Species Transport and Reactive Flows

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Outline

- Quick recap of transport equation
- Species Transport
  - Dispersion
  - Mixing
  - Residence time distribution
  - Phase transfer
- Simulation of reactive flows
  - Species with reaction
  - Homogeneous reactions

Motivation for Modelling

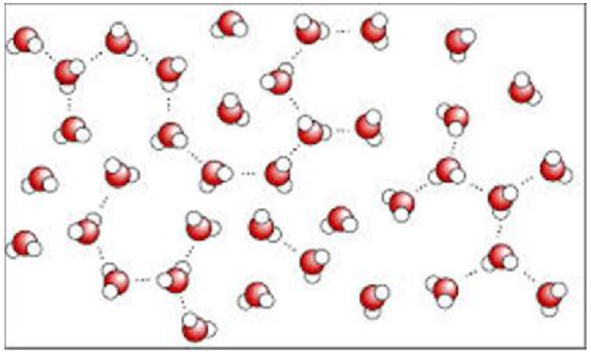
- What are the uses of modelling
  - Applications

Levenspiel
Chemical Reactor Omni Book

- Why systems are modelled
  - Significance and relevance

Continuum

- Continuously fill the domain



Knudsen

- Knudsen number

$$Kn = \frac{\lambda}{L}$$

Governing Equations

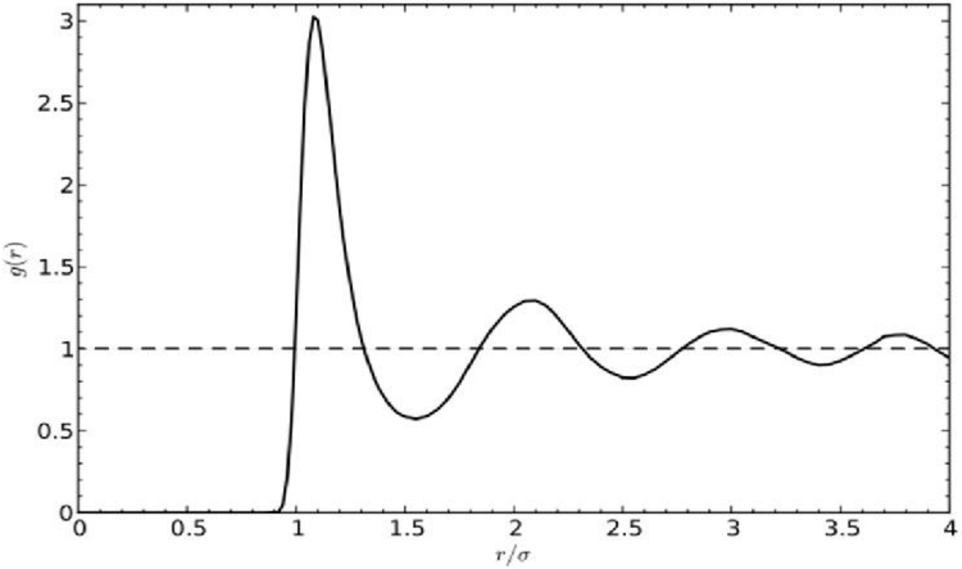
- Conservation of mass
- Conservation of momentum

Transport Equations

- Conservation of energy

- Concept of CV

$$\rho = \lim_{\delta\forall \to \forall^*} \frac{\delta m}{\delta \forall}$$



Generic Transport Equation

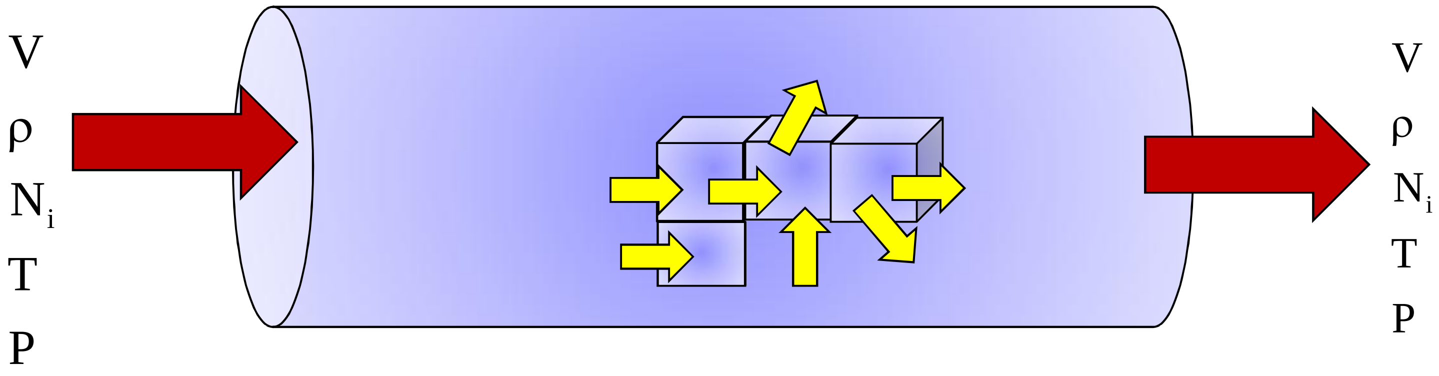
- Transport equation for a quantity ϕ

$$\frac{\partial(\rho\phi)}{\partial t} + \mathrm{div}(\rho\vec{V}\phi) = \mathrm{div}\left(\Gamma\ \mathrm{grad}\,\phi\right) + S_{\phi}$$

$\frac{\phi}{\forall\, t}$ Accumulation + Net outflow = Net Diffusion + Net source $\frac{\phi}{m^3\, s}$

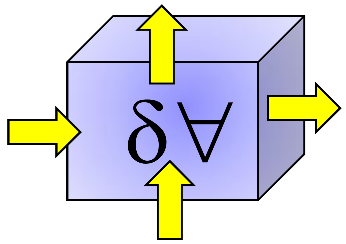
Equation	**Specific quantity f (per unit mass)**	G	**S$_f$**
Mass balance	1	0	0
Momentum balance	u	μ	∇P ρg
Energy balance	C_pT	k	$-\Delta H_R$ $UA\Delta T$
Species balance i	x_i	D	r_i

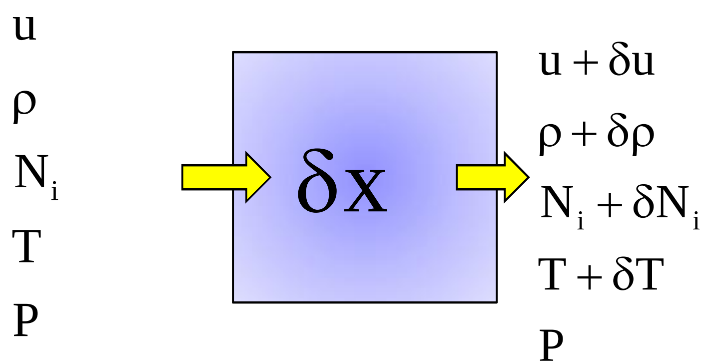
Advection



Balance	**Unit Mass**	**Unit Volume**
$\dot{m} = \rho u A$	1	$\frac{\dot{m}}{\delta\forall} = \rho$
$\dot{P} = \dot{m} u$	u	$\frac{\dot{P}}{\delta\forall} = \rho u$
$\dot{Q} = \dot{m} C_P T$	$C_P T$	$\frac{\dot{Q}}{\delta\forall} = \rho C_P T$
N_i	x_i	$\frac{N_i}{\delta\forall} = C_i = \rho x_i$

How small is this infinitesimally small CV?





Diffusion

- Molecular means of transport
- Newton’s law of Viscosity
- Fick’ law
- Fourier’s law

Not, All That Easy

$$\text{Flux} \propto \frac{\Delta \phi}{\Re} = -\Gamma \; \Delta \phi$$

Reactive flows

- Homogeneous reactions
  - Gas phase reactions
    - ✓ Combustion of gaseous fuel – natural gas (CH_4)
  - Liquid phase reactions
    - ✓ Soap – glycerol – esterification
- Heterogeneous
  - Reactants and products in different phase
    - ✓ Coal combustion
  - Catalytic reactions
    - ✓ Catalytic converter – vehicle exhaust – boiler exhaust
    - ✓ Biodiesel – trans-esterification

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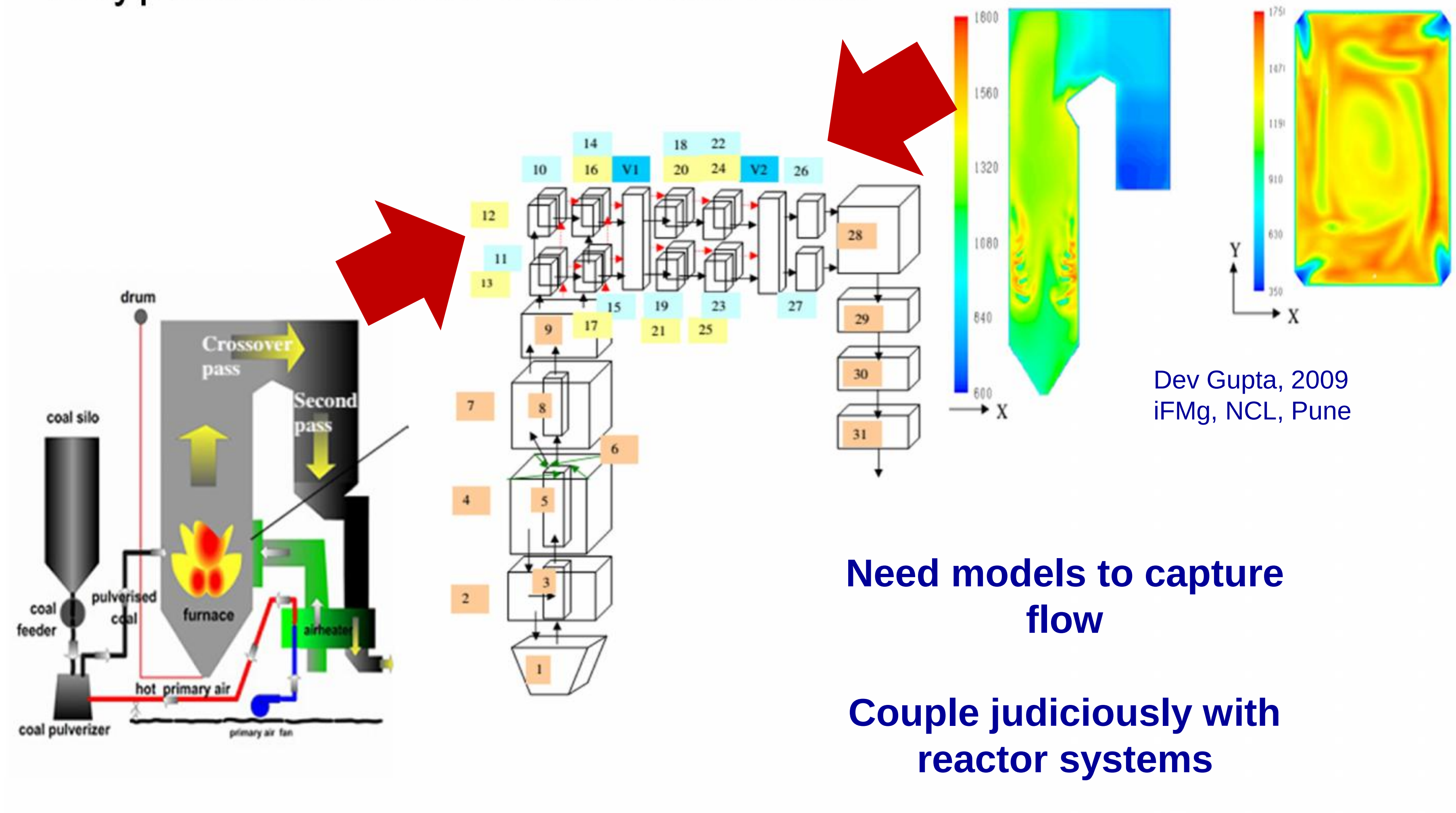
- A typical 200 MWe Coal Fired Boiler



Dev Gupta, 2009
iFMg, NCL, Pune

Need models to capture flow

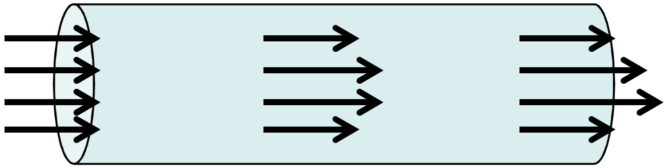
Couple judiciously with reactor systems

Time scale in reactive flows

- Space time τ

$$\tau = \frac{V}{\upsilon} = \frac{L}{\langle u \rangle}$$

- Residence time
  - Different fluid elements spend different time $\bar{t}$



- Finite time required for mixing
  - milk to tea / coffee decoction

- Reaction time

Species Balance

- Convection – bulk motion and diffusion at face x and x+δx

$$\dot{F}_{i,x} = \dot{F}_{i,ad} + \dot{F}_{i,diff} = \left(\dot{m}\ x_{i,x}\right) + \left(-\Gamma\ \nabla\ x_{i,x}\ A_x\right)$$

$$\dot{m}_x\ x_{i,x} = \left(\rho u A\right)_x\ x_{i,x}$$

- Net source

$$\dot{F}_{i,gene} - \dot{F}_{i,disapp} = \left(S_{i,\delta\forall}\right)\delta\forall$$

Accumulation

$$\dot{F}_{i,accu} = \frac{\delta\left(m_i\right)}{\delta t} = \frac{\delta\left(\rho\delta\forall\ x_i\right)}{\delta t}$$

$$\boxed{\dot{F}_{i,x} + \dot{F}_{i,gene} = \dot{F}_{i,x+\delta x} + \dot{F}_{i,disapp} + F_{i,accu}}$$

- Shrink CV to 0

$$\lim \delta\forall \to 0 \qquad \lim \delta t \to 0$$

$$\boxed{\frac{\partial\left(\rho x_i\right)}{\partial t} + \frac{\partial(\rho u\ x_i)}{\partial x} = \frac{\partial\left(\Gamma\ \text{grad}\ x_i\right)}{\partial x} + S_i}$$

$$\boxed{\frac{\partial\left(\rho x_i\right)}{\partial t} + \text{div}(\rho\vec{V}\ x_i) = \text{div}\left(\Gamma\ \text{grad}\ x_i\right) + S_i}$$

Closures

- Source terms for species
  - Reaction
  - Mass transfer / phase transfer

$$a\ A + b\ B \rightarrow c\ C + d\ D$$

- Rate of formation or consumption of species

$$r_i = -\frac{1}{a}\frac{dN_A}{dt} = -\frac{1}{b}\frac{dN_B}{dt} = +\frac{1}{c}\frac{dN_C}{dt} = +\frac{1}{d}\frac{dN_D}{dt} = \frac{1}{\upsilon_i}\frac{dN_i}{dt}$$

$$S_i = \frac{r_i}{\delta \forall}$$

Reaction rate

- Right quantity Right Energy Right place?

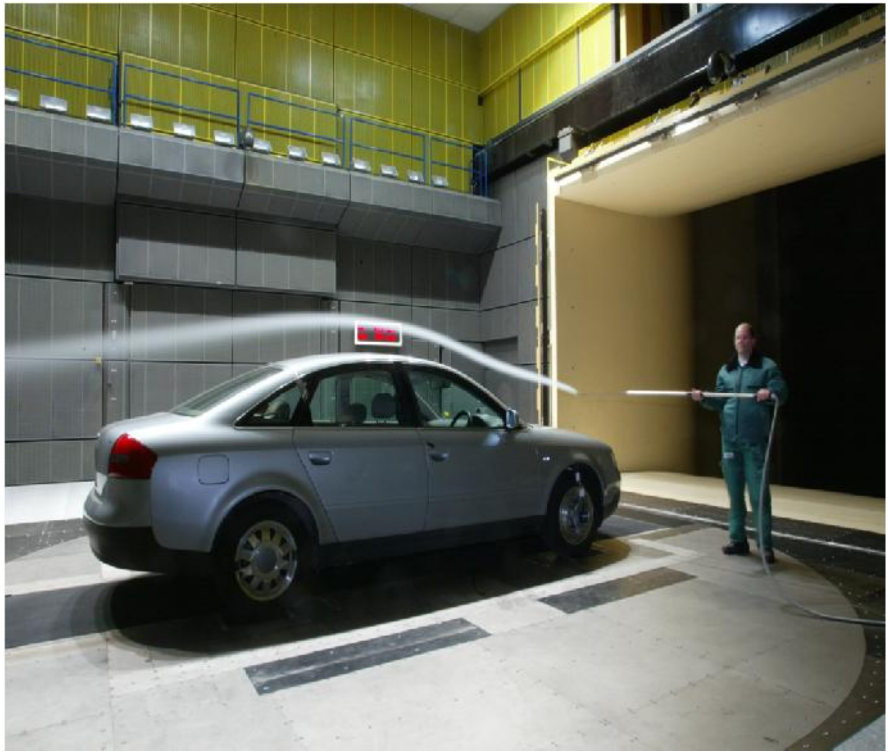
- Reaction rate
  - Availability of the substance
    - ✓ Concentration
  - Energy available

$$r_i = f(C, T) = k \Pi C_i^{\upsilon_i}$$

$$k = k_0 \exp\left(\frac{-E}{RT}\right)$$

Species transport

- Species balance without source term
  - No reaction
  - Only bulk motion (advection) and diffusion
  - Track / trace flow
    - ✓Streamline
    - ✓Streakline
    - ✓Pathline



Building species transport in CFD model

- Define species
  - N_2, CO, CO_2
- Define reaction involving species
  - Reaction stoichiometry
- Source term for reaction
  - Reaction rate
- Inlet mass fraction

Tips: Residence Time

- Define species
  - Same physico-chemical properties as of base fluid
    - ✓A tagged fluid element (or) numerical tracer
- Simulation sequence
  - Enable only “flow” and solve
  - Converge and freeze flow pattern
    - ✓Velocity pattern is established
  - Uncheck/ Disable the “flow” equation
  - Enable the “species equation”

RTD: Simulation Sequence

- Model
  - Enable transient model
- Monitor
  - Set surface monitor at outlet plane
    - ✓ Mol fraction of species at the surface against time
- Pulse input
  - Set mass fraction for species as “1” at inlet boundary
  - Iterate for one time step
    - ✓ check flow time / space time of the model
  - Revert species mass fraction to “0”
  - Continue to solve till mass fraction at outlet drops ~ 1E-12
  - Check species mass balance

Tips on Solving Reactive Flows

- Solve flow sans reaction
  - ✓ Equation – deselect mol fraction
  - – Establish flow structure
  - – Use constant heat capacity

$$C_P \neq fn(T)$$

- Enable reactions
  - ✓ Equation – select mol fraction
    - – May freeze flow
  - ✓ Constant heat capacity
- Include heat effects
  - ✓ Variable heat capacity $C_P = fn(T)$

Few Comments

- Effect of turbulence on reaction rate
  - Reaction is at molecular scale
    - ✓ What if eddies are present ?
- Reversible reactions
- Heterogeneous reactions
- Reactions at wall surface
- Diffusion coefficient
  - Multicomponent diffusion
- Complex reaction network – Multiple reactions
  - Combustion
  - Fluid catalytic cracking

Resources

- Patankar, S. (1980) **Numerical Heat Transfer and Fluid Flow**. Taylor and Francis
- Versteeg, H.K. and Malalasekera, W. (1995) **An Introduction to computational Fluid Dynamics - The Finite Volume Method**. Longman Scientific and Technical
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Web Resources

- http://www.cfd-online.com
- http://en.wikipedia.org/wiki/Computational_fluid_dynamics
- http://www.cfdreview.com/
- https://confluence.cornell.edu/display/SIMULATION/FLUENT+Learning+Modules
- www.google.com
- http://weblab.open.ac.uk/firstflight/forces/#

Gratitude

- Dr. Vivek V. Ranade – My Mentor Guide and Teacher and the research group at NCL, Pune

- Dr. B. Jayaraman, SAP, SoME
  - For providing me a wonderful platform to play with

- Audience
  - For patient hearing
  - For thirst in seeking knowledge

THANK YOU

A person who never made a mistake never tried anything new

- Albert Einstein
- 1879 -1955