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# Front propagation in Rayleigh-Taylor systems with reaction.

**A. Scagliarini<sup>1</sup>, L. Biferale<sup>2,3</sup>, F. Mantovani<sup>4</sup>, M. Pivanti<sup>5</sup>, F. Pozzati<sup>6</sup>,  
M. Sbragaglia<sup>2</sup>, S.F. Schifano<sup>5</sup>, F. Toschi<sup>3,7,8</sup>, R. Tripiccione<sup>5</sup>**

<sup>1</sup> Department of Fundamental Physics, University of Barcelona, Barcelona, Spain

<sup>2</sup> Dept. Physics and INFN University of Rome, Tor Vergata, Italy

<sup>3</sup> Department of Applied Physics Eindhoven University of Technology, The Netherlands

<sup>4</sup> Deutsches Elektronen Synchrotron (DESY), Zeuthen, Germany

<sup>5</sup> University of Ferrara and INFN, Ferrara, Italy

<sup>6</sup> Fondazione Bruno Kessler Trento, Trento, Italy

<sup>7</sup> Department of Mathematics and Computer Science and J.M. Burgers Centre for Fluid Dynamics, Eindhoven University of Technology, The Netherlands

<sup>8</sup> CNR, Istituto per le Applicazioni del Calcolo, Rome, Italy

E-mail: [ascagliarini@gmail.com](mailto:ascagliarini@gmail.com)

**Abstract.** A special feature of Rayleigh-Taylor systems with chemical reactions is the competition between turbulent mixing and the “burning processes”, which leads to a highly non-trivial dynamics. We studied the problem performing high resolution numerical simulations of a 2d system, using a thermal lattice Boltzmann (LB) model. We spanned the various regimes emerging at changing the relative chemical/turbulent time scales, from slow to fast reaction; in the former case we found numerical evidence of an enhancement of the front propagation speed (with respect to the laminar case), providing a phenomenological argument to explain the observed behaviour. When the reaction is very fast, instead, the formation of sharp fronts separating patches of pure phases, leads to an increase of intermittency in the small scale statistics of the temperature field.

## 1. Introduction

Turbulent mixing triggered by a Rayleigh-Taylor (RT) instability has a great relevance in several natural phenomena and experimental setups (Sharp, 1984; Livescu et al, 2009). A situation even more complicated occurs when the mixing fluids can undergo chemical reactions between them, opening the way to a richer phenomenology (Zingale et al, 2005; Khokhlov, 1995; Gamezo et al, 2003; Freeman et al, 1997). In our setup the two mixing/reacting scalar fields are the temperatures of the two superposed blobs of fluid under gravity, thus mimicking the combustion of a cold mixture of actual reactants into a hot mixture of burnt products. In such reactive RT systems a fundamental issue is the competition between mixing, due to the unstable configuration, and burning due to the reaction: in particular we will discuss the crossing over between the different regimes emerging at varying the reaction rate and the effects of turbulence intensity on the flame propagation speed (Koudella & Neufeld, 2004; Biferale et al, 2011). What controls such crossing over is the ratio between the turbulence  $\tau_{turb}(t)$  (which depends on time

since RT turbulence is unsteady (Chertkov et al, 2009)) and reaction  $\tau_R$  time scales, that is called the Damköhler number  $Da(t) = \tau_{turb}(t)/\tau_R$ .

We obtained results (Biferale et al, 2011) concerning the enhancement of the front propagation speed due to the underlying turbulence (for the slow reaction case,  $Da \ll 1$ ), on one hand, and the signature of the strong feedback of reaction on the fluid, observable in the small scale statistics of temperature, on the other.

## 2. Equations of motion and numerical setup

We simulated a 2d system by means of a thermal lattice Boltzmann (LB) algorithm proposed in (Sbragaglia et al, 2009; Scagliarini et al, 2010), where it was shown that the method integrates, with good numerical accuracy (Biferale et al, 2010), the following set of macroscopic equations for the density  $\rho$ , velocity  $u_i$  and temperature  $T$  fields:

$$\begin{cases} D_t \rho = -\rho \partial_{ii} u_i \\ \rho D_t u_i = -\partial_{ii} p - \rho g \delta_{i,z} + \nu \Delta u_i \\ \rho c_v D_t T = -p \partial_i u_i + k \Delta T, \end{cases} \quad (1)$$

(where  $p$  is the pressure,  $k$  the thermal conductivity,  $\tau_R$  the reaction time,  $g$  the gravity and  $c_v = d/2$  the specific heat at constant volume), provided that one applies a suitable *shift* to the thermohydrodynamic fields appearing in the Maxwellian equilibria appearing in the LB equation:

$$\mathbf{u} \rightarrow \mathbf{u} + \tau_{LB} \mathbf{g}; \quad T \rightarrow T + \frac{\tau_{LB}(\Delta t - \tau_{LB})}{d} g^2.$$

In order to incorporate the reaction term  $R(T)$ , we introduced an extra-shift for the temperature field (Biferale et al, 2011), that is<sup>1</sup>

$$T \rightarrow T + \frac{\tau_{LB}(\Delta t - \tau_{LB})}{d} g^2 + \frac{\tau_{LB}}{\tau_R} R(T). \quad (2)$$

A proper reaction term should fulfill  $R(0) = R(1) = 0$ ,  $T = 0$  and  $T = 1$  being the temperatures of the pure cold (at the bottom of the simulation box) and hot (at the top, see figure 1) fluids respectively; moreover it should convert irreversibly the pure cold phase (unstable) into the hot one (stable). A simple expression for  $R(T)$  with these properties can be  $R(T) = T(1 - T)$ , that gives to the temperature equation the following advection-diffusion-reaction form

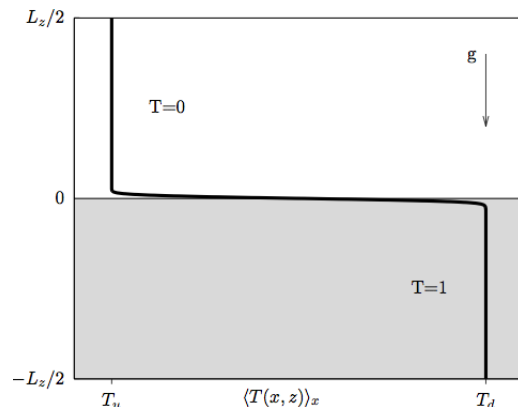
$$\rho c_v D_t T = \kappa \Delta T + \frac{1}{\tau_R} T(1 - T), \quad (3)$$

originally proposed (Fisher, 1937; Kolmogorov et al, 1937) as a model for the propagation of an advantageous gene in a population and as a model for reactions in a Rayleigh–Taylor system in (Chertkov et al, 2009).

Notice that in equation (3) we have subtracted the compression term  $p \partial_i u_i$  (compare with the third of equations (1)), by adding an extra counter-term in the shifted temperature inside equilibrium, in order to avoid effects due to the adiabatic gradient (Biferale et al, 2011b) or extra-heating not coming from the reaction itself.

We performed three high resolution sets of runs (on lattices of  $4096 \times 10000$  grid points, with different reaction times, see table 1 for run parameters) on the QPACE supercomputer, a massively parallel dedicated machine based on PowerXCell 8i processors (Goldrian et al, 2008). For each set we have collected  $\mathcal{O}(10)$  independent runs.

<sup>1</sup> This shift represents a kind of implicit equation, since  $R(T)$  is a function of the “real” hydrodynamic temperature  $T^{(H)}$ , which must be itself shifted (Scagliarini et al, 2010). However, observing that for  $\tau_R \gg \tau_{LB}$  (always true in



**Figure 1.** Initial configuration for the Rayleigh-Taylor system with combustion: cold fluid (fresh fuel) at  $T = 0$  on top and hot fluid (burnt material) at  $T = 1$  on bottom. The temperature jump at the interface is smoothed by a hyperbolic tangent profile with a width of the order of 10 grid points and with a randomly perturbed centre (thus enabling to perform independent runs). We simulated an ideal gas in a two dimensional box of  $L_x \times L_z$  lattice points with periodic boundary conditions applied along the  $x$  direction.

	$At$	$Fr$	$\nu$	$g$	$T_u$	$T_d$	$\tau_R$	$\tau$
run A	0.05	$7.5 \times 10^{-3}$	0.005	$2.67 \times 10^{-5}$	0.95	1.05	$5 \times 10^3$	$5.5 \times 10^4$
run B	0.05	$2.4 \times 10^{-4}$	0.005	$2.67 \times 10^{-5}$	0.95	1.05	$5 \times 10^4$	$5.5 \times 10^4$
run C	0.05	$7.5 \times 10^{-6}$	0.005	$2.67 \times 10^{-5}$	0.95	1.05	$5 \times 10^5$	$5.5 \times 10^4$

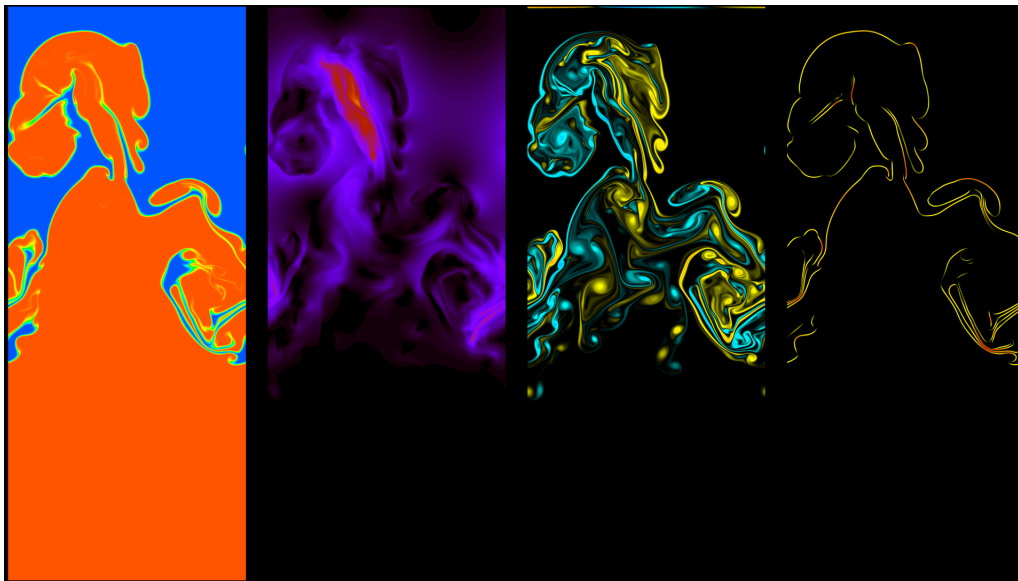
**Table 1.** Parameters for the three sets of runs. Size is  $L_x \times L_z = 4096 \times 10000$  for the three runs; Atwood number,  $At = (T_d - T_u)/(T_d + T_u)$ ; (laminar) Froude number  $Fr = V_f^2/(g L_f)$ , where  $V_f$  and  $L_f$  are the front laminar velocity and thickness (see text), respectively; viscosity  $\nu$ ; thermal diffusivity  $\kappa = \nu$ ; gravity  $g$ ; temperature in the upper half region,  $T_u$ ; temperature in the lower half region,  $T_d$ ; reaction characteristic time  $\tau_R$ ; normalization time,  $\tau = \sqrt{L_x/(g At)}$ .

### 3. Results and discussion

Owing to the fact that in a RT system (as previously pointed out), turbulence slows down adiabatically  $\tau(t) \propto t$ , for any reaction rate (even when  $\tau_R \gg 1$ ), one would eventually reach the “fast reaction limit”,  $Da \gg 1$ , with an active flame propagating. We address, then, in the following the transition between the various regimes.

For large  $Da$ , the mixing is effective only at very small scales (where the characteristic times of the fluid motion are shorter), while the reaction tends to make uniform the mixed regions, leading to a topology of the temperature field made of “patches” of pure phases separated by rather sharp interfaces, which are smoother than the non-reacting RT case (Chertkov et al, 2009); in addition, the front of the hot phase moves, on average, with a non zero mean *propagation* velocity towards the top. In order to better understand these preliminary features, at least on a pictorial level, we show in figure 2 a snapshot, during the mixing/burning evolution, of various fields, namely the temperature, kinetic energy, vorticity and magnitude of the temperature gradient ( $|\nabla T|^2 = ((\partial_x T)^2 + (\partial_z T)^2)$ ), for the fastest reaction rate that we have studied (for which the

actual situations), and that the other shift is  $\mathcal{O}(g^2)$  (hence  $\mathcal{O}(Kn^2)$  (Scagliarini et al, 2010)) we can safely assume that  $R(T^{(H)}) \approx R(T)$ .



**Figure 2.** Snapshot at  $t = 5.5\tau$  of (from left to right) temperature, kinetic energy, vorticity and temperature gradient magnitude fields, for the fastest reaction case  $\tau_R = 5000$  (run A in table 1).

overall dynamics is strikingly different from the standard non-reacting case). On the other hand, the larger the reaction time  $\tau_R$  the closer is the phenomenology to the standard RT case: to see this we compare in figure 3 the evolution of the mean temperature profile

$$\bar{T}(z, t) = \frac{1}{L_x} \int T(x, z; t) dx \quad (4)$$

for the two extreme cases in our database, runs A and C: while for  $\tau_R = 5 \times 10^5$  the evolution is basically undistinguishable from the usual RT dynamics (Scagliarini et al, 2010; Biferale et al, 2010), in the fast reaction case ( $\tau_R = 5 \times 10^3$ ) the center of mass of the system clearly moves upwards, due to the burning processes, inducing a displacement of the mixing region (which becomes asymmetric, too). Correspondingly, the flame leaves behind it a region of homogenized (by the burning processes) mean temperature, where, nevertheless, the turbulence is still active, as one can see from figure 4 where we plot both the mean temperature and mean kinetic energy

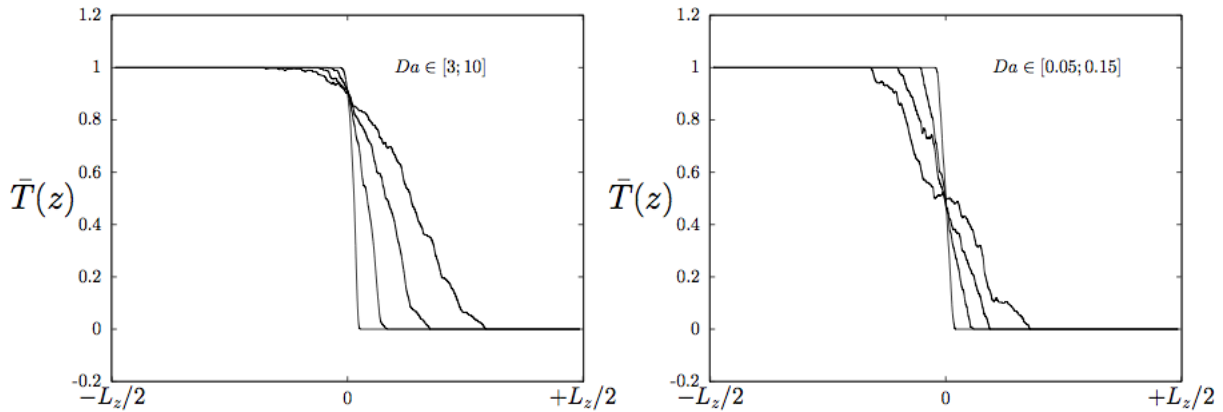
$$\bar{E}_{kin}(z, t) = \frac{1}{L_x} \int \frac{1}{2} \rho (u^2 + v^2)(x, z; t) dx \quad (5)$$

profiles: the latter is significantly non-zero in a belt out of the mixing layer (at strong difference from what typically happens in standard RT).

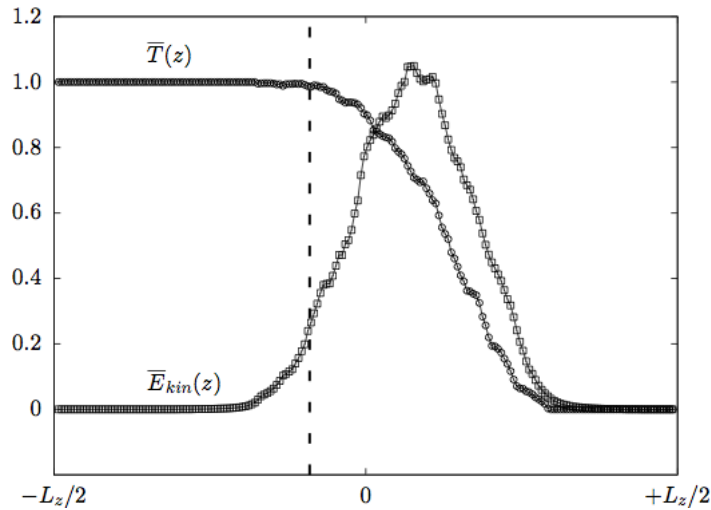
### 3.1. Front propagation speed

Upon integration (and normalization by  $L_x$ ) of eq. (3) over the whole volume we get an exact equation for the propagating front speed:

$$V_f(t) = \partial_t \left( \int_{-L_z/2}^{+L_z/2} \bar{T}(z, t) dz \right) = \frac{1}{\tau_R} \langle T(1 - T) \rangle, \quad (6)$$



**Figure 3.** Mean temperature profiles at various times for run A (left panel) and run C (right panel). The latter case is almost identical to the non-reacting case.



**Figure 4.** Mean vertical profiles of temperature and (normalized) kinetic energy at  $t = 3.5\tau$ . Turbulence remains active (the kinetic energy being significantly non-zero) in a region where the mean temperature profile is homogenized by the burning processes.

(where  $\langle(\cdot)\rangle = (1/L_x) \int \int(\cdot) dx dz$ ) since the boundary terms vanish, owing to the periodic conditions on the lateral walls and to the adiabatic condition at top and bottom plates ( $\nabla T|_{z=\pm L_z/2} = 0$ ). Such integral gives an explicit expression for the speed in the laminar flame case, that is  $V_f \propto L_f/\tau_R$ , where  $L_f$  is the front thickness: as the latter can be estimated to be  $L_f \propto \sqrt{\kappa\tau_R}$ , the well known result

$$V_f \propto \sqrt{\frac{\kappa}{\tau_R}} \quad (7)$$

is recovered (that is the front propagates at constant speed).

The natural question is how turbulence may affect such behaviour. In the small  $Da$  limit, when turbulence has the time to mix the fluids before reaction becomes active, we are in the so-called *pre-mixed combustion* regime. In this case, it has been conjectured (Koudella & Neufeld, 2004;

Damkoehler, 1940) that the simplest way to extend the result of the laminar case is to replace in expression (7) the molecular diffusivity  $\kappa$  with an effective (turbulent) eddy diffusivity  $\kappa_T$ . In terms of the *mixing layer length*, defined as

$$L(t) = \langle \bar{T}(1 - \bar{T}) \rangle,$$

(directly related to the definition usually used in RT turbulence (Cabot & Cook, 2006)), a dimensional estimate for the turbulent diffusivity is  $\kappa_T(t) \sim U(t)L(t)$ , where  $U$  is a large scale characteristic velocity (e.g. the root mean square velocity). Plugging it into (7), we get:

$$V_f(t) \sim \sqrt{\frac{\kappa_T}{\tau_R}} \sim \sqrt{\frac{U(t)L(t)}{\tau_R}} \sim U(t) \sqrt{\frac{L(t)/U(t)}{\tau_R}}, \text{ where } V_f(t) \sim U(t) \sqrt{\frac{\tau_{turb}}{\tau_R}} \equiv U(t) Da(t)^{1/2}. \quad (8)$$

This prediction, probably valid to describe the evolution of slow flames in stationary turbulent flows cannot be expected to apply for RT turbulence. The explanation is that the observation of an eddy-diffusivity driven propagation requires also a scale separation between the turbulent eddies and the flame thickness, something not realized by the evolving RT system. However, it is possible to rewrite (6) exactly as:

$$V_f(t) = \frac{1}{\tau_R} [\langle \bar{T}(1 - \bar{T}) \rangle - \langle \theta^2 \rangle], \quad (9)$$

where with  $\theta = T - \bar{T}$  we denote the fluctuations with respect to the mean vertical profile. It is clear now that for  $Da < 1$ , the front will not have any strong influence on the underlying RT evolution, thus it is possible to identify the first term on the rhs as the mixing layer length  $L(t)$ . Moreover, since in a RT system temperature fluctuations are almost constant in time and homogeneous inside the mixing layer, the second term on the rhs of (9) is proportional to the mixing layer extension, too (Chertkov, 2003). A natural prediction for  $V_f(t)$ , at small  $Da$ , can be therefore (Biferale et al, 2011):

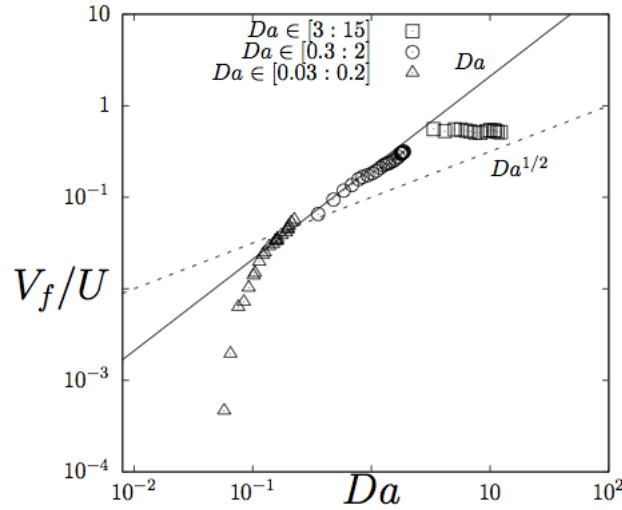
$$V_f(t) \propto \frac{L(t)}{\tau_R}; \quad V_f(t) \propto U(t)Da(t); \quad (10)$$

This result can be easily generalized to different types of reaction term: in fact as long as we may write  $R(T, \tau_R) = (1/\tau_R)f(T)$  (where  $f$  is some smooth function of  $T$ ), we will have, for the front speed

$$V_f(t) = \frac{1}{\tau_R} \langle f(\bar{T}) \rangle;$$

moreover, it is always possible to use  $\overline{f(T)} = f(\bar{T}) + \text{fluctuations}$ , and  $f$  is non-zero (and positive) only in the mixing layer (being a reaction term). Then,  $\langle f(\bar{T}) \rangle \propto L(t)$  and the scaling (10) of  $V_f$  with  $Da$  is recovered.

To check this prediction at varying the reaction/turbulence relative intensity, we can exploit RT non-stationarity and, hence, the Damköhler number time dependence  $Da = Da(t)$ . In figure 5 front speed (normalized with the root mean square velocity) is reported as a function of  $Da$  (which is itself a function of the simulation time) for the three runs. As one can see, our prediction (10) works satisfactorily in a wide range of  $Da(t)$ , showing deviations only for very small times, where turbulence is not yet developed and the front evolution is strongly influenced by the initial configuration, and, of course, for  $Da(t) > 1$ , a regime out of the range of validity of the underlying assumptions. In this latter case, data point flatten. The feedback of the flame on the turbulent mixing shows up with a sort of synchronization between front propagation and evolution of the turbulent kinetic energy toward a value where  $V_f(t) \sim U(t)$ . Such a behaviour turns out to be in agreement with recent theoretical results obtained through a mean-field approach (Brandenburg et al, 2011).



**Figure 5.** Front speed normalized by the root mean square (vertical) fluid velocity for the three runs as a function of the Damköhler number  $Da(t)$ . The solid line represents the theoretically predicted behaviour  $V_f/U \propto Da$ , obtained on the basis that for  $Da < 1$  flame propagates inside the well mixed mixing layer. The prediction  $V_f/U \propto Da^{1/2}$ , obtained from the assumption that in the pre-mixed combustion (slow reaction) regime one can simply substitute the molecular diffusivity with the turbulent one  $\kappa \rightarrow \kappa_T$  in the expression for the laminar front speed, is also plotted (dashed line).

### 3.2. Small scale intermittency

For high reaction rate ( $Da \gg 1$ ), there are no extended regions which are well mixed, since the cold material is rapidly burnt. As a result, the temperature field organizes in patches of pure reactants/products separated by sharp interfaces (being in the so called “segregated regime”), and, consequently, it has been conjectured that an increased intermittency should develop at the small scales (Chertkov et al, 2009). According to a phenomenological prediction (Chertkov et al, 2009), in the asymptotics of  $Da \gg 1$ , the scaling laws of fluid temperature (and velocity) structure functions should obey the following relation

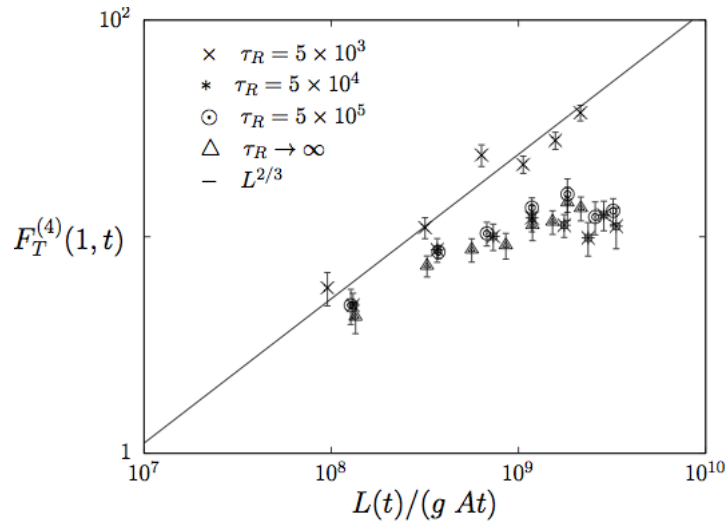
$$S_T^{(p)}(R, t) \equiv \langle |\delta_R T|^p \rangle \sim \left( \frac{R}{L(t)} \right)^{2/3}, \quad (11)$$

(where  $L(t)$  is the mixing length), irrespective of the order  $p$ . From Eqn. (11) the expression for the flatness reads:

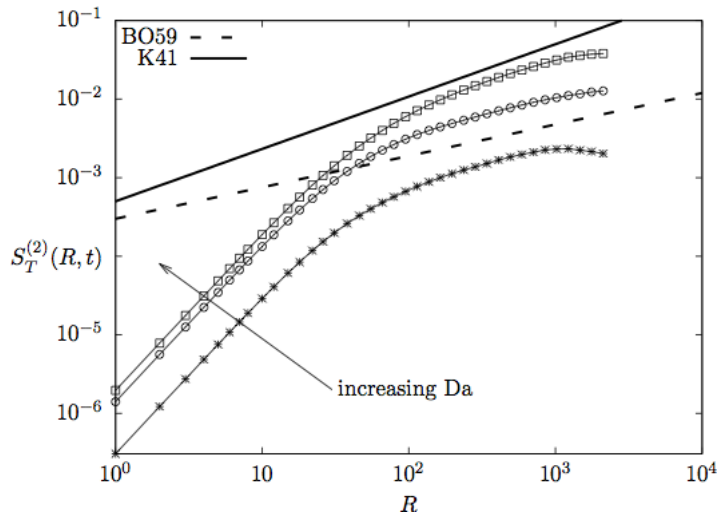
$$F_T^{(p)}(R, t) = \frac{\langle |\delta_R T|^p \rangle}{\langle |\delta_R T|^{p/2} \rangle^2} \sim R^{-2/3} L(t)^{2/3} \quad (12)$$

and so it increases with decreasing  $R$  for all orders, a clear indication of strong small scales intermittency. In figure 6 we show the growth of  $F_T^{(4)}(R = 1, t)$  as function of the mixing length  $L(t)$ , for the three runs: the flatness for run A, corresponding to the smallest reaction time, is in good agreement, within error bars, with the prediction of equation (12),  $F_T^{(4)} \sim L^{2/3}$ ; instead, at increasing  $\tau_R$ , intermittency is depleted and the flatness grows more slowly, at a rate comparable (within error bars) with the non-reacting RT case, whose data are also reported for comparison. Equation (11) was derived in (Chertkov et al, 2009) under the assumption of a K41 scaling for structure functions, as it should be in 3D; actually we show in figure 7 that this is also our case: at increasing  $Da$  (that is going from slower to faster reactions) the scaling of  $S_T^{(2)}(R, t)$  is closer to K41 than to a Bolgiano-Obukhov-like behaviour (as one would expect for a 2D system).





**Figure 6.** The 4-th order ( $\tau_R \rightarrow \infty$ ). Data from run A ( $Da \gg 1$ ) agree well, within error bars, with the prediction given by equation (12)  $F_T^{(4)} \sim L^{2/3}$ .



**Figure 7.** 2-th order structure functions  $S_T^{(2)}(R, t = 5.5\tau)$  for the three reaction rates (the three curves are vertically shifted for the sake of clarity): at increasing  $Da$  one goes from a Bolgiano-Obhukov scaling (dashed line) to a behaviour much closer to the K41 prediction (solid line).

#### 4. Conclusions

We simulated a 2d Rayleigh-Taylor system with a reaction term (of Fisher type) by means of a thermal lattice Boltzmann algorithm. We presented results on the enhancement of the reaction front propagation speed  $V_f$  in the “pre-mixed combustion” regime  $Da \ll 1$ , giving a phenomenological argument to explain the dependence of  $V_f$  on  $Da$ . On the other way round, we showed that when  $Da \gg 1$ , the feedback of the flame on turbulence is that of strongly increasing small scales intermittency in the temperature field (finding nice agreement

with previous theoretical results (Chertkov et al, 2009)) and that the statistics of temperature fluctuations is closer to a K41 phenomenology rather than to a Bolgiano-Obhukov one, typical for two-dimensional standard convective systems.

## 5. Acknowledgments

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