read as

\[
\frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \frac{\partial f^s}{\partial \mathbf{x}} = \nu_s (\mathcal{M}_s - f^s) \quad s = 1, \ldots, 4, \tag{2}
\]

where each of the \( \mathcal{M}_s \) is a local Maxwellian with 5 disposable scalar parameters

\[
\mathcal{M}_s(\mathbf{v}) = n_s \left( \frac{m^s}{2\pi K T_s} \right)^{\frac{3}{2}} \exp \left[ -\frac{m^s}{2K T_s} (\mathbf{v} - \mathbf{u}_s)^2 \right], \quad s = 1, \ldots, 4 \tag{3}
\]

and \( \nu_s \), independent of \( \mathbf{v} \), is the inverse of the \( s \)-th relaxation time (macroscopic collision frequency). We remark that a superscript \( s \) is used as a label of the \( s \)-th species for any actual physical or observable property, whereas fictitious fields relevant to that species are identified by an \( s \) subscript. The auxiliary fields \( n_s, \mathbf{u}_s, T_s \) are determined by requiring that the exchange rates for mass, momentum and energy following from (2) coincide with those deduced from the corresponding Boltzmann equations. The latter rates are known analytically for Maxwell molecules [10], and may be expressed in terms of some physical parameters like masses \( m^s \) (with \( m^1 + m^2 = m^3 + m^4 = M \)), reduced masses \( \mu^{sr} \), energies of chemical link \( E^s \), and energy difference between reactants and products \( \Delta E = -\sum_{s=1}^{4} \lambda^s E^s \) (with \( \lambda^1 = \lambda^2 = -\lambda^3 = -\lambda^4 = 1 \)), conventionally assumed to be positive. Other essential parameters are the microscopic collision frequencies

\[
\nu_k^{sr}(g) = \nu_k^{rs}(g) = 2\pi g \int_0^\pi \sigma^{sr}(g, \chi) (1 - \cos \chi)^k \sin \chi \, d\chi \quad k = 0, 1, \tag{4}
\]

and

\[
\nu_{12}^{34}(g) = 2\pi g \int_0^\pi \sigma_{12}^{34}(g, \chi) \sin \chi \, d\chi, \tag{5}
\]

where \( \sigma \) stands for differential cross section, and \( 0 \leq \nu_1^{sr} \leq 2\nu_0^{sr} \). In our Maxwell molecules assumption, cross sections are inversely proportional to the
impact speed and thus all microscopic collision frequencies are constant with respect to \( g \). The above constraints on the exchange rates result in

\[
n_s = n^s + \frac{\lambda^s}{\nu_s} Q
\]

\[
m^s n_s u_s = m^s n^s u^s + \frac{1}{\nu_s} \sum_{r=1}^{4} \phi^{sr} u^r + \frac{\lambda^s}{\nu_s} m^s u Q
\]

\[
n_s \frac{3}{2} K T_s = n_s \frac{3}{2} K T^s - \frac{1}{2} m^s [n_s u_s^2 - n^s (u^s)^2] + \frac{1}{\nu_s} \sum_{r=1}^{4} \psi^{sr} T^r
\]

\[
+ \frac{1}{\nu_s} \sum_{r=1}^{4} \nu^{sr} \left[ \frac{n^r}{m^r + m^s} n^s n^r (m^s u^s + m^r u^r) \cdot (u^r - u^s) \right]
\]

\[
+ \frac{\lambda^s}{\nu_s} Q \left[ \frac{1}{2} m^s u^2 + \frac{3}{2} K T + \frac{M - m^s}{M} K T \left( \frac{\Delta E}{K T} \right)^{\frac{3}{2}} e^{-\frac{\Delta E}{K T}} \right]
\]

\[
- \frac{1 - \lambda^s}{2} \frac{M - m^s}{M} \Delta E \right] ,
\]

where \( \Gamma \) is an incomplete gamma function \([17]\) and

\[
Q = \nu^{34}_{12} \frac{2}{\sqrt{\pi}} \Gamma \left( \frac{3}{2}, \frac{\Delta E}{K T} \right) \left[ n^3 n^4 \left( \frac{m^1}{m^3} \right)^{\frac{3}{2}} e^{\frac{\Delta E}{K T}} - n^1 n^2 \right] .
\]

The expression of the symmetric singular matrices \( \Phi \) and \( \Psi \) is omitted here for brevity; the interest reader is referred to [7, 8] for their essential properties. Global macroscopic parameters are expressed in terms of single–component parameters by

\[
n = \sum_{s=1}^{4} n^s , \quad \rho = \sum_{s=1}^{4} m^s n^s , \quad u = \frac{1}{\rho} \sum_{s=1}^{4} m^s n^s u^s ,
\]

\[
n K T = \sum_{s=1}^{4} n^s K T^s + \frac{1}{3} \sum_{s=1}^{4} \rho^s (u^s_k u^s_k - u_k u_k).
\]

For a reactive mixture, actual conserved quantities in the Boltzmann collision process, as well as in its present BGK approximation, are in number of seven, and may be chosen as three combinations of number densities like \( n^1 + n^3 \),
\( n^1 + n^4, n^2 + n^4 \), the three components of the mass velocity \( \mathbf{u} \), and the internal (thermal + chemical) energy \( \frac{3}{2} nKT + \sum_{s=1}^{4} E^s n^s \). This yields the same set of 7 scalar exact non-closed macroscopic conservation equations in the two settings, and another indication of the robustness of this approximation is the fact [7] that collision equilibria also coincide with the actual ones, and are provided by a seven-parameter family of Maxwellians

\[
\mathcal{M}^s(\mathbf{v}) = n^s \left( \frac{m^s}{2\pi K T} \right)^{\frac{3}{2}} \exp \left[ - \frac{m^s}{2KT} (\mathbf{v} - \mathbf{u})^2 \right], \quad s = 1, \ldots, 4, 
\]

with equilibrium densities related by the well known mass action law of chemistry

\[
\frac{n^1 n^2}{n^3 n^4} = \left( \frac{\mu^{12}}{\mu^{34}} \right)^{\frac{3}{2}} \exp \left( \frac{\Delta E}{K T} \right) .
\]

The proper Lyapunov functional indicating dissipativity and stability of equilibria for the Boltzmann equations turns out to be the \( H \)-functional [16]

\[
H[f] = \sum_{s=1}^{4} \int f^s(\mathbf{v}) \log \frac{f^s(\mathbf{v})}{(m^s)^3} d\mathbf{v},
\]

where the denominator \((m^s)^3\) may be omitted in the non-reactive case. In such a frame it has been indeed possible to prove that (11) constitutes a Lyapunov functional also for the BGK equations [8], whereas up to now we have only numerical evidence of this fact for reactive mixtures [7].

The point, left open in [7], that will be considered here, at least for a first estimate, is the most convenient choice of the inverse relaxation times \( \nu_s \). In previous papers we followed the option of reproducing the actual average number of collisions (regardless if mechanical or chemical) taking place for each species, which, in the physical frame described in the Introduction (Maxwell molecule interactions, mechanical scale shorter than chemical scale), leads to [7]

\[
\nu_1 = \sum_{r=1}^{4} \nu_0^{1r} n^r + \frac{2}{\sqrt{\pi}} \Gamma \left( \frac{3}{2}, \frac{\Delta E}{K T} \right) \nu_{12} n^2
\]
\begin{align*}
\nu_2 &= \sum_{r=1}^{4} \nu_0^{2r} n^r + \frac{2}{\sqrt{\pi}} \Gamma \left( \frac{3}{2}, \frac{\Delta E}{K T} \right) \nu_{12}^{34} n^1 \\
\nu_3 &= \sum_{r=1}^{4} \nu_0^{3r} n^r + \frac{2}{\sqrt{\pi}} \Gamma \left( \frac{3}{2}, \frac{\Delta E}{K T} \right) \left( \frac{\mu_{12}}{\mu_{34}} \right)^{\frac{3}{2}} e^{\frac{\Delta E}{K T} \nu_{12}^{34} n^4} \\
\nu_4 &= \sum_{r=1}^{4} \nu_0^{4r} n^r + \frac{2}{\sqrt{\pi}} \Gamma \left( \frac{3}{2}, \frac{\Delta E}{K T} \right) \left( \frac{\mu_{12}}{\mu_{34}} \right)^{\frac{3}{2}} e^{\frac{\Delta E}{K T} \nu_{12}^{34} n^3}.
\end{align*}

A nice feature of (12) is that they fulfil the constraint

\[ \nu_s \geq \frac{1}{2} \sum_{r=1}^{4} \nu_1^{sr} n^r \tag{13} \]

that guarantees positivity of temperature fields [8], as well as the condition

\[ \max(-\nu_1 n^1, -\nu_2 n^2) < Q < \min(\nu_3 n^3, \nu_4 n^4), \tag{14} \]

which ensures positivity of density fields for a reactive gas [7]. However, as already pointed out, this option might introduce an excess of collisionality in the model, so that we shall consider in the sequel these reference values divided by a factor \( \alpha \), and study the effect of a varying \( \alpha \) on the dissipativity of the model, described by the \( H \)-functional (11).

If the chemical reaction is switched off, the above algorithm changes only in that one has to formally set \( \nu_{12}^{34} = 0 \) (then \( Q = 0 \)). Implications however are not completely trivial, since now all number densities \( n^s \) are conserved quantities, and consequently collision equilibria constitute a eight-parameter family of Maxwellians, still given by (9), but with uncorrelated equilibrium densities. In addition, no auxiliary density fields are needed (\( n_s = n^s \), for any \( s \)).

3. BKW MODES FOR GAS MIXTURES

We recall here briefly the exact solutions of BKW-type holding for a multi-component gas, whose most general available class was worked out, to our
knowledge, in [13]. They apply to an inert mixture of $N$ different species in space homogeneous conditions with Maxwell molecule collisions and isotropic scattering. This implies existence of $N + 4$ first integrals

$$n^s = \text{constant} \quad \forall s, \quad u = \text{constant}, \quad T = \text{constant}, \quad (15)$$

and, in our notation, we must have then $\nu_0^{sr} = \nu_r^{sr}, \forall (s, r)$. The BKW solutions are isotropic in $v$, so that a priori we may set $u$ as well as all macroscopic velocities equal to zero, and initial conditions determine species densities and global temperature. The search for these solutions goes through a Fourier transformation with respect to the velocity variable of the set of integro–differential nonlinear Boltzmann equations, followed by a systematic similarity analysis of the transformed problem [13]. The BKW modes presented below are obtained by Fourier inversion of suitable invariant solutions with respect to the previously determined Lie groups [18].

More precisely, BKW–mode solutions take, for $s = 1, ..., N$, the form

$$f^s(v, t) = n^s \left[ \frac{m^s}{2\pi KT \theta(t)} \right] \left\{ 1 + a^s \frac{1 - \theta(t)}{\theta(t)} \left[ \frac{m^s v^2}{2 KT \theta(t)} - \frac{3}{2} \right] \right\} \exp \left[ - \frac{m^s v^2}{2 KT \theta(t)} \right], \quad (16)$$

in terms of $N$ scalar parameters $a^s$ and of a scalar function $\theta$, and condition for their existence is the constraint that there exists an integer $p$, with $1 \leq p \leq N - 1$, such that the products $\varepsilon^{sr} \nu_0^{sr}$ are independent of the pair $(s, r) \forall s = 1, ..., p, \forall r > s$, where we have introduced the known dimensionless parameters

$$\varepsilon^{sr} = \frac{4m^s m^r}{(m^s + m^r)^2}, \quad 0 < \varepsilon^{sr} \leq 1. \quad (17)$$

These are $p \left( N - \frac{p + 1}{2} \right) - 1$ independent relations among the $\frac{N(N - 1)}{2}$ off diagonal collision frequencies. It makes sense then defining a positive quantity representing the common value of the above products, and we will set

$$\gamma = \frac{n}{2} \varepsilon^{sr} \nu_0^{sr} \quad s = 1, ..., p, \quad r = s + 1, ..., N. \quad (18)$$
The remaining $N$ diagonal collision frequencies $\nu_0^{sr}$ follow in turn from the requirements

$$\frac{1}{6} \sum_{r=1}^{N} a^r (3 - 2\varepsilon^{sr}) \varepsilon^{sr} \nu_0^{sr} n^r = \gamma, \quad s = 1, \ldots, N,$$

(19)

that bind together coefficients $a^s$ appearing in (16), mass ratios, initial conditions, and the whole matrix of collision frequencies. As regards coefficients $a^s$, the first $p$ of them ($s = 1, \ldots, p$) remain free, whereas the others are provided by

$$a^s = \left[ \sum_{r=p+1}^{N} n^r \right]^{-1} \left( n - \sum_{r=1}^{p} a^r n^r \right) \quad s = p+1, \ldots, N,$$

(20)

and are equal to each other. Finally, the function $\theta$ is given by

$$\theta(t) = 1 - \theta_0 e^{-\gamma t},$$

(21)

where $\theta_0$ is a positive constant ($\theta_0 = 0$ would yield the stationary solution). Notice that the determination (20) of coefficients $a^s$ is such that

$$\sum_{s=1}^{N} a^s n^s = n,$$

(22)

and that, if the first $p$ of them are chosen to be unity, the remaining ones are also unity.

In order to ensure positivity of distribution functions, the $p+1$ free parameters characterizing the BKW solution must obey the additional conditions

$$a^s \geq 0, \quad \forall s = 1, \ldots, p; \quad \sum_{s=1}^{p} a^s n^s < n;$$

$$\theta_0 \leq \min\{\theta_1, \theta_2\},$$

(23)

where

$$\theta_1 = \frac{2}{2 + 3 \max\{a^s\}_{s=1,\ldots,p}}, \quad \theta_2 = \frac{2}{2 + 3a^{p+1}},$$

(24)
with, in particular, $\theta_0 < 1$. These solutions describe relaxation towards the equilibrium Maxwellians

$$f^s_M(v) = n^s \left( \frac{m^s}{2\pi KT} \right)^{3/2} \exp \left( -\frac{m^sv^2}{2KT} \right), \quad s = 1, ..., N \quad (25)$$

starting from initial conditions

$$f^s(v,0) = n^s \left[ \frac{m^s}{2\pi K T (1 - \theta_0)} \right]^{3/2} \left\{ 1 + a^s \frac{\theta_0}{1 - \theta_0} \left[ \frac{m^sv^2}{2KT(1 - \theta_0)} - \frac{3}{2} \right] \right\} \cdot \exp \left( -\frac{m^sv^2}{2KT(1 - \theta_0)} \right). \quad (26)$$

One can observe that, if equal sign holds in the last of (23), then one or more of the initial distributions (26) vanishes at $v = 0$, being positive elsewhere. All distribution functions are instead positive for any positive value of $t$.

Once $p$ is given, the last $N - p$ distribution functions are self-similar, since, except for masses, their shape depends on $s$ via $a^s$ only. In this respect, we can also remark that the option $p = 1$ puts the least constraints on the collision frequencies, but makes all coefficients $a^s$ with $s > 1$ equal, whereas the opposite option $p = N - 1$ allows all different $a^s$, but at the expenses of a strongly conditioned collision frequencies matrix.

Finally, species temperatures are not constant, in general, and can be cast in the very simple form

$$T^s(t) = T \left[ 1 + (a^s - 1)\theta_0 e^{-\gamma t} \right], \quad s = 1, ..., N. \quad (27)$$

4. NUMERICAL EXPERIMENTS AND CONCLUSIONS

BGK and BKW solutions as described in the previous sections have been systematically compared to each other, covering as much as possible the allowed ranges of variation of all physical parameters and initial conditions. Results presented in this section are intended as a sample of the extensive experiments
that have been performed. Numerical values have been selected only for illustrative purposes, and the number of gas components has been chosen as \( N = 4 \), as minimal requirement for a bimolecular reaction like (1) to occur.

We start from a reference test case defined by \( p = 3 \), \( T = 4 \), and by the following tables of parameters, satisfying of course the constraints for existence of BKW modes.

\[
\begin{array}{c|cccc}
\text{ } & 1 & 2 & 3 & 4 \\
\hline
m^s & 11.7 & 3.6 & 8 & 7.3 \\
a^s & 1.3 & 0.5 & 2 & 0.1538 \\
n^s & 10 & 12 & 14 & 13 \\
\end{array}
\]

**Table I.** Initial values and parameters for the reference test case.

\[
\begin{array}{c|cccc}
\nu_{sr}^0 & 1 & 2 & 3 & 4 \\
\hline
1 & 0.5838 & 0.1 & 0.0746 & 0.0761 \\
2 & 0.1 & 1.0579 & 0.0841 & 0.0813 \\
3 & 0.0746 & 0.0841 & 0.3171 & 0.0721 \\
4 & 0.0761 & 0.0813 & 0.0721 & 3.4945 \\
\end{array}
\]

**Table II.** Elastic collision frequencies \( \nu_{sr}^0 \) for the reference test case.

The chosen value of the factor \( \theta_0 \) is given by the equal sign in (23), and turns out to be \( \theta_0 = 0.25 \). Notice that from these values it follows \( \gamma = 1.763 \), and \( n = 49 \), and that the mean collision time is here of the order of \( 10^{-1} \) units on the chosen time scale. The given data determine also initial temperatures \( T^s(0) \) as 4.3, 3.5, 5, 3.154 for \( s = 1, \ldots, 4 \), respectively. BGK calculations are run, to begin with, for \( \alpha = 1 \), namely according to the option (12) for the parameters \( \nu_s \) of the model. As explained above, macroscopic quantities are reproduced exactly, in our assumptions, by the present BGK approximation, and this actually occurs to the single temperatures \( T^s \), which converge to \( T \) according to the relaxation time \( 1/\gamma \approx 0.57 \), reaching their asymptote in approximately 4 time units, as shown in Fig. 1. The time evolution of the profiles of the four distribution functions versus the speed variable \( v \) is depicted in Figs.
2 and 3, where the initial and final shapes are reported together with the different BKW and BGK profiles relevant to some intermediate values of time. Fig. 2 is relevant to the species 1 and 3, whose initial shape is farther from a Maxwellian, because of the relatively high values of $a^1$ and $a^3$, and shows four different time instants. The transition is smoother for the other two species, plotted in Fig. 3 at two intermediate times, because of the smaller values of the pertinent $a^s$. As expected, the two profiles overlap very well, and approach the equilibrium shape, in a time span of order unity, even shorter than the temperatures equalization time. Discrepancies show up only in such initial transient, and are the more significant the larger is the deviation from a Maxwellian at $t = 0$, reaching a maximum for $f^3$ and almost disappearing for $f^4$. Trends of BGK profiles are not necessarily monotonic versus time, nor necessarily closer to the final equilibrium than the corresponding BKW solutions. However, this is instead what actually occurs when the initial distribution is more distorted and deviations are more pronounced. This fact is confirmed and quantified by the time evolution of the $H$-functional (11), computed numerically following the two types of solution, and shown in Fig. 4. They essentially coincide in the bulk region, but it is clear that the BGK solution enhances dissipation with respect to reality, and initially accelerates convergence towards equilibrium, as anticipated in previous sections.

These results motivate then the search for a reduction factor $\alpha > 1$ to be applied to the macroscopic collision frequencies (12) in the BGK approximation in order to achieve a more faithful representation of the actual relaxation process. Therefore, the BGK calculation has been repeated for varying values of $\alpha$, and the relevant $H$-functional as a function of time has been compared to the exact BKW one. The optimal value $\alpha^*$ of the reduction parameter has been selected as the one yielding the best least square approximation. For this test case it turns out to be $\alpha^* \approx 1.975$. The $H$-functional versus time in the initial transient is reported for different values of $\alpha$ in Fig. 5, whereas the trend of the distribution functions versus $v$ and $t$ is shown in Fig. 6, which is
a variant of Fig. 2 relevant to the option $\alpha = \alpha^*$. It is clear that increasing $\alpha$ amounts to slowing down the relaxation process, even making it too slow with respect to reality, until eventually we run into positivity problems since the $\nu_s$ become too small. As regards the distribution functions, overlapping with the exact results has not to be expected, of course, but anyway a significant improvement may be observed with respect to the case $\alpha = 1$ (discrepancies are hardly visible at all for $f^1$). Obviously, analogous improvement is in order for the less critical distributions $f^2$ and $f^4$, which are not shown here for brevity.

The procedure applied above to the reference case has been repeated for a great variety of other possible choices of input parameters, trying to guarantee a complete coverage, with reasonably fine mesh, of the numerical ranges for which an exact BKW solution does exist. Variations have involved masses, microscopic collision frequencies, initial number densities and global temperature, and the parameters underlying the BKW modes themselves, like index $p$, coefficients $a^s$, and factor $\theta_0$. Though in some cases it has been possible to identify and understand the effects of variation of some parameter, it is really impossible to draw general conclusions, in the mess of so many varying constrained parameters. Just to provide some examples concerning the crucial point of this preliminary investigation, namely an estimate of the optimal reduction factor $\alpha^*$, we describe here the effects of some parameter variations with respect to the reference case.

If the string of independent coefficients $a^s$, $s = 1, 2, 3$, is changed to $3.0, 1.1, 0.1$, keeping all other free parameters, including $\nu_0^{12}$, unchanged, then $\gamma$ does not vary, but $\theta_0$, still determined by the equal sign in (23), decreases to 0.1818 and the final result of our least square test is $\alpha^* \approx 1.850$. If, in addition to the $a^s$, also $\nu_0^{12}$ were varied in all admissible ways, the optimal value of $\alpha^*$ would not change from 1.850, since it is easy to see that such a variation would simply produce the same BGK and BKW solutions on a different time scale. Another variation that has no consequences on $\alpha^*$, exactly for the same reason, is a change of $n$ with constant ratios among the $n^s$. 

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Starting again from the reference case, if we change only $\theta_0$, by setting it equal to a half of the maximum allowed to it, we observe a sensible increase of $\alpha^*$, which becomes 2.175. If $\theta_0$ is decreased further, $\alpha^*$ keeps increasing, but seems to approach a saturation value. A parameter that has been observed not to affect appreciably the optimal value of $\alpha$ is the global temperature $T$. Such a value appears instead to be quite sensitive to a non-proportional variation of the single densities $n^s$. If their string is changed to 0.1, 1.2, 1.4, 13, leaving all the rest unchanged with respect to the reference case, then we get $\alpha^* \approx 2.225$. The same occurs for variation of masses: if the reference values of $m^s$ are changed only in that $m^3$ is reduced by a factor of 5, we observe an increase of $\alpha^*$ from 1.975 to 2.425. Of course we have mostly run cases in which more than one type of parameters are varied. As an example, starting again from the reference case, if the independent $a^s$ are changed to 0.9, 0.1, 3 and simultaneously the densities become 15, 7, 8, 20, the optimal reduction factor reduces to 1.825. Another crucial parameter to investigate is the index $p$. With the opposite extreme option $p = 1$, only $a^1$ among the $a^s$ is free, and four of the $\nu^s_{gr}$ are independent, namely those corresponding to the pairs $(1,2), (2,3), (2,4), (3,4)$. Taking $a^1 = 1.3$ and $\nu^0_{12} = 0.1$ like in the reference case, $\nu^0_{23} = \nu^0_{24} = 0, \nu^0_{34} = 0.5$, and leaving all other input parameters unchanged, yields the result $\alpha^* \approx 2.350$, which seems to remain essentially constant to any admissible variation of independent microscopic collision frequencies, as long as $\nu^0_{12}$ remains equal to 0.1. If we take this last example as new reference case and only change $n^2$ from 12 to 1.2, we get the slight variation $\alpha^* \approx 2.325$, whereas changing only $a^1$ from 1.3 to 4.3 would yield $\alpha^* \approx 1.825$. Finally, if instead $a^1$ is taken to be unity, so that the special case of all equal $a^s$ is generated, we observe a growth of $\alpha^*$ up to 2.275.

Collecting the results of all cases that have been run, the quite cumbersome numerical campaign shows that the optimal reduction factor ranges in an interval whose rough lower and upper bounds are approximately 1.75 and 2.50. With that factor, our BGK equations yield an entropy production
that best approximates the actual entropy production that can be evaluated exactly for the selected values of input parameters. Such a conclusion is certainly useful for future developments of the present BGK model for mixtures. However it is clear that it is quite loose, and at the same time largely incomplete, coming from comparison with a very special class of test functions, holding under certain restrictions on physical parameters. We hope to be able to perform more accurate and fancy tests in our future investigations, and to include more realistic physical conditions, eventually also chemical reactions.

It is worth concluding this paper with a short remark. As pointed out in [8], for a chemically inert mixture the so-called indifferentiability principle should hold. In the same article it was proved that this is not always the case, if macroscopic collision parameters are chosen according to the general consistency condition (13). In order to guarantee that such principle holds, one should actually take the equal sign in the quoted equation. In our case, one must just apply a reduction factor \( \alpha = 2 \) to the actual average collision frequencies of the components. Or, in other words, factors providing the best approximation of entropy production in different physical conditions range not far around the factor 2 that ensures indifferentiability.

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REFERENCES


Figure 1: Trends of temperatures $T^s$ versus time for the reference case.
Figure 2: Velocity profiles of $f^1$ (top) and $f^3$ (bottom) at different time instants for BKW and BGK solutions. Initial shape: dash-dotted line; final shape: dotted line.
Figure 3: Velocity profiles of $f^2$ (left) and $f^4$ (right) at different time instants for BKW and BGK solutions. Initial shape: dash-dotted line; final shape: dotted line.
Figure 4: $H$-functional versus time for BGK solution with $\alpha = 1$ (dashed line) and for BKW mode (solid line).
Figure 5: Zoom of the trend of $H$-functionals versus time: BGK solutions with different values of $\alpha$ compared to the exact BKW mode.
Figure 6: Velocity profiles of $f^1$ (top) and $f^3$ (bottom) at different time instants for BKW and BGK solutions with $\alpha = \alpha^*$. Initial shape: dash-dotted line; final shape: dotted line.