## Animation of Reactive Gaseous Fluids through Chemical Kinetics

Insung Ihm Byungkwon Kang Deukhyun Cha

Department of Computer Science Sogang University, Seoul, Korea

#### Abstract

Although chemically reactive fluids may be used effectively to increase the reality of visual effects, little work has been done with the general modeling of chemical reactions in computer animation. In this paper, we attempt to extend an established, physically based fluid simulation technique to handle reactive gaseous fluids. The proposed technique exploits the theory of chemical kinetics to account for a variety of chemical reactions that are frequently found in everyday life. In extending the existing fluid simulation method, we introduce a new set of physically motivated control parameters that allow an animator to control intuitively the behavior of reactive fluids. Our method is straightforward to implement, and is flexible enough to create various interesting visual effects including explosions and catalysis. We demonstrate the effectiveness of our new simulation technique by generating several animation examples with user control.

Categories and Subject Descriptors (according to ACM CCS): I.3.5 [Computer Graphics]: Computational Geometry and Object Modeling – Physically Based Modeling; I.3.7 [Computer Graphics]: Three-Dimensional Graphics and Realism – Animation; I.6.8 [Simulation and Modeling]: Type of Simulation – Animation

#### 1. Introduction

While recent research has made great advances in the production of realistic fluid effects, physically based fluid animation still remains one of the most challenging tasks in computer graphics. Among a variety of fluids, chemically reacting flows abound in the real world, and can be used to create a diverse class of interesting visual effects in computer animation, ranging from weathering effects to explosions.

In computational fluid dynamics, reactive flows containing multiple chemical species have been generally modeled by extending the Navier–Stokes equations to include the appropriate chemical reactions [Chu02, Fed97]. These equations tightly couple the chemical reactions with the conservation equations for mass, momentum, and energy, resulting in a complex system of nonlinear conservation laws. While effective numerical techniques have been developed with proper assumptions (for instance, refer to [Fed97]), they are often too complicated to apply directly to the production of animation effects.

In the computer graphics community, many researchers

have attempted to visualize special effects of reactive flows. Explosions are among the most commonly used phenomena of reactive fluids in the entertainment industry. Numerous studies have been directed at developing practical techniques for modeling realistic explosions using various physically based and/or ad hoc fluid mod-[NF99, MMA99, YOH00, BY01, FOA03, RNGF03]. els Fire and flame are another kind of dramatic special effects frequently employed in fluid animation, and have been modeled in several previous researches [CMTM94, SF95, BPP01, NFJ02, LF02, WLMK02, HK03]. The concept of chemical reaction has also been utilized to synthesize textures on arbitrary surfaces [Tur91, WK91], to model patterns on seashells [FMP92], and to generate stone weathering effects [DEJ\*99].

While all these related works concern the chemical phenomena, little work has been done with the general modeling of chemical reactions in computer animation. The only attempt (to the best of our knowledge) is found in [Gat02], where transport and reaction processes of chemical species were expressed through a system of differen-

<sup>©</sup> The Eurographics Association 2004.

tial equations  $\frac{\partial C_i}{\partial t} + \mathbf{v} \cdot \nabla C_i = \lambda_i \nabla^2 C_i + Q_i - L_i C_i$ . In this transport–reaction system, chemical reactions are undertaken through the production and loss rates  $Q_i - L_i C_i$ , while the reactive species are transported by flow through convection  $\mathbf{v} \cdot \nabla C_i$  and diffusion  $\lambda_i \nabla^2 C_i$ . A simple form of equation was used to describe the conservation of energy that describes changes in temperature caused by the convection and diffusion of heated fluids  $\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \lambda_T \nabla^2 T + q$ , where q is the heat generated from the chemical reactions.

The goal of this work is to develop a simplified framework that allows an animator to generate animation effects pertaining to reactive fluids easily. Our method is based on the numerical simulation technique proposed in [Sta99, FSJ01], which successfully generates the motion of gases such as smoke. The concepts of chemical kinetics are applied to the simulation process to handle gases containing a set of real or hypothetical chemical species that react with each other. While compressibility was often assumed to model reactive fluids, especially in a variety of combustion problems [NF99, YOH00], our method considers incompressible fluids, as in [FSJ01, NFJ02, FOA03], which provide a relatively stable and easy-to-compute numerical solution.

Our extension is simple to implement, and is flexible enough to enable an animator to create a wide range of visual effects concerning chemical reactions. In extending the existing fluid simulation method, a new set of physically motivated control parameters for the chemical reaction is introduced. Using examples, we show how they can be manipulated effectively to adjust reaction effects.

This paper is organized as follows. After the theory of chemical kinetics is briefly reviewed in Section 2, we explain how the concepts of chemical kinetics are integrated with an existing fluid simulation system in Section 3. Next, the effectiveness of our method is demonstrated by applying it to a number of interesting scenarios in Section 4, and then the paper is concluded in the last section.

### 2. A brief introduction to chemical kinetics

Chemical kinetics or reaction kinetics is a branch of kinetics that studies the rates and mechanisms of chemical reactions, and describes the nonequilibrium states of fluid systems containing several reactive substances [Lev02]. Consider a simple chemical reaction

$$aA + bB \longrightarrow eE + fF$$
,

where A, B, E, and F stand for the chemical species and a, b, e, and f are, respectively, their stoichiometric coefficients. The chemical reaction is described by a differential equation

$$r = -\frac{1}{a}\frac{d[A]}{dt} = -\frac{1}{b}\frac{d[B]}{dt} = \frac{1}{e}\frac{d[E]}{dt} = \frac{1}{f}\frac{d[F]}{dt}$$

for the rate of change of the concentrations of the reactants and products ([\*] denotes the molar concentration of species in mol/L).

The rate of reaction r is also called the rate law, and is a time-dependent function  $r = f_r([A], [B], [E], [F])$  of the concentrations of species present at time t. For a large class of chemical reactions, it is experimentally found to be proportional to the concentration of each reactant/product raised to some power. For instance, if only a forward reaction occurs, it can be expressed in the form  $r = k[A]^{\alpha}[B]^{\beta}$  for some orders  $\alpha$  and  $\beta$ . Here, the rate constant k is a function of temperature and pressure. While the pressure dependence is usually ignored, the constant relies strongly on temperature where the Arrhenius equation of the form  $k = Ae^{-\frac{L_a}{RT}}$  holds well for many homogeneous reactions. The rate law is determined from measurements by following the concentrations of reactants and/or products as a function of time. The overall rate of a reaction is a net rate  $r = r_f - r_b$  where  $r_f$  and  $r_b$ are, respectively, the forward rate and the reverse rate.

A given stoichiometric equation does not necessarily imply the actual mechanism by which the reaction actually occurs. A simple reaction can occur in a single elementary step. On the other hand, most reactions are composite in that they consist of a series of elementary steps. For instance, the gas-phase decomposition of  $N_2O_5$  with the overall stoichiometric equation  $2N_2O_5 \longrightarrow 4NO_2 + O_2$  is known to occur by the three-step mechanism:

$$\begin{array}{l} N_2O_5 \longrightarrow NO_2 + NO_3 \\ NO_2 + NO_3 \longrightarrow NO + O_2 + NO_2 \\ NO + NO_3 \longrightarrow 2NO_2 \end{array}$$

Catalytic reactions form a class of composite reactions that may interest an animator. They are formed by a sequence of steps in which a reactive intermediate (or catalyst) is consumed, reactants are converted to products, and the intermediate is regenerated. Regeneration of the intermediate allows the reaction cycle to be iterated over and over again, so a small quantity of catalyst produces a large amount of product. Most combustion reactions and explosions, which are important ingredients of animation productions, belong to this class of reactions and usually involve free radicals as intermediates.

#### 3. The proposed simulation method

In this section, we present a detailed description that proposes how an existing fluid simulation model can easily be extended to create visual effects relating to chemical reactions. In the explanation, we only consider reactive flows represented by a simple type of stoichiometric equation  $aA + bB \longrightarrow eE + fF$  with negligible reverse reaction. Slight modifications to our technique can handle a wider range of chemical reactions.

#### 3.1. [Stage 1] Computation of the fluid's velocity field

As explained in previous studies, the basic motion of an incompressible fluid is described by the Navier–Stokes system of two governing equations. First, momentum is conserved by enforcing the equation:

$$\frac{\partial \mathbf{u}}{\partial t} = -(\mathbf{u} \cdot \nabla)\mathbf{u} - \frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}, \tag{1}$$

where **u** is the fluid velocity, *p* pressure,  $\rho$  density,  $\nu$  viscosity, and **f** is the external force acting on the fluid. In [FSJ01], gases were assumed to be inviscid, constant density fluids, which can be represented in the equation simply by setting  $\rho = 1$  and  $\nu = 0$ .

The next governing equation is for mass conservation, requiring the velocity divergence to be zero:  $\nabla \cdot \mathbf{u} = 0$ . This incompressibility condition states that mass is neither created nor destroyed in the flows. Sometimes it is useful to vary this equation to have fluids move outward or inward as a reflection of activities in the flows. In [FOA03], a modified equation was employed to model the introduction of additional gaseous products that are generated as the explosive vaporizes:

$$\nabla \cdot \mathbf{u} = \phi. \tag{2}$$

Rather than modeling the computationally expensive blast wave of compressible fluids, as in [YOH00], an incompressible fluid model was adopted where the expansive flow caused by the explosion was produced by appropriately controlling the value of  $\phi$ .

To take care of the expansion or contraction of gases because of chemical reactions, we too use the same equation where the divergence constraint  $\phi$  is determined for each fluid cell according to the reaction process that occurs in the corresponding region. The fluid in a cell will flow outward or expand if its  $\phi$  value is positive, and flow inward or contract if  $\phi$  is negative. As the fluid may no longer be divergent-free for some cells, the pressure of each cell is computed through the modified Poisson equation

$$\nabla^2 p = \frac{\rho}{\Delta t} (\nabla \cdot \mathbf{u} - \phi).$$

## **3.2.** [Stage 2] Evolution of the density and temperature through the velocity field

After the fluid's velocity field is computed, the density *d* of the gas mixture is evolved using an advection–diffusion equation with diffusion constant  $\kappa_d$ :

$$\frac{\partial d}{\partial t} = -(\mathbf{u} \cdot \nabla)d + \kappa_d \nabla^2 d. \tag{3}$$

Note that the density d of the gas is  $\frac{m}{V}$ , where m and V are its mass and volume. Assume that the molar masses of the four gases A, B, E, and F are respectively  $M_A$ ,  $M_B$ ,  $M_E$ , and  $M_F$ . If there are  $n_A$ ,  $n_B$ ,  $n_E$ , and  $n_F$  moles of each substance in the mixture, then the following equation holds:

$$d = \frac{M_A n_A + M_B n_B + M_E n_E + M_F n_F}{V}$$

C The Eurographics Association 2004.

$$= M_A \frac{n_A}{V} + M_B \frac{n_B}{V} + M_E \frac{n_E}{V} + M_F \frac{n_F}{V}$$
$$= M_A \cdot [A] + M_B \cdot [B] + M_E \cdot [E] + M_F \cdot [F].$$

That is, the density of a mixture of gases is the sum of molar concentrations weighted by the corresponding molar masses.

In moving the substances in the gas mixture, we evolve them separately. That is, given a molar concentration vector  $\mathbf{c} = ([A], [B], [E], [F])$  of a unit cell, Eq. (3) is applied for each substance with its density  $d_A = M_A \cdot [A], d_B = M_B \cdot [B],$  $d_E = M_E \cdot [E]$ , or  $d_F = M_F \cdot [F]$ . After all substances are moved, the new tare concentration vector for a cell is set to  $\mathbf{c} = (\frac{d_A}{M_A}, \frac{d_B}{M_B}, \frac{d_F}{M_F}, \frac{d_F}{M_F}).$ 

In addition to the density, the temperature *T* is also transferred using a similar equation with thermal diffusivity  $\kappa_T$ :

$$\frac{\partial T}{\partial t} = -(\mathbf{u} \cdot \nabla)T + \kappa_T \nabla^2 T + \sigma_T, \qquad (4)$$

which can be viewed as a simple form of the energy conservation equation as used in [Gat02]. Here,  $\sigma_T$  represents a heat source that is useful to control the temperature change because of the chemical reaction. In our framework, only the advection and diffusion terms are computed at this stage. The heat source term is updated at a later stage to reflect the chemical reaction that is considered in the next stage.

#### 3.3. [Stage 3] Application of the chemical kinetics

After the gaseous fluid is evolved, the reaction process  $aA + bB \rightarrow eE + fF$  takes place. In this stage, the reaction rate function  $r = f_r([A], [B], [E], [F])$  must be carefully designed to produce desirable animation effects. In reality, it is determined from various kinds of measurements, and is strictly correct only for ideal systems. In general, the theory assumes that the reaction rate is the same in all parts of a closed system where a reaction takes place. However, such a condition is hard to satisfy when reaction kinetics are applied to a fluid animation. To simulate nonuniform reactions, we discretize the entire reaction system, creating cells aligned with the computational grid on which the fluids are simulated. The molar concentration vector  $\mathbf{c} = ([A], [B], [E], [F])$  is defined at the center of each cell, and the reaction rate is assumed to be constant in the cell.

Once the reaction rate function is defined by an animator, the new concentration **c** is obtained from the old one by integrating the following differential equations over  $\Delta t$ :

$$\frac{d[A]}{dt} = -a \cdot r, \ \frac{d[B]}{dt} = -b \cdot r, \ \frac{d[E]}{dt} = e \cdot r, \ \frac{d[F]}{dt} = f \cdot r. \ (5)$$

When the reaction rate law r is simple, the system of differential equations can be integrated analytically. If it is complicated, a numerical integration technique must be applied. We find that the modified Euler method of order two generally suffices for this purpose, although higher-order methods

I. Ihm, B. Kang & D. Cha / Reactive Gaseous Fluids

Control parameter	Description
$aA + bB \longrightarrow eE + fF$	the chemical reaction type
A, B, E, F	the stoichiometric coefficients
$M_A, M_B, M_E, M_F$	the molar masses
$r = f_r([A], [B], [E], [F])$	the reaction rate law
$k = f_k(T, \cdots)$	the reaction rate constant
$\sigma_T = f_T(r,\cdots)$	the heat source term
$\varepsilon$ (or $\frac{d\varepsilon}{dt}$ ) = $f_{\varepsilon}(r, \cdots)$	the vorticity confinement coefficient
$\phi(\operatorname{or} \frac{d\phi}{dt}) = f_{\phi}(r, \cdots)$	the divergence control factor

**Table 1:** The new control parameters pertaining to chemical reactions. These parameters are introduced in the extension of the fluid simulation method. The last five functional parameters may be defined by simple mathematical expressions or by possibly non-physically based, user-defined procedures. It is also possible to have the stoichiometric coefficients time-dependent for a flexible animation control.

such as the Rosenbrock methods may have to be used for a very stiff system [PTVF92].

#### 3.4. [Stage 4] Update of the external force and $\phi$ value

The fluid's velocity, density, and temperature interact with each other. The density and the temperature are evolved through the velocity field. On the other hand, the updated density and temperature alternately influence the velocity through the external force **f** and the  $\phi$  value, which is a function of pressure.

In the fluid animation, various external forces are possibly applied to affect the way the fluid flows. One of the most frequently used forces is the buoyancy force, which is given in [FM97b, FSJ01] by the weighted combination

$$\mathbf{f}_{buoy} = -\alpha d\mathbf{z} + \beta (T - T_{amb})\mathbf{z},\tag{6}$$

where  $\mathbf{z}$  and  $T_{amb}$  are, respectively, the direction opposite to gravity and the ambient temperature of the environment. In our frame, we apply the same buoyancy force. However, we use the density and temperature values that have been updated as a result of the chemical reaction.

In particular, we allow the reaction process to directly update the temperatures of substances. Temperature is closely related to the heat energy transferred into the system. In [FOA03], a term  $\frac{1}{\rho c_V} \dot{H}$  was added to the equation for temperature evolution to handle the energy transferred because of combustion. We assume that the temperature change rate is a function of any variable including the reaction rate *r*. As the reaction proceeds, the temperature update in Eq. (4) is completed by taking care of the heat source term  $\sigma_T$  according to a user-defined function  $\sigma_T = f_T(r, \cdots)$ .

Another useful force is the vorticity confinement force  $\mathbf{f}_{conf} = \varepsilon h(\mathbf{N} \times \omega)$ , proposed in [FSJ01], which puts the small-scale details back into the simulated fluid. It is possible for the occurring reaction to affect the magnitude of the force by defining  $\varepsilon = f_{\varepsilon}(r, \cdots)$  or  $\frac{d\varepsilon}{dt} = f_{\varepsilon}(r, \cdots)$ , although its influence is not as great as that of the buoyancy force.

After the density *d*, the temperature *T*, and the scale parameter  $\varepsilon$  are updated to reflect the chemical reaction, the resulting force  $\mathbf{f} = \mathbf{f}_{user} + \mathbf{f}_{buoy} + \mathbf{f}_{conf}$  is applied back to the solution of Eq. (1) in the next time frame.

In addition to the external force, we provide another way of controlling the fluid's flow through the  $\phi$  value in Eq. (2), which is set by yet another control function  $\phi = f_{\phi}(r, \cdots)$  or  $\frac{d\phi}{dt} = f_{\phi}(r, \cdots)$  of the reaction rate and other parameters. By defining this function adequately, an animator can freely adjust the fashion in which the gaseous fluid expands or contracts as a result of the chemical reaction.

#### 4. Animation results

We have implemented our simulation technique and applied it to the production of a variety of animation effects involving reactive gaseous fluids. For an effective production, it is quite important to develop a straightforward control mechanism that allows an animator to model desirable effects easily. Since a control mechanism in fluid animation was described in [FM97a], several researchers have attempted to control the motion of fluids. Recently, very interesting techniques for controlling animated fluids have been proposed in [TMPS03, MTPS04, FL04].

As the fluid simulation method is extended, additional physically motivated control parameters, summarized in



**Figure 1:** Two examples of a simple reaction  $A + B \rightarrow 2E$ . The first sequence shows a natural animation in which two gases react with each other producing a third. In the second example, we made the produced gas heavier by controlling its molar mass, inducing the gases to move downwards.

Table 1, are introduced. Once a chemical reaction type  $aA + bB \longrightarrow eE + fF$ , which is to be applied in the animation is determined, the remaining parameters must be set carefully to describe the reaction effects that the animator desires to create. Each parameter may be defined by a simple mathematical expression, or it may be any procedure written by the animator, as in [FM97a] and subsequent papers. Also, it may be designed to be time-dependent for a flexible animation control. The definition of these parameters may not be necessarily physically based. In our experimentation, we often find that an ad hoc, non-physically based definition of the control procedures that characterizes a desired reaction effect produces very realistic looking and interesting animation results.

We now present some examples of animations that demonstrate how the proposed simulation method with a proper setup of control parameters can be used effectively to create realistic reactive fluid effects.

### 4.1. A simple reaction of two gases

The frames in the first row of Figure 1 illustrate an animation of two reactive gases A (in white) and B (in light blue) simulated on a  $60 \times 60 \times 60$  grid. As they are mixed, another gas E (in pink) is produced according to the stoichiometric equation  $A + B \longrightarrow 2E$ . The resulting animation demonstrates that a straightforward addition of this simple chemical reaction in the fluid simulation method successfully creates a very natural visual effect of reacting fluids.

In the next animation, in the second row of Figure 1, we tried to make the produced gas *E* heavier by adjusting its molar mass  $M_E$ . Recall that the density of the gas mixture is  $d = M_A \cdot [A] + M_B \cdot [B] + M_E \cdot [E]$ . When a larger value of  $M_E$ 

is applied, the total density increases as the reaction continues. At some point, the gravity force term of the buoyancy force  $\mathbf{f}_{buoy}$  in Eq. (6) starts dominating the buoyancy force term, inducing an external force towards the floor. As the force is reflected in the velocity field through the Navier– Stokes equations, the gases move towards the floor as expected. It should be mentioned that all the gases move down together rather than the relatively lighter gases *A* and *B* continuing to rise. This is because our method maintains only one velocity field, even though many gases are involved in the simulation. More natural animations could be possible if the velocity fields were computed independently for each gas, as is often done in computational fluid dynamics, although this has higher computational costs.

## 4.2. Gas-phase explosion-like effects using a simple reaction

Figure 2 demonstrates several scenes animating two highly reactive gases simulated using a  $80 \times 80 \times 80$  grid. In this scenario, a gas *A* (in light blue) descends into the pool where another gas *B* (in white) exists. As the two gases contact, they burn and generate a gas *C* (in red) as a product. The energy released by the burning process increases the temperature of the gases, resulting in thermal buoyancy. While most phenomena of combustion and explosion are known to be catalytic chain reactions that usually involve free radicals as intermediates, we used an elementary reaction of the form  $aA + bB \longrightarrow eE$  in an attempt to minimize the computational cost for the simulation of gas-phase explosion effects.

The first animation sequence in the top row was simulated with a = b = 1 and e = 2. In this animation, we employed a reaction rate law  $r = f_r([A], [B], [E]) = k[A][B]$  of overall order two, where the choice of the rate constant k is dis-

<sup>©</sup> The Eurographics Association 2004.



**Figure 2:** Generation of gas-phase explosion-like effects using a simple reaction. The first three animation sequences illustrate how the stoichiometric coefficients in the base equation  $aA + bB \rightarrow eE$  can affect the behavior of the reactive fluids. For a fixed pair (a,b) = (1,1), they were simulated using e = 2, 5, and 7, respectively. The frames in the fourth row were created in an attempt to control the buoyancy force with the reaction rate constant  $k = f_k(T) = \gamma_1 e^{-\frac{\gamma_2}{T}}$ . Using a larger  $\gamma_2$ , it is possible to take longer for the gases to start to move upwards (compare these frames with those in the second row). Finally, we tried to control the heat source term  $\sigma_T$  so that the temperature increases somewhat exponentially. As a result, the gases rise more quickly as shown in the last animation frames (compare these frames with those in the first row).

cussed shortly. We also used a linear heat source function  $\sigma_T = f_T(r) = 30r$ , intending that the temperature increases proportionally to the rate at which the two gases react. As expected, the appearance of the reaction is strongly influenced by the stoichiometric coefficients *a*, *b*, and *e*. When the coefficient *e* increases with fixed *a* and *b*, implying that more molecules are produced than consumed in the reaction process, we observe that the gases start rising more abundantly.

The effect of varying stoichiometric coefficients is reflected in the simulation through the user-defined divergence control function

$$\phi = f_{\phi}([A], [B], [E], T)$$
  
=  $\gamma_0([A] + [B] + [E])(T - T_{amb})$ 

for some control factor  $\gamma_0$ . The functional value is connected to the pressure value *P* in the equation for the ideal gas mix-

© The Eurographics Association 2004.

![](_page_6_Figure_1.jpeg)

**Figure 3:** Two choices of the reaction rate constant  $k = f_k(T) = \gamma_1 e^{-\frac{\gamma_2}{T}}$ . The graphs of the function with two different  $(\gamma_1, \gamma_2)$  pairs are depicted. By adjusting the coefficients  $\gamma_1$  and  $\gamma_2$ , it is possible to control the way the temperature and the buoyancy force vary.

ture  $P = \frac{n_{tot}RT}{V}$ , where  $\frac{n_{tot}}{V}$  corresponds to [A] + [B] + [E], and R is the gas constant. We used this pressure-related quantity as a measure that determines how fast the reacting gases expand. Note that the coefficient e, with e > a + b, causes the total concentration [A] + [B] + [E] to increase, which in turn induces the gases to expand. See the next two animation frames in the second and third rows that were created with e = 5 and 7, respectively. Note that it is also possible to vary the respective speeds at which the reacting gases A and B disappear by controlling the relative magnitude of a and b.

In producing these three examples, we used the rate constant defined by  $k = f_k(T) = \gamma_1 e^{-\frac{\gamma_2}{T}}$  with coefficient values  $\gamma_1 = 30$  and  $\gamma_2 = 24$ , following the Arrhenius equation. We observed that the appearance of the animation can be also controlled intuitively by adjusting these coefficients. Figure 3 depicts two curves corresponding to the different assignments of  $\gamma_2$ . For the larger  $\gamma_2$ , the functional value of the rate constant increases less steeply with respect to temperature. Notice the cycle formed between the heat source term ( $\sigma_T = f_T(r)$ ), the temperature ( $k = f_k(T)$ ), and then the reaction rate  $(r = f_r([A], [B], [E]) = k[A][B])$ . By increasing the value of  $\gamma_2$ , it is possible to restrain the temperature from rising too fast. In other words, it is possible to control the way the buoyancy force increases as a result of the reaction. The animation frames in the fourth row were created using the new  $\gamma_2 = 90$  for the reaction  $A + B \longrightarrow 5E$  (compare these frames with those in the second row). Unlike the previous case, in which the gases rise up as soon as the gases A and B meet, it takes a little longer to start to move upwards because of the relatively slower increase in the buoyancy force.

Another control parameter that greatly affects the appearance of the reaction is the heat source function. In addition to the linear function, we also tested an exponential rate:

$$\sigma_T = f_T(r) = \gamma_3 (e^{\frac{r - r_{min}}{r_{max} - r_{min}}} - 1)$$

where  $[r_{min}, r_{max}]$  is the actual range of the reaction rate and  $\gamma_3$  is a constant. As the reaction proceeds, this exponential function starts to heat up the gases rapidly, which makes the reaction go faster. That heats up the gases more rapidly, and so on. This reaction cycle causes a faster increase in the buoyancy force so that the gases rise more quickly. Compare the frames in the bottom row with ones in the first row.

# **4.3.** Gas-phase explosion-like effects using a chain reaction

When the simple reaction in the previous subsection occurs, the heated gases expand, which causes their concentrations to decrease quickly. The gases also cool down as the heat energy dissipates from the reaction site. These effects tend to prevent an explosive reaction. Such a thermal explosion does not produce a very fast reaction effect unless the entire reaction is contained in a vessel, although some interesting explosion-like effects were made through the simple reaction.

Many very rapid reactions such as explosions are known to proceed by a chain mechanism. In a chain reaction, highly reactive radicals are formed as intermediary species in an initiating step. In the next branching-and-propagating step, these intermediates react with the original reactants, generating more radicals and products. As the reaction proceeds, the radicals are recycled, and build up to produce very fast reaction rates, thus inducing an explosion.

Borrowing an idea from the gas-phase hydrogen and oxygen explosion  $(2H_2 + O_2 \rightarrow 2H_2O)$  [LvE87], we modeled an explosion using a hypothetical reaction  $A + B \rightarrow 5E$ , which occurs by the following chain mechanism:

$$A \longrightarrow 2I$$
  

$$B \longrightarrow 2J$$
  

$$I + B \longrightarrow K + J$$
  

$$J + A \longrightarrow K + I$$
  

$$A + B + K \longrightarrow K + 5E$$

Note that radicals I and J are produced in the initiating step for some reason; for instance, induced by light (the first two reactions), then another radical K is generated rapidly in the next branching step (the next two reactions). The radical Kin turn reacts with the reactants A and B to create the product E in the propagating step (the last reaction).

To simulate this chain reaction, a system of five differential equations was solved on a  $50 \times 60 \times 50$  grid. In this experiment, we used the respective reaction rate functions having partial order one with respect to each reactant. Figure 4

<sup>(</sup>C) The Eurographics Association 2004.

![](_page_7_Figure_1.jpeg)

Figure 4: Generation of gas-phase explosion-like effects using a chain reaction. The first two animation sequences were generated under the identical scenario except that the initial distributions of the reacting gases are different: their concentrations were distributed somewhat uniformly (the first row) and randomly (the second row), respectively. In the third animation, we put the gases in a container from which a fireball came out.

shows some animation results. When the explosion was simulated, the reaction proceeded so rapidly that we had to use a shorter time step  $\Delta t$  until the initial surge in the reaction rates disappears. To create a glowing effect, we employed a spectrum of color ranging from red (low temperature) to orange (high temperature) in rendering the produced gas *E*.

The image frames in the first two rows were produced under the same scenario: a concentrated mass of two explosive gases A and B sits on the ground. When light induces dissociation of the gases, they start to turn into the radicals, then an explosion occurs. As they burst, a rising cloud of gases is generated. A major difference in the setups is the initial distribution of concentrations of A and B. In the first animation, the reacting gases were distributed pretty uniformly. On the other hand, we used a noise function to make their concentrations distributed somewhat randomly, which resulted in a more interesting effect. In the third example, the gases were initially put in a container. As demonstrated in the animation, interaction with the object created a different motion of the fireball.

In the simulation of these examples, we find that small changes in initial values of the control parameters often cause a great impact on the appearance and behavior of gas explosions. Although it was possible to create quite realistic effects using a chain reaction, we feel that more investigation is necessary to develop an effective control mechanism. In this experiment, we did not consider the last terminating step of a chain reaction where the intermediates are removed by one or more inhibiting reactions, completing the reaction. We expect that the reactions in the last stage can be used effectively to control the appearance of the explosive effect.

### 4.4. Catalytic effects

A substance that increases the rate of a reaction and can be recovered chemically unchanged at the end of the reaction is called a catalyst. In other words, the catalyst can be viewed as a substance that increases the reaction rate but does not appear in the overall chemical equation. The animations in Figure 5 illustrate an example of a catalyzed reaction, simulated on a  $60 \times 60 \times 60$  grid, where a solid ball floating through the velocity field in a closed room behaves as a catalyst.

In this simulation, we used a simple reaction equation  $A + B \longrightarrow B + 5C$  so that the gas A (in light blue) turns into another gas C (in red) at the moment it contacts the solid object B. The animation sequence in the first row was produced with a reaction rate function  $r = f_r([A], [B]) = k[A][B]$  of order two. Here, [B] is set to null except in the cells where the object appears. We see that the red gas is generated very realistically along the trace of the moving object.

![](_page_8_Figure_1.jpeg)

Figure 5: Three examples of catalysis. The ball moving in a closed room behaves as a catalyst. As it floats through the velocity field, the red gas is produced along its trace. In the first animation frame, we set up the scene so that the occurring reaction does not affect the temperature. On the other hand, the temperature was made to increase or decrease as a result of the catalyzed reaction in the second and the third frames, respectively. We wanted the ball to ascend or descend as the reaction occurs rather than just float through the velocity field. This control effort is reflected evidently in the created animations.

In the first example, the occurring reaction does not cause any temperature change, but it is again possible to have the reaction process act on the moving object by heating or cooling down the gases. In the second animation sequence, the heat source function  $\sigma_T = f_T(r) = 30r$  was selected to heat the gases near the object where the reaction occurs. The generated heat induces the increased buoyancy force that influences the computation of the velocity fields through the Navier–Stokes equations. As a result of the catalysis, both the gases and the ball rise up. As a contrast, we also tried a negative heat source function  $\sigma_T = f_T(r) = -30r$  to cool down the gases near the ball. As illustrated in the third set of animation frames in the figure, the ball tends to sink rather than proceed through the velocity field as time passes.

#### 5. Conclusions and future work

We have extended a well-accepted fluid simulation method in an attempt to create realistic visual effects for chemically reactive fluids. In our technique, the theory of chemical kinetics was exploited to account for a variety of chemical reactions that are frequently found. We have also described the newly introduced control parameters, and demonstrated how they can be used to generate desired effects intuitively.

Our experience with the animation controls indicates

that a non-physically based characterization of these control parameters often results in very natural and interesting fluid effects. For instance, a heat source function such as  $\sigma_T = f_T(r) = \gamma_4 e^{\gamma_5 r}$  can make the gases rise up and disappear instantly, although this function is physically incorrect (note that the temperature increases for a positive  $\gamma_4$ even if no reaction occurs). It would be worthwhile spending more time to understand how the reaction-related parameters affect the simulation computation. Such an effort will be very valuable in developing an intuitive and easy-tocontrol interface for an animator. Most animation examples in this paper were produced using simple chemical reactions. In fact, there is an abundance of theory in chemical kinetics. Our method is promising in that more complicated chemical reactions may be utilized to create a wider range of special effects. Finding additional classes of chemical reactions appropriate for computer animation is left as a topic of future work.

## References

[BPP01] BEAUDOIN P., PAQUET S., POULIN P.: Realistic and controllable fire simulation. In Proc. of Graphics Interface 2001 (2001), pp. 159– 166. 1

- [BY01] BASHFORTH B., YANG Y.-H.: Physics-based explosion modeling. *Graphical Models* 63, 1 (2001), 21–44. 1
- [Chu02] CHUNG T.: Computational Fluid Dynamics. Cambridge University Press, ISBN 0-521-59416-2, 2002. 1
- [CMTM94] CHIBA N., MURAOKA K., TAKAHASHI H., MIURA M.: Two dimensional visual simulation of flames, smoke and the spread of fire. *Journal of Visualization and Computer Animation 5* (1994), 37–53. 1
- [DEJ\*99] DORSEY J., EDELMAN A., JENSEN H., LEGAKIS J., PEDERSEN H.: Modeling and rendering of weathered stone. In *Proc. of ACM SIGGRAPH 1999* (1999), pp. 225–234. 1
- [Fed97] FEDKIW R.: A Survey of Chemically Reacting, Compressible Flows. PhD thesis, Dept. of Mathematics, Univ. of California, Los Angeles, 1997. 1
- [FL04] FATTAL R., LISCHINSKI D.: Target-driven smoke animation. ACM Transactions on Graphics (ACM SIGGRAPH 2004) 23, 3 (2004). (to appear). 4
- [FM97a] FOSTER N., METAXAS D.: Controlling fluid animation. In Proc. of Computer Graphics International 1997 (1997), pp. 178–188. 4, 5
- [FM97b] FOSTER N., METAXAS D.: Modeling the motion of a hot, turbulent gas. In Proc. of ACM SIGGRAPH 1997 (1997), pp. 181–188. 4
- [FMP92] FOWLER D., MEINHARDT H., PRUSINKIEWICZ P.: Modeling seashells. In Proc. of ACM SIGGRAPH 1992 (1992), pp. 379–387. 1
- [FOA03] FELDMAN B., O'BRIEN J., ARIKAN O.: Animating suspended particle explosions. ACM Transactions on Graphics (ACM SIGGRAPH 2003) 22, 3 (2003), 708–715. 1, 2, 3, 4
- [FSJ01] FEDKIW R., STAM J., JENSEN H.: Visual simulation of smoke. In Proc. of ACM SIGGRAPH 2001 (2001), pp. 23–30. 2, 3, 4
- [Gat02] GATES W.: Animation of Reactive Fluids. PhD thesis, Dept. of Computer Science, The Univ. of British Columbia, 2002. 1, 3
- [HK03] HASINOFF S., KUTULAKOS K.: Photoconsistent 3D fire by flame-sheet decomposition. In Proc. of the Ninth IEEE International Conference on Computer Vision (2003), pp. 1184–1191. 1
- [Lev02] LEVINE I.: *Physical Chemistry*, 5th ed. McGraw-Hill, Inc., ISBN 0-07-253495-8, 2002. 2
- [LF02] LAMORLETTE A., FOSTER N.: Structural

modeling of flames for a production environment. ACM Transactions on Graphics (ACM SIGGRAPH 2002) 21, 3 (2002), 729–735. 1

- [LvE87] LEWIS B., VON ELBE G.: Combustion, Flames and Explosions of Gases, 3rd ed. Academic Press, ISBN 0-12-446751-2, 1987. 7
- [MMA99] MAZARAK O., MARTINS C., AMANATIDES J.: Animating exploding objects. In *Proc. of Graphics Interface 1999* (1999), pp. 211–218.
- [MTPS04] MCNAMARA A., TREUILLE A., POPOVIĆ Z., STAM J.: Fluid control using the adjoint method. ACM Transactions on Graphics (ACM SIGGRAPH 2004) 23, 3 (2004). (to appear). 4
- [NF99] NEFF M., FIUME E.: A visual model for blast waves and fracture. In *Proc. of Graphics Interface 1999* (1999), pp. 193–202. 1, 2
- [NFJ02] NGUYEN D., FEDKIW R., JENSEN H.: Physically based modeling and animation of fire. ACM Transactions on Graphics (ACM SIG-GRAPH 2002) 21, 3 (2002), 721–728. 1, 2
- [PTVF92] PRESS W., TEUKOLSKY S., VETTERLING W., FLANNERY B.: Numerical Recipes in C: The Art of Scientific Computing, 2nd ed. Cambridge University Press, ISBN 0-521-43108-5, 1992. 4
- [RNGF03] RASMUSSEN N., NGUYEN D., GEIGER W., FEDKIW R.: Smoke simulation for large scale phenomena. ACM Transactions on Graphics (ACM SIGGRAPH 2003) 22, 3 (2003), 703–707. 1
- [SF95] STAM J., FIUME E.: Depicting fire and other gaseous phenomena using diffusion processes. In *Proc. of ACM SIGGRAPH 1995* (1995), pp. 129–136. 1
- [Sta99] STAM J.: Stable fluids. In *Proc. of ACM SIG-GRAPH 1999* (1999), pp. 121–128. 2
- [TMPS03] TREUILLE A., MCNAMARA A., POPOVIĆ Z., STAM J.: Keyframe control of smoke simulations. ACM Transactions on Graphics (ACM SIGGRAPH 2003) 22, 3 (2003), 716–723. 4
- [Tur91] TURK G.: Generating textures on arbitrary surfaces using reaction-diffusion. In *Proc. of ACM SIGGRAPH 1991* (1991), pp. 289–298. 1
- [WK91] WITKIN A., KASS M.: Reaction-diffusion textures. In Proc. of ACM SIGGRAPH 1991 (1991), pp. 299–308. 1
- [WLMK02] WEI X., LI W., MUELLER K., KAUFMAN A.: Simulating fire with texture splats. In *Proc. of IEEE Visualization 2002* (2002), pp. 227–234.
- [YOH00] YNGVE G., O'BRIEN J., HODGINS J.: Animating explosions. In Proc. of ACM SIG-GRAPH 2000 (2000), pp. 29–36. 1, 2, 3

© The Eurographics Association 2004.