NO Formation during Ignition of One Dimensional Laminar Flamelets

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Abstract

NO formation during ignition of combustible mixtures has been calculated in non–stationary two-dimensional systems by coupling the fluid flow and chemical reactions using “interactive flamelets”. The fluid flow was calculated by the PISO (Pressure–Implicit with Splitting of Operators) method to solve the Navier–Stokes equations. Further a convection–diffusion equation for the mixture fraction $Z(x, y, t)$ has been solved to calculate the scalar dissipation rate χ, needed for the flamelet calculations. The one dimensional flamelet code solves the flamelet equation in the mixture fraction space. The stiffness of the system of equations describing the 1D non–stationary flamelets requires a fully-implicit calculation. It has been shown in the past, that Newton's method, damped and modified, is suitable to solve this class of equations. A backward difference scheme (BDF) with automatic order selection strategies is utilized. The grid resolving the 1D–flamelet supports high accuracy by using a moving grid method. Back transformation of the calculated species mass fractions from the flamelet space gives a two dimensional distribution of all chemical species included in the large chemical system.

1 Introduction

In the high Damköhler number regime of combustion turbulent diffusion flames can be conceived as an ensemble of laminar diffusion flamelets [1]. This concept has been realized assuming the laminar flamelets to be stationary [2]. The calculated flow field was coupled with chemical reactions by the help of flamelet libraries describing the dependence of flamelets on several parameters, e.g. the scalar dissipation rate χ and the mixture fraction Z. The flamelet libraries are calculated in advance using detailed chemical mechanisms for the combustion reactions under consideration. It is obvious that ignition and extinction phenomena in turbulent diffusion flames cannot be modeled with stationary flamelets. On the other hand, the calculation of the non–stationary conservation equations for temperature and species mass fractions on each grid point in the flow field cannot be realized for large chemical systems in more than one dimension. Therefore, it has been proposed recently [3], to calculate several unsteady flamelets interactively with the calculation of the flow field. Each flamelet is representative for a

certain domain of the flame. This concept allows to couple large chemical systems with the flow field by “interactive flamelets”.
In the present work the system of ammonia/air is considered. This system is described by a set of 148 chemical reactions between 19 chemical species. To attain high accuracy of the calculated solution for temperature and species mass fractions in the flamelet calculations a moving grid method is used. For each chemical system the motion of grid points due to a weight function resolving the pyrolysis of the fuel, the ignition process, the propagating flame fronts and the stationary solution of the diffusion flame is presented. The spatial distribution of mass fractions is retrieved via the mixture fraction/scalar dissipation rate field, which is calculated with the flow field.

2 Modelling

2.1 Modelling of the Flow Field

The PISO (Pressure–Implicit with Splitting of Operators) algorithm is a non-iterative method for solving the implicitly discretised, time dependent Navier–Stokes equations [4]. The method is based on the use of pressure and velocity as dependent variables and is, hence, applicable for the compressible formulation of the transport equations. The main feature of the technique is the splitting of the solution process into a series of steps whereby operations on pressure are decoupled from those on velocity at each step, with the split sets of equations being amenable to solution by standard techniques. At each time–step, the procedure yields solutions which approximate the exact solution of the difference equations.
The governing equations are written here in Cartesian tensor notation. The equations for continuity, momentum and total energy in laminar compressible flows are

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0, \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_j}\left[\mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij})\right] \tag{2}$$

and

$$\begin{aligned}\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_j}(\rho u_j e) = \frac{\partial}{\partial x_j}\left(\frac{\mu}{Pr}\frac{\partial T}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(P u_j) \\ + \frac{\partial}{\partial x_j}\left[u_i \mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij})\right] + Q,\end{aligned} \tag{3}$$

where μ is the laminar viscosity and Pr is the Prandtl number. The total energy e is related to the temperature by

$$e = C_v T + \frac{1}{2}u_i u_i \tag{4}$$

where C_v is the constant volume specific heat. The equation of state taken here is that of perfect gas

$$\rho = p/RT \tag{5}$$

where R is the gas constant. Q contains the external source of energy.

The discretisation of the equations in time and space is obtained by a finite difference scheme. The predictor and corrector steps of the PISO algorithm lead to the new velocities u_i^{n+1} and the new pressure p^{n+1} by solving the momentum, continuity and energy equations. The poisson equation is solved by a Block–LU decomposition, an ADI technique with operator splitting leads to the velocities.

2.2 Modelling of the Chemical System

For laminar diffusion flamelets ,under the condition that equal diffusivities of chemical species and temperature can be assumed, all Lewis numbers

$$Le_i = \lambda / c_p \rho D_i = 1 \qquad (i = 1, 2, ..., n) \tag{6}$$

are unity, such that a common diffusion coefficient $D = \lambda/(c_p\rho)$ can be introduced. The conservation equation for the mixture fraction Z, the temperature T and the species mass fraction are given in cartesian coordinates:

$$\rho \frac{dZ}{dt} + \rho u \frac{dZ}{dx} = \frac{d}{dx}\left(\rho D \frac{dZ}{dx}\right) \tag{7}$$

$$\rho c_p \frac{dT}{dt} + \rho u c_p \frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) + \sum_{i=1}^{n} h_i M_i \sum_{k=1}^{N_r} \nu_{i,k} w_k \tag{8}$$

$$\rho \frac{dY_i}{dt} + \rho u \frac{dY_i}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_i}{dx}\right) + M_i \cdot \sum_{k=1}^{N_r} \nu_{i,k} w_k \tag{9}$$

Eq.(8) and (9) can be transformed into the mixture fraction space according to [1]. The mixture fraction Z is a function of space and time. Then the surface of the stoichiometric mixture can be determined from

$$Z(x,t) = Z_{st}. \tag{10}$$

Combustion takes place in a thin layer in the vicinity of this surface if the local mixture fraction gradient is sufficiently high. To introduce a coordinate system attached to the surface of a stoichiometric mixture, we replace the coordinate x by the mixture fraction Z and define the original coordinate system such that the coordinate x does not lie within this surface. By definition the new coordinate Z is normal to the surface of the stoichiometric mixture. With the help of the transformation rules

$$\frac{d}{dt} = \frac{d}{d\tau} + \frac{dZ}{dt}\frac{d}{dZ} \tag{11}$$

und

$$\frac{d}{dx} = \frac{dZ}{dx}\frac{d}{dZ}. \tag{12}$$

and introducing the new variable χ

$$\chi = 2D\left(\frac{dZ}{dx}\right)^2 \tag{13}$$

for the scalar dissipation rate to describe the influence of the flow field, the flamelet equations for temperature and species mass fractions in the mixture fraction space are obtained.

$$\rho c_p \frac{dT}{d\tau} = \rho c_p \frac{\chi}{2}\frac{d^2T}{dZ^2} + \sum_{i=1}^{n} h_i M_i \sum_{k=1}^{N_r} \nu_{i,k} w_k \tag{14}$$

$$\rho \frac{dY_i}{d\tau} = \rho \frac{\chi}{2} \frac{d^2 Y_i}{dZ^2} + M_i \cdot \sum_{k=1}^{N_r} \nu_{i,k} w_k \tag{15}$$

The stiffness of the system of equations describing the 1D non–stationary flamelets requires a fully-implicit calculation. It has been shown in the past, that Newton's method, damped and modified, is suitable to solve this class of equations. The semi–discrete partial differential equations approximation is written in the form $U_t = F(U)$, where F is a nonlinear operator. To reduce CPU–time, needed for each timestep, a backward difference scheme (BDF) with automatic order selection strategies is utilized [5]. Finally the grid resolving the 1D–flamelet has to support this approach.

2.3 Coupling of Fluid Flow and Chemical Reactions

The non–stationary flow field is computed by means of the PISO–procedure. According to the Navier–Stokes equations a convection–diffusion equation

$$\rho \frac{dZ}{dt} + \rho u_k \frac{dZ}{dx_k} = \frac{d}{dx_k}\left(\rho D \frac{dZ}{dx_k}\right) \tag{16}$$

is implemented for the mixture fraction $Z(x, y, t)$ in the fluid dynamic code to attain the scalar dissipation rate χ as a function of Z for the flamelet calculation. The scalar dissipation rate

$$\chi = 2D\left(\frac{dZ}{dx_k}\right)^2 = 2D\left[\left(\frac{dZ}{dx}\right)^2 + \left(\frac{dZ}{dy}\right)^2\right], \tag{17}$$

which describes the influence of the flow field on the chemistry, is needed for the calculation of the species mass fractions. The heat release, calculated in the flamelet code, serves as the external source of energy Q in the equation of total energy to feed back the chemical relation to the flow field [6].

Back transformation of the calculated species mass fractions from the flamelet space gives a two dimensional distribution of all chemical species included in the large chemical system.

2.4 Moving grid method

Several types of grid–generators are discussed. The most simple class of grids are fixed grids. The initial distribution of the grid points, equidistant or best guess problem oriented, is maintained for all timesteps. The order selection of the BDF method is not influenced by the grid. Either the resolution in Z of those grids is low or a high number of gridpoints is needed to resolve all species profiles in the flame. It is not possible to follow a propagating flame front after an ignition process, that means that this method is only accurate for stationary problems.

In contrast to this method, irregular grids allow to resolve steep gradients. Those adaptive grids are calculated at each time step according to a weight function describing the local truncation error of the applied discretisation scheme. Unfortunately, the unknown variables, known at the old gridpoints, have to be interpolated on the new adaptive grid. This method influences the selection of the order of the BDF method. Hence the stepsize of the timesteps has to be reduced whenever the grid is adapted.

Moving grid techniques [7] are able to avoid the problems of interpolation and low resolution. For moving grid techniques an additional convective term has to be introduced as given in the following. The non-stationary system of conservation equations for species mass fractions and temperature in Z formulate a parabolic system of time dependent partial differential equations

$$\vec{u_t} = \vec{f}(\vec{u}, \vec{u_x}, \vec{u_{xx}}, x, t). \tag{18}$$

Discretisation in Z leads to the following system of ordinary differential equation

$$U_t = F(U), \tag{19}$$

where F is a nonlinear operator.
The motion of the grid points introduces an additional convective term to the system of equations

$$U_t = F(U) + U_x X_t, \tag{20}$$

where X_t is calculated from the corresponding weight function. The weight function W is calculated as a function of the gradients of U and the solution of U. The proportion of the gradients of U to the solution U can be varied and has to be adapted for each combustion problem. An interpolation of the solution is avoided. The order of accuracy is determind by the applied BDF method. The stepsize of each timestep is only slightly influenced by the velocity of the grid motion. The moving grid techniques are able to resolve steep gradients by using only a minimum number of grid points.

3 Results and Discussion

The grid motion for an ammonia/air flamelet is given in figure 1. In this example the ammonia stream is diluted by air in a ratio of 1:1. The figure includes the time dependent grid motion of every 5th gridpoint.

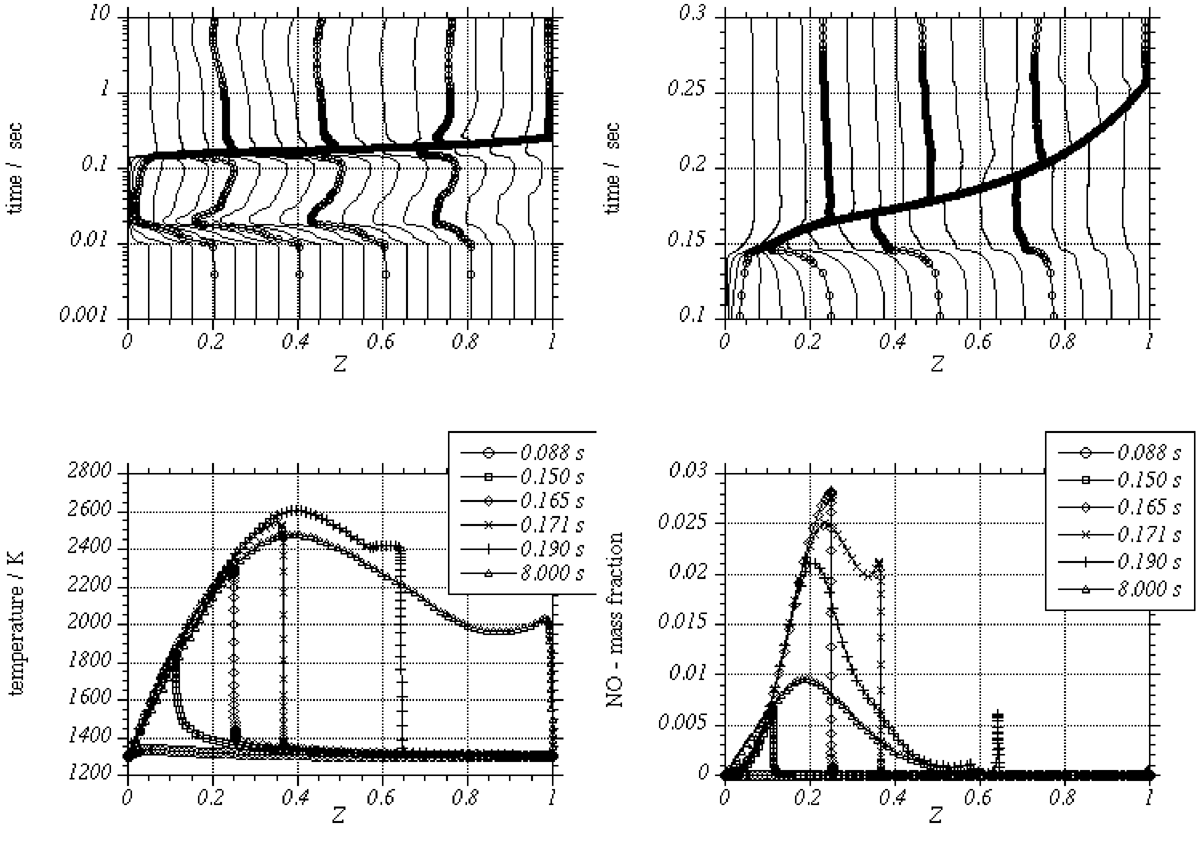

Figure 1: Non–stationary grid motion, temperature and NO profiles during the ignition of an ammonia/air flamelet.

The mechanism for the ignition of ammonia includes the mechanism for the formation of NO. The initial boundary conditions are $T = 1300\text{K}$ and $p = 1\text{bar}$. During the first phase of ignition, the grid has to resolve the pyrolysis of ammonia. Then the grid has to be adapted to the formation of intermediate species, e.g. HO_2 and OH. The ignition delay time is found to be t $\approx$ 0.15sec at mixture fraction $Z = 0.065$. It is obvious from figure 1, that the grid is contracted very rapidly during the ignition process. Then the grid resolves the evolution of two flames. One flame is a fuel–lean flame burning at the fuel lean side of the flamelet. The other flame is a fuel–rich flame burning at the fuel–rich side of the flamelet. The propagation of this flame is indicated by the motion of contracted grid points. In the stationary solution the grid only has to resolve the stationary diffusion flame.

Further the non-stationary profiles of the NO mass fraction and the temperature in the mixture fraction space Z are obvious from fig.1. The high resolution of the time dependent profiles indicate the propagating flames.

A two dimensional non–stationary distribution of NO has been calculated by using interactive flamelets. The domain of computation consists of a quadratic combustion chamber, where the fuel is injected into hot air. The temperature of the air and the fuel is 1300 K. The diameter of the inlet tube is 60 mm. The fuel is injected with a velocity of 10 cm/s, the injection time is 0.2 sec.

Figure 2 shows the non–stationary evolution of the mixture fraction Z in the flow field. The mixture fraction represents the contour of the injected fuel.

According to the mixture fraction Z, the velocities u and w were calculated in the compressible PISO code. The time dependent distribution of the velocity field is given in fig.3. The velocity field at t= 0.39 sec shows the fluid flow after the injection of the fuel into the hot air.

In fig. 4 the non–stationary evolution of the NO mass fraction is shown. After the injection of ammonia, the formation of NO near Z= 0.07 can be recognized in the mass fraction plot of NO at t= 0.39 sec. For the next time steps the NO formation during the flame propagation into the middle of the injected fuel can be shown.

4 Conclusions

Numerical modelling of NO formation in a quadratic combustion chamber has been performed using an “interactive flamelets” model to couple the non–stationary fluid flow with a detailed chemical mechanism.

An additional transport equation for the mixture fraction was solved to calculate the scalar dissipation rate χ as input for the flamelet model. The heat release, calculated in the flamelet code, serves as the external source of energy in the equation of total energy in the fluid flow calculation.

The concept of “interactive flamelets” allows to couple large chemical systems with the flow field. A two dimensional distribution of all chemical species, included in the chemical mechanism, can be calculated for the ignition - as far as ignition occurs in the flamelet regime - and combustion process.

Using moving grid methods a high accuracy of the calculated species is attained. This method is able to resolve time dependent steep gradients. Interpolation errors or high numbers of grid points are avoided.

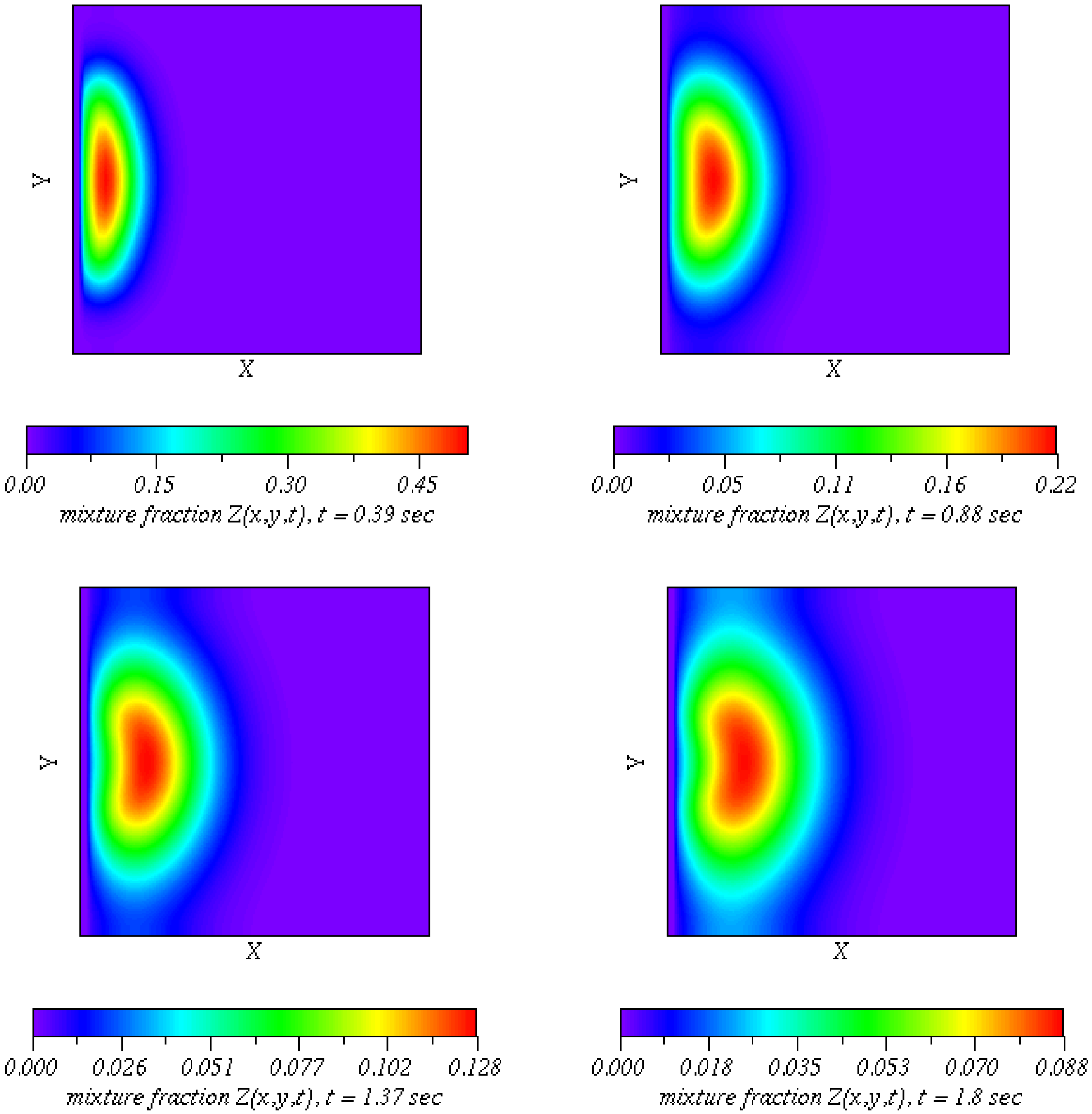

Figure 2: Non–stationary two dimensional distribution of the mixture fraction.

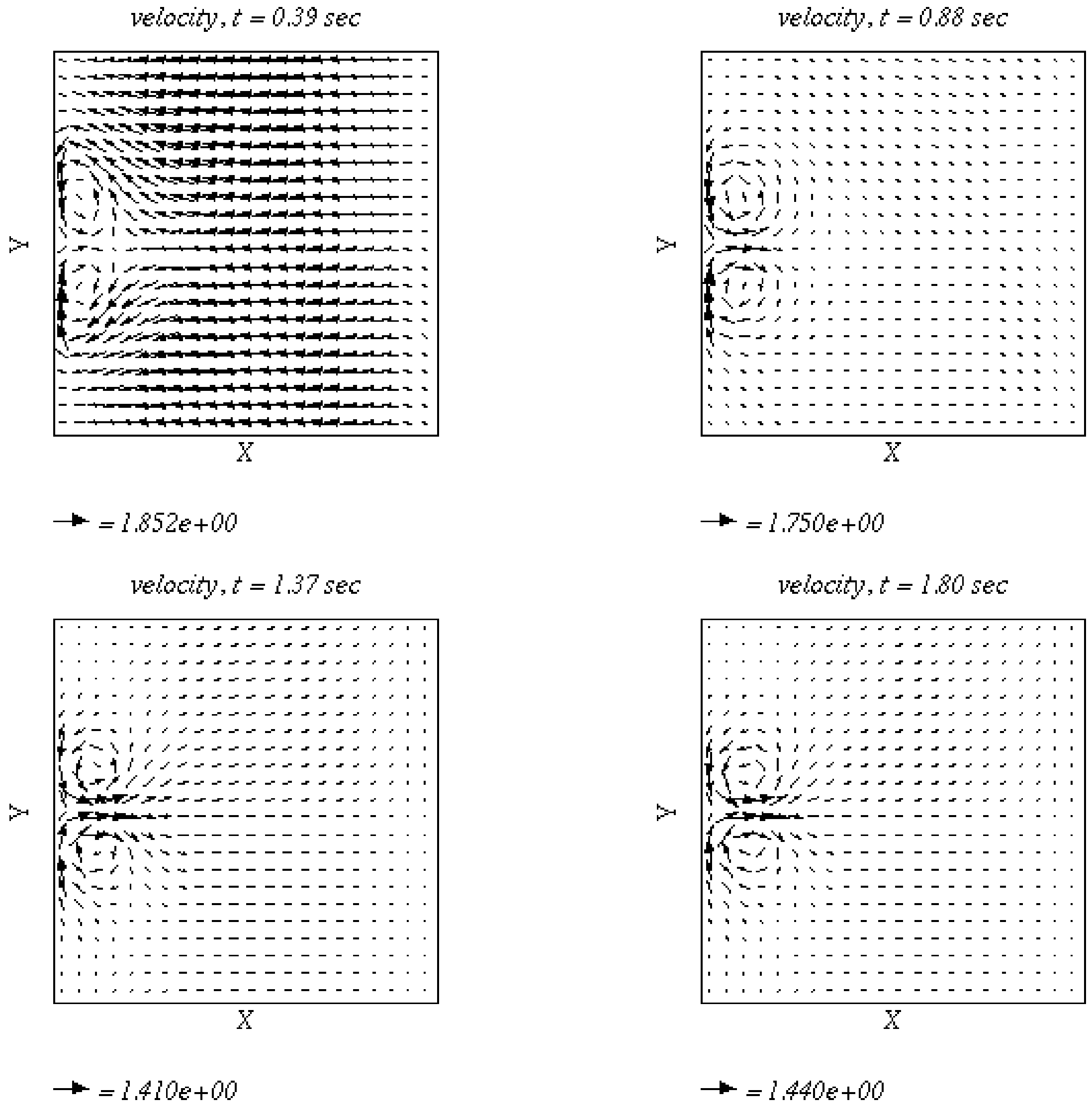

Figure 3: Non–stationary two dimensional velocity field.

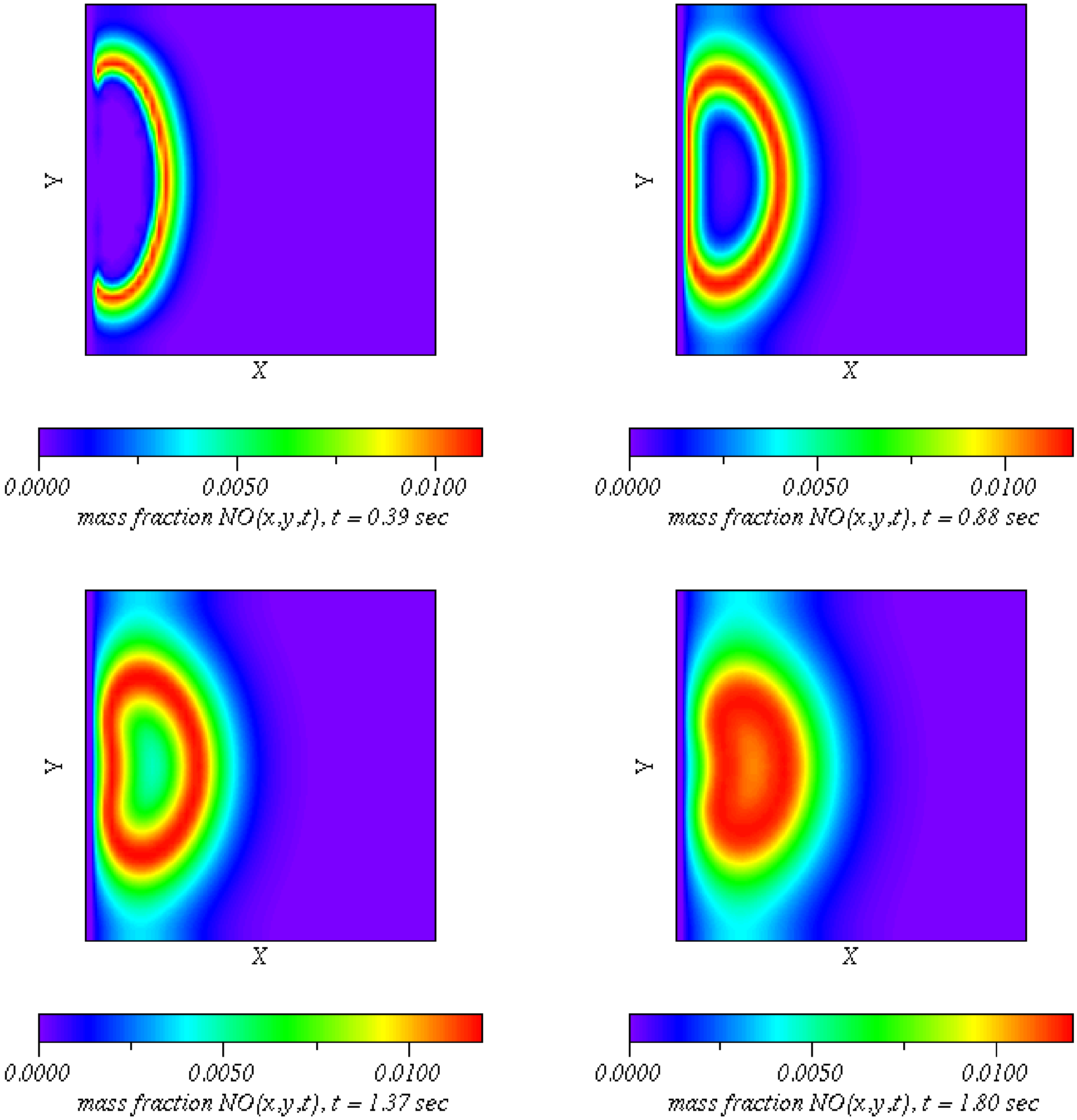

Figure 4: Non–stationary evolution of the NO mass fraction.

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