

Introduction to Reactive Fluid Dynamics

Toshihisa Ueda
School of Science
for Open and Environmental Systems
Keio University, Japan

- *Basic concept of reactive flows*
- *Combustion*
- *Mixing and reaction in high viscous fluid*
- *Application of Chaos*

- *Basic concept of reactive flows*

Basic concept of reactive flows

What is reactive flows ?



- *The flows with reactions*
 - *combustion*
 - *air pollution*
 - *chemical reactor*
 - *bio reactor*

Basic concept of reactive flows

Most important point of reactive fluids



- **multi-component fluid**
 - fluid consists of reactants and products
 - species concentration changes locally and temporally
 - with heat release or absorption

Basic concept of reactive flows

Basis of Reactive Fluid Dynamics



- **Chemical reaction mechanism**
- **Fluid dynamics**
- **Thermodynamics**
- **Transport phenomena**

Basic concept of reactive flows

Concentration and fraction



- **Concentration: amount / unit volume**
 - mass concentration m_i [kg/m³]
 - molar concentration c_i [mol/m³]
- **Fraction: ratio of concentration**
 - mass fraction $Y_i = m_i / \sum m_j$
 - molar fraction $X_i = c_i / \sum c_j$

Basic concept of reactive flows

Understanding reactive flows



- **flow motion**
 - velocity and pressure u, v, w, p
- **energy transport**
 - temperature T
- **species transport**
 - mass fraction of chemical species Y_i

Basic concept of reactive flows

Governing equations



- Conservation equations of physical motion
 - mass, momentum, energy, chemical species
- Equations of chemical variations
 - Chemical reaction formula
 - Rate equations for chemical reaction
 - concentration dependence
 - temperature dependence

Basic concept of reactive flows

Conservation equations of physical motion



$$\text{Mass: } \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0$$

$$\text{Momentum: } \rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}$$

$$\text{energy: } \rho \frac{Dh}{Dt} = -\nabla \cdot \left(q + \sum_i \rho_i U_i h_i \right) + \frac{Dp}{Dt} + \Phi$$

($dh = C_p dT$: for perfect gases)

$$\text{chemical species: } \rho \frac{DY_i}{Dt} = -\nabla \cdot (\rho_i U_i) + w_i$$

Basic concept of reactive flows

Reaction model



Reaction model



Reaction rate equation

$$\text{Concentration : } \omega_{\text{CH}_4} [\text{kmol/m}^3\text{s}] = -\frac{dc_{\text{CH}_4}}{dt} = -kc_{\text{CH}_4}^a c_{\text{O}_2}^b$$

$$\text{Temperature } k = A \exp\left(-\frac{E_a}{R_0 T}\right) = AT^n \exp\left(-\frac{E_a}{R_0 T}\right)$$

;

Basic concept of reactive flows

Passive scalar or active scalar ?



- Passive scalar : scalar variables passive for flow motion
- Active scalar : scalar variables active for flow motion
- constant properties \Rightarrow Passive scalar
- variable properties \Rightarrow Active scalar

Basic concept of reactive flows

Passive: constant property

$$\text{Mass: } \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0$$

$$\text{Momentum: } \rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}$$

u, v, w, p

$$\text{energy: } \rho \frac{Dh}{Dt} = -\nabla \cdot \left(q + \sum_i \rho_i U_i h_i \right) + \frac{Dp}{Dt} + \Phi$$

$$\text{chemical species: } \rho \frac{DY_i}{Dt} = -\nabla \cdot (\rho_i U_i) + w_i$$

Basic concept of reactive flows

Active: variable property

$$\text{Mass: } \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0$$

$$\text{Momentum: } \rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}$$

$(Y_i, T), \mu(Y_i, T)$

u, v, w, p

$$\text{energy: } \rho \frac{Dh}{Dt} = -\nabla \cdot \left(q + \sum_i \rho_i U_i h_i \right) + \frac{Dp}{Dt} + \Phi$$

$$\text{chemical species: } \rho \frac{DY_i}{Dt} = -\nabla \cdot (\rho_i U_i) + w_i$$

Basic concept of reactive flows

Non-dimensional parameter for reactive flows

$$\text{Damköhler number: } Da = \frac{\tau_f}{\tau_c}$$

τ_f : characteristic time of fluid motion (mixing)

τ_c : characteristic time of chemical reaction

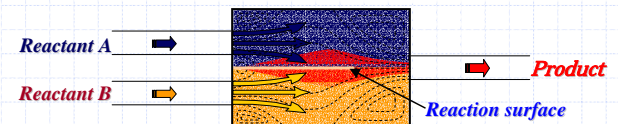
Basic concept of reactive flows

Damköhler number

$$\tau_f \gg \tau_c \quad Da \rightarrow \infty \quad Da = \frac{\tau_f}{\tau_c}$$

The chemical reaction is much faster than the fluid motion,
e.g. engines, high temperature chemical reactors
Fluid motion (mixing) determines
the progress in chemical reaction

the chemical reaction instantly occurs in reaction surface,
as soon as reactants meet



Basic concept of reactive flows

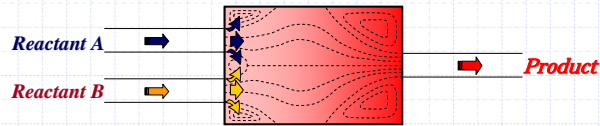
Damköhler number

$$\tau_f \ll \tau_c \quad Da \rightarrow 0 \quad Da = \frac{\tau_f}{\tau_c}$$

The fluid motion is much faster than the chemical reaction,
e.g. low temperature chemical reactors, bioreactors

Rate of chemical reaction determines
the progress in chemical reaction

Chemical reaction gradually occurs
after Reactants mix well



Basic concept of reactive flows

Mixing

Mixing due to Molecular diffusion

➡ Molecular level mixing
necessary for chemical reaction

➡ Newton's law for momentum transfer $\tau = \mu \frac{du}{dy} = v \frac{d(\rho u)}{dy}$

Fourier's law for heat conduction $q = k \frac{dT}{dy} = \alpha \frac{d(\rho C_p T)}{dy}$

Fick's law for species diffusion $j_i = D \frac{dm_i}{dy}$

Basic concept of reactive flows

Mixing

Mixing due to advection

- ➡ Turbulent advection (Turbulent mixing)
mixing by multi-scale vortex motion
- Chaotic advection (Chaotic mixing)
mixing by stretching and folding

Basic concept of reactive flows

Mixing

When the viscosity is low

➡ Mixing due to turbulence is effective

When the viscosity is high

➡ It is not easy to make the flow turbulent
It is necessary to enhance the mixing
even in laminar flow condition

➡ Chaotic mixing

Basic concept of reactive flows

Non-steady motion opens new world

- **Periodic motion**
 - *precise control is possible*
- **Turbulent motion**
 - *transport, such as mixing, is enhanced*
 - *most reactive systems use turbulent motion*
 - *engines*
 - *furnaces*
 - *reactors*

Basic concept of reactive flows

Non-steady motion opens new world

- **Chaotic advection**
 - *enhance laminar mixing*
 - *in low Reynolds number area*
 - *low velocity* ⇒ *heat island issue*
 - *low shear* ⇒ *bio reactor*
 - *small area* ⇒ *micro reactor*
 - *high viscous fluids* ⇒ *polymer technology*
 - *non-Newtonian fluids* ⇒ *artificial organs*

- **Combustion**

Combustion

Combustion plays a key role in many energy devices

- **Engines**
- **Furnaces**

“Dynamics of Combustion” is a future technology for improving combustion

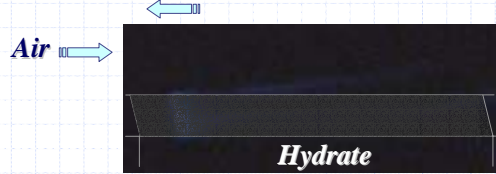


Bunsen flame with burner rotation

Combustion

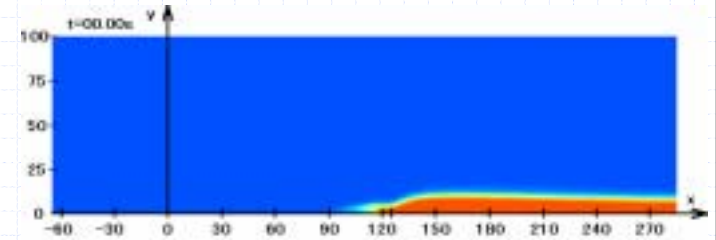
Combustion over a Clathrate Hydrate

The flame front propagates upstream direction



Combustion

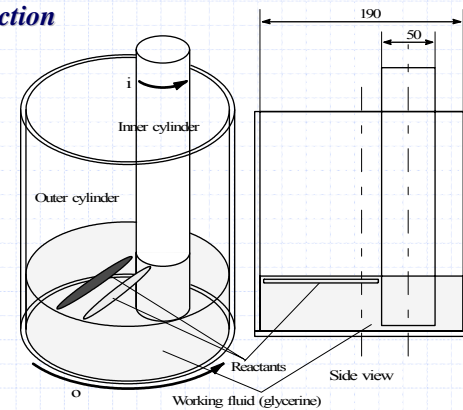
Combustion over a hydrate can be predicted numerically



□ Mixing and reaction in high viscous fluid

Mixing and reaction in high viscous fluids

Test section



Mixing and reaction in high viscous fluids

Parameters

Working fluid; Glycerin 1300ml (98wt%)

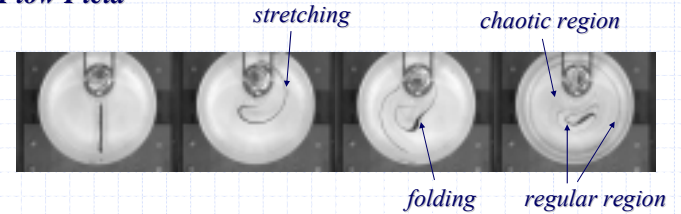
Ratio of radii;
 $\frac{R_i}{R_o} = 0.26$

Eccentricity;
 $\varepsilon \equiv \frac{d}{R_o - R_i}$

Chemical reaction; $\text{Fe}^{3+} + \text{K}_4[\text{Fe}(\text{CN})_6] \rightarrow \text{KFe}[\text{Fe}(\text{CN})_6] + 3\text{K}^+$
Yellow Red Dark blue

Mixing and reaction in high viscous fluids

Flow Field



Chaotic region \Rightarrow The mixing occurs well

Regular region \Rightarrow The mixing occurs scarcely

Mixing and reaction in high viscous fluids

Effect of initial locations



Both reactants are initially located in the regular region



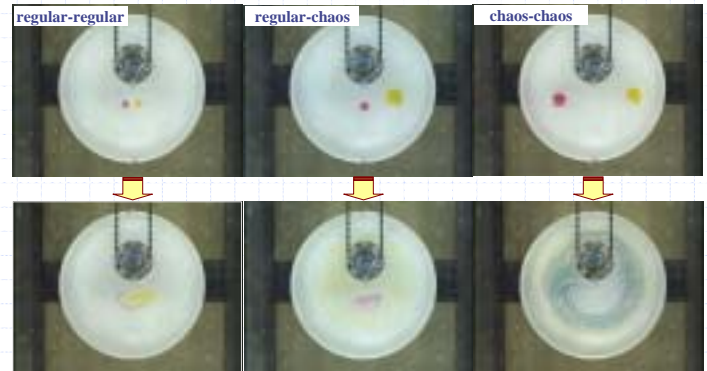
One reactant is in regular, the other in chaotic region



Both reactants are initially located in the chaotic region

Mixing and reaction in high viscous fluids

Effect of initial locations



□ Application of Chaos

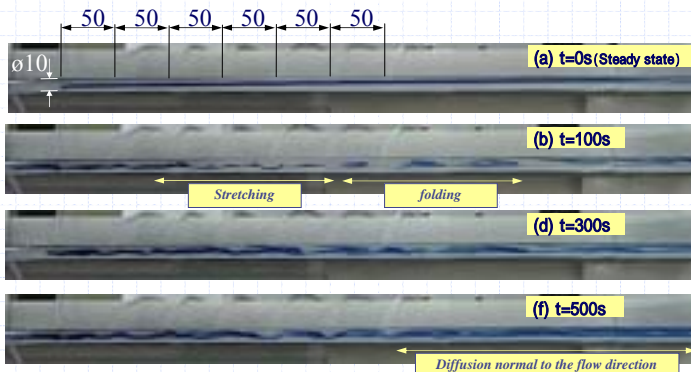
Application of Chaos

Non-element mixer and reactor

Non-element mixer and reactor is realized by using chaotic advection (chaotic mixing)

- *High viscosity*
 - *mixing and reaction in laminar flow condition*
- *Micro scale and low speed*
 - *Micro, millimeter scale machines*
- *Low shear*
 - *polymer fluid, bio fluid*

Application of Chaos



Summary

Reactive Fluid Dynamics

Combustion

Mixing and reaction in laminar flow condition

Micro, millimeter scale machines

Application of chaos

Reactive Fluid Dynamics is an important, interesting and challenging field