Animation of Reactive Gaseous Fluids through Chemical Kinetics

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Insung Ihm, Byungkwon Kang, Deukhyun Cha
Dept. of Computer Science, Sogang University
Seoul, Korea

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Motivation

- There are a variety of natural phenomena related to chemical reaction.
  - Combustion, explosion, erosion, catalytic effect, etc.
- These are very useful for producing interesting fluid effects in computer animation.

An Example of
Gas-Phase Explosion

(Side View)

A gas-phase explosion

- However, little work has been done in the general modeling of chemical reactions in the fluid animation field.

Contribution of this paper

- We extend the well-accepted fluid animation technique by [Sta99] and [FSJ01] to effectively handle reactive gaseous fluids.

- We present a set of physically motivated control parameters to control the behavior of reactive fluids.

- The proposed technique generates several interesting fluid effects related to chemical reaction with user control.

Related works

- Gas and smoke

  [FM97b] Foster, N., and Metaxas, D., "Modeling the motion of a hot, turbulent gas," *ACM SIGGRAPH '97*, pp. 181-188, 1997.

  [Sta99] Stam, J., "Stable fluids," *ACM SIGGRAPH '99*, pp. 121-128, 1999.

  [FSJ01] Fedkiw, R., Stam, J., and Jensen, H., "Visual simulation of smoke," *ACM SIGGRAPH '01*, pp. 23-30, 2001.

  [TMPS03] Treuille, A., Mcnamara, A., Popović, Z., and Stam, J., "Keyframe control of smoke simulation," *ACM Transactions on Graphics (ACM SIGGRAPH '03)*, Vol. 22, No. 3, pp. 716-723, 2003.

- Fire, flame, and explosion

[YOH00] Yngve, G., O'Brien, J., and Hodgins, J., "Animating explosions," *ACM SIGGRAPH '00,* pp. 29-36, 2000.

Courtesy of [FOA03]

[NFJ02] Nguyen, D., Fedkiw, R., and Jensen, H., "Physically based modeling and animation of fire", *ACM Transactions on Graphics (ACM SIGGRAPH '02)*, Vol. 21, No. 3, pp. 721-728, 2002.

[FSJ03] Feldman, R., Stam, J., and Jensen, H. "Animating suspended particle explosions," *ACM Transactions on Graphics* (*ACM SIGGRAPH '03*), pp.708-715, 2003.

- Reactive fluids

  [Fed97] R. Fedkiw, “A survey of chemically reacting, compressible flows,” PhD thesis, Dept. of Mathematics, Univ. of California, Los Angeles, 1997.

  [Gat02] W. Gates, “Animation of Reactive fluids,” PhD thesis, Dept. of Computer Science, Univ. of British Columbia, 2002.

Introduction to chemical kinetics

- What is chemical kinetics?
  - ✓ A branch of kinetics that studies the rates and mechanisms of chemical reactions.

- Stoichiometric equation

$$\boxed{aA + bB \rightarrow eE + fF}$$

  - A, B, E, F : chemical species (reactants & products)
  - a, b, e, f : stoichiometric coefficients

- Reaction rate (a.k.a. rate law)

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

  - Describes the rate r of change of the concentrations, denoted by [*], of reactants and products.

- How to decide the reaction rate r :
  - r : a function of the concentrations of species present at time t, which is usually measured experimentally.
  - For a large class of chemical reactions, it is proportional to the concentration of each reactant/product raised to some power.
    - When, for example, only a forward reaction occurs,

$$\boxed{r = f_r([A],[B],[E],[F]) = k[A]^{\alpha}[B]^{\beta}}$$

  - Once the rate is determined, $[A]$, $[B]$, $[C]$ and $[D]$ are updated by integrating the rate law over time interval.

- Rate constant k
  - Is a function of both temperature and pressure.
  - Usually, the pressure dependence is ignored.

  - For many homogeneous reactions,

$$\boxed{k = Ae^{-\frac{Ea}{RT}}}$$

Arrhenius equation

The Navier-Stokes equations for gaseous fluids

- The simulation technique by [Sta99] and [FSJ01] are well-accepted in computer animation.

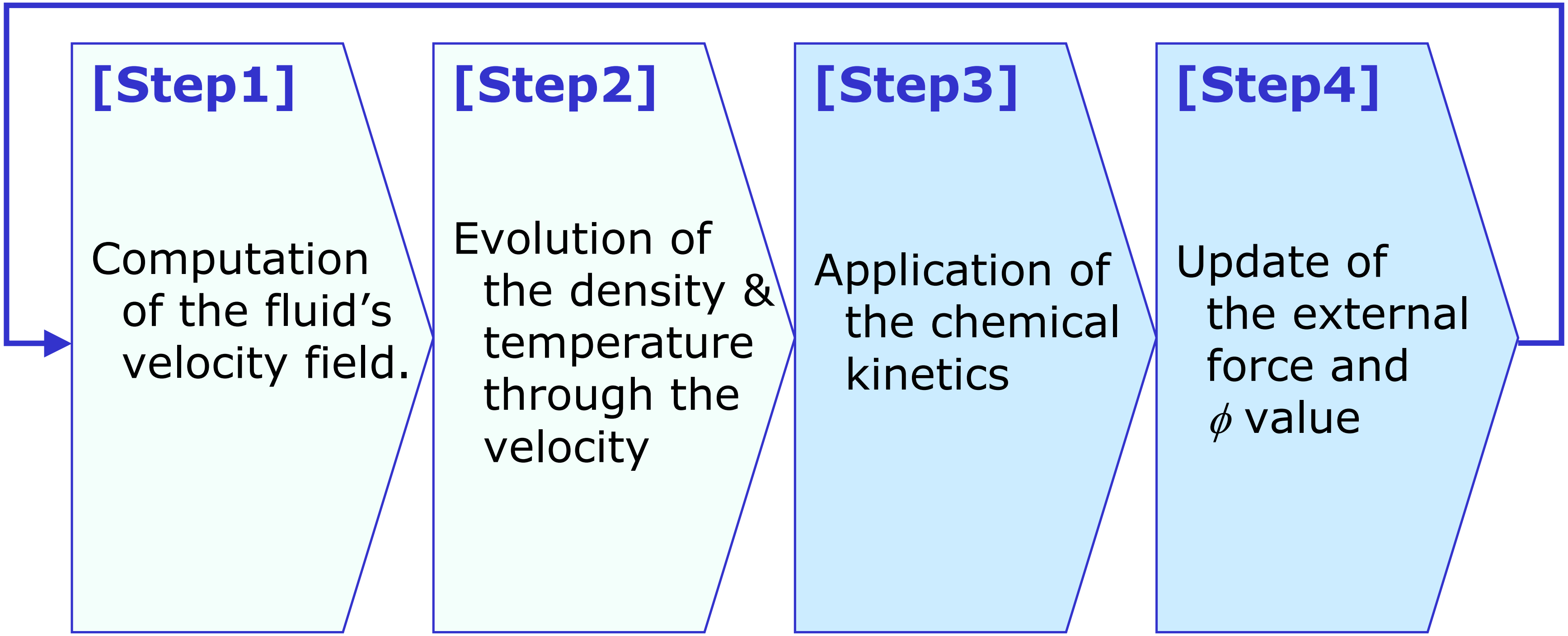
- The incompressible Navier-Stokes equations for inviscid fluids
  - Conservation of mass

$$\boxed{\nabla \cdot u = 0}$$

  - Conservation of momentum

$$\boxed{\frac{\partial u}{\partial t} = -(u \cdot \nabla)u + v\nabla \cdot (\nabla u) - \frac{1}{\rho}\nabla p + f}$$

The proposed simulation method



[Step1]

Computation of the fluid's velocity field.

[Step2]

Evolution of the density & temperature through the velocity

[Step3]

Application of the chemical kinetics

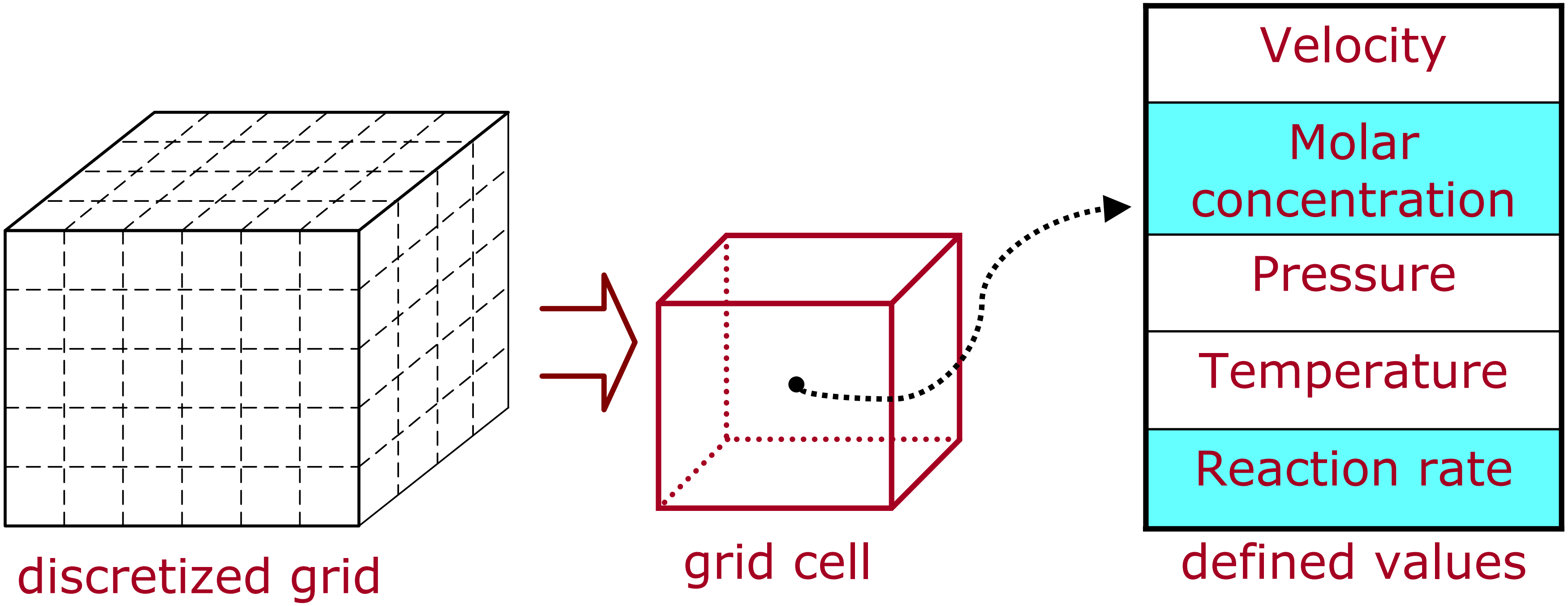
[Step4]

Update of the external force and ϕ value

The simulation technique by [Sta99] and [FSJ01], as slightly modified, comprises **[Step1]** and **[Step2]**.

Grid values used in this method

- Several values are defined at the center of the grid cell



[Step1] Computation of the fluid’s velocity field

- Uses a modified mass conservation equation, as in [FOA03], to control the expansion/contraction of reactive gases:

$$\boxed{\nabla \cdot u = \phi}$$

- The divergence constraint ϕ is determined for each cell according to the reaction process that occurs in the region.
  - Determined in **[Step4]** after the application of chemical kinetics.
- The pressure is computed through the modified Poisson equation:

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

[Step2] Evolution of the density and temperature through the velocity

- Density field
  - Similarly as in [Sta99] and [FSJ01] except that multiple substances in the gas mixture are handled:

$$\boxed{\frac{\partial d}{\partial t} = -(u \cdot \nabla)d + \kappa_d \nabla^2 d}$$

- Each substance is evolved separately.
  - Molar concentrations and densities are related by molar masses M_A, M_B, M_E, M_F.

$$\boldsymbol{c} = ([A],[B],[C],[D])$$

$$\downarrow$$

$$\boldsymbol{d} = (d_A, d_B, d_E, d_F) = (M_A \cdot [A], M_B \cdot [B], M_E \cdot [E], M_F \cdot [F])$$

$$\downarrow$$

Evolve d_A, d_B, d_E, d_F .

$$\downarrow$$

$$\boldsymbol{c} = (\frac{d_A}{M_A}, \frac{d_B}{M_B}, \frac{d_E}{M_E}, \frac{d_F}{M_F})$$

- Temperature field
  - Similarly as in [Sta99] and [FSJ01] except that a heat source term σ_T is added.

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

  - The heat source term is updated for each cell in **[Step4]** to reflect the occurring chemical reaction in the region.

[Step3] Application of the chemical kinetics

- The reaction process $aA + bB \rightarrow eE + fF$ is applied for each cell in the reaction system.

① Determine the reaction rate $r = f_r([A],[B],[E],[F])$ as designed by an animator.

② Then, the new concentration vector $\boldsymbol{c}$ is updated by integrating the differential equations over Δt:

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

[Step4] Update of the external force and ϕ value

- The updated density d, temperature T, and reaction rate r influence the velocity through the external force $\mathbf{f}$ and the ϕ value..

① The temperature update is completed by taking care of the heat source term σ_T, defined by $\sigma_T = f_T(r,\cdots)$.

② The buoyancy force, as proposed in [FSJ01], is updated:

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

③ The vorticity confinement force, as proposed in [FSJ01], is updated according to $\varepsilon = f_{\varepsilon}(r,\cdots)$ or $\frac{d\varepsilon}{dt} = f_{\varepsilon}(r,\cdots)$:

$$\boxed{\mathbf{f}_{conf} = \varepsilon h(N \times \omega)}$$

④ The resulting external force $\mathbf{f} = \mathbf{f}_{user} + \mathbf{f}_{buoy} + \mathbf{f}_{conf}$ is applied to the momentum conservation equation in the next time frame.

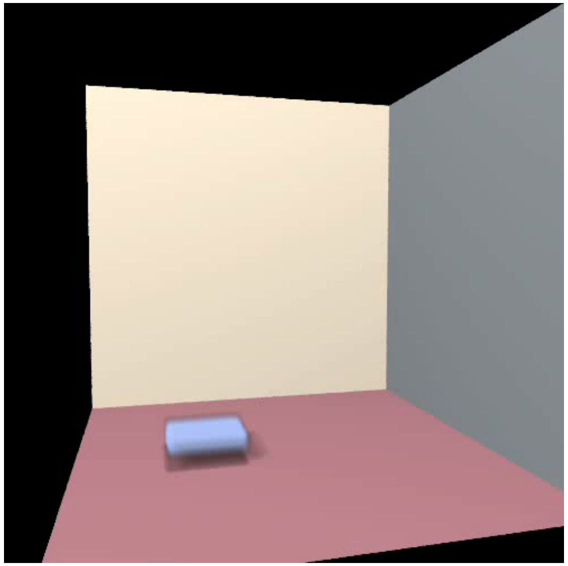
⑤ The ϕ value, determined by $\phi = f_{\phi}(r,\cdots)$ or $\frac{d\phi}{dt} = f_{\phi}(r,\cdots)$, is applied to the modified mass conservation equation in the next time frame.

Added control factors

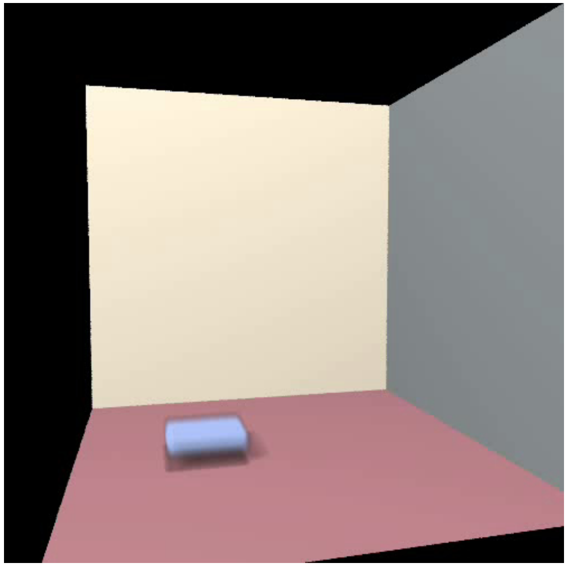
Control parameter	Description
$aA + bB \rightarrow eE + fF$	the chemical reaction type
A, B, E, F	the stoichiometric coefficients
M_A, M_B, M_E, M_F	the molar masses
$r = f_r([A],[B],[E],[F])$	the reaction rate law
$k = f_k(T, \cdots)$	the reaction rate constant
$\sigma_T = f_T(r, \cdots)$	the heat source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

[Animation ex. 1] A simple reaction $A+B\rightarrow 2E$ of two gases

- Control factor: Molar mass M_E to generate a heavier smoke



An example

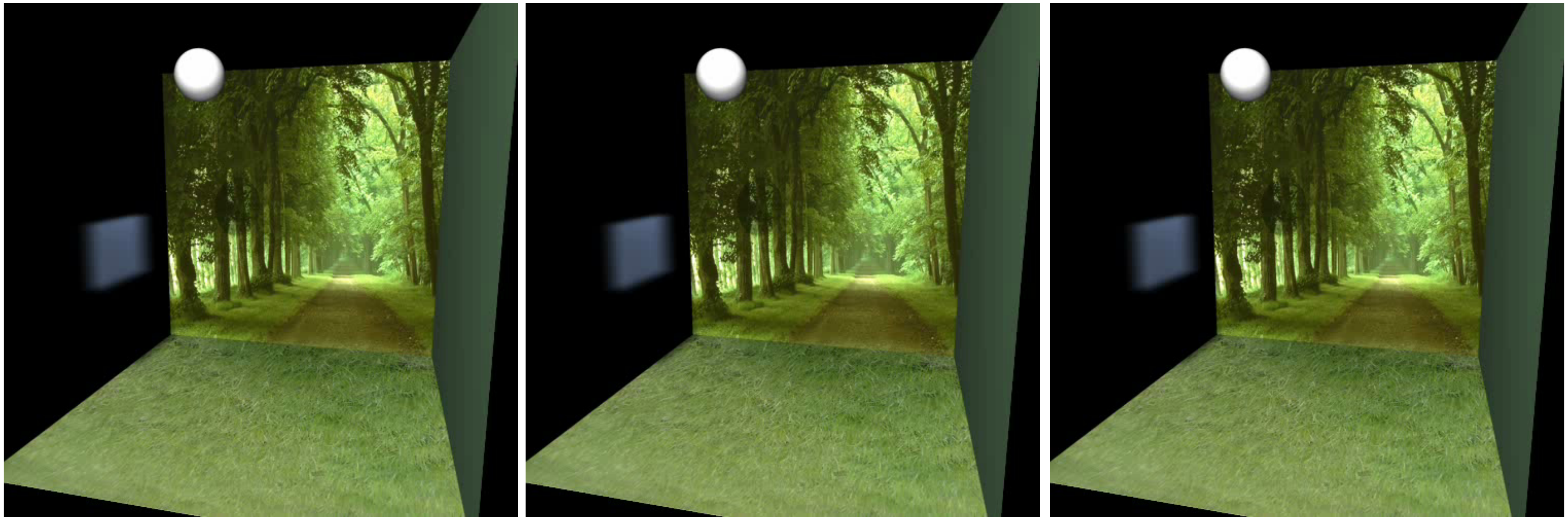


With an increased M_E

Note that the density d affecting the buoyancy force $\mathbf{f}_{buoy}$ is defined as $d = M_A \cdot [A] + M_B \cdot [B] + M_E \cdot [E]$.

[Animation ex. 2]
A catalytic reaction $A + B \rightarrow B + 5C$

- Control factor: the heat source term σ_T



No heat source

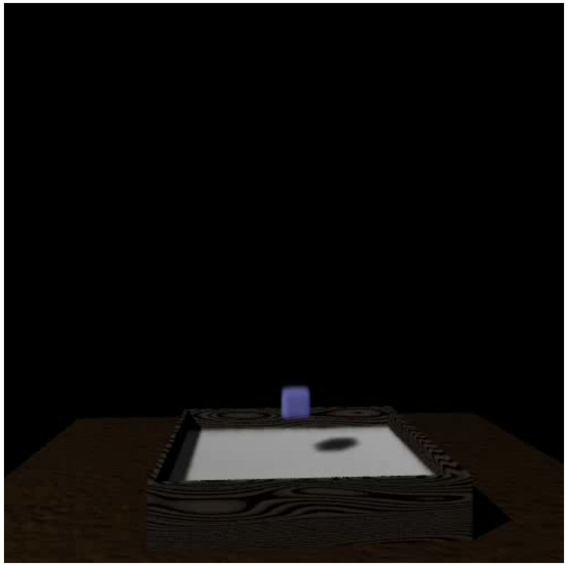
$\sigma_T = f_T(r, \cdots) = 30r$

$\sigma_T = f_T(r, \cdots) = -30r$

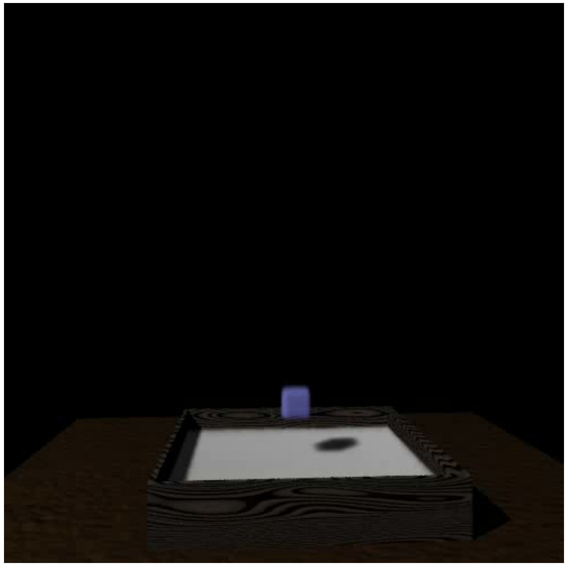
B denotes a catalyst that is the floating ball in this example.

[Animation ex. 3] Gas-phase explosion-like effects using a simple reaction $aA + bB \rightarrow eE$

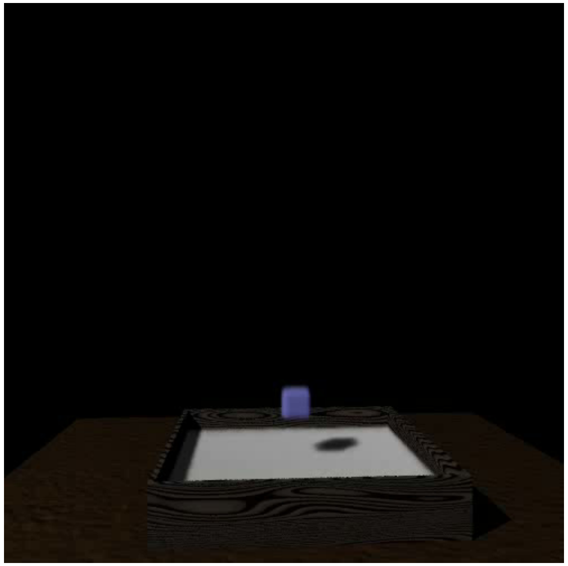
- Control factor: stoichiometric coefficients a, b, and e



$a = 1, b = 1, e = 2$



$a = 1, b = 1, e = 5$

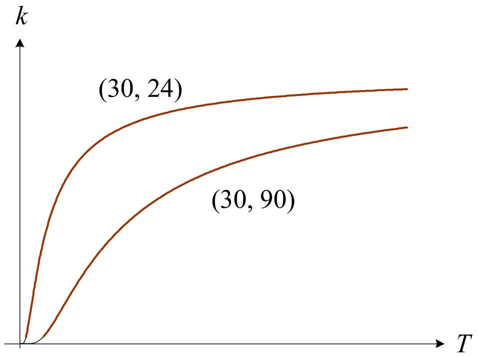


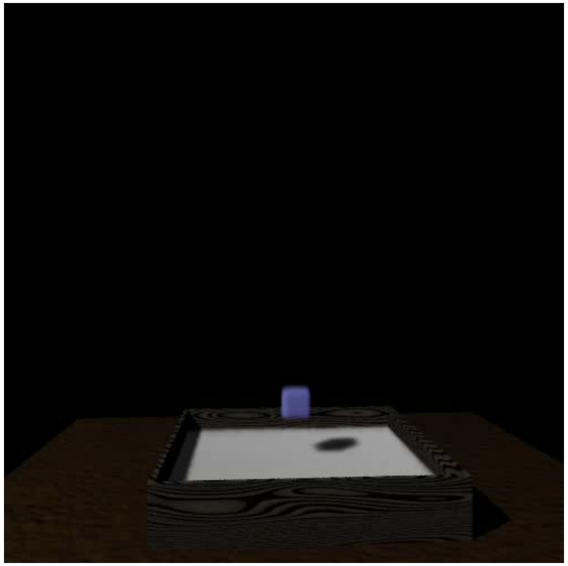
$a = 1, b = 1, e = 7$

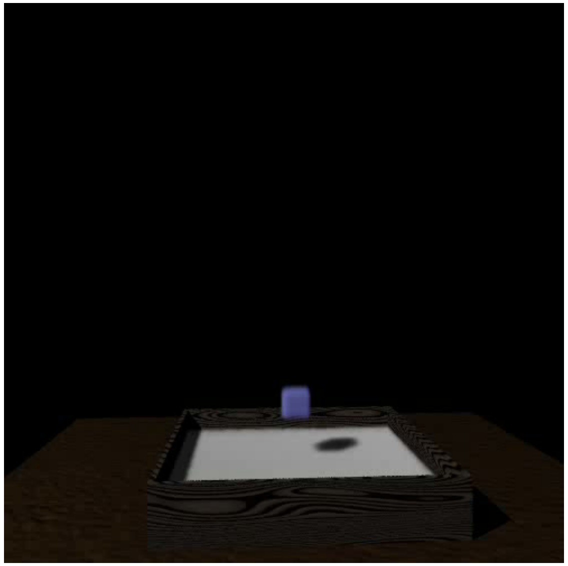
The same control parameters except the stoichiometric coefficients were applied to these animations:

$$r = k[A][B],\ \sigma_T = 30r,\ \phi = \gamma_0([A]+[B]+[C])(T - T_{amb}),\ k = 30e^{-\frac{24}{T}}$$

- Control factor: rate constant $k = \gamma_1 e^{-\frac{\gamma_2}{T}}$

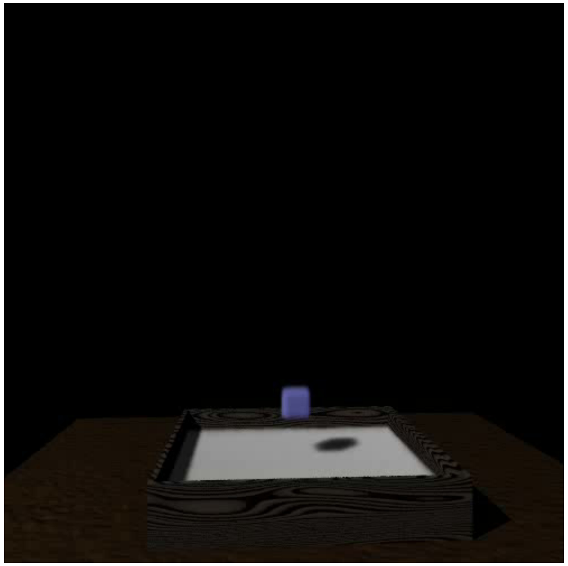



With $\gamma_1 = 30,\ \gamma_2 = 24$

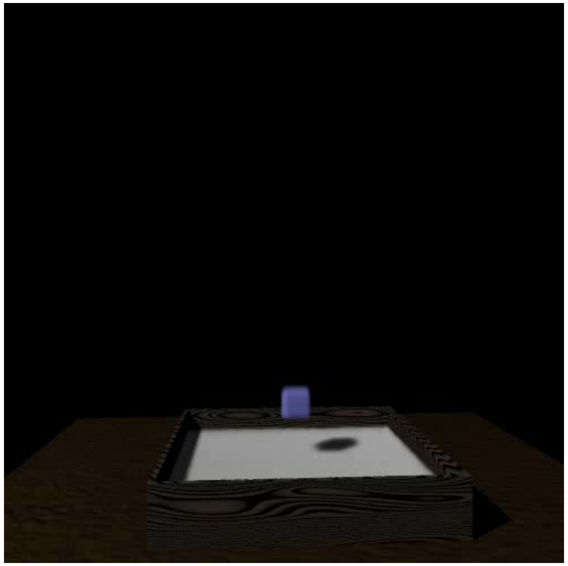

With $\gamma_1 = 30,\ \gamma_2 = 90$

For the larger γ_2, the rate constant k increases less steeply w.r.t. temperature, resulting that the temperature, hence the gases, are restrained from rising too fast.

- Control factor : heat source term σ_T



With $\sigma_T = 30r$



With $\sigma_T = e^r$

The exponential heat source function heats up the gases rapidly, which makes the reaction go faster. As a result, the gases rise very quickly.

[Animation ex. 4] Gas-phase explosion-like effects using a chain reaction

- Control factor: the chemical reaction type
  - Most combustion reactions and explosions are known to proceed by a chain mechanism.
  - Ex.: the gas-phase hydrogen and oxygen explosion
    - Highly reactive radicals are formed as intermediary species.
    - They build up to produce very fast reaction rates as they are recycled.

$$2H_2 + O_2 \rightarrow 2H_2O$$

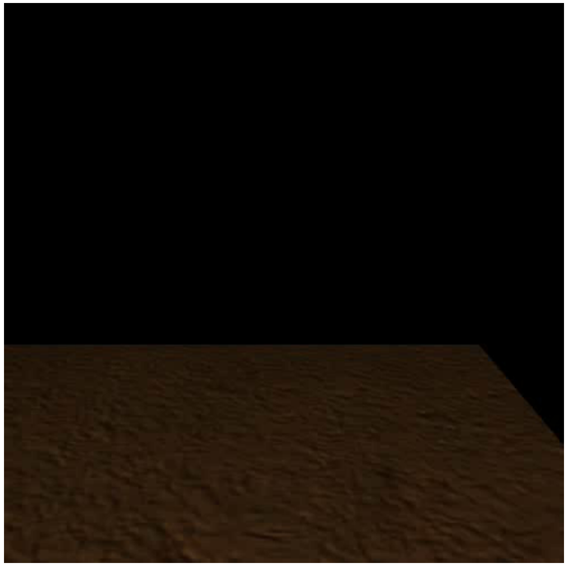
$$\downarrow$$

Reaction	Stage
$\mathrm{H_2 \rightarrow H\bullet + H\bullet}$	Initiation
$\mathrm{H\bullet + O_2 \rightarrow \bullet OH + O\bullet}$ $\mathrm{O\bullet + H_2 \rightarrow \bullet OH + H\bullet}$	Branch
$\mathrm{\bullet OH + H_2 \rightarrow H_2O + H\bullet}$ $\mathrm{H\bullet + O_2 \rightarrow HO_2\bullet}$ $\mathrm{HO_2\bullet + H_2 \rightarrow H_2O + \bullet OH}$	Propagation
$\mathrm{H\bullet + H\bullet \rightarrow H_2}$	Termination

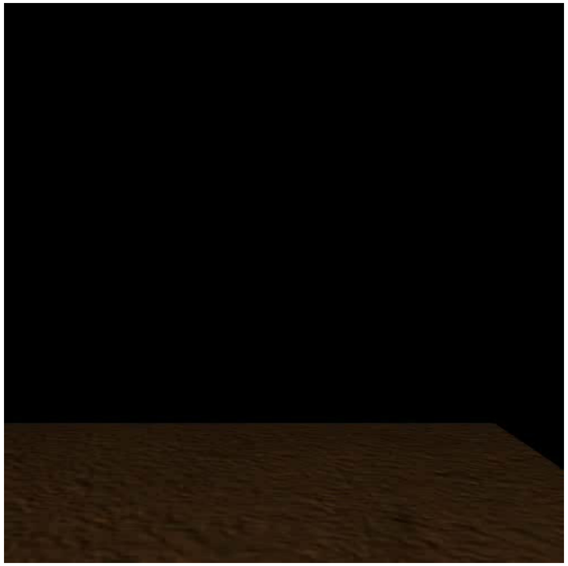
– A hypothetical chain reaction

$$A + B \to 5E \quad \longrightarrow \quad \begin{aligned} &A \to 2I \\ &B \to 2J \\ &I + B \to K + J \\ &J + A \to K + I \\ &A + B + K \to K + 5E \end{aligned}$$

✓ Note that I, J, and K are radicals.



Uniform initial distribution of A and B



Random initial distribution of A and B

Conclusions & Future works

- We proposed a new simulation method handling chemical reaction.
- We proposed several new control factors and demonstrated how they can be used to generate realistic visual effects.
- More chemical reactions may be utilized to create a wider range of special effects.
- More realistic rendering scheme for explosion, flame, and other natural phenomena can be further researched and developed.

Thank you!

An Example of
Gas-Phase Explosion

(Side view)