COMMUN. MATH. SCI.
Vol. 20, No. 3, pp. 763–801

© 2022 International Press

REACTION–DIFFUSION EQUATIONS DERIVED FROM KINETIC MODELS AND THEIR TURING INSTABILITY*

MARZIA BISI† AND ROMINA TRAVAGLINI‡

Abstract. We consider a binary mixture composed by a polyatomic (diatomic) and a monatomic gas, diffusing in a gaseous background (typically, the atmosphere), and undergoing reversible and irreversible chemical reactions. We show the derivation of proper reaction–diffusion equations for the number densities of the constituents, starting from suitably rescaled kinetic Boltzmann equations. The dominant process is assumed to be the elastic scattering with the host medium, while we present two different scalings for the various chemical reactions: the first option leads to a system of three reaction–diffusion equations, while the second regime leads to two reaction–diffusion equations similar to the classical Brusselator system. Then, we study the Turing instability properties of such macroscopic systems, showing their dependence on particle masses, on collision frequencies of the Boltzmann operators, and, above all, on particle internal energies.

Keywords. Kinetic equations; Diffusive limits; Reaction-diffusion equations; Turing instability.

AMS subject classifications. 35K57; 82C40; 76P05.

1. Introduction

Reaction–diffusion equations are extensively used in mathematical physics, since they often constitute simple but reliable models able to describe time and space evolution of physical quantities. An excursus of the basic models of this type used in mathematical biology, with particular reference to the epidemiology (diffusion of infectious diseases), may be found in the books [29–31,46]. Reaction–diffusion systems appear also in ecology [8], in the physics of hot plasmas [47], in astrophysics [48], and of course in chemistry [23].

Mathematical aspects of these systems, as existence and uniqueness of solutions for Cauchy–Dirichlet problems, stability of solutions, symmetry properties have been extensively investigated, see for instance [22,34,45]. An important feature worth to be analyzed is the Turing instability [44], occurring when a steady state which is stable in space homogeneous conditions becomes unstable in presence of diffusion. This situation generates the formation of patterns, namely solutions of the reaction–diffusion equations that turn out to be heterogeneous in space (with some regular or periodic structure) and stable in time. This kind of instability has been recovered in several problems, as models for morphogenesis [27], prey–predator systems [26], epidemic models [14], neural networks [50], models for metal growth [7] or for multiple sclerosis [28], just to mention some of them.

Many of such reaction–diffusion systems have been built up starting from phenomenological considerations, therefore diffusion coefficients and parameters appearing in the reaction part are taken as arbitrary constants, and are not directly related to microscopic interactions between cells, preys and predators, etc. Even the physical or biological meaning of some reaction terms sometimes is not very clear, and some tools enabling to relate them to the microscopic activities would be very welcome.

In this respect, kinetic theory, originally proposed by Boltzmann to describe rarefied gas dynamics, may be useful. Indeed, it is based on a mesoscopic approach, providing

---

[*] Received: April 09, 2021; Accepted (in revised form): September 05, 2021. Communicated by Lorenzo Pareschi.

[†] Corresponding author. Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, Parco Area delle Scienze 53/A, I-43124 Parma, Italy (marzia.bisi@unipr.it).

[‡] Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, Parco Area delle Scienze 53/A, I-43124 Parma, Italy (romina.travaglini@unipr.it).

the evolution of the distribution function of particles (or individuals); the Boltzmann collision term is an integral operator taking into account the interaction mechanisms at the microscopic level. Major macroscopic fields can be recovered as suitable moments of the distribution function. In proper hydrodynamic regimes, a closure of macroscopic equations may be obtained resorting to an asymptotic Chapman–Enskog procedure [10]. In fluid–dynamics, the most common hydrodynamic systems are Euler and Navier–Stokes equations [9].

In the framework of reacting gas mixtures, the connection between reactive kinetic equations and reaction–diffusion systems has been explored starting from BGK or Fokker–Planck models [41, 42], from discrete velocity models [49], and also from Boltzmann operators for a single bimolecular chemical reaction [5]. Rigorous results on this kind of limit have been recently proved in [16, 33]. Under suitable assumptions on the macroscopic fields and on the distribution functions, the diffusive asymptotic limit leads to reaction–diffusion systems of Maxwell–Stefan type [1, 2]. Also, in different physical frameworks, some attempts to derive reaction–diffusion equations from kinetic equations or as mean–field limit of interacting particle systems have been performed [11, 43].

This paper fits into this research line. We consider a gaseous mixture with several species, undergoing elastic collisions, inelastic transitions and chemical reactions, and, following the strategy suggested in the paper [5], we derive reaction–diffusion equations from the kinetic level in two different hydrodynamic limits. Specifically, we consider two species, one monatomic and the other polyatomic (diatomic) diffusing in a background medium (typically, the atmosphere). The host medium is itself a mixture, constituted by particles with different masses, and as a whole it is assumed accommodated at a Maxwellian distribution, with fixed mean velocity and temperature. The kinetic system is composed by three Boltzmann equations, one for the distribution of the monatomic species and the others for the distributions of the two components of the diatomic gas, each one with its value of internal energy. Intra–species and inter–species elastic scattering is allowed, as well as elastic scattering with the background medium. Inelastic transitions may also occur, where polyatomic particles pass from one energy state to the other. Moreover, two bimolecular and reversible chemical reactions are taken into account, involving the considered monatomic and polyatomic constituents and the host medium as well. In the diffusive limit, the dominant process is assumed to be, as usual, the elastic scattering with the background. Two different regimes are explored, corresponding to different scales assumed for the chemical reactions. The first one, where all reactions have the same order of magnitude, leads to a system of three reaction–diffusion equations for the number densities of the monatomic gas and the two components of the polyatomic one. The second one, where a reaction is assumed to be faster than the other chemical and inelastic interactions, allows to explicitly get one density in terms of the other two, so that the final reaction–diffusion system is constituted by only two equations, similar to the classical Brusselator system [35]. This reduction resembles the classical quasi–steady–state approximation, a standard procedure in the study of chemical reaction kinetics in situations where certain species have a very short time of existence and therefore their variation may be neglected, thus reducing the number of equations. A detailed description of such kind of reductions can be found in [39, 40] and it is applied in the particular case of the Brusselator in [12].

Diffusion coefficients and reaction terms of our macroscopic systems explicitly depend on particle masses, background density, collision frequencies of all interaction phenomena, and internal energies of the species. We investigate the occurrence of Turing instability by varying these microscopic parameters. More precisely, for the system of two reaction–diffusion equations we are able to find explicit conditions on the internal energies allowing (or preventing) the pattern formation; the analytical results are also validated by some numerical simulations. An analogous study is then performed also for the system of three equations, that is much more involved, since the number of coefficients is higher and the Turing instability conditions are more complicated. We apply, in this case, results derived in [38], where a generalization for Turing bifurcation under certain conditions in n-dimensional systems is provided. Analogies and differences between the instability properties of our two systems are commented on.

In more detail, the paper is organized as follows. In Section 2 we present the physical setting we are considering, and the kinetic Boltzmann equations with explicit collision operators for elastic, inelastic, and chemical encounters for involved components are written. Section 3 is devoted to the diffusive asymptotic limit leading from the kinetic level to a closed set of three reaction–diffusion equations for species number densities. Then, in Section 4 a modified hydrodynamic regime is explored, obtaining a reduced set of only two macroscopic equations. In Section 5, the analysis of stability properties of the systems derived in Sections 3 and 4 is shown. Finally, Section 6 contains some concluding remarks.

2. Physical setting and Boltzmann equations

We consider a mixture of two rarefied gases diffusing in a background medium: one species Y is supposed to have two possible energy levels, E_1 and E_2, thus, according to the way of modelling proposed in [19, 21], it can be decomposed into two different components, Y_1 and Y_2; the other gas Z is monatomic and has only one energy level, E_Z. Particle masses of these gases are denoted by m_Y and m_Z, respectively.

The host medium, which from the physical point of view could be seen as the atmosphere, is a gaseous mixture and is much denser than the considered species Y_1, Y_2, Z. Specifically, in this model the background is provided by a mixture of three gas species A, B and C, with different particle masses m_A, m_B, m_C. These background species are supposed to have only one possible energy level, expressed by E_A, E_B, E_C, respectively. Their distributions are supposed to be fixed Maxwellians, with constant number densities n_A, n_B, n_C, temperature equal to one and zero mean velocity:

$$f_J(\mathbf{v}) = n_J M_J(\mathbf{v}) \qquad M_J(\mathbf{v}) = n_J \left(\frac{m_J}{2\pi}\right)^{\frac{3}{2}} \exp\left(-\frac{m_J|\mathbf{v}|^2}{2}\right) \qquad J = A, B, C.$$

We shall write and investigate (in different asymptotic limits) kinetic Boltzmann equations for the evolution of distribution functions of species Y_1, Y_2, Z, denoted by f_1, f_2, f_Z, respectively. Besides on molecular velocity $\mathbf{v}$, they depend also on time t and on the space variable $\mathbf{x}$. Particles, in addition to elastic collisions with the background medium and among themselves, are subject to the following inelastic transitions or chemical reactions

$$A + Y_1 \to A + Y_2, \tag{2.1}$$
$$Z + Y_2 \to Z + Y_1, \tag{2.2}$$
$$B + Y_1 \leftrightarrows A + C, \tag{2.3}$$
$$Y_1 + Y_1 \leftrightarrows Z + B. \tag{2.4}$$

The interactions (2.1) and (2.2) are inelastic transitions where particles of species Y, colliding with the background (in (2.1)) or with the other species Z (in (2.2)), pass from one energy state to the other, namely a particle of the component Y_1 transforms itself into a particle of the component Y_2 or vice versa. The collisions (2.3) and (2.4) represent bimolecular and reversible chemical reactions: (2.3) describes creation or disappearance of a particle of species Y_1 through interactions with the background medium; in (2.4) a pair of particles Y_1 produces a particle Z and a background particle or the other way round. From the physical point of view, the reactions (2.1)–(2.4) represent a simple set of bimolecular interactions (that can be easily modelled by Boltzmann operators) allowing to recover, in a suitable hydrodynamic limit that will be detailed in Section 4, the well known Brusselator system [35]. External production of particles is provided by chemical interactions with the fixed background, and passages from one component to another (with the same mass) occur through inelastic transitions. The possibility of modelling auto–catalytic reactions of the Brusselator system introducing an intermediate unstable state Z has also been outlined in [24], by one of the authors of the original paper [35].

The kinetic Boltzmann equations for distributions $f_I(t,\mathbf{x},\mathbf{v})$, with $I=1,2,Z$, may be cast as

$$\frac{\partial f_I}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}} f_I=\sum_{J=A,B,C} Q^I_{EL}(f_I,n_J M_J)+\sum_{K=1,2,Z} Q^I_{EL}(f_I,f_K)+Q^I_{IN}(\mathbf{f})+Q^I_{CH}(\mathbf{f}). \tag{2.5}$$

Here $Q^I_{EL}(f_I,n_J M_J)$ denotes the collision operator for the elastic scattering between the considered species I and one background species $J=A,B,C$. Then, the operator $Q^I_{EL}(f_I,f_K)$ describes the elastic collisions between particles of the species I and particles of only one other species $K=1,2,Z$, including of course the case $K=I$. Finally, the operator $Q^I_{IN}(\mathbf{f})$ takes into account the effects on species I due to inelastic transitions (2.1), (2.2), and $Q^I_{CH}(\mathbf{f})$ takes into account the effects due to the chemical reactions (2.3), (2.4); here $\mathbf{f}$ denotes the whole set of distributions, the precise dependencies will be specified here below.

Elastic operators between a gas component I and the background are

$$Q^I_{EL}(f_I,n_J M_J)(\mathbf{v})=\int_{\mathbb{R}^3\times S^2}\sigma_{IJ}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g\Big[f_I(\mathbf{v}')n_J M_J(\mathbf{w}')-f_I(\mathbf{v})n_J M_J(\mathbf{w})\Big]d\mathbf{w}d\hat{\mathbf{\Omega}}' \tag{2.6}$$

for $I=1,2,Z$ and $J=A,B,C$, while elastic operators between a gas component I and another component K are

$$Q^I_{EL}(f_I,f_K)(\mathbf{v})=\int_{\mathbb{R}^3\times S^2}\sigma_{IK}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g\Big[f_I(\mathbf{v}')f_K(\mathbf{w}')-f_I(\mathbf{v})f_K(\mathbf{w})\Big]d\mathbf{w}d\hat{\mathbf{\Omega}}'. \tag{2.7}$$

Here, $(\mathbf{v},\mathbf{w})$ stand for the pre–collision velocities and $(\mathbf{v}',\mathbf{w}')$ for the post–collision ones; in addition, $\mathbf{g}=g\hat{\mathbf{\Omega}}=\mathbf{v}-\mathbf{w}$ is the relative velocity vector, where g is its modulus and $\hat{\mathbf{\Omega}}$ its direction, and $\hat{\mathbf{\Omega}}'$ is thus the direction of the post–collision relative velocity. The functions $\sigma_{IJ}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')$ and $\sigma_{IK}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')$ denote the so–called differential cross sections, depending on the relative speed and on the impact parameter of the collision. More details on such operators may be found in classical kinetic theory books [9, 10]. A Maxwell molecule assumption will be adopted throughout the paper, implying that

$$\int_{S^2}\sigma_{IJ}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g\,d\hat{\mathbf{\Omega}}':=\nu_{IJ}, \qquad \int_{S^2}\sigma_{IK}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g\,d\hat{\mathbf{\Omega}}':=\nu_{IK}, \tag{2.8}$$

where ν_{IJ} and ν_{IK} are constant collision frequencies.

As concerns inelastic transitions, components Y_1 and Y_2 are involved in both interactions (2.1) and (2.2), therefore their inelastic operators may be split into two parts

$$Q^I_{IN}(\mathbf{f})=Q^I_{IN}(f_1,f_2,n_A M_A)+Q^I_{IN}(f_1,f_2,f_Z), \qquad I=1,2.$$

Inelastic collision operator for Y_1 related to the collision (2.1) is simply provided by a loss term as

$$Q^1_{IN}(f_1,f_2,n_AM_A)(\mathbf{v}) = -\int_{\mathbb{R}^3\times S^2} H\left(g^2-\delta^{A2}_{A1}\right)\sigma^{A2}_{A1}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\,g\,f_1(\mathbf{v})n_AM_A(\mathbf{w})\,d\mathbf{w}d\hat{\mathbf{\Omega}}'. \tag{2.9}$$

Here and below the notation δ^{HK}_{IJ} stands for

$$\delta^{HK}_{IJ} = \frac{2\,\Delta E^{HK}_{IJ}}{\mu_{IJ}}, \tag{2.10}$$

where $\mu_{IJ}=m_Im_J/(m_I+m_J)$ is the reduced mass and $\Delta E^{HK}_{IJ}=E_H+E_K-E_I-E_J$. Moreover, in (2.9) the symbol $H(\cdot)$ is the unit step Heaviside function, taking into account the fact that an inelastic transition $A_I+A_J\to A_H+A_K$ occurs only if the ingoing kinetic energy $\frac{1}{2}\mu_{IJ}g^2$ overcomes the potential barrier ΔE^{HK}_{IJ}. Again $\sigma^{HK}_{IJ}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')$ denotes the differential cross section of the considered transition.

On the other hand, collision (2.1) produces a gain term for component Y_2, that, according to the derivation of reacting operators presented in [36], may be cast as

$$Q^2_{IN}(f_1,f_2,n_AM_A)(\mathbf{v}) = \int_{\mathbb{R}^3\times S^2} H\left(g^2-\delta^{A1}_{A2}\right)\sigma^{A2}_{A1}(g',\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\frac{(g')^2}{g}f_1(\mathbf{v}')n_AM_A(\mathbf{w}')d\mathbf{w}d\hat{\mathbf{\Omega}}'. \tag{2.11}$$

Analogous operators are in order for transition (2.2), with a gain term for Y_1 and a loss term for Y_2:

$$Q^1_{IN}(f_1,f_2,f_Z)(\mathbf{v}) = \int_{\mathbb{R}^3\times S^2} H\left(g^2-\delta^{Z2}_{Z1}\right)\sigma^{Z1}_{Z2}(g',\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\frac{(g')^2}{g}f_2(\mathbf{v}')f_Z(\mathbf{w}')\,d\mathbf{w}d\hat{\mathbf{\Omega}}', \tag{2.12}$$

$$Q^2_{IN}(f_1,f_2,f_Z)(\mathbf{v}) = -\int_{\mathbb{R}^3\times S^2} H\left(g^2-\delta^{Z1}_{Z2}\right)\sigma^{Z1}_{Z2}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\,g\,f_2(\mathbf{v})f_Z(\mathbf{w})\,d\mathbf{w}d\hat{\mathbf{\Omega}}'. \tag{2.13}$$

The species Z is involved only in the inelastic transition (2.2), and its inelastic Boltzmann operator may be cast as

$$\begin{aligned} Q^Z_{IN}(\mathbf{f}) = Q^Z_{IN}(f_1,f_2,f_Z)(\mathbf{v}) = \int_{\mathbb{R}^3\times S^2} \Big[& H\left(g^2-\delta^{Z2}_{Z1}\right)\sigma^{Z1}_{Z2}(g',\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\frac{(g')^2}{g}f_Z(\mathbf{v}')f_2(\mathbf{w}') \\ & - H\left(g^2-\delta^{Z1}_{Z2}\right)\sigma^{Z1}_{Z2}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\,g\,f_Z(\mathbf{v})f_2(\mathbf{w})\Big]\,d\mathbf{w}d\hat{\mathbf{\Omega}}'. \end{aligned} \tag{2.14}$$

More details on the construction of the Boltzmann gain and loss terms for non–conservative interactions may be found, for instance, in [19, 36]. In this paper we shall need only the computations of contributions appearing in number density equations, that, for Maxwell molecules, become manageable resorting to the Jacobian of the transformation between pre- and post–collision velocities:

$$H\left((g')^2-\delta^{IJ}_{HK}\right)d\mathbf{v}'d\mathbf{w}'d\hat{\mathbf{\Omega}} = \frac{g'}{g}H\left(g^2-\delta^{HK}_{IJ}\right)d\mathbf{v}d\mathbf{w}d\hat{\mathbf{\Omega}}'. \tag{2.15}$$

Boltzmann collision operators relevant to chemical reactions (2.3) and (2.4) are more standard, since bimolecular reversible reactions have been extensively studied in kinetic theory [5, 6, 21]. Component Y_1 is involved in both reactions (2.3) and (2.4), therefore the relevant operator is the sum of two terms

$$Q^1_{CH}(\mathbf{f}) = Q^1_{CH}(f_1,n_AM_A,n_BM_B,n_CM_C) + Q^1_{CH}(f_1,f_Z,n_BM_B),$$

where the first one, taking into account the reaction (2.3), is provided by

$$Q_{CH}^{1}(f_1,n_AM_A,n_BM_B,n_CM_C)(\mathbf{v})=\int_{\mathbb{R}^3\times S^2}H\left(g^2-\delta_{B1}^{AC}\right)\sigma_{B1}^{AC}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g$$
$$\times\left[\left(\frac{m_Bm_Y}{m_Am_C}\right)^3 n_CM_C(\mathbf{v}')n_AM_A(\mathbf{w}')-f_1(\mathbf{v})n_BM_B(\mathbf{w})\right]d\mathbf{w}d\hat{\mathbf{\Omega}}', \tag{2.16}$$

and the second one, accounting for the effects of (2.4), reads as

$$Q_{CH}^{1}(f_1,f_Z,n_BM_B)(\mathbf{v})=\int_{\mathbb{R}^3\times S^2}H\left(g^2-\delta_{11}^{ZB}\right)\sigma_{11}^{ZB}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g$$
$$\times\left[\left(\frac{m_Y^2}{m_Zm_B}\right)^3 f_Z(\mathbf{v}')n_BM_B(\mathbf{w}')-f_1(\mathbf{v})f_1(\mathbf{w})\right]d\mathbf{w}d\hat{\mathbf{\Omega}}'. \tag{2.17}$$

In the construction of such operators [36], use has been made of the microreversibility condition relating the cross sections of the direct and of the reverse reaction. The ratio between the reduced masses of reactants and of products appearing in front of the gain term is due to the Jacobian of the transformation between pre- and post–collision velocities, that is explicitly reported for a generic encounter in the Appendix, as well as the expressions of post–collision velocities.

The other component Y_2 of the polyatomic gas is not involved in reactions (2.3) and (2.4), therefore $Q_{CH}^2(\mathbf{f})=0$. The monatomic gas Z appears only in reaction (2.4), and we have

$$Q_{CH}^{Z}(\mathbf{f})=Q_{CH}^{Z}(f_1,f_Z,n_BM_B)(\mathbf{v})=\int_{\mathbb{R}^3\times S^2}H\left(g^2-\delta_{ZB}^{11}\right)\sigma_{ZB}^{11}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g$$
$$\times\left[\left(\frac{m_Zm_B}{m_Y^2}\right)^3 f_1(\mathbf{v}')f_1(\mathbf{w}')-f_Z(\mathbf{v})n_BM_B(\mathbf{w})\right]d\mathbf{w}d\hat{\mathbf{\Omega}}'. \tag{2.18}$$

Even for inelastic transitions (2.1), (2.2) and for the direct reactions in (2.3), (2.4), cross sections will be assumed of Maxwell molecule type as

$$\int_{S^2}\sigma_{IJ}^{HK}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g\,d\hat{\mathbf{\Omega}}':=\nu_{IJ}^{HK}, \tag{2.19}$$

with ν_{IJ}^{HK} denoting constant collision frequencies.

3. Derivation of a three–component reaction–diffusion system

In this section we derive a reaction–diffusion system for the number densities of the two components Y_1 and Y_2 of the polyatomic gas, and of the monatomic constituent Z as well, in a suitable hydrodynamic limit. To this aim, we rescale the set of Boltzmann equations (2.5) in terms of a small parameter ϵ, standing for the Knudsen number (ratio of the particle mean free path to a macroscopic length). We assume different time scales for collisions among particles, as follows: The dominant phenomenon is provided by the elastic collisions with the much denser background medium, that are taken of order $1/\epsilon$; binary elastic collisions between particles of the species Y_1, Y_2, Z are less frequent, of order ϵ^p with $p\geq 0$; inelastic and chemical encounters (2.1), (2.2), (2.3) and (2.4) are assumed to be slow processes of order ϵ. Since we are interested also in the effects on species number densities of inelastic or chemical interactions, we take the same $O(\epsilon)$

scaling in front of the temporal derivatives. Thus, the rescaled Boltzmann equations for distribution functions of Y_1, Y_2 and Z read as

$$\begin{aligned}
&\epsilon\frac{\partial f_1^\epsilon}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}f_1^\epsilon\\
&=\frac{1}{\epsilon}\sum_{J=A,B,C}Q_{EL}^1(f_1^\epsilon,n_JM_J)+\epsilon^p\sum_{I=1,2,Z}Q_{EL}^1(f_1^\epsilon,f_I^\epsilon)+\epsilon\,Q_{IN}^1(\mathbf{f})+\epsilon Q_{CH}^1(\mathbf{f}), \qquad (3.1)\\
&\epsilon\frac{\partial f_2^\epsilon}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}f_2^\epsilon\\
&=\frac{1}{\epsilon}\sum_{J=A,B,C}Q_{EL}^2(f_2^\epsilon,n_JM_J)+\epsilon^p\sum_{I=1,2,Z}Q_{EL}^2(f_2^\epsilon,f_I^\epsilon)+\epsilon\,Q_{IN}^2(\mathbf{f}), \qquad (3.2)\\
&\epsilon\frac{\partial f_Z^\epsilon}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}f_Z^\epsilon\\
&=\frac{1}{\epsilon}\sum_{J=A,B,C}Q_{EL}^Z(f_Z^\epsilon,n_JM_J)+\epsilon^p\sum_{I=1,2,Z}Q_{EL}^Z(f_Z^\epsilon,f_I^\epsilon)+\epsilon\,Q_{IN}^Z(\mathbf{f})+\epsilon Q_{CH}^Z(\mathbf{f}). \qquad (3.3)
\end{aligned}$$

In order to stress the fact that the solution of this system depends on the scaling parameter ϵ, distribution functions are denoted by f_I^ϵ, $I=1,2,Z$, and the corresponding number densities will be given by n_1^ϵ, n_2^ϵ, n_Z^ϵ, respectively. We have skipped here the rigorous dimensional analysis leading to the rescaled system (3.1), (3.2), (3.3). A detailed derivation of dimensionless Boltzmann–like or BGK kinetic equations may be found in several references, as for instance [3,4,9,32,37].

We immediately note that in the kinetic Equations (3.1), (3.2) and (3.3) the Boltzmann operators describing collisions with the background play the dominant role, namely

$$\sum_{J=A,B,C}Q_{EL}^I(f_I^\epsilon,n_JM_J)=O(\epsilon), \qquad I=1,2,Z.$$

Consequently, taking into account the well known mathematical properties of the linear Boltzmann operator (boundedness, self–adjointness, and validity of the Fredholm alternative) [5,9], distributions f_I^ϵ, for $I=1,2,Z$, may be seen as perturbations of their collision equilibrium:

$$f_I^\epsilon(t,\mathbf{x},\mathbf{v})=n_I^\epsilon(t,\mathbf{x})M_I(\mathbf{v})+\epsilon h_I^\epsilon(t,\mathbf{x},\mathbf{v}), \qquad I=1,2,Z, \tag{3.4}$$

with

$$M_I(\mathbf{v})=\left(\frac{m_I}{2\pi}\right)^{\frac{3}{2}}\exp\left(-\frac{m_I|\mathbf{v}|^2}{2}\right)$$

being a Maxwellian distribution sharing the same zero mean velocity and unit temperature as the host medium. The function h_I^ϵ is of order $O(1)$ and, without loss of generality, we may assume that it fulfills the constraint

$$\int_{\mathbb{R}^3}h_I^\epsilon(\mathbf{v})\,d\mathbf{v}=0.$$

Indeed, as already noted in [5], if we suppose $f_I^\epsilon(\mathbf{v})=\tilde{n}_I^\epsilon M_I(\mathbf{v})+\epsilon\tilde{h}_I^\epsilon(\mathbf{v})$ such that $\epsilon\int_{\mathbb{R}^3}\tilde{h}_I^\epsilon(\mathbf{v})\,d\mathbf{v}=n_I^\epsilon-\tilde{n}_I^\epsilon$, we may recover (3.4) setting $h_I^\epsilon(\mathbf{v})=\tilde{h}_I^\epsilon(\mathbf{v})+\frac{1}{\epsilon}(\tilde{n}_I^\epsilon-n_I^\epsilon)M_I(\mathbf{v})$.

Therefore, in this hydrodynamic regime, in order to describe the evolution of distribution functions f_I^ϵ at leading order accuracy, it is enough to build up consistent evolution equations for number densities n_1^ϵ, n_2^ϵ, n_Z^ϵ.

3.1. Equation for n_1^ϵ.

By integrating (3.1) with respect to the kinetic variable $\mathbf{v}$, we get

$$\epsilon\frac{\partial}{\partial t}\int_{\mathbb{R}^3} f_1^\epsilon d\mathbf{v}+\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}f_1^\epsilon d\mathbf{v}=\epsilon\int_{\mathbb{R}^3}\left(Q_{IN}^1(\mathbf{f})+Q_{CH}^1(\mathbf{f})\right)d\mathbf{v}, \tag{3.5}$$

since elastic contributions obviously vanish [9] (the nature of particles does not change in elastic collisions):

$$\int_{\mathbb{R}^3} Q_{EL}^1(f_1^\epsilon,n_J M_J)d\mathbf{v}=0,\quad J=A,B,C,\quad \text{and}\quad \int_{\mathbb{R}^3} Q_{EL}^1(f_1^\epsilon,f_I^\epsilon)d\mathbf{v}=0,\quad I=1,2,Z.$$

Bearing in mind the expression of the distribution functions provided in (3.4), the Equation (3.5) becomes

$$\epsilon\frac{\partial}{\partial t}n_1^\epsilon+\epsilon\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}h_1^\epsilon d\mathbf{v}=\epsilon\int_{\mathbb{R}^3}\left(Q_{IN}^1(\mathbf{nM})+Q_{CH}^1(\mathbf{nM})\right)d\mathbf{v}+O(\epsilon^2), \tag{3.6}$$

with $\mathbf{nM}$ the whole set of Maxwellian distributions $n_I^\epsilon M_I$ $(I=1,2,Z)$ and $n_J M_J$ $(J=A,B,C)$.

Inelastic and chemical collision contributions may be explicitly computed (for Maxwell molecules interactions) when distributions are accommodated at a Maxwellian shape [6,19,21]. Detailed calculations for a general bimolecular and reactive encounter are reported in the Appendix, here we summarize the results relevant to species Y_1. Contributions due to inelastic transitions (2.1) and (2.2) read as

$$\int_{\mathbb{R}^3} Q_{IN}^1(n_1^\epsilon M_1,n_2^\epsilon M_2,n_A M_A)(\mathbf{v})\,d\mathbf{v}=-\nu_{A1}^{A2}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)n_A n_1^\epsilon, \tag{3.7}$$

$$\int_{\mathbb{R}^3} Q_{IN}^1(n_1^\epsilon M_1,n_2^\epsilon M_2,n_Z^\epsilon M_Z)(\mathbf{v})\,d\mathbf{v}=\nu_{Z2}^{Z1}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{Z2}^{Z1})\right)n_Z^\epsilon n_2^\epsilon, \tag{3.8}$$

respectively. As expected, contribution (3.7) is negative, since transitions (2.1) produce a loss of particles Y_1, while term (3.8) is positive, since in encounters (2.2) one gains a particle Y_1. Reactive source terms due to collisions (2.3) and (2.4) are provided, respectively, by

$$\begin{aligned}&\int_{\mathbb{R}^3} Q_{CH}^1(n_1^\epsilon M_1,n_A M_A,n_B M_B,n_C M_C)(\mathbf{v})\,d\mathbf{v}\\&=\nu_{B1}^{AC}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{B1}^{AC})\right)\left[\left(\frac{m_B m_Y}{m_A m_C}\right)^{\frac{3}{2}}\exp(\Delta E_{B1}^{AC})n_A n_C-n_B n_1^\epsilon\right],\end{aligned} \tag{3.9}$$

$$\begin{aligned}&\int_{\mathbb{R}^3} Q_{CH}^1(n_1^\epsilon M_1,n_Z^\epsilon M_Z,n_B M_B)(\mathbf{v})\,d\mathbf{v}\\&=\nu_{11}^{ZB}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{11}^{ZB})\right)\left[\left(\frac{m_Y^2}{m_B m_Z}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_Z^\epsilon n_B-(n_1^\epsilon)^2\right],\end{aligned} \tag{3.10}$$

and they turn out to be a balance between a gain and a loss term, since reactions (2.3) and (2.4) are reversible. In (3.7)–(3.10), symbols ν_{IJ}^{HK} denote collision frequencies defined in (2.19), while Γ is the incomplete Euler gamma function

$$\Gamma(\alpha,y)=\int_y^{+\infty}\tau^{\alpha-1}e^{-\tau}d\tau, \tag{3.11}$$

and $\Theta(y)=\max\{y,0\}$. The presence of these functions is due to the fact that if a reaction is endothermic (namely with a positive internal energy gap $\Delta E_{IJ}^{HK}>0$), it occurs only if the kinetic energy of the ingoing particles is enough, as already explained in Section 2.

By inserting results (3.7)–(3.10) into Equation (3.6), we get

$$\begin{aligned}
&\frac{\partial}{\partial t}n_1^\epsilon+\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}h_1^\epsilon d\mathbf{v}\\
&=-\nu_{A1}^{A2}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)n_A n_1^\epsilon+\nu_{Z2}^{Z1}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{Z2}^{Z1})\right)n_Z^\epsilon n_2^\epsilon\\
&\quad+\nu_{B1}^{AC}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{B1}^{AC})\right)\left[\left(\frac{m_B m_Y}{m_A m_C}\right)^{\frac{3}{2}}\exp(\Delta E_{B1}^{AC})n_A n_C-n_B n_1^\epsilon\right]\\
&\quad+\nu_{11}^{ZB}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{11}^{ZB})\right)\left[\left(\frac{m_Y^2}{m_B m_Z}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_Z^\epsilon n_B-(n_1^\epsilon)^2\right]+O(\epsilon).
\end{aligned}\tag{3.12}$$

We would like to express even the integral $\int_{\mathbb{R}^3}\mathbf{v}h_1^\epsilon d\mathbf{v}$ in terms of our unknown macroscopic fields (number densities); to this aim we resort to the momentum equation for species Y_1. More precisely, we multiply (3.1) by the weight function $\mathbf{v}$ and integrate in $d\mathbf{v}$:

$$\begin{aligned}
&\epsilon\frac{\partial}{\partial t}\int_{\mathbb{R}^3}\mathbf{v}f_1^\epsilon d\mathbf{v}+\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}(\mathbf{v}\otimes\mathbf{v})f_1^\epsilon d\mathbf{v}\\
&=\frac{1}{\epsilon}\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(f_1^\epsilon,n_J M_J)d\mathbf{v}+\epsilon^p\sum_{I=1,2,Z}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(f_1^\epsilon,f_I^\epsilon)d\mathbf{v}\\
&\quad+\epsilon\int_{\mathbb{R}^3}\mathbf{v}Q_{IN}^1(\mathbf{f})\,d\mathbf{v}+\epsilon\int_{\mathbb{R}^3}\mathbf{v}Q_{CH}^1(\mathbf{f})\,d\mathbf{v}.
\end{aligned}\tag{3.13}$$

By substituting the expansions (3.4) for $I=1,2,Z$, we obtain

$$\begin{aligned}
&\nabla_{\mathbf{x}}\cdot\frac{n_1^\epsilon}{m_Y}\mathbb{I}+\epsilon\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}(\mathbf{v}\otimes\mathbf{v})h_1^\epsilon\,d\mathbf{v}\\
&=\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(h_1^\epsilon,n_J M_J)d\mathbf{v}+\epsilon^{p+1}\sum_{I=1,2,Z}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(h_1^\epsilon,n_I^\epsilon M_I)d\mathbf{v}\\
&\quad+\epsilon^{p+1}\sum_{I=1,2,Z}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(n_1^\epsilon M_1,h_I^\epsilon)d\mathbf{v}+\epsilon\int_{\mathbb{R}^3}\mathbf{v}\left(Q_{IN}^1(\mathbf{nM})+Q_{CH}^1(\mathbf{nM})\right)d\mathbf{v}+O(\epsilon^2).
\end{aligned}\tag{3.14}$$

Here it has been taken into account that, since all Maxwellians share the same zero mean velocity, it clearly holds

$$\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(n_1^\epsilon M_1,n_J M_J)d\mathbf{v}=\sum_{I=1,2,Z}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(n_1^\epsilon M_1,n_I^\epsilon M_I)d\mathbf{v}=\mathbf{0},\tag{3.15}$$

and use has been made also of the trivial results

$$\int_{\mathbb{R}^3}\mathbf{v}n_1^\epsilon M_1 d\mathbf{v}=\mathbf{0},\qquad\int_{\mathbb{R}^3}(\mathbf{v}\otimes\mathbf{v})n_1^\epsilon M_1 d\mathbf{v}=\frac{n_1^\epsilon}{m_Y}\mathbb{I}.\tag{3.16}$$

Neglecting $O(\epsilon)$ terms, (3.14) may be cast as

$$\nabla_{\mathbf{x}}\cdot\frac{n_1^\epsilon}{m_Y}\mathbb{I}=\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(h_1^\epsilon,n_J M_J)d\mathbf{v}+O(\epsilon).\tag{3.17}$$

We aim now at computing the elastic contribution on the right-hand side of (3.17), bearing in mind that the weak form of the bi–species elastic Boltzmann operator reads as [9]

$$\int_{\mathbb{R}^3} \varphi(\mathbf{v}) Q_{EL}(f_I,f_J) d\mathbf{v} = \int_{S^2}\int_{\mathbb{R}^3\times\mathbb{R}^3} \Big[\varphi(\mathbf{v}') - \varphi(\mathbf{v})\Big] \sigma_{IJ}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\, g\, f_I(\mathbf{v})\, f_J(\mathbf{w})\, d\mathbf{v}\, d\mathbf{w}\, d\hat{\mathbf{\Omega}}', \tag{3.18}$$

where $\mathbf{v}'$ is the post–collision velocity provided by $\mathbf{v}' = \alpha_{IJ}\mathbf{v} + \alpha_{JI}\mathbf{w} + \alpha_{JI}\, g\hat{\mathbf{\Omega}}'$, with α_{IJ} being the mass ratio $\alpha_{IJ} = m_I/(m_I+m_J)$. In our case we have

$$\int_{\mathbb{R}^3} \mathbf{v} Q^1_{EL}(h^\epsilon_1, n_J M_J) d\mathbf{v} = \int_{S^2}\int_{\mathbb{R}^3\times\mathbb{R}^3} (\mathbf{v}'-\mathbf{v})\, \sigma_{1J}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\, g\, h^\epsilon_1(\mathbf{v}) n_J M_J(\mathbf{w})\, d\mathbf{v}\, d\mathbf{w}\, d\hat{\mathbf{\Omega}}', \tag{3.19}$$

where $\mathbf{v}' = \alpha_{YJ}\mathbf{v} + \alpha_{JY}\mathbf{w} + \alpha_{JY}\, g\hat{\mathbf{\Omega}}'$, therefore we have to compute

$$\int_{S^2}\int_{\mathbb{R}^3\times\mathbb{R}^3} \sigma_{1J}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\, g\alpha_{JY}(g\hat{\mathbf{\Omega}}' - \mathbf{v} + \mathbf{w})\, h^\epsilon_1(\mathbf{v}) n_J M_J(\mathbf{w})\, d\mathbf{v}\, d\mathbf{w}\, d\hat{\mathbf{\Omega}}'.$$

With Maxwell molecules assumption we have that the following quantity is constant

$$\int_{S^2} \sigma_{1J}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\, g\, d\hat{\mathbf{\Omega}}' := \nu_{1J},$$

and by parity arguments

$$\int_{S^2} \sigma_{1J}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')\, g\hat{\mathbf{\Omega}}'\, d\hat{\mathbf{\Omega}}' = \mathbf{0}.$$

Consequently, in the integral (3.19) we have to compute

$$-\nu_{1J}\alpha_{JY}\int_{\mathbb{R}^3} \mathbf{v} h^\epsilon_1(\mathbf{v}) d\mathbf{v} \int_{\mathbb{R}^3} n_J M_J(\mathbf{w}) d\mathbf{w} + \nu_{1J}\alpha_{JY}\int_{\mathbb{R}^3} h^\epsilon_1(\mathbf{v}) d\mathbf{v} \int_{\mathbb{R}^3} \mathbf{w} n_J M_J(\mathbf{w}) d\mathbf{w};$$

last term obviously vanishes, and in conclusion we get

$$\int_{\mathbb{R}^3} \mathbf{v} Q^1_{EL}(h^\epsilon_1, n_J M_J) d\mathbf{v} = -\nu_{1J} n_J \alpha_{JY} \int_{\mathbb{R}^3} \mathbf{v} h^\epsilon_1(\mathbf{v}) d\mathbf{v}. \tag{3.20}$$

By inserting this result into (3.17) we obtain

$$\nabla_{\mathbf{x}}\cdot \frac{n^\epsilon_1}{m_Y}\mathbb{I} = -\left(\sum_{J=A,B,C} \nu_{1J} n_J \alpha_{JY}\right) \int_{\mathbb{R}^3} \mathbf{v} h^\epsilon_1(\mathbf{v}) d\mathbf{v} + O(\epsilon). \tag{3.21}$$

In this way we have expressed the sought streaming contribution appearing in (3.12) in terms of masses, collision frequencies and number densities; more precisely, by substituting (3.21) into (3.12), we get the reaction–diffusion equation

$$\frac{\partial}{\partial t} n^\epsilon_1 - \frac{\Delta_{\mathbf{x}} n^\epsilon_1}{m_Y \displaystyle\sum_{J=A,B,C} \nu_{1J} n_J \alpha_{JY}}$$
$$= -\nu^{A2}_{A1} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E^{A2}_{A1})\right) n_A n^\epsilon_1 + \nu^{Z1}_{Z2} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E^{Z1}_{Z2})\right) n^\epsilon_Z n^\epsilon_2$$

$$+\nu_{B1}^{AC}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{B1}^{AC})\right)\left[\left(\frac{m_B m_Y}{m_A m_C}\right)^{\frac{3}{2}}\exp(\Delta E_{B1}^{AC})n_A n_C - n_B n_1^{\epsilon}\right]$$
$$+\nu_{11}^{ZB}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{11}^{ZB})\right)\left[\left(\frac{m_Y^2}{m_B m_Z}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_Z^{\epsilon} n_B - (n_1^{\epsilon})^2\right] + O(\epsilon). \qquad (3.22)$$

It's important to remark that an evolution equation of this kind could be obtained also without Maxwell molecule assumptions on collision kernels. At first, even for hard potentials or for hard spheres with cutoff, the spectral properties of the linear Boltzmann operator [9] allow to conclude that distributions functions in the present scaling take the form (3.4). Moreover, looking at the detailed computations of inelastic and reactive contributions outlined in the Appendix, we note that their dependence on species number densities may be recovered without any assumption on cross sections σ_{IJ}^{HK} (see formula (A.9)); the Maxwellian potential allows only to explicitly compute the coefficient in front of the classical Arrhenius term, vanishing at chemical equilibrium. The major additional difficulty arising for non–Maxwell collisions concerns the computation of the integral $\int_{\mathbb{R}^3}\mathbf{v}h_1^{\epsilon}d\mathbf{v}$, since in general it is not directly amenable to the moment of the linear operator $\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(h_1^{\epsilon},n_J M_J)d\mathbf{v}$ as in (3.20). By inserting expansions (3.4) into the rescaled Boltzmann Equation (3.1), we get that h_1^{ϵ} should be a solution to the linear problem

$$\sum_{J=A,B,C} Q_{EL}^1(h_1^{\epsilon},n_J M_J)(\mathbf{v}) = \mathbf{v}M_1(\mathbf{v})\cdot\nabla_{\mathbf{x}} n_1^{\epsilon} + O(\epsilon).$$

It can be proved [5, 13] that the problem $Q_{EL}^1(k_{1J},n_J M_J)(\mathbf{v}) = \mathbf{v}M_1(\mathbf{v})$ has a unique solution that may be cast as $k_{1J}(\mathbf{v}) = -\tilde{k}_{1J}(|\mathbf{v}|)\mathbf{v}$, where $\tilde{k}_{1J}(|\mathbf{v}|)$ depends only on the modulus of $\mathbf{v}$. Consequently, the sought perturbation takes the form $h_1^{\epsilon} = -\left(\sum_{J=A,B,C}\tilde{k}_{1J}(|\mathbf{v}|)\right)\mathbf{v}\cdot\nabla_{\mathbf{x}} n_1^{\epsilon} + O(\epsilon)$, and the streaming term of the macroscopic equation for n_1^{ϵ} becomes

$$\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}h_1^{\epsilon}d\mathbf{v} = -\left(\sum_{J=A,B,C}\int_{\mathbb{R}^3}\tilde{k}_{1J}(|\mathbf{v}|)\frac{|\mathbf{v}|^2}{3}d\mathbf{v}\right)\Delta_{\mathbf{x}} n_1^{\epsilon},$$

therefore it is again a diffusion operator, but with a non-explicit diffusion coefficient. Since the final aim of our work is to investigate the stability properties of reaction–diffusion systems derived from the kinetic level, in this paper we consider only the case of Maxwell molecule interactions, in order to have diffusion and reaction coefficients completely explicit in terms of the microscopic parameters of the gas mixture.

3.2. Equation for n_2^{ϵ}.

Now we perform the same procedure in order to obtain an equation for density n_2^{ϵ}. By integrating (3.2) in $d\mathbf{v}$ we get

$$\epsilon\frac{\partial}{\partial t}\int_{\mathbb{R}^3} f_2 d\mathbf{v} + \nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3} f_2 d\mathbf{v} = \epsilon\int_{\mathbb{R}^3} Q_{IN}^2(\mathbf{f})d\mathbf{v}, \qquad (3.23)$$

since

$$\int_{\mathbb{R}^3} Q_{EL}^2(f_2^{\epsilon},n_J M_J)d\mathbf{v} = 0, \quad J=A,B,C \quad \text{and} \quad \int_{\mathbb{R}^3} Q_{EL}^2(f_2^{\epsilon},f_I)d\mathbf{v} = 0, \quad I=1,2,Z.$$

Substituting again for $I=1,2,Z$ the asymptotic expansions (3.4) we have

$$\epsilon\frac{\partial}{\partial t}n_2^{\epsilon} + \epsilon\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}h_2^{\epsilon}d\mathbf{v} = \epsilon\int_{\mathbb{R}^3} Q_{IN}^2(\mathbf{nM})d\mathbf{v} + O(\epsilon^2). \qquad (3.24)$$

Inelastic collision contributions may be computed as described in the Appendix, giving

$$\begin{aligned}&\frac{\partial}{\partial t}n_2^\epsilon+\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}h_2^\epsilon d\mathbf{v}\\&=\nu_{A1}^{A2}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)n_A n_1^\epsilon-\nu_{Z2}^{Z1}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{Z2}^{Z1})\right)n_Z^\epsilon n_2^\epsilon+O(\epsilon),\end{aligned}\tag{3.25}$$

where the first term appearing on the right side is due to encounters (2.1) and the second one due to interactions (2.2). In order to have an explicit expression for the streaming term, similarly to previous subsection we multiply (3.2) by $\mathbf{v}$ and integrate in $d\mathbf{v}$, getting

$$\begin{aligned}&\epsilon\frac{\partial}{\partial t}\int_{\mathbb{R}^3}\mathbf{v}f_2^\epsilon d\mathbf{v}+\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}(\mathbf{v}\otimes\mathbf{v})f_2 d\mathbf{v}\\&=\frac{1}{\epsilon}\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^2(f_2^\epsilon,n_J M_J)d\mathbf{v}+\epsilon^p\sum_{I=1,2,Z}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^2(f_2^\epsilon,f_I)d\mathbf{v}+\int_{\mathbb{R}^3}\mathbf{v}Q_{IN}^2(\mathbf{f})d\mathbf{v}.\end{aligned}\tag{3.26}$$

We again substitute, for $I=1,2,Z$, the expansions (3.4) for the distribution functions obtaining, as above,

$$\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}(\mathbf{v}\otimes\mathbf{v})n_2^\epsilon M_2 d\mathbf{v}=\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^2(h_2^\epsilon,n_J M_J)d\mathbf{v}+O(\epsilon),$$

since all elastic contributions vanish to the leading order accuracy. This leads, as for the component Y_1, to

$$\nabla_{\mathbf{x}}\cdot\frac{n_2^\epsilon}{m_Y}\mathbb{I}=-\left(\sum_{J=A,B,C}\nu_{2J}n_J\alpha_{JY}\right)\int_{\mathbb{R}^3}\mathbf{v}h_2^\epsilon(\mathbf{v})d\mathbf{v}+O(\epsilon).\tag{3.27}$$

Finally, inserting (3.27) into Equation (3.25) we have the reaction–diffusion equation

$$\begin{aligned}&\frac{\partial}{\partial t}n_2^\epsilon-\frac{\Delta_{\mathbf{x}}n_2^\epsilon}{m_Y\displaystyle\sum_{J=A,B,C}\nu_{2J}n_J\alpha_{JY}}\\&=\nu_{A1}^{A2}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)n_A n_1^\epsilon-\nu_{Z2}^{Z1}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{Z2}^{Z1})\right)n_Z^\epsilon n_2^\epsilon+O(\epsilon).\end{aligned}\tag{3.28}$$

3.3. Equation for n_Z^ϵ. Once again, we start from the rescaled kinetic equation (3.3) and integrate in $d\mathbf{v}$, obtaining

$$\epsilon\frac{\partial}{\partial t}\int_{\mathbb{R}^3}f_Z^\epsilon d\mathbf{v}+\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}f_Z^\epsilon d\mathbf{v}=\epsilon\int_{\mathbb{R}^3}\left(Q_{IN}^Z(\mathbf{f})+Q_{CH}^Z(\mathbf{f})\right)d\mathbf{v},\tag{3.29}$$

being

$$\int_{\mathbb{R}^3}Q_{EL}^Z(f_Z^\epsilon,n_J M_J)d\mathbf{v}=0,\quad J=A,B,C\quad\text{and}\quad\int_{\mathbb{R}^3}Q_{EL}^Z(f_Z^\epsilon,f_I)d\mathbf{v}=0,\quad I=1,2,Z.$$

Substituting the asymptotic expansions (3.4) we have

$$\epsilon\frac{\partial}{\partial t}n_Z^\epsilon+\epsilon\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}h_Z^\epsilon d\mathbf{v}=\epsilon\int_{\mathbb{R}^3}\left(Q_{IN}^Z(\mathbf{nM})+Q_{CH}^Z(\mathbf{nM})\right)d\mathbf{v}+O(\epsilon^2).\tag{3.30}$$

We note that the contribution given by the inelastic encounter (2.2) is null, since there is no net production of particles of species Z; we compute the chemical integral due to the bimolecular and reversible reaction (2.4) and we get

$$\begin{aligned}&\frac{\partial}{\partial t}n_Z^\epsilon+\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}h_Z^\epsilon d\mathbf{v}\\&=-\nu_{11}^{ZB}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{11}^{ZB})\right)\left[\left(\frac{m_Y^2}{m_B m_Z}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_Z^\epsilon n_B-(n_1^\epsilon)^2\right]+O(\epsilon).\end{aligned}\tag{3.31}$$

By multiplying (3.3) by $\mathbf{v}$ and integrating in $d\mathbf{v}$ we have

$$\begin{aligned}&\epsilon\frac{\partial}{\partial t}\int_{\mathbb{R}^3}\mathbf{v}f_Z^\epsilon d\mathbf{v}+\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}(\mathbf{v}\otimes\mathbf{v})f_Z^\epsilon d\mathbf{v}\\&=\frac{1}{\epsilon}\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^Z(f_Z^\epsilon,n_J M_J)d\mathbf{v}+\epsilon^p\sum_{I=1,2,Z}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^Z(f_Z^\epsilon,f_I^\epsilon)d\mathbf{v}\\&\quad+\epsilon\int_{\mathbb{R}^3}\mathbf{v}\left(Q_{IN}^Z(\mathbf{f})+Q_{CH}^Z(\mathbf{f})\right)d\mathbf{v},\end{aligned}\tag{3.32}$$

and use of expansions (3.4) now gives

$$\begin{aligned}&\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}(\mathbf{v}\otimes\mathbf{v})n_Z^\epsilon M_Z d\mathbf{v}\\&=\frac{1}{\epsilon}\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^Z(n_Z^\epsilon M_Z,n_J M_J)d\mathbf{v}+\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^Z(h_Z^\epsilon,n_J M_J)d\mathbf{v}\\&\quad+\epsilon\int_{\mathbb{R}^3}\left(Q_{IN}^Z(\mathbf{nM})+Q_{CH}^Z(\mathbf{nM})\right)d\mathbf{v}+O(\epsilon^2),\end{aligned}\tag{3.33}$$

leading again to the equality

$$\nabla_{\mathbf{x}}\cdot\frac{n_Z^\epsilon}{m_Z}\mathbb{I}=-\left(\sum_{J=A,B,C}\nu_{ZJ}n_J\alpha_{JZ}\right)\int_{\mathbb{R}^3}\mathbf{v}h_Z^\epsilon(\mathbf{v})d\mathbf{v}+O(\epsilon).\tag{3.34}$$

We have now obtained the third reaction-diffusion equation for the density of species Z

$$\begin{aligned}&\frac{\partial}{\partial t}n_Z^\epsilon-\frac{\Delta_{\mathbf{x}}n_Z^\epsilon}{m_Z\displaystyle\sum_{J=A,B,C}\nu_{ZJ}n_J\alpha_{JZ}}\\&=-\nu_{11}^{ZB}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{11}^{ZB})\right)\left[\left(\frac{m_Y^2}{m_B m_Z}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_Z^\epsilon n_B-(n_1^\epsilon)^2\right]+O(\epsilon).\end{aligned}\tag{3.35}$$

3.4. Reaction–diffusion system.

By passing to the limit $\epsilon\to 0$ in Equations (3.22), (3.28), and (3.35), and denoting by (n_1,n_2,n_Z) the limit of the sequence of density functions $(n_1^\epsilon,n_2^\epsilon,n_Z^\epsilon)$, we have that (n_1,n_2,n_Z) is a solution of the system of reaction–diffusion equations:

$$\frac{\partial}{\partial t}n_1-\frac{1}{m_Y\displaystyle\sum_{J=A,B,C}\nu_{1J}n_J\alpha_{JY}}\Delta_{\mathbf{x}}n_1=\tilde{a}-(\tilde{b}+\tilde{c})n_1+\tilde{\eta}n_Z n_2+\tilde{e}n_Z-\tilde{f}n_1^2$$

$$\frac{\partial}{\partial t}n_2 - \frac{1}{m_Y \displaystyle\sum_{J=A,B,C} \nu_{2J} n_J \alpha_{JY}} \Delta_{\mathbf{x}} n_2 = \tilde{b} n_1 - \tilde{\eta} n_Z n_2$$

$$\frac{\partial}{\partial t}n_Z - \frac{1}{m_Z \displaystyle\sum_{J=A,B,C} \nu_{ZJ} n_J \alpha_{JZ}} \Delta_{\mathbf{x}} n_Z = \tilde{f} n_1^2 - \tilde{e} n_Z, \tag{3.36}$$

with

$$\tilde{a} = \nu_{B1}^{AC} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{B1}^{AC})\right) \left(\frac{m_B m_Y}{m_A m_C}\right)^{\frac{3}{2}} \exp(\Delta E_{B1}^{AC}) n_A n_C \tag{3.37}$$

$$\tilde{b} = \nu_{A1}^{A2} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{A1}^{A2})\right) n_A \tag{3.38}$$

$$\tilde{c} = \nu_{B1}^{AC} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{B1}^{AC})\right) n_B \tag{3.39}$$

$$\tilde{\eta} = \nu_{Z2}^{Z1} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{Z2}^{Z1})\right) \tag{3.40}$$

$$\tilde{e} = \nu_{11}^{ZB} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{11}^{ZB})\right) \left(\frac{m_Y^2}{m_Z m_B}\right)^{\frac{3}{2}} \exp(\Delta E_{11}^{ZB}) n_B \tag{3.41}$$

$$\tilde{f} = \nu_{11}^{ZB} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{11}^{ZB})\right). \tag{3.42}$$

In Section 5, the stability properties of system (3.36) will be investigated in a regular open space domain Ω. If we suppose that the rescaled distribution functions f_I^ϵ, $I = 1,2,Z$, satisfy the initial conditions

$$f_I^\epsilon(0,\mathbf{x},\mathbf{v}) = f_I^0(\mathbf{x},\mathbf{v}), \quad I = 1,2,Z, \tag{3.43}$$

and the specular reflection boundary conditions

$$f_I^\epsilon(t,\mathbf{x},\mathbf{v}) = f_I^\epsilon(t,\mathbf{x},R\mathbf{v}) \qquad \forall t > 0, \quad \mathbf{x} \in \partial\Omega, \quad \mathbf{v} \in \mathbb{R}^3, \quad I = 1,2,Z, \tag{3.44}$$

with $R\mathbf{v} = \mathbf{v} - 2(\mathbf{v}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}$, with $\hat{\mathbf{n}}(\mathbf{x})$ being the outward normal vector to $\partial\Omega$ at a point $\mathbf{x}$, then, as proved in [5], by integrating the rescaled kinetic system (3.1)–(3.3) over $(t,\mathbf{x},\mathbf{v}) \in (0,+\infty) \times \Omega \times \mathbb{R}^3$ and passing to the limit $\epsilon \to 0$, we get exactly the weak form of the reaction–diffusion system (3.36), with initial data

$$n_I(0,\mathbf{x}) = \int_{\mathbb{R}^3} f_I^0(\mathbf{x},\mathbf{v}) d\mathbf{v}, \quad I = 1,2,Z, \tag{3.45}$$

and homogeneous Neumann boundary conditions

$$\hat{\mathbf{n}} \cdot \nabla_{\mathbf{x}} n_I = 0 \quad \text{on} \quad (0,+\infty) \times \partial\Omega, \quad I = 1,2,Z, \tag{3.46}$$

that will be assumed valid in Section 5.

Changing the time variable $\tilde{t} = \tilde{c}t$ and defining

$$a = \frac{\tilde{a}}{\tilde{c}}, \qquad b = \frac{\tilde{b}}{\tilde{c}}, \qquad \eta = \frac{\tilde{\eta}}{\tilde{c}}, \qquad e = \frac{\tilde{e}}{\tilde{c}}, \qquad f = \frac{\tilde{f}}{\tilde{c}}, \tag{3.47}$$

$$D_1=\left[\tilde{c}m_Y\sum_{J=A,B,C}\nu_{1J}n_J\alpha_{JY}\right]^{-1},\qquad D_2=\left[\tilde{c}m_Y\sum_{J=A,B,C}\nu_{2J}n_J\alpha_{JY}\right]^{-1},$$
$$D_Z=\left[\tilde{c}m_Z\sum_{J=A,B,C}\nu_{ZJ}n_J\alpha_{JZ}\right]^{-1}, \tag{3.48}$$

we have that the system (3.36) for n_1, n_2 and n_Z may be rewritten as

$$\begin{aligned}
&\frac{\partial n_1}{\partial t}-D_1\Delta_{\mathbf{x}}n_1=a-(b+1)n_1+\eta n_Z n_2+e n_Z-f n_1^2\\
&\frac{\partial n_2}{\partial t}-D_2\Delta_{\mathbf{x}}n_2=b n_1-\eta n_Z n_2\\
&\frac{\partial n_Z}{\partial t}-D_Z\Delta_{\mathbf{x}}n_Z=f n_1^2-e n_Z.
\end{aligned} \tag{3.49}$$

Diffusion coefficients D_1, D_2, D_Z are essentially due to the very frequent interactions with the host medium; indeed, they depend on collision frequencies of such dominant collisions, on number densities of background species, and on masses of the colliding particles. The terms on the right-hand sides are due to inelastic transitions and chemical reactions (2.1)–(2.4). Notice that, besides quadratic contributions due to binary reactions involving a pair of the considered components Y_1, Y_2, Z, there are linear terms caused by non–conservative interactions with background particles, and in the equation for n_1 there appears also a constant source term, taking into account the production of particles Y_1 due to the background only (see the reverse reaction in (2.3)). As we will show in Section 5, the occurrence of this “external” particle source allows the system to have a unique homogeneous state, independent of initial data. A great advantage of the present derivation from the kinetic level is that diffusion and reaction coefficients are explicitly provided in terms of the microscopic parameters of the colliding system, namely particle masses, collision frequencies and internal energy.

4. Derivation of a reduced two–component reaction–diffusion system

In this section we present a derivation from our kinetic model of a closed system of reaction–diffusion equations for the two components Y_1, Y_2 of the polyatomic gas only. In this hydrodynamic regime, the other gas Z will play the role of a very unstable particle state, quickly disappearing through proper interactions. The final macroscopic system will turn out to be similar to the classical Brusselator system; the presence of an intermediate unstable state Z in the Brusselator–type reaction has been already explored in [12], where such intermediate gas is assumed non–diffusive and at an almost steady configuration, namely with the reaction term vanishing at leading order accuracy.

We show that it is possible to derive such a reduction for system (3.49) assuming faster time scales for elastic collisions between the background and the species Z, and for the reaction (2.4). In particular, we prove that in the considered scaling the number density n_Z^ϵ is completely determined in terms of the number density n_1^ϵ and other fixed parameters (masses, internal energies, and background density), therefore it will suffice to derive a system of two coupled reaction–diffusion equations for n_1^ϵ, n_2^ϵ.

In the present scaling, elastic scattering with the host medium is again the dominant process: Collisions of the two components of the gas Y with the background are taken of order $1/\epsilon$ as in the previous section, while scattering between the monatomic gas Z and the background is assumed faster, of order $1/\epsilon^2$. All other bi–species elastic collisions are of order ϵ^p, $p\geq 0$, as above. Inelastic encounters (2.1), (2.2) and chemical reaction (2.3) are of order ϵ (slow as above), while the bimolecular reaction (2.4), involving the unstable state Z, is faster, of order 1. This means that a pair of particles Y_1 easily recombines to give rise to a particle Z, and then such particle Z, colliding with the host medium, very quickly dissociates again into a pair (Y_1,Y_1). We use here a separate notation for the chemical collision operator for reactions (2.3) and (2.4), respectively:

$$\begin{aligned}
&Q^{1^*}_{CH}(\mathbf{f})=Q^1_{CH}(f_1^\epsilon,n_AM_A,n_BM_B,n_CM_C),\quad Q^{1^{**}}_{CH}(\mathbf{f})=Q^1_{CH}(f_1^\epsilon,f_Z^\epsilon,n_BM_B),\\
&Q^{Z^{**}}_{CH}(\mathbf{f})=Q^Z_{CH}(f_1^\epsilon,f_Z^\epsilon,n_BM_B).
\end{aligned}\tag{4.1}$$

Thus, rescaled Boltzmann equations for Y_1, Y_2 and Z read as:

$$\begin{aligned}
&\epsilon\frac{\partial f_1^\epsilon}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}f_1^\epsilon\\
&=\frac{1}{\epsilon}\sum_{J=A,B,C}Q^1_{EL}(f_1^\epsilon,n_JM_J)+\epsilon^p\sum_{I=1,2,Z}Q^1_{EL}(f_1^\epsilon,f_I^\epsilon)+\epsilon\, Q^1_{IN}(\mathbf{f})+\epsilon\, Q^{1^*}_{CH}(\mathbf{f})+Q^{1^{**}}_{CH}(\mathbf{f}),
\end{aligned}\tag{4.2}$$

$$\begin{aligned}
&\epsilon\frac{\partial f_2^\epsilon}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}f_2^\epsilon\\
&=\frac{1}{\epsilon}\sum_{J=A,B,C}Q^2_{EL}(f_2^\epsilon,n_JM_J)+\epsilon^p\sum_{I=1,2,Z}Q^2_{EL}(f_2^\epsilon,f_I^\epsilon)+\epsilon\, Q^2_{IN}(\mathbf{f}),
\end{aligned}\tag{4.3}$$

$$\begin{aligned}
&\epsilon\frac{\partial f_Z^\epsilon}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}f_Z^\epsilon\\
&=\frac{1}{\epsilon^2}\sum_{J=A,B,C}Q^Z_{EL}(f_Z^\epsilon,n_JM_J)+\epsilon^p\sum_{I=1,2,Z}Q^Z_{EL}(f_Z^\epsilon,f_I^\epsilon)+\epsilon\, Q^Z_{IN}(\mathbf{f})+Q^{Z^{**}}_{CH}(\mathbf{f}).
\end{aligned}\tag{4.4}$$

Also in this case the dynamics is dominated by collisions with the background, and specifically it means that

$$\sum_{J=A,B,C}Q^I_{EL}(f_I^\epsilon,n_JM_J)=O(\epsilon)\quad I=1,2,\qquad \sum_{J=A,B,C}Q^I_{EL}(f_I^\epsilon,n_JM_J)=O(\epsilon^2)\quad I=Z.$$

Consequently, the perturbed expressions of distributions are

$$f_I^\epsilon(t,\mathbf{x},\mathbf{v})=n_I^\epsilon(t,\mathbf{x})M_I(\mathbf{v})+\epsilon h_I^\epsilon(t,\mathbf{x},\mathbf{v}),\qquad I=1,2,\tag{4.5}$$

$$f_I^\epsilon(t,\mathbf{x},\mathbf{v})=n_I^\epsilon(t,\mathbf{x})M_I(\mathbf{v})+\epsilon^2 h_I^\epsilon(t,\mathbf{x},\mathbf{v}),\qquad I=Z,\tag{4.6}$$

where we may assume

$$\int_{\mathbb{R}^3}h_I^\epsilon(\mathbf{v})\,d\mathbf{v}=0,\qquad I=1,2,Z.\tag{4.7}$$

4.1. Equation for n_1^ϵ. By integrating the Boltzmann equation (4.2) with respect to the velocity variable $\mathbf{v}$, and substituting the expressions (4.5) and (4.6) for distributions we get, eliminating vanishing terms,

$$\epsilon\frac{\partial}{\partial t}n_1^\epsilon+\epsilon\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}h_1^\epsilon d\mathbf{v}=\epsilon\int_{\mathbb{R}^3}\Big(Q^1_{IN}(\mathbf{nM})+Q^{1^*}_{CH}(\mathbf{nM})\Big)d\mathbf{v}+\int_{\mathbb{R}^3}Q^{1^{**}}_{CH}(\mathbf{nM})\,d\mathbf{v}$$

$$+\epsilon\int_{\mathbb{R}^3}\tilde{Q}^{1^{**}}_{CH}(h_1^\epsilon,n_1^\epsilon M_1)d\mathbf{v}+O(\epsilon^2), \tag{4.8}$$

where $\tilde{Q}^{1^{**}}_{CH}(h_1^\epsilon,n_1^\epsilon M_1)$ is the first order ($O(\epsilon)$) correction of the dominant chemical term $Q^{1^{**}}_{CH}(\mathbf{f})$ given in (2.17), that turns out to be

$$\tilde{Q}^{1^{**}}_{CH}(h_1^\epsilon,n_1^\epsilon M_1)=-2\int_{\mathbb{R}^3}\int_{S^2}H\left(g^2-\delta_{11}^{ZB}\right)\sigma_{11}^{ZB}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g\,h_1^\epsilon(\mathbf{v})n_1^\epsilon M_1(\mathbf{w})d\mathbf{w}d\hat{\mathbf{\Omega}}'. \tag{4.9}$$

Leading order of Equation (4.8) provides

$$\int_{\mathbb{R}^3}Q^{1^{**}}_{CH}(\mathbf{nM})\,d\mathbf{v}=O(\epsilon), \tag{4.10}$$

which after the explicit computation of collision contribution, following the lines outlined in the Appendix, becomes

$$\nu_{11}^{ZB}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{11}^{ZB})\right)\left[\left(\frac{m_Y^2}{m_Z m_B}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_Z^\epsilon n_B-(n_1^\epsilon)^2\right]=O(\epsilon). \tag{4.11}$$

We note that this provides an explicit expression for number density n_Z^ϵ, to the leading order accuracy, as function of n_1^ϵ:

$$n_Z^\epsilon=(n_1^\epsilon)^2\left[\left(\frac{m_Y^2}{m_Z m_B}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_B\right]^{-1}+O(\epsilon). \tag{4.12}$$

With this result at hand, by writing explicitly next order ($O(\epsilon)$) of Equation (4.8) we get

$$\begin{aligned}&\frac{\partial}{\partial t}n_1^\epsilon+\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}\mathbf{v}h_1^\epsilon d\mathbf{v}\\&=\int_{\mathbb{R}^3}\left(Q^1_{IN}(\mathbf{nM})+Q^{1^*}_{CH}(\mathbf{nM})\right)d\mathbf{v}+\int_{\mathbb{R}^3}\tilde{Q}^{1^{**}}_{CH}(h_1^\epsilon,n_1^\epsilon M_1)d\mathbf{v}+O(\epsilon).\end{aligned} \tag{4.13}$$

Under a Maxwell molecule assumption for the direct reaction in (2.4), the last integral in (4.13) is explicitly provided by

$$\begin{aligned}&\int_{\mathbb{R}^3}\tilde{Q}^{1^{**}}_{CH}(h_1^\epsilon,n_1^\epsilon M_1)\,d\mathbf{v}\\&=-2\nu_{11}^{ZB}n_1^\epsilon\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}H\left(g^2-\delta_{11}^{ZB}\right)h_1^\epsilon(\mathbf{v})M_1(\mathbf{w})\,d\mathbf{v}d\mathbf{w}.\end{aligned} \tag{4.14}$$

If we suppose that the quantity $\Delta E_{11}^{ZB}=E_B+E_Z-2E_1<0$, we have $H\left(g^2-\delta_{11}^{ZB}\right)\equiv 1$ and thus the whole integral is zero, owing to (4.7). In the opposite case, the contribution cannot be made explicit without further assumptions on the perturbation $h_1^\epsilon(\mathbf{v})$. Anyway, we expect that such contribution would be very small (bearing in mind (4.7)), and therefore negligible in the final macroscopic equation; moreover, we will see in next section that the assumption $\Delta E_{11}^{ZB}<0$ is almost not restrictive in determining the configurations of masses and energy values allowing pattern formation, therefore it may be reasonably adopted.

Also in Equation (4.13) we need an expression for $\int_{\mathbb{R}^3}\mathbf{v}\,h_I^\epsilon d\mathbf{v}$ in terms of number densities; we multiply (4.2) by $\mathbf{v}$ and integrate in $d\mathbf{v}$. Substituting again expansions (4.5) and (4.6) and taking only the leading order terms, we obtain

$$\nabla_{\mathbf{x}}\cdot\int_{\mathbb{R}^3}(\mathbf{v}\otimes\mathbf{v})n_1^\epsilon M_1 d\mathbf{v}=\sum_{J=A,B,C}\int_{\mathbb{R}^3}\mathbf{v}Q_{EL}^1(h_1^\epsilon,n_J M_J)d\mathbf{v}+\int_{\mathbb{R}^3}\mathbf{v}Q_{CH}^{1^{**}}(\mathbf{nM})\,d\mathbf{v}+O(\epsilon). \tag{4.15}$$

But for $\Delta E_{11}^{ZB}<0$ we easily get

$$\int_{\mathbb{R}^3}\mathbf{v}Q_{CH}^{1^{**}}(\mathbf{nM})\,d\mathbf{v}=\mathbf{0}, \tag{4.16}$$

since it is enough to perform the change of variables $(\mathbf{v},\mathbf{w})\to(\mathbf{g},\mathbf{G})$ expressed in the Appendix and to observe that

$$\int_{\mathbb{R}^3}\mathbf{G}\exp\left(-m_Y G^2\right)d\mathbf{G}=\int_{\mathbb{R}^3}\mathbf{g}\exp\left(-\frac{1}{4}m_Y g^2\right)d\mathbf{g}=\mathbf{0}.$$

Thus the following relation holds again

$$\nabla_{\mathbf{x}}\cdot\frac{n_1^\epsilon}{m_Y}\mathbb{I}=-\left(\sum_{J=A,B,C}\nu_{1J}n_J\alpha_{JY}\right)\int_{\mathbb{R}^3}\mathbf{v}h_1^\epsilon(\mathbf{v})d\mathbf{v}+O(\epsilon). \tag{4.17}$$

It is now sufficient to insert this into the Equation (4.13) and to compute inelastic and chemical collision integrals in order to obtain the reaction–diffusion equation

$$\begin{aligned}&\frac{\partial}{\partial t}n_1^\epsilon-\frac{\Delta_{\mathbf{x}}n_1^\epsilon}{m_Y\sum_{J=A,B,C}\nu_{1J}n_J\alpha_{JY}}\\&=-\nu_{A1}^{A2}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)n_A n_1^\epsilon+\nu_{Z2}^{Z1}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{Z2}^{Z1})\right)n_Z^\epsilon n_2^\epsilon\\&\quad+\nu_{B1}^{AC}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{B1}^{AC})\right)\left[\left(\frac{m_B m_Y}{m_A m_C}\right)^{\frac{3}{2}}\exp(\Delta E_{B1}^{AC})n_A n_C-n_B n_1^\epsilon\right]+O(\epsilon).\end{aligned} \tag{4.18}$$

Substituting on the right-hand side the expression (4.12) for the density of the unstable state n_Z^ϵ, it becomes

$$\begin{aligned}&\frac{\partial}{\partial t}n_1^\epsilon-\frac{\Delta_{\mathbf{x}}n_1^\epsilon}{m_Y\sum_{J=A,B,C}\nu_{1J}n_J\alpha_{JY}}\\&=-\nu_{A1}^{A2}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)n_A n_1^\epsilon\\&\quad+\nu_{Z2}^{Z1}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{Z2}^{Z1})\right)\left[\left(\frac{m_Y^2}{m_Z m_B}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_B\right]^{-1}(n_1^\epsilon)^2 n_2^\epsilon\\&\quad+\nu_{B1}^{AC}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{B1}^{AC})\right)\left[\left(\frac{m_B m_Y}{m_A m_C}\right)^{\frac{3}{2}}\exp(\Delta E_{B1}^{AC})n_A n_C-n_B n_1^\epsilon\right]+O(\epsilon).\end{aligned} \tag{4.19}$$

4.2. Equation for n_2^ϵ. Since the component Y_2 is not involved in reaction (2.4), that is the only one with a modified scaling with respect to previous section, the derivation of the reaction–diffusion equation for density n_2^ϵ is really analogous to the one performed in Section 3, thus we skip the details here. With the usual asymptotic procedure we derive the equation

$$\begin{aligned}&\frac{\partial}{\partial t}n_2^\epsilon-\frac{\Delta_{\mathbf{x}}n_2^\epsilon}{m_Y\sum_{J=A,B,C}\nu_{2J}n_J\alpha_{JY}}\\&=\nu_{A1}^{A2}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)n_An_1^\epsilon-\nu_{Z2}^{Z1}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{Z2}^{Z1})\right)n_Z^\epsilon n_2^\epsilon+O(\epsilon).\end{aligned}\tag{4.20}$$

Again we substitute the expression for n_Z^ϵ provided by (4.12), obtaining

$$\begin{aligned}&\frac{\partial}{\partial t}n_2^\epsilon-\frac{\Delta_{\mathbf{x}}n_2^\epsilon}{m_Y\sum_{J=A,B,C}\nu_{2J}n_J\alpha_{JY}}\\&=\nu_{A1}^{A2}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)n_An_1^\epsilon\\&\quad-\nu_{Z2}^{Z1}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{Z2}^{Z1})\right)\left[\left(\frac{m_Y^2}{m_Zm_B}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_B\right]^{-1}(n_1^\epsilon)^2n_2^\epsilon+O(\epsilon).\end{aligned}\tag{4.21}$$

4.3. Reaction-diffusion system. We pass to the limit $\epsilon\to0$ in (4.19) and (4.21) obtaining the following reaction–diffusion system for the unknown number densities n_1, n_2, which denote the limiting values of the sequences n_1^ϵ, n_2^ϵ:

$$\begin{aligned}&\frac{\partial n_1}{\partial t}-\frac{1}{m_Y\sum\limits_{J=A,B,C}\nu_{1J}n_J\alpha_{JY}}\Delta_{\mathbf{x}}n_1=\tilde{a}-(\tilde{b}+\tilde{c})n_1+\tilde{d}n_1^2n_2\\&\frac{\partial n_2}{\partial t}-\frac{1}{m_Y\sum\limits_{J=A,B,C}\nu_{2J}n_J\alpha_{JY}}\Delta_{\mathbf{x}}n_2=\tilde{b}n_1-\tilde{d}n_1^2n_2,\end{aligned}\tag{4.22}$$

with

$$\tilde{a}=\nu_{B1}^{AC}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{B1}^{AC})\right)\left(\frac{m_Bm_Y}{m_Am_C}\right)^{\frac{3}{2}}\exp(\Delta E_{B1}^{AC})n_An_C\tag{4.23}$$

$$\tilde{b}=\nu_{A1}^{A2}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)n_A\tag{4.24}$$

$$\tilde{c}=\nu_{B1}^{AC}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{B1}^{AC})\right)n_B\tag{4.25}$$

$$\tilde{d}=\nu_{Z2}^{Z1}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{Z2}^{Z1})\right)\left[\left(\frac{m_Y^2}{m_Zm_B}\right)^{\frac{3}{2}}\exp(\Delta E_{11}^{ZB})n_B\right]^{-1}.\tag{4.26}$$

Notice that coefficients $\tilde{a}$, $\tilde{b}$, $\tilde{c}$ coincide with the ones obtained in the previous section for the system of three equations (see formulas (3.37), (3.38), (3.39)). The coefficient $\tilde{d}$ may be instead recovered from (3.40), (3.41), (3.42) as $\tilde{d}=\tilde{\eta}\tilde{f}/\tilde{e}$. Indeed, system (4.22) could also be formally obtained from the macroscopic system (3.36) in a suitable scaling. In order to do this, one has to carefully check the implications at the macroscopic level of the additional assumption $\Delta E_{11}^{ZB} < 0$ introduced in this section. Specifically, this requirement makes the chemical contribution (4.14) vanish, implying that $n_Z^\epsilon = \tilde{f}(n_1^\epsilon)^2/\tilde{e} + O(\epsilon^2)$. For this reason, the right scaling allowing to derive (4.22) from (3.36) consists in putting $1/\epsilon^2$ in front of the right-hand side of equation for n_Z^ϵ in (3.36) and in the analogous contribution appearing in the equation for n_1^ϵ. The derivation of a system of type (4.22) as a reduction of a system of three equations may be found also in [12], where one of the species (Z) is assumed non–diffusing and unstable, so that it may be considered accommodated at an equilibrium configuration, with its number density related to the ones of other constituents as in (4.12).

We will investigate Turing instability of system (4.22) in a bounded domain Ω, and to this aim, as already motivated in Subsection 3.4, we set an initial datum

$$n_I(0,\mathbf{x}) = \int_{\mathbb{R}^3} f_I^0(\mathbf{x},\mathbf{v})d\mathbf{v}, \quad I = 1,2, \tag{4.27}$$

and we assume Neumann boundary conditions

$$\hat{\mathbf{n}} \cdot \nabla_{\mathbf{x}} n_I = 0 \quad \text{on} \quad (0,\infty) \times \partial\Omega, \quad I = 1,2. \tag{4.28}$$

For convenience, we perform again the change of time variable $\tilde{t} = \tilde{c}t$ and define

$$a = \frac{\tilde{a}}{\tilde{c}}, \qquad b = \frac{\tilde{b}}{\tilde{c}}, \qquad d = \frac{\tilde{d}}{\tilde{c}}, \tag{4.29}$$

$$D_1 = \left[\tilde{c} m_Y \sum_{J=A,B,C} \nu_{1J} n_J \alpha_{JY} \right]^{-1}, \quad D_2 = \left[\tilde{c} m_Y \sum_{J=A,B,C} \nu_{2J} n_J \alpha_{JY} \right]^{-1}; \tag{4.30}$$

in this way, the evolution system for n_1 and n_2 reads as

$$\begin{aligned} &\frac{\partial n_1}{\partial t} - D_1 \Delta_{\mathbf{x}} n_1 = a - (b+1) n_1 + d {n_1}^2 n_2, \\ &\frac{\partial n_2}{\partial t} - D_2 \Delta_{\mathbf{x}} n_2 = b n_1 - d {n_1}^2 n_2. \end{aligned} \tag{4.31}$$

The system (4.31) is similar to the classical Brusselator model, whose stability properties were investigated for the first time in [35] and [24] (the only difference is the presence of our coefficient d instead of 1). In that context, coefficients of the system were expressed in terms of the kinetic constants of the individual reaction steps of the auto–catalytic process and of concentrations of constant reactants involved. Here, coefficients of the system play a similar role; indeed, their dependence is on microscopic quantities that, besides masses and energy levels, are collision frequencies (determining the interaction rates between elements of the mixture) and densities of the background species.

5. Discussion of Turing instability of reaction–diffusion systems

The classical Brusselator was introduced in order to model the behavior of cross–activator–inhibitor chemical reactions for which pattern formation predicted by Turing [44] could be observed. One example is the chloriteiodide–malonic acid (CIMA) reaction [25] and other analogous models, and results can be found in [20]. Analytical conditions on the parameters involved in the equations leading to Turing instability were originally given in [35]. The target was to find a homogeneous stationary state that in presence of diffusion turns into spatially non–homogeneous structures.

In this section, we want to proceed in the same direction with systems (3.49) and (4.31), that have been consistently derived from kinetic equations. We start from the reduced system of two equations, that allows us to derive completely explicit conditions on internal energies and other microscopic parameters giving rise to Turing instability. Then we take into account the more complicated system of three equations (3.49), involving a higher number of parameters, and both an analytical investigation and a numerical study are performed in order to deduce its stability properties.

5.1. Turing instability for the reduced two–component system. Considering system (4.31), we first look for conditions on the coefficients a, b, d and on diffusion coefficients D_1, D_2 in order to have Turing instability, then we discuss the fulfillment of such conditions for varying microscopic quantities, energy levels in particular. The first step consists in imposing the stability of a space homogeneous steady state, and to this aim we consider the system in absence of diffusion:

$$\begin{aligned} \frac{\partial n_1}{\partial t} &= a-(b+1)n_1+d{n_1}^2 n_2 \\ \frac{\partial n_2}{\partial t} &= b n_1 - d{n_1}^2 n_2. \end{aligned} \tag{5.1}$$

We note that this set of ODEs admits a unique stationary state, provided by

$$(\bar{n}_1,\bar{n}_2)=\left(a,\frac{b}{ad}\right).$$

Uniqueness of the equilibrium is due to the presence of a source term a, related to chemical interactions with the host medium. Indeed, in self–contained reacting systems, involving for instance four gases undergoing only a bimolecular and reversible chemical reaction, one has that the collision contribution in equations for number densities is provided by an Arrhenius–type law, having a manifold of steady equilibria (of the form $n_1 n_2 = K n_3 n_4$) [5, 36].

In order to study the equilibrium stability in spatially homogeneous conditions, we linearize the system (5.1) getting

$$\frac{\partial \mathbf{W}}{\partial t}=A\mathbf{W}, \tag{5.2}$$

with $\mathbf{W}=\begin{pmatrix} n_1-\bar{n}_1 \\ n_2-\bar{n}_2\end{pmatrix}$ and $A=\begin{pmatrix} b-1 & a^2 d \\ -b & -a^2 d\end{pmatrix}$. Conditions to have the stability of the stationary state are $tr\,A<0$ and $det\,A>0$. Since in our model coefficients of the system are all positive quantities, the determinant is trivially positive while for the sign of the trace we get the constraint

$$b<1+a^2 d. \tag{5.3}$$

The linearized system including diffusive terms in a space domain $\Omega\in\mathbb{R}^N$ with zero–flux boundary conditions reads as

$$\begin{cases} \dfrac{\partial \mathbf{W}}{\partial t}=D\Delta_{\mathbf{x}}\mathbf{W}+A\mathbf{W} & \text{on } (0,\infty)\times\Omega \\ \hat{\mathbf{n}}\cdot\nabla_{\mathbf{x}}\mathbf{W}=0 & \text{on } (0,\infty)\times\partial\Omega \end{cases} \tag{5.4}$$

with diffusion matrix $D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}$. We look for solutions of this system represented in Fourier series as

$$\mathbf{W}(\mathbf{x},t) = \sum_k c_k e^{\lambda_k t} \tilde{\mathbf{W}}_k(\mathbf{x}), \tag{5.5}$$

with $k \in \mathbb{N}$ and the eigenfunction $\tilde{\mathbf{W}}_k(\mathbf{x})$ denoting a solution of the time–independent problem

$$\begin{cases} \Delta_{\mathbf{x}} \tilde{\mathbf{W}} + k^2 \tilde{\mathbf{W}} = \mathbf{0} & \text{on } (0,\infty) \times \Omega \\ \hat{\mathbf{n}} \cdot \nabla_{\mathbf{x}} \tilde{\mathbf{W}} = 0 & \text{on } (0,\infty) \times \partial\Omega. \end{cases} \tag{5.6}$$

In our numerical simulations we will consider as domain Ω a one-dimensional segment $\Omega = [0, L]$, and solutions of (5.6) in this case are

$$\tilde{\mathbf{W}}_{k_n}(x) = \mathbf{C}_n \cos(k_n x) \tag{5.7}$$

with wavenumbers k_n given by

$$k_n = \frac{n\pi}{L}, \qquad n \in \mathbb{N}. \tag{5.8}$$

Going back to (5.4), the linear PDE provides

$$\sum_k \lambda_k c_k e^{\lambda_k t} \tilde{\mathbf{W}}_k(\mathbf{x}) = D \sum_k (-k^2) c_k e^{\lambda_k t} \tilde{\mathbf{W}}_k(\mathbf{x}) + A \sum_k c_k e^{\lambda_k t} \tilde{\mathbf{W}}_k(\mathbf{x}), \tag{5.9}$$

and this means that, for each k, λ_k is an eigenvalue of the matrix $A - k^2 D$. Imposing $det(A - k^2 D - \lambda_k \mathbb{I}) = 0$, we find

$$\lambda_{k\,1,2} = \frac{1}{2} \left[trA - k^2(D_1 + D_2) \pm \sqrt{[trA - k^2(D_1 + D_2)]^2 - 4h(k^2)} \right], \tag{5.10}$$

being the function

$$h(k^2) = k^4 D_1 D_2 + k^2 [D_2(1-b) + D_1 a^2 d] + a^2 d. \tag{5.11}$$

Turing instability occurs if there exists at least one wavenumber $\bar{k}$ such that the corresponding solution $\mathbf{W}_{\bar{k}}(\mathbf{x},t)$ has $Re\lambda_{\bar{k}} > 0$ [30]. This implies that $h(k^2)$ is needed to attain a negative value for some $k \neq 0$. To this aim, we have to require firstly that

$$D_2(1-b) + D_1 a^2 d < 0. \tag{5.12}$$

If we introduce the quantity $\delta := \frac{D_1}{D_2}$, conditions (5.3) and (5.12) may be recast as

$$\delta < \frac{b-1}{a^2 d} < 1, \tag{5.13}$$

and consequently it must be $\delta < 1$ and $b > 1$. Compared to the classical theory of Turing systems [31,44], this result states that the component Y_2 of gas species Y corresponding to the energy level E_2 plays the role of “inhibitor”, while the component Y_1 plays the role of “activator” in the reaction–diffusion dynamics, being known that Turing patterns may appear only below a critical value for the parameter δ, representing the ratio of the diffusion constants of the activator to the inhibitor. A second condition to be satisfied in order to have $h(k^2)<0$ is that $h_{min}<0$, and being

$$h_{min} = -\frac{[D_2(1-b)+D_1a^2d]^2-4D_1D_2a^2d}{4D_1D_2}, \tag{5.14}$$

it becomes

$$\delta^2a^4d^2-2\delta(1+b)a^2d+(1-b)^2>0. \tag{5.15}$$

By solving this algebraic equation with respect to the parameter δ, we get

$$\delta<\frac{(\sqrt{b}-1)^2}{a^2d} \quad \vee \quad \delta>\frac{(\sqrt{b}+1)^2}{a^2d}, \tag{5.16}$$

but, bearing in mind (5.13), only the first of the two inequalities above provides admissible values for δ.

In conclusion, necessary conditions to have unstable modes can be summed up as follows

$$\begin{gathered} 0<\frac{b-1}{a^2d}<1, \\ \delta<\frac{(\sqrt{b}-1)^2}{a^2d}. \end{gathered} \tag{5.17}$$

The range of possible wavenumbers $\bar{k}$ such that $Re\lambda_{\bar{k}}>0$ is then $k_1<\bar{k}<k_2$, where k_1^2, k_2^2 are the solutions of the equation $h(k^2)=0$, reading as

$$k_{1,2}^2 = \frac{b-1-\delta a^2d \pm \sqrt{(1-b+\delta a^2d)^2-4a^2d}}{2D_1}. \tag{5.18}$$

We should bear in mind that for finite domains the relevant wavenumbers are discrete (see (5.8) for a one–dimensional problem), therefore Turing instability occurs only if at least one of them belongs to the interval (k_1,k_2).

We investigate now conditions (5.17) in terms of the parameters of the mixture. Before proceeding in this direction, we introduce some assumptions, especially concerning the fixed parameters of the host medium. Indeed, since the background may be considered as a unique external medium, we may suppose that collision frequencies relevant to elastic scattering of species Y_1 with the background take a unique value, independently of the species A, B, C of the colliding molecule: $\nu_{1A}=\nu_{1B}=\nu_{1C}=\bar{\nu}_1$, and analogously for scattering involving species Y_2 and the background: $\nu_{2A}=\nu_{2B}=\nu_{2C}=\bar{\nu}_2$. Also, for background number densities we assume for simplicity $n_A=n_B=n_C=\bar{n}$. We fix particle masses of background species and of gases Y and Z, bearing in mind the obvious conservations of masses prescribed by encounters (2.1)–(2.4). We fix also background energies, and for convenience we pick a value for E_1 in such a way that $\Delta E_{B1}^{AC}\le 0$. This implies $\Gamma\left(\frac{3}{2},\Theta(\Delta E_{B1}^{AC})\right)=\frac{\sqrt{\pi}}{2}$, but the presence of a different value would not change the main results of the investigation below.

With these assumptions, the analysis of Turing instability depends only on the difference E_2-E_1 and on E_Z, which has to be chosen such that $\Delta E_{11}^{ZB}\le 0$ in order to have an exact (not approximated) computation of integral (4.14). Reaction coefficients of system (4.31) may be recast as

$$a=\left(\frac{m_Bm_Y}{m_Am_C}\right)^{\frac{3}{2}}\exp(\Delta E_{B1}^{AC})\bar{n} \tag{5.19}$$

$$b = \frac{\nu_{A1}^{A2}}{\nu_{B1}^{AC}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{A1}^{A2})\right) \frac{2}{\sqrt{\pi}} \tag{5.20}$$

$$d = \frac{\nu_{Z2}^{Z1}}{\nu_{B1}^{AC}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{Z2}^{Z1})\right) \left[\frac{\sqrt{\pi}}{2}\left(\frac{m_Y^2}{m_Z m_B}\right)^{\frac{3}{2}} \exp(\Delta E_{11}^{ZB}) \bar{n}^2\right]^{-1}, \tag{5.21}$$

while the ratio between diffusion coefficients is simply provided by

$$\delta = \frac{D_1}{D_2} = \frac{\bar{\nu}_2}{\bar{\nu}_1}. \tag{5.22}$$

By defining the following functions

$$\mathcal{G}(E_2 - E_1) := \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{A1}^{A2})\right) - \frac{\nu_{B1}^{AC}}{\nu_{A1}^{A2}} \frac{\sqrt{\pi}}{2} \tag{5.23}$$

$$\mathcal{H}(E_2 - E_1) := \left[\sqrt{\Gamma\left(\frac{3}{2}, \Theta(\Delta E_{A1}^{A2})\right)} - \sqrt{\frac{\nu_{B1}^{AC}}{\nu_{A1}^{A2}} \frac{\sqrt{\pi}}{2}}\right]^2 \tag{5.24}$$

$$\mathcal{N}(E_2 - E_1) := \gamma\, \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{Z2}^{Z1})\right) \tag{5.25}$$

with

$$\gamma = \left(\frac{m_B^3 m_Z}{m_C^2 m_A^2}\right)^{\frac{3}{2}} \exp\Big(2(E_A + E_C) - 3E_B\Big) \frac{\nu_{Z2}^{Z1}}{\nu_{B1}^{AC}}, \tag{5.26}$$

conditions (5.17) can be written as

$$0 < \frac{\mathcal{G}(E_2 - E_1)}{\mathcal{N}(E_2 - E_1)} e^{E_Z} < 1 \tag{5.27}$$

$$\delta < \frac{\mathcal{H}(E_2 - E_1)}{\mathcal{N}(E_2 - E_1)} e^{E_Z}. \tag{5.28}$$

We observe that $\mathcal{H}(E_2 - E_1) \geq 0$ and $\mathcal{N}(E_2 - E_1) > 0$, thus the first requirement to have Turing instability is

$$\mathcal{G}(E_2 - E_1) > 0. \tag{5.29}$$

This is possible only if the ratio $\frac{\nu_{B1}^{AC}}{\nu_{A1}^{A2}}$ is less than one. More precisely, for $E_2 - E_1 \leq 0$ we have $\mathcal{G} \equiv \frac{\sqrt{\pi}}{2}\left(1 - \frac{\nu_{B1}^{AC}}{\nu_{A1}^{A2}}\right)$, while in the range $E_2 - E_1 > 0$ the function $\mathcal{G}$ is decreasing and $\lim_{E_2 - E_1 \to +\infty} \mathcal{G} = -\frac{\sqrt{\pi}}{2} \frac{\nu_{B1}^{AC}}{\nu_{A1}^{A2}} < 0$. Therefore, if $\frac{\nu_{B1}^{AC}}{\nu_{A1}^{A2}} < 1$, there exists a unique value E^* such that $\mathcal{G} > 0$ for every $E_2 - E_1 < E^*$ and $\mathcal{G}$ is negative after this threshold.

In this admissible range, conditions (5.27) and (5.28) can be summarized as

$$\delta \frac{\mathcal{N}(E_2 - E_1)}{\mathcal{H}(E_2 - E_1)} < e^{E_Z} < \frac{\mathcal{N}(E_2 - E_1)}{\mathcal{G}(E_2 - E_1)}. \tag{5.30}$$

At this point, we notice that there could be admissible values for E_Z only if the inequality

$$\delta \frac{\mathcal{G}(E_2 - E_1)}{\mathcal{H}(E_2 - E_1)} < 1 \tag{5.31}$$

holds. It's easy to check that the function $\delta\frac{\mathcal{G}}{\mathcal{H}}$ is increasing where $\mathcal{G}$ is positive, and its limit for $E_2-E_1\to E^*$ is $+\infty$. Since for $E_2-E_1\le 0$ we have $\delta\frac{\mathcal{G}}{\mathcal{H}}\equiv \delta\left(1+\sqrt{\frac{\nu_{B1}^{AC}}{\nu_{A1}^{A2}}}\right)\left(1-\sqrt{\frac{\nu_{B1}^{AC}}{\nu_{A1}^{A2}}}\right)^{-1}$, only if collision frequencies are chosen in such a way that this quantity is less than one we can find a nonnegative value $\overline{E}$ (less than E^*) such that $\delta\frac{\mathcal{G}}{\mathcal{H}}<1$ for every $E_2-E_1<\overline{E}$. Another condition for the existence of values for the energy E_Z fulfilling (5.30) is that the right-hand side has to be greater than one (since energy E_Z is positive):

$$\frac{\mathcal{N}(E_2-E_1)}{\mathcal{G}(E_2-E_1)}>1. \tag{5.32}$$

But, the function $\frac{\mathcal{N}}{\mathcal{G}}$ being increasing where $\mathcal{G}$ is positive and ranging from zero (for $E_2-E_1\to-\infty$) to $+\infty$ (for $E_2-E_1\to E^*$), we get that there exists a unique $\widetilde{E}$ such that $\frac{\mathcal{N}}{\mathcal{G}}(\widetilde{E})=1$, and $\frac{\mathcal{N}}{\mathcal{G}}>1$ for $E_2-E_1>\widetilde{E}$. Thus, we can conclude that Turing instability may occur only if $\widetilde{E}<\overline{E}$ and we take values for E_2-E_1 in the interval $\left(\widetilde{E},\overline{E}\right)$. With E_2-E_1 in this range, inequalities (5.30) are fulfilled for E_Z such that

$$\begin{aligned}&\log(\delta)+\log(\mathcal{N}(E_2-E_1))-\log(\mathcal{H}(E_2-E_1))<E_Z\\&<\log(\mathcal{N}(E_2-E_1))-\log(\mathcal{G}(E_2-E_1)).\end{aligned} \tag{5.33}$$

As test case, we choose the following set of masses and background energies for the mixture:

$$m_A=2 \quad m_B=3.5 \quad m_C=4 \quad m_Y=2.5 \quad m_Z=1.5, \tag{5.34}$$

$$E_A=4.5 \quad E_B=3.6 \quad E_C=4 \tag{5.35}$$

and we fix $E_1=7.2$. We remark that masses fulfill conservations prescribed by chemical reactions (2.3)–(2.4), namely $m_B+m_Y=m_A+m_C$ and $2m_Y=m_Z+m_B$. Collision frequencies are the ones listed below

$$\nu_{A1}^{A2}=0.004, \quad \nu_{Z2}^{Z1}=0.3, \quad \nu_{B1}^{AC}=0.0001, \quad \nu_{11}^{ZB}=1, \quad \bar\nu_1=150, \quad \bar\nu_2=20. \tag{5.36}$$

Elastic collisions frequencies $\bar\nu_1$, $\bar\nu_2$ are much higher than the others in order to take into account that scattering with the host medium is the dominant process; concerning the other collision rates, $\nu_{11}^{ZB}=1$ is the highest (recall the assumption that the chemical reaction (2.4) is faster).

The region of energy parameters allowing Turing instability is depicted in Figure 5.1. The first value that we highlight is $E^*\approx 4.77$, for which $\mathcal{G}(E^*)=0$. Then we plot the critical curve given by

$$\mathcal{C}^1: E_Z=\log(\mathcal{N}(E_2-E_1))-\log(\mathcal{G}(E_2-E_1)), \tag{5.37}$$

whose intersection with the E_2-E_1 axis is at the point $\widetilde{E}\approx-9.03$. For points (E_2-E_1,E_Z) in the region under this curve we have linear stability of the stationary state. Moreover, we have the other critical curve

$$\mathcal{C}^2: E_Z=\log(\delta)+\log(\mathcal{N}(E_2-E_1))-\log(\mathcal{H}(E_2-E_1)), \tag{5.38}$$

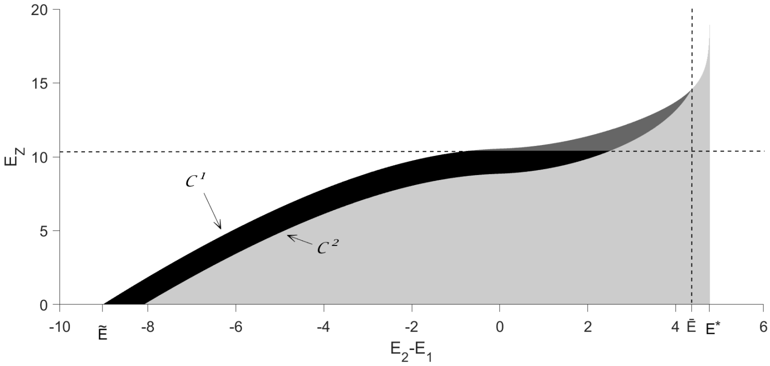

Fig. 5.1. *Values for E_Z and E_2-E_1 satisfying requirements for Turing instability in system* (4.31)*. Values for masses as in* (5.34)*, background energies as in* (5.35)*, frequencies as in* (5.36) *and $E_1=7.2$. The region allowing Turing instability is depicted in black. The meaning of the plotted curves is explained in the text.*

and the intersection of curves $\mathcal{C}^1$ and $\mathcal{C}^2$ occurs at $\overline{E}\approx 4.36$. For (E_2-E_1, E_Z) in the region between curves $\mathcal{C}^2$ and $\mathcal{C}^1$, conditions (5.17) for Turing instability hold. We should recall that we have to take $E_Z<2E_1-E_B=10.8$ to have the computation of (4.14) explicit, therefore, in conclusion, energy levels for which pattern formation can be expected are the ones in the black area of the picture. It is worth noticing that Turing instability may occur both if E_2-E_1 is positive, namely with the inelastic transition (2.1) endothermic and (2.2) exothermic, and also if E_2-E_1 is negative, thus with (2.1) exothermic and (2.2) endothermic.

We perform some numerical simulations for the system (4.31) in a one-dimensional domain $\Omega=[0,L]$, taking values for masses, background energies and collision frequencies as in (5.34), (5.35) and (5.36), and fixing energy of component Y_1 as $E_1=7.2$. Initial data are random perturbations of the space homogeneous equilibrium state. We take values for the difference of energy values E_2-E_1 and for E_Z in the region where Turing instability is expected. It is important to remark that pattern formation occurs only if at least a squared wavenumber $k_n^2=(n\pi/L)^2$ belongs to the interval individuated by the roots (5.18); in our simulations we fix $L=30$.

Firstly, we choose $E_2-E_1=1$ and take three possible values for E_Z. The results of this case are shown in Figure 5.2. In the panels (a), (b), (c), we plot the configuration at time $t=30$ of number densities n_1, n_2, compared with the relevant space homogeneous equilibrium value. We see that the density of the two components is considerably heterogeneous and we notice that the two distributions oscillate around the homogeneous equilibrium values. As E_Z increases, we observe for the quantity n_1 a bigger fluctuation from the equilibrium, giving rise to regions where n_1 is nearly zero alternated to regions with higher density. For n_2, instead, oscillations are not equally sharp and for higher values of E_Z its plot remains mostly under the equilibrium value. In the other plots of Figure 5.2 we show the time and space behaviour of number densities (panels (d), (e), (f) for n_1 and panels (g), (h), (i) for n_2): in the trend from the initial data to the oscillating configurations at $t=30$ one can appreciate the formation of space periodic patterns.

Analogous behaviours appear in different tests, we show here two of them focusing the attention mainly on density n_1, which shows higher oscillations. In Figure 5.3 we

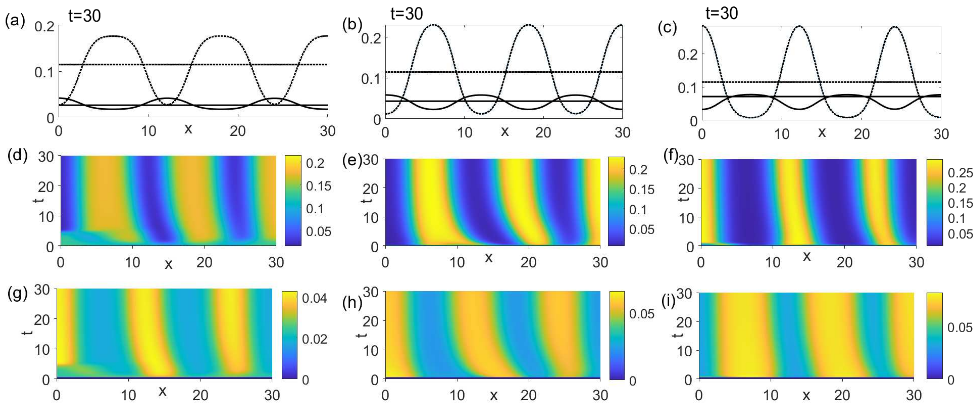

FIG. 5.2. *Panels (a), (b), (c): Configuration at time* $t=30$ *of the densities compared to their equilibrium state* n_1 *(dotted line) and* n_2 *(solid line) taking* $E_2-E_1=1$ *and* $E_Z=9.3,9.8,10.3$*, respectively. Panels (d), (e), (f): behaviour of density* n_1 *in space and time for the energy levels taken above. Panels (g), (h), (i): behaviour of density* n_2 *in space and time. Values for masses as in* (5.34)*, background energies as in* (5.35)*, frequencies as in* (5.36) *and* $E_1=7.2$*.*

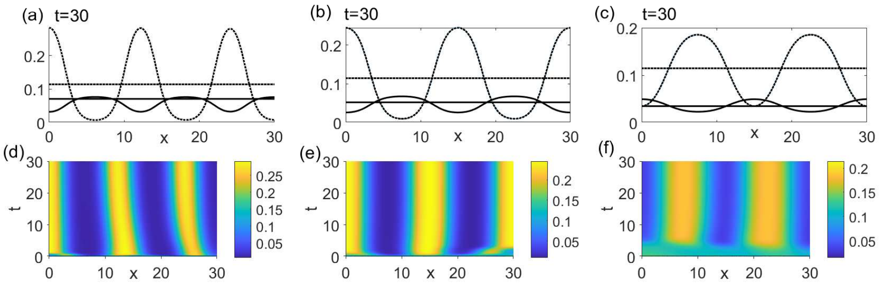

FIG. 5.3. *Panels (a), (b), (c): Configuration at time* $t=30$ *of the densities compared to their equilibrium state* n_1 *(dotted line) and* n_2 *(solid line) taking* $E_Z=10.3$ *and* $E_2-E_1=1,1.6,2.2$*, respectively. Panels (d), (e), (f): behaviour of density* n_1 *in space and time for the energy levels taken above. Values for masses as in* (5.34)*, background energies as in* (5.35)*, frequencies as in* (5.36) *and* $E_1=7.2$*.*

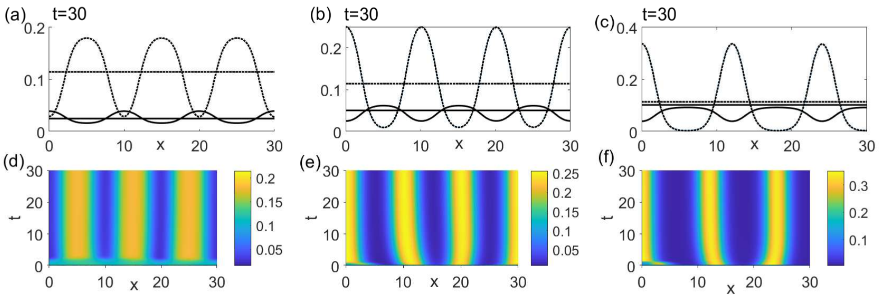

FIG. 5.4. *Panels (a), (b), (c): Configuration at time* $t=30$ *of the densities compared to their equilibrium state* n_1 *(dotted line) and* n_2 *(solid line) taking* $E_2-E_1=-2$ *and* $E_Z=8.2,8.9,9.6$*, respectively. Panels (d), (e), (f): behavior of density* n_1 *in space and time for the energy levels taken above. Values for masses as in* (5.34)*, background energies as in* (5.35)*, frequencies as in* (5.36) *and* $E_1=7.2$*.*

fix $E_Z=10.3$ and we increase E_2-E_1 starting from 1 to a value close to the highest one allowing Turing instability. We note that for higher values of E_2-E_1, the number of space oscillations for n_1 decreases, but the space amplitude of the peaks increases. Fixing, instead, in Figure 5.4, a negative value for $E_2-E_1=-2$, when E_Z is higher we observe that the number of oscillations for n_1 is lower, but peaks are high and narrow, thus the component Y_1 is highly concentrated in few points.

5.2. Turing instability for the complete three–components system. This subsection is devoted to the investigation of stability properties and pattern formation for system (3.49). First of all, we look for stationary states for our model in absence of diffusion, given by the system

$$\begin{aligned}\frac{\partial n_1}{\partial t}&=a-(b+1)n_1+\eta n_Z n_2+en_Z-fn_1^2\\ \frac{\partial n_2}{\partial t}&=bn_1-\eta n_Z n_2\\ \frac{\partial n_Z}{\partial t}&=fn_1^2-en_Z.\end{aligned}\tag{5.39}$$

By imposing in the system above $\frac{\partial n_1}{\partial t}=\frac{\partial n_2}{\partial t}=\frac{\partial n_Z}{\partial t}=0$, we get a unique steady state

$$(\bar n_1,\bar n_2,\bar n_Z)=\left(a,\frac{be}{a\eta f},\frac{fa^2}{e}\right).$$

The state $(\bar n_1,\bar n_2,\bar n_Z)$ is Turing unstable if it is locally stable for the homogeneous system (5.39), but unstable for the system with diffusion (3.49). We linearize at first the system in spatially homogeneous conditions, writing it in the following form

$$\frac{\partial \mathbf{W}}{\partial t}=B\mathbf{W},\tag{5.40}$$

with $\mathbf{W}=\begin{pmatrix}n_1-\bar n_1\\ n_2-\bar n_2\\ n_Z-\bar n_Z\end{pmatrix}$ and

$$B=\begin{pmatrix}-b-1-2af & \dfrac{a^2\eta f}{e} & e\left(\dfrac{b}{af}+1\right)\\ b & -\dfrac{a^2\eta f}{e} & -\dfrac{be}{af}\\ 2af & 0 & -e\end{pmatrix}.\tag{5.41}$$

The stability of the stationary state is achieved if all the eigenvalues of B have negative real part. They are provided by the roots of the characteristic polynomial

$$-\lambda^3+\lambda^2 trB-\lambda\tilde\Lambda+detB,\tag{5.42}$$

with

$$\begin{aligned}trB&=-b-1-2af-\frac{a^2\eta f}{e}-e<0,\\ \tilde\Lambda&=2\frac{a^3\eta f^2}{e}+a^2\eta f+\frac{a^2\eta f}{e}-eb+e\end{aligned}$$

and $detB = -a^2\eta f < 0$. Applying the Routh–Hurwitz criterion [18], all roots have negative real part if the condition

$$\tilde{\Lambda}\, trB < detB \tag{5.43}$$

is satisfied. Of course this is possible only if the term $\tilde{\Lambda}$ is positive; more precisely, since in this case we would have $\tilde{\Lambda}\, trB = detB + \tilde{\Gamma}$ with $\tilde{\Gamma}$ a negative quantity, the condition $\tilde{\Lambda} > 0$, that we rewrite as

$$\left[\frac{2af+1}{e^2} + \frac{1}{e}\right] a^2\eta f > b-1, \tag{5.44}$$

is also sufficient for the equilibrium stability.

Now we consider the linearized system including diffusive terms in Ω with zero–flux boundary conditions

$$\begin{cases} \dfrac{\partial \mathbf{W}}{\partial t} = D\Delta_{\mathbf{x}}\mathbf{W} + B\mathbf{W} & \text{on } (0,\infty)\times\Omega \\ \hat{\mathbf{n}}\cdot\nabla_{\mathbf{x}}\mathbf{W} = 0 & \text{on } (0,\infty)\times\partial\Omega \end{cases} \tag{5.45}$$

with diffusion matrix

$$D = \begin{pmatrix} D_1 & 0 & 0 \\ 0 & D_2 & 0 \\ 0 & 0 & D_Z \end{pmatrix}.$$

As in the subsection above, we look for solutions in the form

$$\mathbf{W}(\mathbf{x},t) = \sum_k c_k e^{\lambda_k t}\tilde{\mathbf{W}}_k(\mathbf{x}), \tag{5.46}$$

with $\tilde{\mathbf{W}}_k(\mathbf{x})$ being a solution of the time–independent problem. Choosing as domain Ω a one–dimensional segment of length L it can be checked that wavenumbers allowing the existence of a solution to the time–independent problem are again $k_n = \pi n/L$, with $n \in \mathbb{N}$. Concerning the global problem (5.45), for each k, the exponent λ_k has to be an eigenvalue of the matrix $B - k^2 D$, hence a root of the characteristic polynomial

$$-\lambda^3 + \lambda^2 tr\left(B - k^2 D\right) - \lambda\Lambda + det\left(B - k^2 D\right), \tag{5.47}$$

with $tr\left(B - k^2 D\right) = trB - k^2(D_1 + D_2 + D_Z) < 0$,

$$\begin{aligned} \Lambda = {} & (D_1D_2 + D_1D_Z + D_2D_Z)k^4 \\ & + \left(D_2 + 2afD_2 + D_1\frac{a^2\eta f}{e} + 2D_Z af + D_Z b + D_Z + 2D_1D_Z\frac{a^2\eta f}{e} + D_2 e\right)k^2 \\ & + \frac{a^2\eta f}{e} + 2\frac{a^3\eta f^2}{e} + a^2\eta f - eb + e \end{aligned} \tag{5.48}$$

and

$$\begin{aligned} \beta(k^2) := det(B - k^2 D) = {} & -D_1D_2D_Z k^6 \\ & - \left(D_1D_Z\frac{a^2\eta f}{e} + 2D_2D_Z af + eD_1D_2 + bD_2D_Z + D_2D_Z\right)k^4 \end{aligned}$$

$$-\left(2D_Z\frac{a^3\eta f^2}{e}+D_1a^2\eta f+D_Z\frac{a^2\eta f}{e}-D_2eb+eD_2\right)k^2-a^2\eta f. \tag{5.49}$$

Turing instability may occur only if for some k the characteristic polynomial (5.47) has roots with positive real part. Again for the Routh–Hurwitz criterion, this happens if there exists k such that

$$det(B-k^2D)>0 \tag{5.50}$$

or

$$\Lambda tr(B-k^2D)>det(B-k^2D). \tag{5.51}$$

We notice that last five terms of Λ in (5.48) are exactly the quantity $\tilde{\Lambda}$ that we have supposed to be positive in (5.44) for the stability in the homogeneous problem, and consequently we have $\Lambda>0$. Since we have

$$\Lambda tr(B-k^2D)=det(B-k^2D)+\Gamma, \tag{5.52}$$

Γ being a negative quantity, we see that (5.51) can never be satisfied. It means that the matrix $B-k^2D$ has eigenvalues with positive real part only if condition (5.50) holds.

We aim at finding more specific conditions on the parameters of the system (3.49). As in Subsection 5.1, we suppose that collision frequencies for the elastic scattering with the background take a unique value for each species: $\nu_{1A}=\nu_{1B}=\nu_{1C}=\bar{\nu}_1$, $\nu_{2A}=\nu_{2B}=\nu_{2C}=\bar{\nu}_2$, $\nu_{ZA}=\nu_{ZB}=\nu_{ZC}=\bar{\nu}_Z$, and also background number densities have the common value $n_A=n_B=n_C=\bar{n}$. We fix energies E_A, E_B, E_C, and E_1 in such a way that $\Delta E^{AC}_{B1}\leq 0$, so that $\Gamma\left(\frac{3}{2},\Theta(\Delta E^{AC}_{B1})\right)=\frac{\sqrt{\pi}}{2}$. The analysis of conditions allowing pattern formation still depends on the difference E_2-E_1 and on E_Z: We restrict our investigation to E_Z such that $\Delta E^{ZB}_{11}\leq 0$ (just for convenience, in order to be able to compare results with the ones obtained for the two–component system in the previous subsection). Moreover, as usual in kinetic models dealing with energy levels [19, 21], we assume $E_2>E_1$, then also $\Gamma\left(\frac{3}{2},\Theta(\Delta E^{Z1}_{Z2})\right)=\frac{\sqrt{\pi}}{2}$. With these assumptions at hand, the parameters appearing in the reaction–diffusion system (3.49) read as

$$a=\left(\frac{m_Bm_Y}{m_Am_C}\right)^{\frac{3}{2}}\exp(\Delta E^{AC}_{B1})\bar{n} \tag{5.53}$$

$$b=\frac{\nu^{A2}_{A1}}{\nu^{AC}_{B1}}\Gamma\left(\frac{3}{2},\Theta(\Delta E^{A2}_{A1})\right)\frac{2}{\sqrt{\pi}} \tag{5.54}$$

$$\eta=\frac{\nu^{Z1}_{Z2}}{\nu^{AC}_{B1}}\frac{1}{\bar{n}} \tag{5.55}$$

$$e=\frac{\nu^{ZB}_{11}}{\nu^{AC}_{B1}}\left(\frac{m_Y^2}{m_Zm_B}\right)^{\frac{3}{2}}\exp(\Delta E^{ZB}_{11}) \tag{5.56}$$

$$f=\frac{\nu^{ZB}_{11}}{\nu^{AC}_{B1}}\frac{1}{\bar{n}}, \tag{5.57}$$

$$D_1=\left[\nu^{AC}_{B1}m_Y\bar{n}\bar{\nu}_1\sum_{J=A,B,C}n_J\alpha_{JY}\right]^{-1},\quad D_2=\frac{\bar{\nu}_1}{\bar{\nu}_2}D_1,$$

$$D_Z = \left[\nu_{B1}^{AC} m_Z \bar{n} \bar{\nu}_Z \sum_{J=A,B,C} n_J \alpha_{JZ} \right]^{-1}. \tag{5.58}$$

Our first purpose is to find suitable values for energies $E_2 - E_1$ and E_Z in order to have condition (5.44) for the linear stability in the space homogeneous problem satisfied. We find convenient rewriting condition (5.44) as

$$(1-b)e^2 + ea^2\eta f + (2af+1)a^2\eta f > 0. \tag{5.59}$$

If $b<1$ this inequality is obviously fulfilled, while the case $b>1$ is much more involved. The condition $b>1$ means

$$\mathcal{L}(E_2-E_1) := \frac{\nu_{A1}^{A2}}{\nu_{B1}^{AC}} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{A1}^{A2})\right) - 1 > 0; \tag{5.60}$$

the function $\mathcal{L}$ has the same behavior as that of the function $\mathcal{G}$ introduced in the previous subsection, thus also in this case there exists a unique value E^* such that $\mathcal{L}>0$ for every $E_2 - E_1 < E^*$. Notice that in the inequality (5.59) the dependence on E_Z is included only in the parameter e. Therefore, by defining a second function

$$\mathcal{T}(E_2-E_1) := \frac{\gamma}{2}\left[1 + \sqrt{1 + 4\chi\left(\frac{\nu_{A1}^{A2}}{\nu_{B1}^{AC}} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{A1}^{A2})\right) - 1\right)}\right], \tag{5.61}$$

with γ as in (5.26) and

$$\chi = 2\left[\left(\frac{m_B m_Y}{m_A m_C}\right)^{\frac{3}{2}} \exp(\Delta E_{B1}^{AC}) \frac{\nu_{Z2}^{Z1}}{\nu_{B1}^{AC}}\right]^{-1} + \left[\left(\frac{m_B m_Y}{m_A m_C}\right)^{3} \exp\left(2\Delta E_{B1}^{AC}\right) \frac{\nu_{Z2}^{Z1}\nu_{11}^{ZB}}{(\nu_{B1}^{AC})^2}\right]^{-1}, \tag{5.62}$$

condition (5.59) leads to the explicit constraint:

$$e^{E_Z} < \frac{\mathcal{T}(E_2-E_1)}{\mathcal{L}(E_2-E_1)}. \tag{5.63}$$

Since we are dealing with positive energies, we have $e^{E_Z} > 1$, so we must require that the right-hand side of (5.63) is greater than one. But, being $\mathcal{L}' > 0$ and

$$\left(\frac{\mathcal{T}}{\mathcal{L}}\right)' = \frac{\gamma}{2}\left(\frac{-\sqrt{1+4\chi\mathcal{L}} - 1 - 2\chi\mathcal{L}}{\mathcal{L}^2\sqrt{1+4\chi\mathcal{L}}}\right)\mathcal{L}', \tag{5.64}$$

the function $\frac{\mathcal{T}}{\mathcal{L}}$ is increasing where $\mathcal{L}$ is positive, and its limit for $E_2 - E_1 \to E^*$ is $+\infty$, while for $E_2 - E_1 = 0$ we have

$$\frac{\mathcal{T}}{\mathcal{L}} \equiv \frac{\gamma\left[1 + \sqrt{1 + 4\chi\left(\frac{\nu_{A1}^{A2}}{\nu_{B1}^{AC}} - 1\right)}\right]}{2\left(\frac{\nu_{A1}^{A2}}{\nu_{B1}^{AC}} - 1\right)}. \tag{5.65}$$

Consequently, if masses, background energies and collision frequencies are chosen in such a way that the quantity above is less than one, then there exists a unique $\widetilde{E} < E^*$ for which $\mathcal{T}/\mathcal{L} > 1$ is satisfied for every $E_2 - E_1 > \widetilde{E}$; otherwise, if the same quantity is greater than one, then $\mathcal{T}/\mathcal{L} > 1$ holds for every $E_2 - E_1 > 0$. In conclusion, for $E_2 -$

$E_1 \in (\max\{\widetilde{E},0\},E^*)$, condition (5.59) guaranteeing stability of the steady state of the homogeneous problem is fulfilled for

$$E_Z < \log\left(\mathcal{T}(E_2-E_1)\right) - \log\left(\mathcal{L}(E_2-E_1)\right).$$

As concerns Turing instability, it has been proved in [38] that it is prevented if all minors of order q of the matrix B given in (5.41) have a determinant with the same sign as $(-1)^q$ (with $1 \le q \le 3$, in our three equations system). Consequently, it's easy to check that in our problem a bifurcation leading to Turing instability is possible only when the determinant of the submatrix extracted from B by eliminating the second row and second column, given by

$$\begin{pmatrix} -b-1-2af & e\left(\dfrac{b}{af}+1\right) \\ 2af & -e \end{pmatrix}, \tag{5.66}$$

is negative. This implies the condition $b>1$, namely $E_2-E_1<E^*$, analogously to the result obtained in previous subsection for the reduced two–component system. In this region, we are able to find a necessary condition on parameters E_Z and E_2-E_1 for Turing instability, recalling that unstable modes are possible only if the determinant of the matrix $B-k^2D$, given by (5.49), is positive for some k. According to the Descartes rule, the cubic function $\beta(k^2)$ may have two positive roots (and consequently it may assume positive values) only if the coefficient of k^2 in (5.49) is positive, which means

$$(1-b)e^2 + \frac{D_1}{D_2}a^2\eta f e + \frac{D_Z}{D_2}a^2\eta f(2af+1) < 0. \tag{5.67}$$

Keeping in mind (5.44) (that has to be valid for the stability of the homogeneous equilibrium), the above relation implies that at least one of coefficients D_1 and D_Z must be smaller than D_2. Defining the function

$$\mathcal{S}(E_2-E_1) := \frac{\gamma}{2}\frac{D_1}{D_2}\left[1+\sqrt{1+4\frac{D_Z}{D_1}\chi\left(\frac{\nu_{A1}^{A2}}{\nu_{B1}^{AC}}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\Theta(\Delta E_{A1}^{A2})\right)-1\right)}\,\right], \tag{5.68}$$

condition (5.67) becomes

$$e^{E_Z} > \frac{\mathcal{S}(E_2-E_1)}{\mathcal{L}(E_2-E_1)}. \tag{5.69}$$

The behaviour of the ratio $\frac{\mathcal{S}}{\mathcal{L}}$ is analogous to that of $\frac{\mathcal{T}}{\mathcal{L}}$ discussed above. We point out that condition (5.69) is compatible with (5.63) only if

$$\frac{\mathcal{T}(E_2-E_1)}{\mathcal{S}(E_2-E_1)} > 1, \tag{5.70}$$

but this is ensured if we take also $D_1 > D_Z$.

One should also check that the cubic β assumes a positive value in correspondence of its positive stationary point, but with this analysis we are not provided with any information about the sign of $det(B-k^2D)$ as function of k. Nevertheless, as proved in [38], a wider range of k for which $det(B-k^2D)>0$ can be obtained taking the diffusion coefficients D_1 and D_Z sufficiently smaller than D_2. More precisely, taking $D_1 = \alpha D_Z \approx \omega$, with ω small positive quantity, we have

$$det(B-k^2D) = D_2 e(b-1)k^2 - a^2\eta f - O(\omega). \tag{5.71}$$

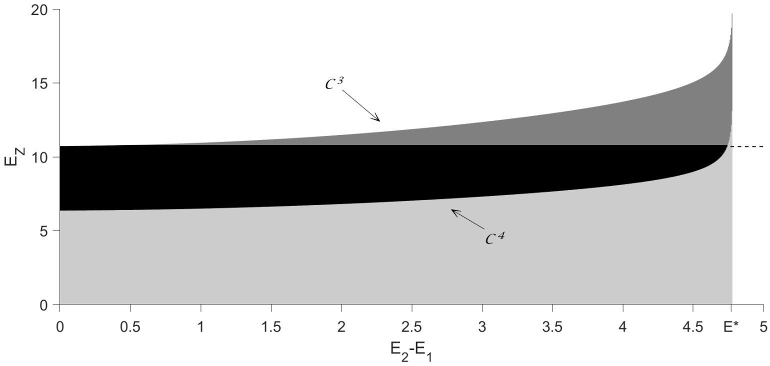

FIG. 5.5. *Values for E_Z and E_2-E_1 satisfying* (5.63) *and* (5.69). *Values for masses as in* (5.34), *background energies as in* (5.35), *frequencies as in* (5.72), (5.73) *and* $E_1=7.2$.

In this case, the component Y_2 can be seen as inhibitor and component Y_1 and gas species Z as activators.

Just for illustrative purpose, we report the conditions established in this subsection in Figure 5.5, choosing as particle masses and background energies the same as in (5.34) and (5.35), fixing $E_1=7.2$, taking as collision frequencies for the inelastic and the chemical collisions the ones below

$$\nu_{A1}^{A2}=0.004, \qquad \nu_{Z2}^{Z1}=0.3, \qquad \nu_{B1}^{AC}=0.0001, \qquad \nu_{11}^{ZB}=0.1, \tag{5.72}$$

and adopting the following choice for collision frequencies with the background

$$\bar{\nu}_1=1.5\times 10^3, \qquad \bar{\nu}_2=2, \qquad \bar{\nu}_Z=3\times 10^3, \tag{5.73}$$

in order to have diffusion coefficients given in (5.58) such that $D_1>D_Z$ and $D_1 \ll D_2$. With these data we have again $E^* \approx 4.77$ such that $\mathcal{L}(E^*)=0$, and Turing instability is prevented for $E_2-E_1>E^*$. In Figure 5.5 we show the critical curve given by

$$\mathcal{C}^3: E_Z=\log(\mathcal{T}(E_2-E_1))-\log(\mathcal{L}(E_2-E_1)), \tag{5.74}$$

under which we have linear stability of the stationary state, and also the second curve

$$\mathcal{C}^4: E_Z=\log(\mathcal{S}(E_2-E_1))-\log(\mathcal{L}(E_2-E_1)), \tag{5.75}$$

above of which the determinant of the matrix $B-k^2D$ might have positive roots. We also plot the line $E_Z=2E_1-E_B$, below of which the assumption $\Delta E_{11}^{ZB}\leq 0$ is satisfied, and the region where Turing instability might occur is thus the black one.

We may compute $det(B-k^2D)$ numerically: In Figure 5.6 we plot it versus k for some values of E_Z and E_2-E_1, and in Table 5.1 we show its maximal value in the right half–plane.

We notice that for $E_Z=10$ and $E_2-E_1=2.5$ there is a particularly wide range in which there could exist wavenumbers k leading to unstable modes. For these values we perform a simulation of the behaviour in time and space for functions n_1, n_2, n_Z in a one–dimensional domain of size $L=0.15$ and we report the result in Figure 5.7. We see that for a time $t=50$ the component Y_1 and the gas species Z, characterized by a very low diffusion coefficient, turn out to be concentrated in one point of the domain, while we have a low but nearly uniform concentration of component Y_2, due to the much higher diffusion coefficient.

E_Z	E_2-E_1	Max $det(B-k^2D)$
7.5	1	1.16×10^6
10	2.5	5×10^7
6.4	2.5	6.27×10^5
8	3.5	-3.1×10^4

TABLE 5.1. *Maximal values of determinant $det(B-k^2D)$ as function of k picking some values for E_Z and E_2-E_1 when values for masses are as in (5.34), background energies as in (5.35), frequencies as in (5.72), (5.73) and $E_1=7.2$.*

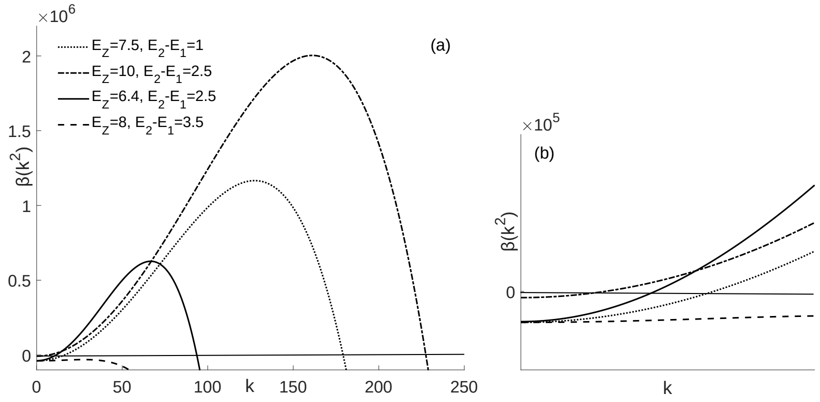

FIG. 5.6. *Panel (a): Behavior of the quantity in (5.49) as function of wavenumbers k, taking values of E_Z and E_2-E_1 as in Table 5.1 (the graph corresponding to the values $E_Z=10, E_2-E_1=2.5$ is reduced by a factor 5). Panel (b): Zoom of the area close to $k=0$ of panel (a).*

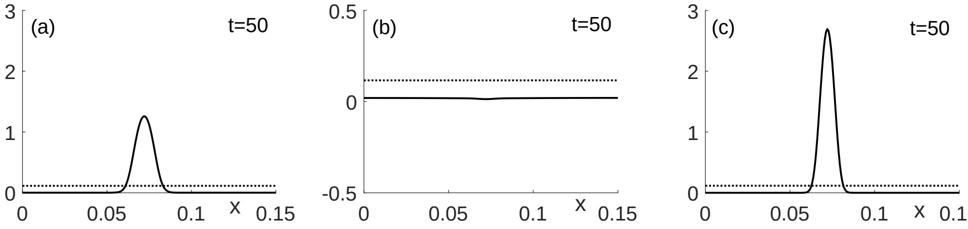

FIG. 5.7. *Panels (a), (b), (c): Configuration at time $t=300$ of the densities n_1, n_2 and n_Z (solid lines) compared to their equilibrium state (dotted lines), respectively, taking $E_Z=10$ and $E_2-E_1=2.5$. Values for masses as in (5.34), background energies as in (5.35), frequencies as in (5.72), (5.73) and $E_1=7.2$.*

6. Conclusions

We have derived reaction–diffusion equations from the kinetic level for a mixture of two gas species in a dense background medium in two different hydrodynamic limits. The mixture is assumed to be composed of a monatomic and a polyatomic gas, this last one having two possible internal energy levels, thus it is considered to be separated into two different components. Different interactions between particles have been taken into account. In particular, apart from elastic scattering with the background (the dominant process), intra–species or inter–species elastic collisions (both less frequent), also two inelastic transitions and two reversible chemical reactions have been supposed to take place among particles at different time scales. In the first scenario, all inelastic and chemical transitions have been assumed of the same order. This has allowed to derive from the rescaled Boltzmann equations suitable macroscopic equations for the number densities of the monatomic gas and of the two components of the polyatomic one. In the system of reaction–diffusion equations obtained, coefficients of both the diffusive and the reactive part are actually functions of microscopic quantities such as particle masses, background densities, collision frequencies and internal energy amounts. The same asymptotic procedure has been repeated in a second case in which one of the two chemical reactions has been considered faster. In this case, in the derivation of the reaction-diffusion system the number density of the monatomic component can be expressed in terms of the other two concentrations. This has led to a system similar to the classical Brusselator, known to exhibit Turing instability for particular choices of the coefficients.

In this framework, a natural step has been the investigation of Turing instability for our reaction–diffusion systems and its discussion upon the dependence of the coefficients on microscopic quantities. We started from the two equations system and we focused our analysis on collision frequencies and energy levels. First of all, we pointed out that, as in any system showing formation of Turing patterns, the diffusion coefficient of the inhibitor species has to be bigger than the one of the activator, and in our case this means that collision frequencies of the inhibitor component with the background have to be less than the ones relevant to the activator. We have explicitly individuated a region that provides values for the internal energy of the monatomic gas and for the difference of the two energy levels of the polyatomic species leading to spatial oscillations in the equilibrium configuration. We have also verified the appearance of a spatial non–homogeneous solution owing to some numerical simulations, and we have discussed the dependence of the number of oscillations on the values of the energy levels. Moreover we noted, as expected, that the component with the higher diffusion coefficient shows a more homogeneous profile at equilibrium. Concerning the complete system of three equations, we have been able to derive necessary conditions on microscopic parameters allowing Turing instability, but, the number of parameters involved being higher than those in the two–component Brusselator–type system, it has not been possible to verify analytically when such conditions really lead to unstable modes. To this aim we have numerically simulated a test case, obtaining as final state a configuration in which the polyatomic component having the lower energy is concentrated in a small region, as well as the monatomic species, while the density of the second polyatomic component, characterized by a much higher diffusion coefficient, is basically constant in space.

The derivation performed in this paper, based on a diffusive asymptotic limit of a system of kinetic equations, has provided reaction–diffusion systems in which the diffusion matrix is diagonal and constant. Actually, in many physical situations the Brusselator–type dynamics is better described if the diffusive part is nonlinear, as for instance in [17], or if there is also a cross diffusion term, as in [15]. In these cases the discussion of Turing instability requires a deeper analysis of parameters appearing in the diffusion part. Our future aim is to look for a different set of possible interactions among particles of the mixture and also to investigate different hydrodynamic limits of the kinetic equations, that may lead to the appearance of nonlinear diffusion or cross diffusion terms, in order to study their dependence on microscopic quantities.

Acknowledgements. This work has been performed in the framework of activities supported by the University of Parma (Italy), the Italian National Group of Mathematical Physics (GNFM-INdAM), and the Italian National Research Project *Multiscale phenomena in Continuum Mechanics: singular limits, off-equilibrium and transitions* (Prin 2017YBKNCE).

Appendix. Computation of chemical collision contributions. We consider here a generic chemical encounter

$$C_1+C_2 \leftrightarrows C_3+C_4. \tag{A.1}$$

For the purposes of this paper (see Sections 3 and 4), we may suppose to have Maxwellian distributions, that are

$$f_I(\mathbf{v})=n_I M_I(\mathbf{v}), \quad M_I(\mathbf{v})=n_I\left(\frac{m_I}{2\pi}\right)^{\frac{3}{2}}\exp\left(-\frac{m_I|\mathbf{v}|^2}{2}\right), \qquad I=1,2,3,4. \tag{A.2}$$

We want to calculate the net production of particles of species C_1, provided by

$$\int_{\mathbb{R}^3} Q^1(\mathbf{nM})(\mathbf{v})d\mathbf{v}. \tag{A.3}$$

It's easy to check [21,36] that the following relations are in order for the source terms of the four gases:

$$\int_{\mathbb{R}^3} Q^1(\mathbf{nM})(\mathbf{v})d\mathbf{v}=\int_{\mathbb{R}^3} Q^2(\mathbf{nM})(\mathbf{v})d\mathbf{v}=-\int_{\mathbb{R}^3} Q^3(\mathbf{nM})(\mathbf{v})d\mathbf{v}=-\int_{\mathbb{R}^3} Q^4(\mathbf{nM})(\mathbf{v})d\mathbf{v}, \tag{A.4}$$

since in each direct reaction in (A.1), to the disappearance of a pair of particles (C_1,C_2) there corresponds the creation of a pair of particles (C_3,C_4), and vice versa in the reverse reaction.

The reactive Boltzmann operator Q^1 is provided by [36]

$$\begin{aligned} Q^1(\mathbf{nM})(\mathbf{v})=&\int_{\mathbb{R}^3}\int_{S^2} H(g^2-\delta_{12}^{34})\sigma_{12}^{34}(g,\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}')g \\ &\times\left[\left(\frac{m_1m_2}{m_3m_4}\right)^3 n_3M_3(\mathbf{v}')n_4M_4(\mathbf{w}')-n_1M_1(\mathbf{v})n_2M_2(\mathbf{w})\right]d\mathbf{w}\,d\hat{\mathbf{\Omega}}', \end{aligned} \tag{A.5}$$

where, as already explained in Section 2, $H(\cdot)$ is the unit step function, σ_{12}^{34} is the differential cross section of the direct reaction, and $\delta_{12}^{34}=2\Delta E_{12}^{34}/\mu_{12}$, being $\Delta E_{12}^{34}=E_3+E_4-E_1-E_2$ and $\mu_{12}=m_1m_2/(m_1+m_2)$.

We denote by $\mathbf{g}$ the relative velocity, by $\mathbf{G}$ the velocity of the center of mass, and by $\mathbf{g}'$, $\mathbf{G}'$ the corresponding post–collision quantities, defined as

$$\begin{cases}\mathbf{g}=\mathbf{v}-\mathbf{w}\\ \mathbf{G}=\alpha_{12}\mathbf{v}+\alpha_{21}\mathbf{w}\end{cases} \qquad \begin{cases}\mathbf{g}'=\mathbf{v}'-\mathbf{w}'\\ \mathbf{G}'=\alpha_{34}\mathbf{v}'+\alpha_{43}\mathbf{w}',\end{cases} \tag{A.6}$$

with $\alpha_{ij}=\frac{m_i}{m_i+m_j}$. From the conservations of global momentum and energy, one deduces that $\mathbf{G}=\mathbf{G}'$ and

$$g'=\left[\frac{m_1m_2}{m_3m_4}(g^2-\delta_{12}^{34})\right]^{\frac{1}{2}}H(g^2-\delta_{12}^{34}), \qquad g=\left[\frac{m_3m_4}{m_1m_2}({g'}^2-\delta_{34}^{12})\right]^{\frac{1}{2}}H({g'}^2-\delta_{34}^{12}), \tag{A.7}$$

and consequently one has the relations allowing to pass from pre–collision to post–collision quantities and vice versa

$$\begin{cases} \mathbf{v}' = \alpha_{12}\mathbf{v} + \alpha_{21}\mathbf{w} + \alpha_{43} g' \hat{\mathbf{\Omega}}' \\ \mathbf{w}' = \alpha_{12}\mathbf{v} + \alpha_{21}\mathbf{w} - \alpha_{34} g' \hat{\mathbf{\Omega}}'. \end{cases} \tag{A.8}$$

Using the conservation of total energy:

$$\frac{1}{2}m_1 v^2 + E_1 + \frac{1}{2}m_2 w^2 + E_2 = \frac{1}{2}m_3 (v')^2 + E_3 + \frac{1}{2}m_4 (w')^2 + E_4,$$

the integral of the Boltzmann operator Q^1 can be expressed as

$$\begin{aligned} &\int_{\mathbb{R}^3} Q^1(\mathbf{nM})(\mathbf{v}) d\mathbf{v} \\ &= \frac{(m_1 m_2)^{\frac{3}{2}}}{(2\pi)^3} \int_{\mathbb{R}^3\times\mathbb{R}^3} \int_{S^2} H(g^2 - \delta_{12}^{34}) \sigma_{12}^{34}(g, \hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}') g \exp\left(-\frac{1}{2}m_1 v^2 - \frac{1}{2}m_2 w^2\right) d\mathbf{w}\, d\mathbf{v}\, d\hat{\mathbf{\Omega}}' \\ &\quad \times \left[\left(\frac{m_1 m_2}{m_3 m_4}\right)^{\frac{3}{2}} \exp(\Delta E_{12}^{34}) n_3 n_4 - n_1 n_2\right]. \end{aligned} \tag{A.9}$$

We adopt a Maxwell molecules assumption on the differential cross section of the direct reaction, setting

$$\int_{S^2} \sigma_{12}^{34}(g, \hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}') g\, d\hat{\mathbf{\Omega}}' := \nu_{12}^{34} \quad \text{constant}. \tag{A.10}$$

Inside the six–folds remaining integral

$$\int_{\mathbb{R}^3\times\mathbb{R}^3} H(g^2 - \delta_{12}^{34}) \exp\left(-\frac{1}{2}m_1 v^2 - \frac{1}{2}m_2 w^2\right) d\mathbf{w}\, d\mathbf{v} \tag{A.11}$$

we perform the change of variables $(\mathbf{v},\mathbf{w}) \to (\mathbf{g},\mathbf{G})$, obtaining

$$\begin{aligned} &\int_{\mathbb{R}^3} \exp\left(-\frac{1}{2}G^2(m_1+m_2)\right) d\mathbf{G} \int_{g^2 > \delta_{12}^{34}} \exp\left(-\frac{1}{2}g^2 \frac{m_1 m_2}{m_1+m_2}\right) d\mathbf{g} \\ &= 16\pi^{\frac{5}{2}} \frac{1}{(m_1 m_2)^{\frac{3}{2}}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{12}^{34})\right), \end{aligned} \tag{A.12}$$

with $\Gamma(\alpha, y)$ being the incomplete Euler gamma function defined in (3.11) and $\Theta(\Delta E_{12}^{34}) = \max\{\Delta E_{12}^{34}, 0\}$. In conclusion we get

$$\begin{aligned} &\int_{\mathbb{R}^3} Q^1(\mathbf{nM})(\mathbf{v}) d\mathbf{v} \\ &= \nu_{12}^{34} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{12}^{34})\right) \left[\left(\frac{m_1 m_2}{m_3 m_4}\right)^{\frac{3}{2}} \exp(\Delta E_{12}^{34}) n_3 n_4 - n_1 n_2\right]. \end{aligned} \tag{A.13}$$

In case of an irreversible reaction of the type

$$C_1 + C_2 \to C_3 + C_4, \tag{A.14}$$

in the production rate for Q^1 only the loss term remains

$$\int_{\mathbb{R}^3} Q^1(\mathbf{nM})(\mathbf{v}) d\mathbf{v} = -\nu_{12}^{34} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \Theta(\Delta E_{12}^{34})\right) n_1 n_2, \tag{A.15}$$

and relations (A.4) are still in order for the other species.

REFERENCES

[1] B. Anwasia, M. Bisi, F. Salvarani, and A.J. Soares, *On the Maxwell–Stefan diffusion limit for a reactive mixture of polyatomic gases in non–isothermal setting*, Kinet. Relat. Models, 13:63–95, 2020. 1

[2] B. Anwasia, P. Goncalves, and A.J. Soares, *On the formal derivation of the reactive Maxwell–Stefan equations from the kinetic theory*, Europhys. Lett., 129:40005, 2020. 1

[3] K. Aoki, M. Bisi, M. Groppi, and S. Kosuge, *Two-temperature Navier-Stokes equations for a polyatomic gas derived from kinetic theory*, Phys. Rev. E, 102:023104, 2020. 3

[4] C. Bardos, F. Golse, and C.D. Levermore, *Fluid dynamic limits of kinetic equations II-Convergence proofs for the Boltzmann equation*, Commun. Pure Appl. Math., 46:667–753, 1993. 3

[5] M. Bisi and L. Desvillettes, *From reactive Boltzmann equations to reaction–diffusion systems*, J. Stat. Phys., 124:881–912, 2006. 1, 2, 3, 3, 3.1, 3.4, 5.1

[6] M. Bisi, M. Groppi, and G. Spiga, *Grad's distribution functions in the kinetic equations for a chemical reaction*, Contin. Mech. Thermodyn., 14:207–222, 2002. 2, 3.1

[7] B. Bozzini, G. Gambino, D. Lacitignola, S. Lupo, M. Sammartino, and I. Sgura, *Weakly nonlinear analysis of Turing patterns in a morphochemical model for metal growth*, Comput. Math. Appl., 70:1948–1969, 2015. 1

[8] R.S. Cantrell and C. Cosner, *Spatial Ecology via Reaction–Diffusion Equations*, John Wiley & Sons, Ltd., 2003. 1

[9] C. Cercignani, *The Boltzmann Equation and its Applications*, Springer, New York, 1988. 1, 2, 3, 3.1, 3.1, 3.1

[10] S. Chapman and T.G. Cowling, *The Mathematical Theory of Non–Uniform Gases*, Cambridge University Press, Cambridge, 1970. 1, 2

[11] A. Chauviere, L. Preziosi, and H. Byrne, *A model of cell migration within the extracellular matrix based on a phenotypic switching mechanism*, Math. Med. Biol., 27:255–281, 2010. 1

[12] N. Dalchau and S. Smith, *Model reduction enables Turing instability analysis of large reaction-diffusion models*, J.R. Soc. Interface, 15:20170805, 2018. 1, 4, 4.3

[13] L. Desvillettes and F. Golse, *A remark concerning the Chapman-Enskog asymptotics*, Ser. Adv. Math. Appl. Sci., 22:191–203, 1992. 3.1

[14] M. Duan, L. Chang, and Z. Jin, *Turing patterns of an SI epidemic model with cross–diffusion on complex networks*, Phys. A: Stat. Mech. Appl., 533:122023, 2019. 1

[15] D. Fanelli, C. Cianci, and F. Di Patti, *Turing instabilities in reaction-diffusion systems with cross diffusion*, Eur. Phys. J. B, 86:142, 2013. 6

[16] G. Favre and C. Schmeiser, *Hypocoercivity and fast reaction limit for linear reaction networks with kinetic transport*, J. Stat. Phys., 178:1319–1335, 2020. 1

[17] G. Gambino, M.C. Lombardo, M. Sammartino, and V. Sciacca, *Turing pattern formation in the Brusselator system with nonlinear diffusion*, Phys. Rev. E, 88:042925, 2013. 6

[18] F.R. Gantmacher and J.L. Brenner, *Applications of the Theory of Matrices*, Interscience Publishers, New York, 1959. 5.2

[19] V. Giovangigli, *Multicomponent Flow Modeling*, Series on Modeling and Simulation in Science, Engineering and Technology, Birkhäuser, Boston, 1999. 2, 2, 3.1, 5.2

[20] P. Gray and S.K. Scott, *Chemical Oscillations and Instabilities*, Oxford University Press, Oxford, 1990. 5

[21] M. Groppi and G. Spiga, *Kinetic approach to chemical reactions and inelastic transitions in a rarefied gas*, J. Math. Chem., 26:197–219, 1999. 2, 2, 3.1, 5.2, 6

[22] J. Guckenheimer and P. Holmes, *Nonlinear Oscillations, Dynamical Systems and Bifurcations of Vector Fields*, Springer, Berlin, 1984. 1

[23] Y. Kuramoto, *Chemical Oscillations, Waves and Turbulence*, Springer, Berlin, 1984. 1

[24] R. Lefever, G. Nicolis, and P. Borckmans, *The brusselator: it does oscillate all the same*, J. Chem. Soc., Faraday Trans. 1: Phys. Chem. Cond. Phases, 84:1013–1023, 1988. 2, 4.3

[25] I. Lengyel and I.R. Epstein, *Modeling of Turing structures in the chlorite–iodide–malonic acid–starch reaction system*, Science, 251:650–652, 1991. 5

[26] X. Li, W. Jiang, and J. Shi, *Hopf bifurcation and Turing instability in the reaction–diffusion Holling–Tanner predator–prey model*, IMA J. Appl. Math., 78:287–306, 2013. 1

[27] G. Liu and Y. Wang, *Pattern formation of a coupled two-cell Schnakenberg model*, Discrete Contin. Dyn. Syst. Ser. S, 10:1051–1062, 2017. 1

[28] M.C. Lombardo, R. Barresi, E. Bilotta, F. Gargano, P. Pantano, and M. Sammartino, *Demyelination patterns in a mathematical model of multiple sclerosis*, J. Math. Biol., 75:373–417, 2017. 1

[29] M. Martcheva, *An Introduction to Mathematical Epidemiology*, Springer, Berlin, 2015. 1

[30] J.D. Murray, *Mathematical Biology. I. An Introduction*, (Third Edition), Springer, Berlin, 2002. 1, 5.1

[31] J.D. Murray, *Mathematical Biology. II. Spatial Models and Biomedical Applications*, Springer, Berlin, 2003. 1, 5.1

[32] M. Nedjalkov, S. Selberherr, D.K. Ferry, D. Vasileska, P. Dollfus, D. Querlioz, I. Dimov, and P. Schwaha, *Physical scales in the Wigner–Boltzmann equation*, Ann. Phys., 328:220–237, 2013. 3

[33] L. Neumann and C. Schmeiser, *A kinetic reaction model: decay to equilibrium and macroscopic limit*, Kinet. Relat. Models, 9:571–585, 2016. 1

[34] A.G. Nikitin and R.J. Wiltshire, *Systems of reaction diffusion equations and their symmetry properties*, J. Math. Phys., 42:1667–1688, 2001. 1

[35] I. Prigogine and R. Lefever, *Symmetry breaking instabilities in dissipative systems. II*, J. Chem. Phys., 48:1695–1700, 1968. 1, 2, 4.3, 5

[36] A. Rossani and G. Spiga, *A note on the kinetic theory of chemically reacting gases*, Phys. A, 272:563–573, 1999. 2, 2, 2, 5.1, 6, 6

[37] L. Saint-Raymond, *Hydrodynamic Limits of the Boltzmann Equation*, Springer, Berlin, 2009. 3

[38] R. Satnoianu, M. Menzinger, and P. Maini, *Turing instabilities in general systems*, J. Math. Biol., 41:493–512, 2000. 1, 5.2, 5.2

[39] L.A. Segel and M. Slemrod, *The quasi-steady-state assumption: a case study in perturbation*, SIAM Rev., 31:446–477, 1989. 1

[40] T.J. Snowden, P.H. Van der Graaf, and M.J. Tindall, *Methods of model reduction for large-scale biological systems: a survey of current methods and trends*, Bull. Math. Biol., 79:1449–1486, 2017. 1

[41] R. Spigler and D.H. Zanette, *Reaction-diffusion models from the Fokker-Planck formulation of chemical processes*, IMA J. Appl. Math., 49:217–229, 1992. 1

[42] R. Spigler and D.H. Zanette, *Asymptotic analysis and reaction-diffusion approximation for BGK kinetic models of chemical processes in multispecies gas mixtures*, J. Appl. Math. Phys., 44:812–827, 1993. 1

[43] E. Trélat, J. Zhu, and E. Zuazua, *Allee optimal control of a system in ecology*, Math. Mod. Meth. Appl. Sci., 28:1665–1697, 2018. 1

[44] A.M. Turing, *The chemical basis of morphogenesis*, Philos. Trans. R. Soc. London Ser. B, 237:37–72, 1952. 1, 5, 5.1

[45] V. Volpert, *Elliptic Partial Differential Equations Volume 2: Reaction-Diffusion Equations*, Birkhauser, Basel, 2014. 1

[46] J. Wei and M. Winter, *Mathematical Aspects of Pattern Formation in Biological Systems*, Springer, Berlin, 2014. 1

[47] H. Wilhelmsson and E. Lazzaro, *Reaction-Diffusion Problems in the Physics of Hot Plasmas*, Taylor & Francis, Milton Park, 2000. 1

[48] A. Wolff, *Diffusion-reaction-models and their application to biological and astrophysical problems*, PhD thesis, Universität zu Köln, Germany, 2011. 1

[49] D.H. Zanette, *Linear and nonlinear diffusion and reaction-diffusion equations from discrete-velocity kinetic models*, J. Phys. A: Math. Gen., 26:5339–5349, 1993. 1

[50] H. Zhao, X. Huang, and X. Zhang, *Turing instability and pattern formation of neural networks with reaction-diffusion terms*, Nonlinear Dyn., 76:115–124, 2014. 1