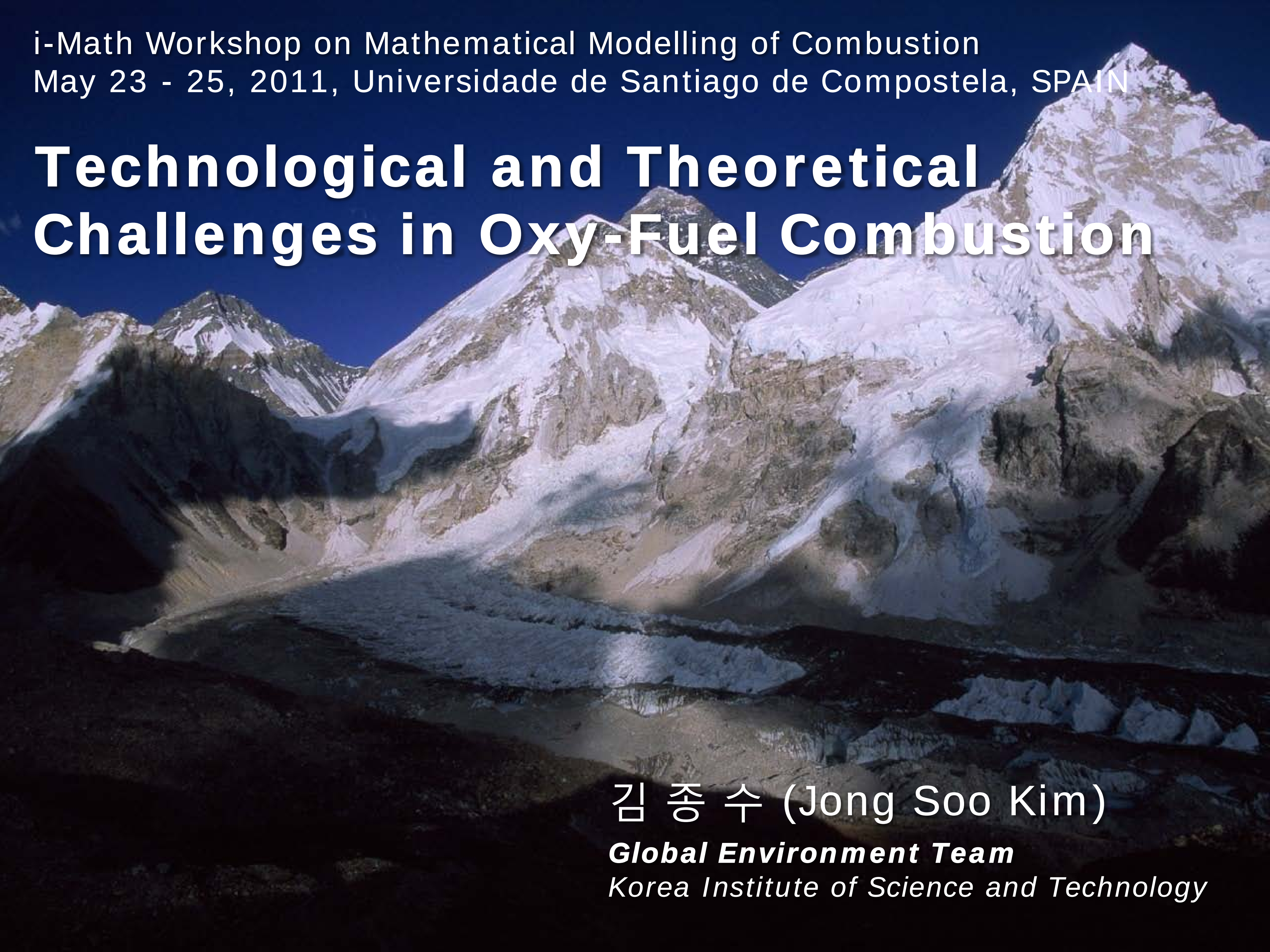

i-Math Workshop on Mathematical Modelling of Combustion
May 23 - 25, 2011, Universidade de Santiago de Compostela, SPAIN

Technological and Theoretical Challenges in Oxy-Fuel Combustion

김 종 수 (Jong Soo Kim)
Global Environment Team
Korea Institute of Science and Technology

Climate Change & Combustion

- Two Outstanding Issues

- **Oxy-Fuel Combustion** for CCS
  - CCS = CO_2 Capture & Storage

- Climate Forcing By Black Carbon
  - Particularly on the Arctic Climate

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Numerical Modelling ?

- Numerical Prediction
- Numerical Model
- Numerical Computation
- Numerical Simulation
- CFD
- ...

- Are They the Same ?

What is Modelling ?

- Modelling
  - Simplify
  - The Complex Real-World Problems
  - To a Tractable Form
  - While Maintaining the Physical Essence

- Modelling Procedure
  - Physical Modelling
  - Mathematical (or Experimental) Modelling
  - Numerical (or Experimental) Realization

Contents

What is Oxy-Fuel Combustion ?

- Applications

Physical Essence of Oxy-Fuel Combustion

- Theoretical Challenges

Mathematical Modelling Issues

Technological Challenges

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What is Oxy-Fuel Combustion ?

Stoichiometry

- Oxy-Fuel : $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$
- Air-Fuel : $CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2$

Higher Flame Temperature (~ 3000K)

Improved Heat Transfer & Thermal Efficiency

- Enhanced Heat Transfer ← High Temperature & Concentrations of CO_2 and H_2O
- Less Energy-Loss through Exhaust Gas
- Need to Overcome the Oxygen Production Cost

Significant Increase in Flame Stability

Easy to Capture CO_2

Oxy-Fuel Combustion

- Where do we use it ?

Application	Why ?
Industrial Furnace	➢ Higher Thermal Efficiency ➢ Higher Productivity
Gasification or Fuel Reforming	➢ **Rich Oxy-Fuel Combustion** ➢ Maintaining the Gasifying Reaction
Oxy-PC Combustion with FGR	➢ **CO_2 Capture** ➢ Retrofitting the Existing PC Power Plant
Oxy-PC Combustion w/o FGR	➢ **CO_2 Capture** ➢ High Performance CCS-Capable PC Power Plant ➢ Only Conceptually Exists

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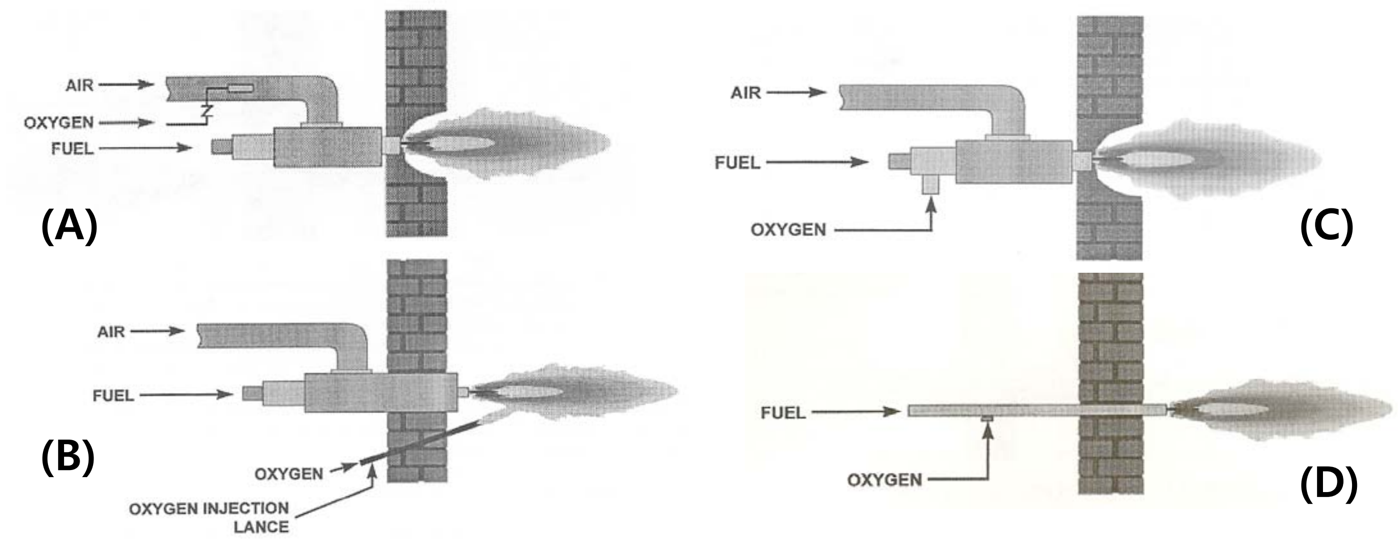
OFC for Industrial Furnace

- Mainly For Metal Heating & Glass Melting
- High Exit Temperature > 1000K
  - Air-Fuel Flame : $T_f < 2000K$ ➔ $\eta < 50\%$
- Oxy-Fuel Flame Temperature ~ 3000K : **$\eta \sim 70\%$**
- Low NOx, Higher Productivity and Quality
- Enough to Cover the Oxygen Cost

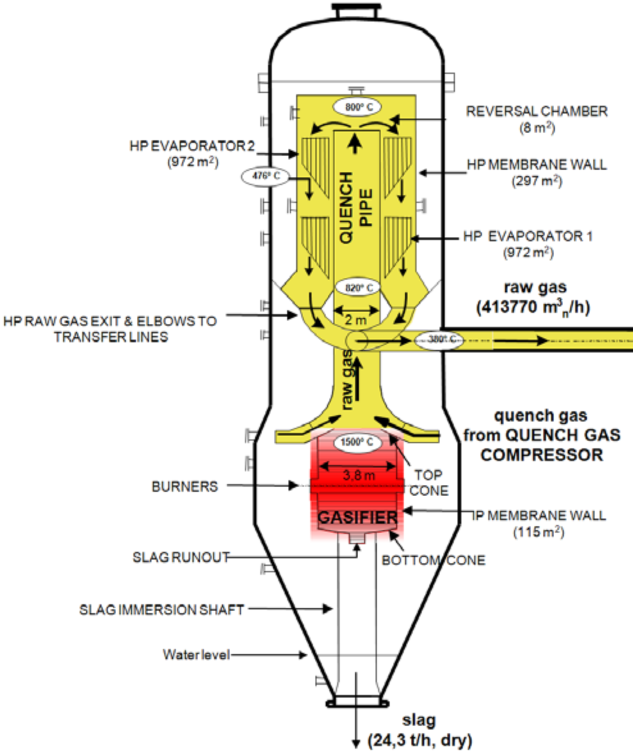


Source : Oxygen-Enhanced Combustion (CRC Press)

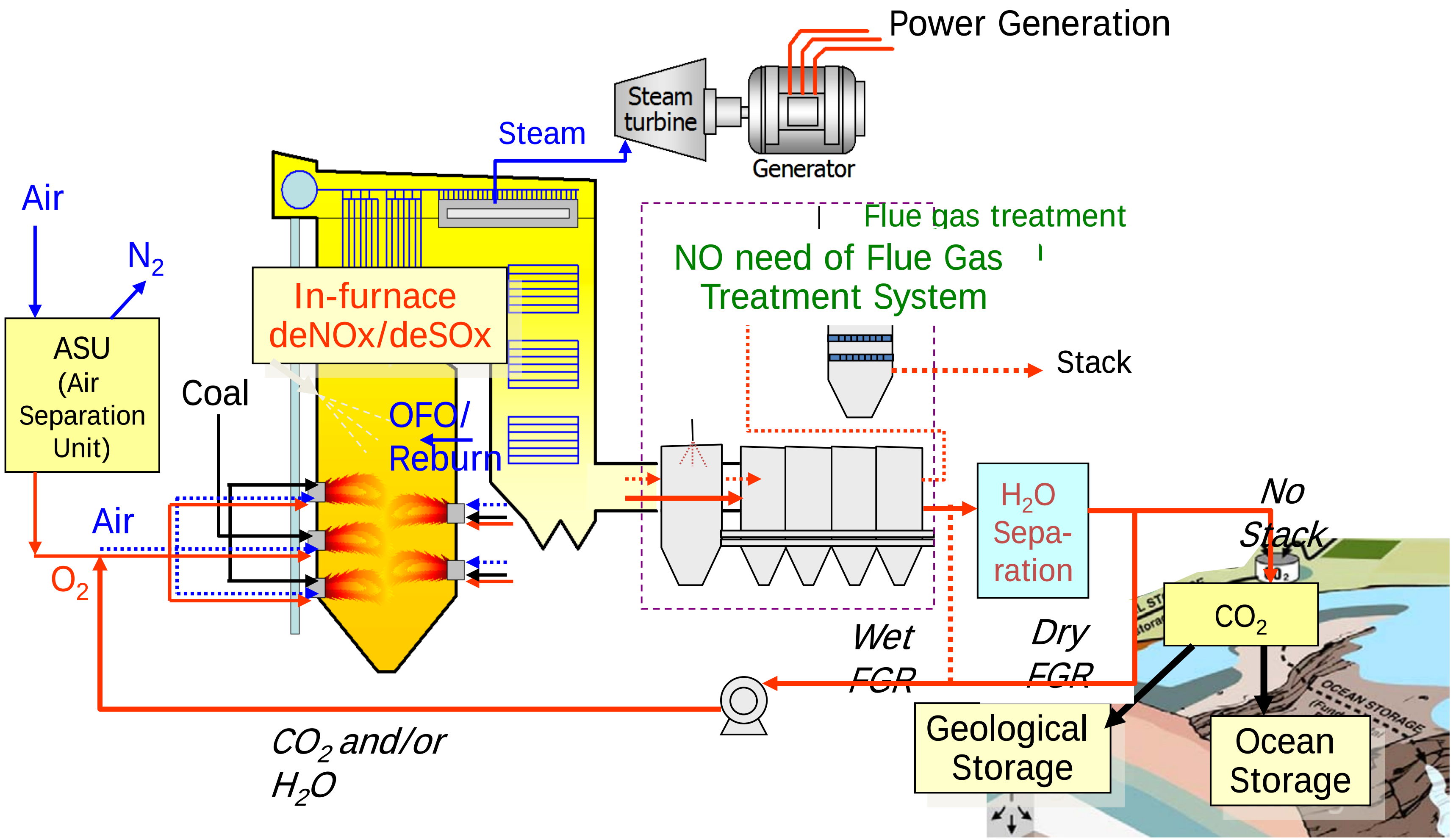
OFC Gasifier

Elcogas IGCC Gasifier

- Gasification by <u>Partial Oxidation</u>
  - C + ½ $O_2 \rightarrow CO$
  - **Rich Oxy-Fuel Combustion**
  - Pure Oxygen to Maintain the Reaction Temperature



OFC for PC Power Plant



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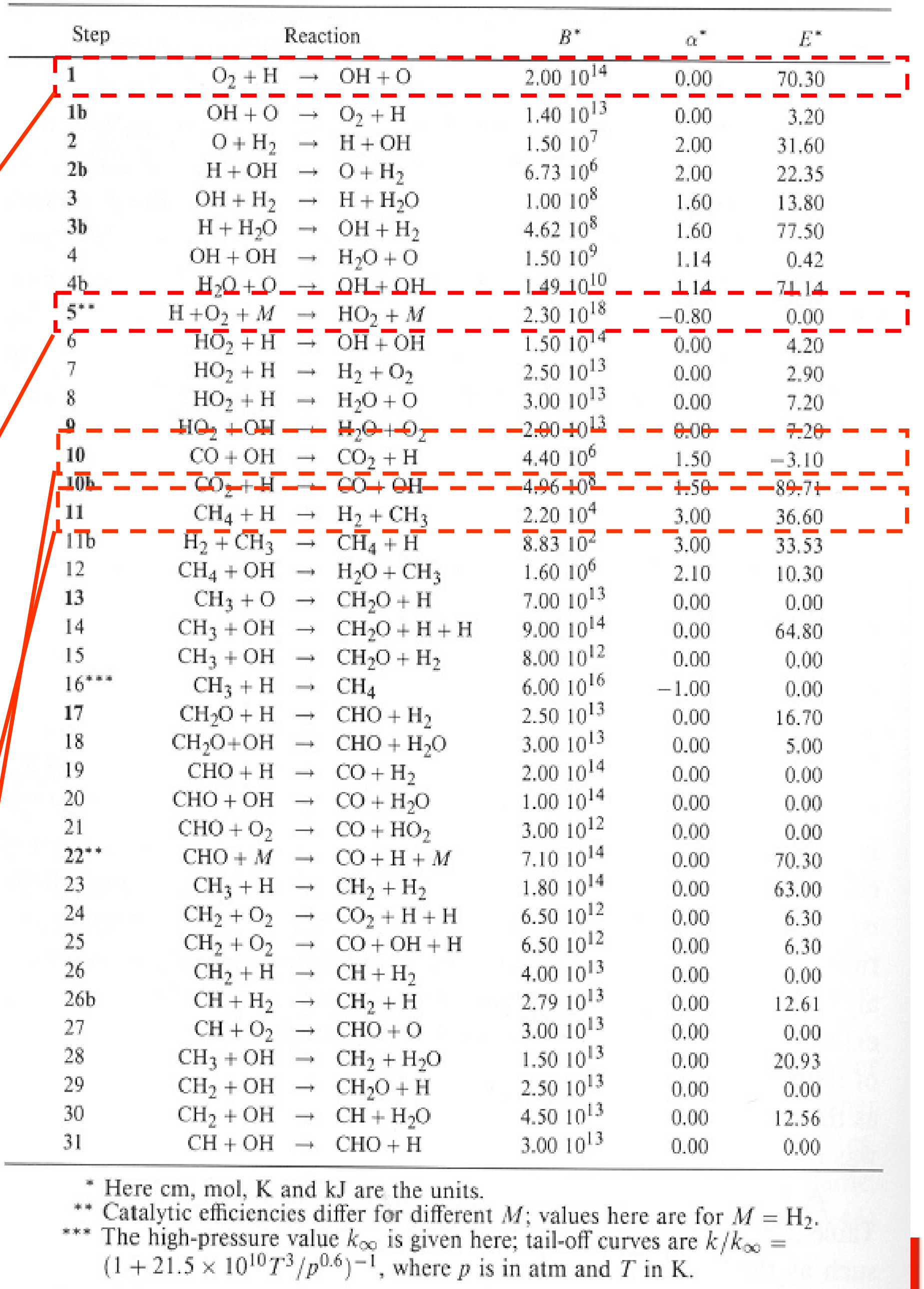
Physical Essence

- Chemical Kinetics
- Flame Structure
- Heterogeneous Combustion

Chemistry

- ❖ Radicals
  - ➢ Chain Branching
    - ◆ **1** : $O_2 + H \rightarrow OH + O$
  - ➢ Radical Recombination
    - ◆ **5** : $O_2 + H + M \rightarrow HO_2 + M$
  - ➢ **Crossover Temperature**
    - ◆ $\omega_1 = \omega_5$

- ❖ Methane oxidation
  - ➢ Fuel decomposition
    - ◆ $CH_4 + 1.5O_2 \rightarrow CO + H_2O$
    - ◆ Dominated by reaction #11
    - ◆ **11** : $CH_4 + H \rightarrow CH_3 + H_2$
  - ➢ CO oxidation
    - ◆ $CO + 0.5O_2 \rightarrow CO_2$
    - ◆ Dominated by reaction #10
    - ◆ **10** : $CO + OH \rightarrow CO_2 + H$



Step	Reaction	B*	α*	E*
1	$O_2 + H \rightarrow OH + O$	$2.00\ 10^{14}$	0.00	70.30
1b	$OH + O \rightarrow O_2 + H$	$1.40\ 10^{13}$	0.00	3.20
2	$O + H_2 \rightarrow H + OH$	$1.50\ 10^{7}$	2.00	31.60
2b	$H + OH \rightarrow O + H_2$	$6.73\ 10^{6}$	2.00	22.35
3	$OH + H_2 \rightarrow H + H_2O$	$1.00\ 10^{8}$	1.60	13.80
3b	$H + H_2O \rightarrow OH + H_2$	$4.62\ 10^{8}$	1.60	77.50
4	$OH + OH \rightarrow H_2O + O$	$1.50\ 10^{9}$	1.14	0.42
4b	$H_2O + O \rightarrow OH + OH$	$1.49\ 10^{10}$	1.14	71.14
5**	$H + O_2 + M \rightarrow HO_2 + M$	$2.30\ 10^{18}$	−0.80	0.00
6	$HO_2 + H \rightarrow OH + OH$	$1.50\ 10^{14}$	0.00	4.20
7	$HO_2 + H \rightarrow H_2 + O_2$	$2.50\ 10^{13}$	0.00	2.90
8	$HO_2 + H \rightarrow H_2O + O$	$3.00\ 10^{13}$	0.00	7.20
9	$HO_2 + OH \rightarrow H_2O + O_2$	$2.00\ 10^{13}$	0.00	7.20
10	$CO + OH \rightarrow CO_2 + H$	$4.40\ 10^{6}$	1.50	−3.10
10b	$CO_2 + H \rightarrow CO + OH$	$4.96\ 10^{8}$	1.50	89.71
11	$CH_4 + H \rightarrow H_2 + CH_3$	$2.20\ 10^{4}$	3.00	36.60
11b	$H_2 + CH_3 \rightarrow CH_4 + H$	$8.83\ 10^{2}$	3.00	33.53
12	$CH_4 + OH \rightarrow H_2O + CH_3$	$1.60\ 10^{6}$	2.10	10.30
13	$CH_3 + O \rightarrow CH_2O + H$	$7.00\ 10^{13}$	0.00	0.00
14	$CH_3 + OH \rightarrow CH_2O + H + H$	$9.00\ 10^{14}$	0.00	64.80
15	$CH_3 + OH \rightarrow CH_2O + H_2$	$8.00\ 10^{12}$	0.00	0.00
16***	$CH_3 + H \rightarrow CH_4$	$6.00\ 10^{16}$	−1.00	0.00
17	$CH_2O + H \rightarrow CHO + H_2$	$2.50\ 10^{13}$	0.00	16.70
18	$CH_2O + OH \rightarrow CHO + H_2O$	$3.00\ 10^{13}$	0.00	5.00
19	$CHO + H \rightarrow CO + H_2$	$2.00\ 10^{14}$	0.00	0.00
20	$CHO + OH \rightarrow CO + H_2O$	$1.00\ 10^{14}$	0.00	0.00
21	$CHO + O_2 \rightarrow CO + HO_2$	$3.00\ 10^{12}$	0.00	0.00
22**	$CHO + M \rightarrow CO + H + M$	$7.10\ 10^{14}$	0.00	70.30
23	$CH_3 + H \rightarrow CH_2 + H_2$	$1.80\ 10^{14}$	0.00	63.00
24	$CH_2 + O_2 \rightarrow CO_2 + H + H$	$6.50\ 10^{12}$	0.00	6.30
25	$CH_2 + O_2 \rightarrow CO + OH + H$	$6.50\ 10^{12}$	0.00	6.30
26	$CH_2 + H \rightarrow CH + H_2$	$4.00\ 10^{13}$	0.00	0.00
26b	$CH + H_2 \rightarrow CH_2 + H$	$2.79\ 10^{13}$	0.00	12.61
27	$CH + O_2 \rightarrow CHO + O$	$3.00\ 10^{13}$	0.00	0.00
28	$CH_3 + OH \rightarrow CH_2 + H_2O$	$1.50\ 10^{13}$	0.00	20.93
29	$CH_2 + OH \rightarrow CH_2O + H$	$2.50\ 10^{13}$	0.00	0.00
30	$CH_2 + OH \rightarrow CH + H_2O$	$4.50\ 10^{13}$	0.00	12.56
31	$CH + OH \rightarrow CHO + H$	$3.00\ 10^{13}$	0.00	0.00

* Here cm, mol, K and kJ are the units.

** Catalytic efficiencies differ for different M; values here are for $M = H_2$.

*** The high-pressure value k_∞ is given here; tail-off curves are $k/k_\infty = (1 + 21.5 \times 10^{10} T^3/p^{0.6})^{-1}$, where p is in atm and T in K.

A. Liñán and F. A. Williams
Fundamental Aspects of Combustion, 1993, p.50

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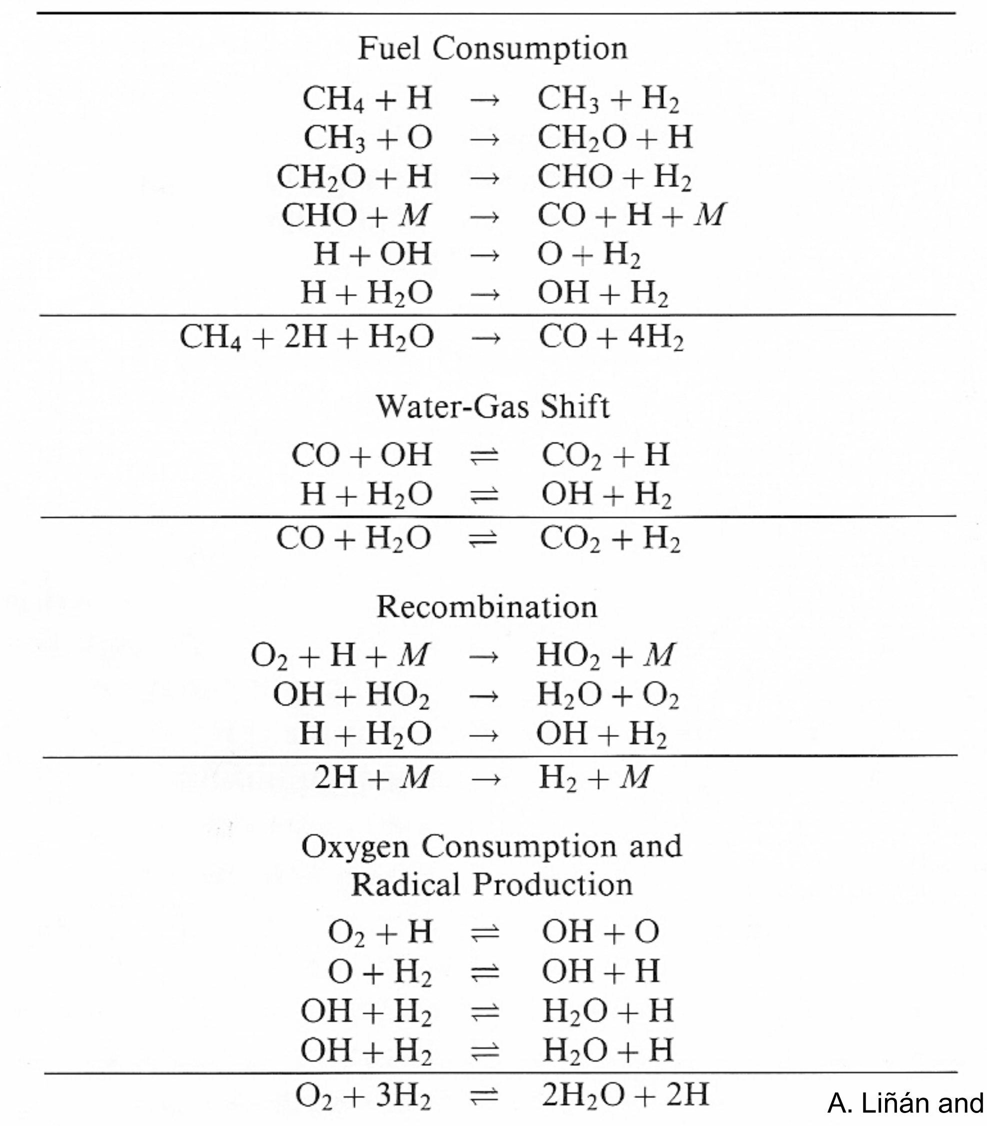
4-Step Mechanism



Fuel Consumption

$$\begin{aligned} CH_4 + H &\rightarrow CH_3 + H_2 \\ CH_3 + O &\rightarrow CH_2O + H \\ CH_2O + H &\rightarrow CHO + H_2 \\ CHO + M &\rightarrow CO + H + M \\ H + OH &\rightarrow O + H_2 \\ H + H_2O &\rightarrow OH + H_2 \end{aligned}$$

$$CH_4 + 2H + H_2O \rightarrow CO + 4H_2$$

Water-Gas Shift

$$\begin{aligned} CO + OH &\rightleftharpoons CO_2 + H \\ H + H_2O &\rightleftharpoons OH + H_2 \end{aligned}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

Recombination

$$\begin{aligned} O_2 + H + M &\rightarrow HO_2 + M \\ OH + HO_2 &\rightarrow H_2O + O_2 \\ H + H_2O &\rightarrow OH + H_2 \end{aligned}$$

$$2H + M \rightarrow H_2 + M$$

Oxygen Consumption and Radical Production

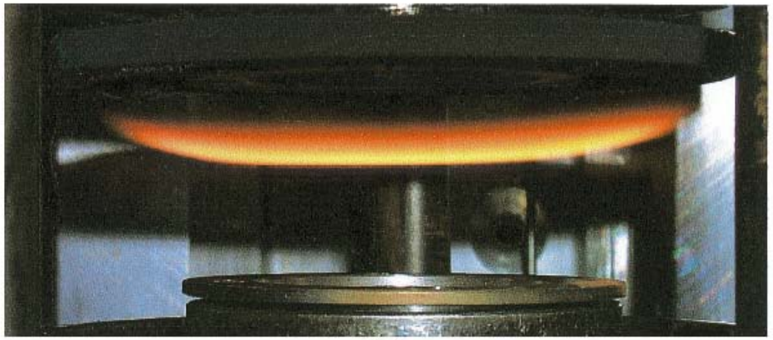
$$\begin{aligned} O_2 + H &\rightleftharpoons OH + O \\ O + H_2 &\rightleftharpoons OH + H \\ OH + H_2 &\rightleftharpoons H_2O + H \\ OH + H_2 &\rightleftharpoons H_2O + H \end{aligned}$$

$$O_2 + 3H_2 \rightleftharpoons 2H_2O + 2H$$

A. Liñán and F. A. Williams
Fundamental Aspects of Combustion, 1993, p.51

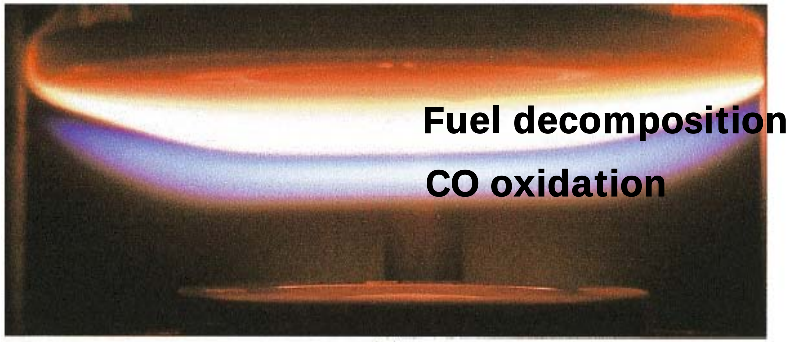
Flame Structure

- **Air-Fuel Flame**

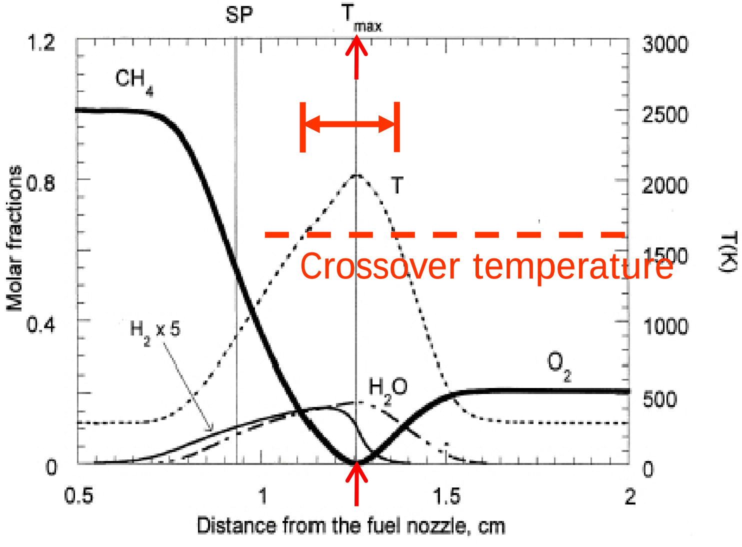


(a)

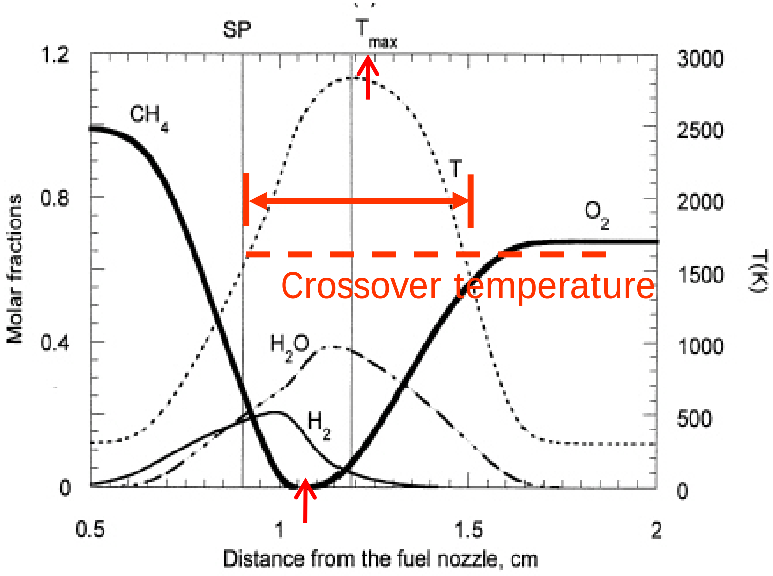
- **Oxy-Fuel Flame**



(b)



(a)



(b)

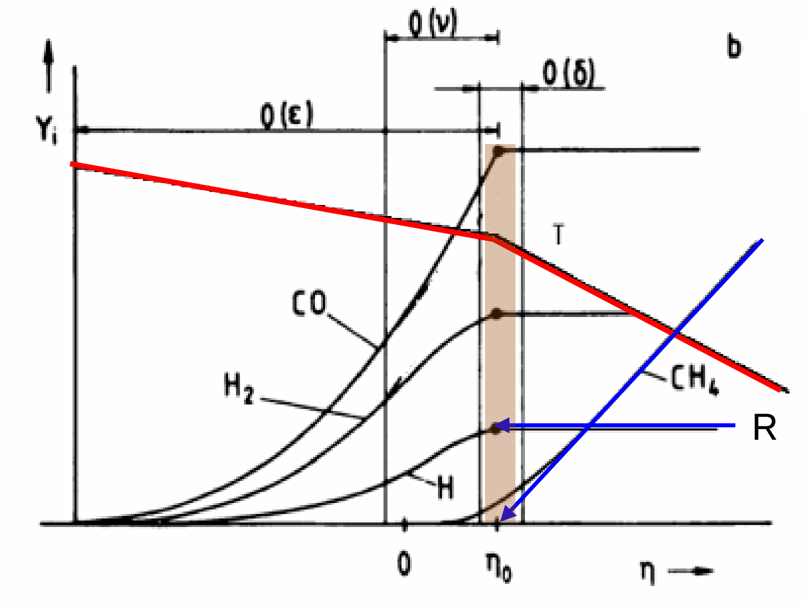
CF124:295-310
Kennedy (Illinois Chicago)

Two-Zone Structure

Thin “fuel decomposition region”

- Similar structure to the premixed flame of CH_4 and radicals

Thick “CO oxidation region”



➢**CH_4–R Premixed Flame**
➢**Super-Adiabatic Downstream**
➢**AEA by Linan**
 ➔**No Extinction**
 ➔**Improved Flame Stability**

Robust Flame

Thin Fuel Decomposition Layer

- No Quenching ← Superadiabatic

Thick CO Oxidation Layer

- $\delta_{\text{Oxy-Fuel}} \gg \delta_{\text{Air-Fuel}}$
- Longer Residence Time : $t_{\text{Diff}} \sim \delta^2$
- Higher Temperature → Shorter Chemical Time t_{Ch}
- **$t_{\text{Diff}} >> t_{\text{Ch}}$ → Extremely Difficult to Quench**
- **Providing the Superadiabatic Thermal Shield**

Fuel Reforming

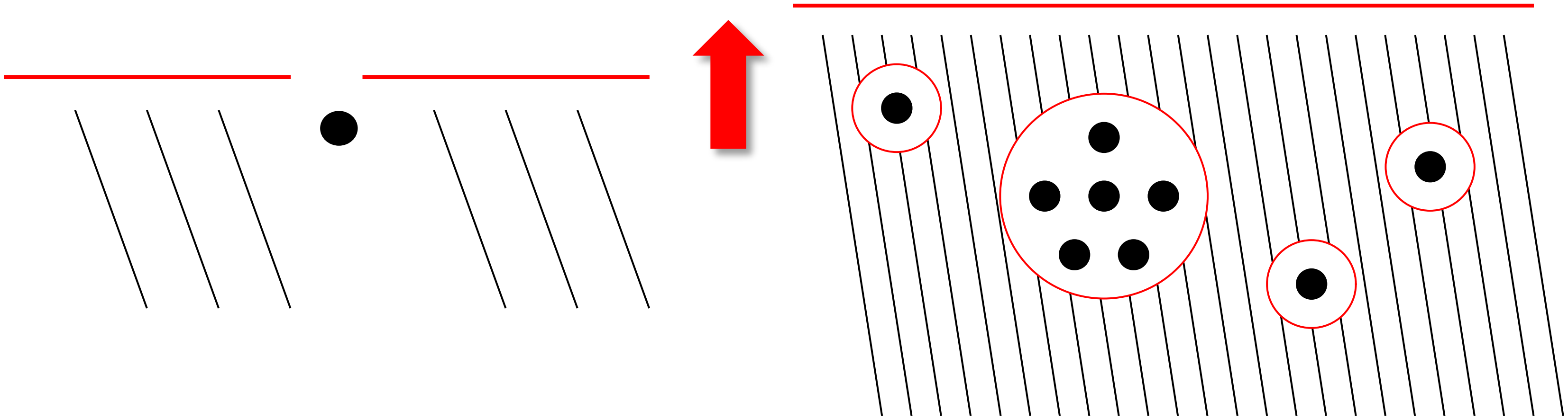
Thinner CO Oxidation Layer

- **Less Thermal Shielding** for the Fuel Decomposition Layer
- Much Weaker to Outer Disturbances

What Happens if the Fuel Decomposition Layer is Percolated ?

- Can Occur for Heterogeneous Combustion
    - Fuel : Pulverized Coal or Heavy Fuel Oil
- **Partial Oxidation** vs **Partial Combustion** ?

Heterogeneous Combustion



- ❖ Percolated by Fuel Spray
- ❖ Partial Combustion
  - ➢ Completely Burnt or Unburnt
- ❖ **Poor Gasification**

- ❖ Percolated but Self-Healed
  - ➢ Repaired by Strong Reaction Structure
- ❖ **Complete Combustion or Gasification**

➢ Key Issue : Prevention of the Fuel-Decomposition Reaction-Front Percolation

Numerical Modelling

Transport : Strong Turbulence

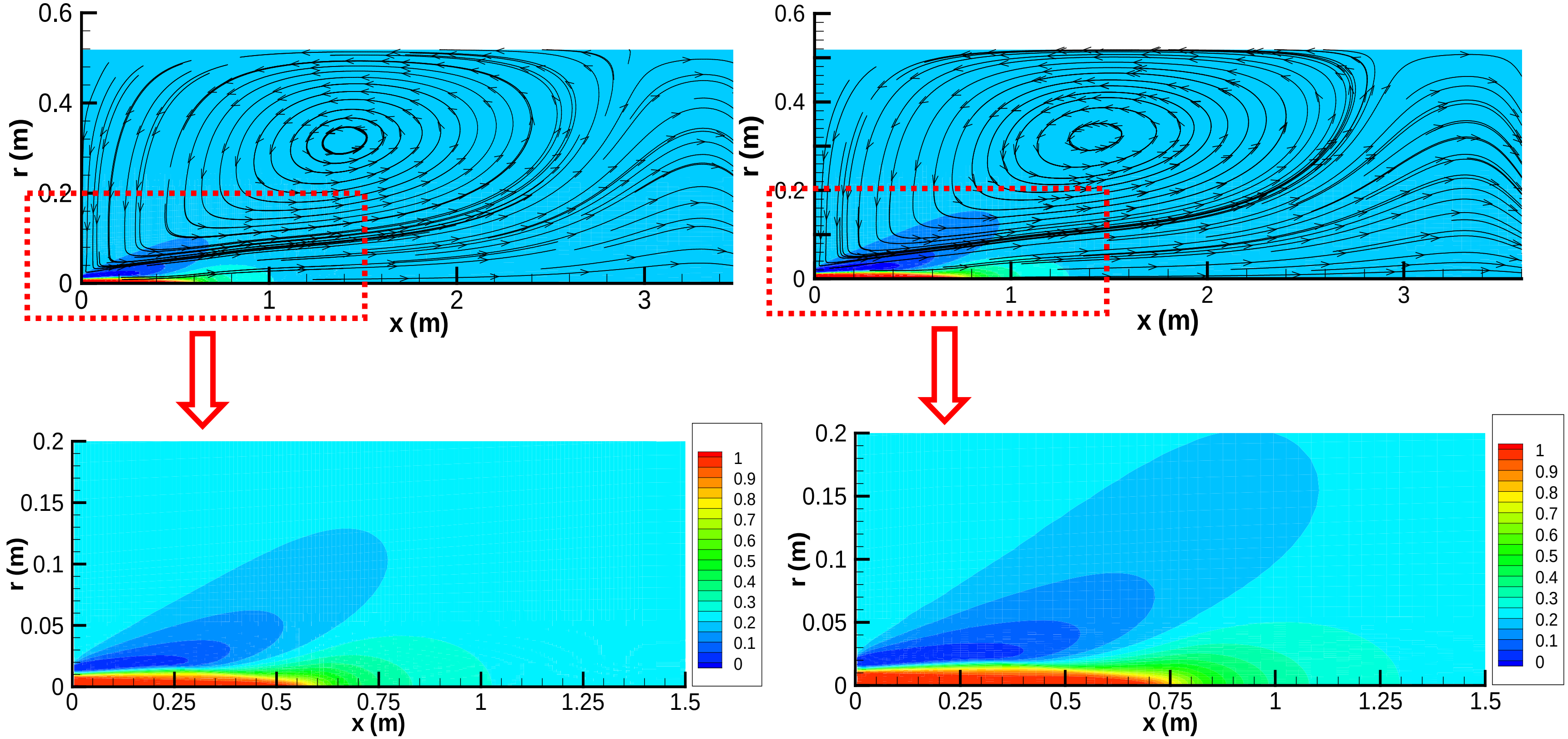
- Oxy-Fuel Burner ~ Simple Co-Axial Pipes
- High Injection Velocity
  - Better Burner Tip Cooling
  - Better Recirculation Region ➔ Better NOx Control
  - Improved Heat Transfer Properties

Kinetics : Thin Flame or Distributed Reaction ?

- Flamelet Model , CMC , PDF , ...

CMC Calculation Results

Velocity and Mixture Fraction Fields



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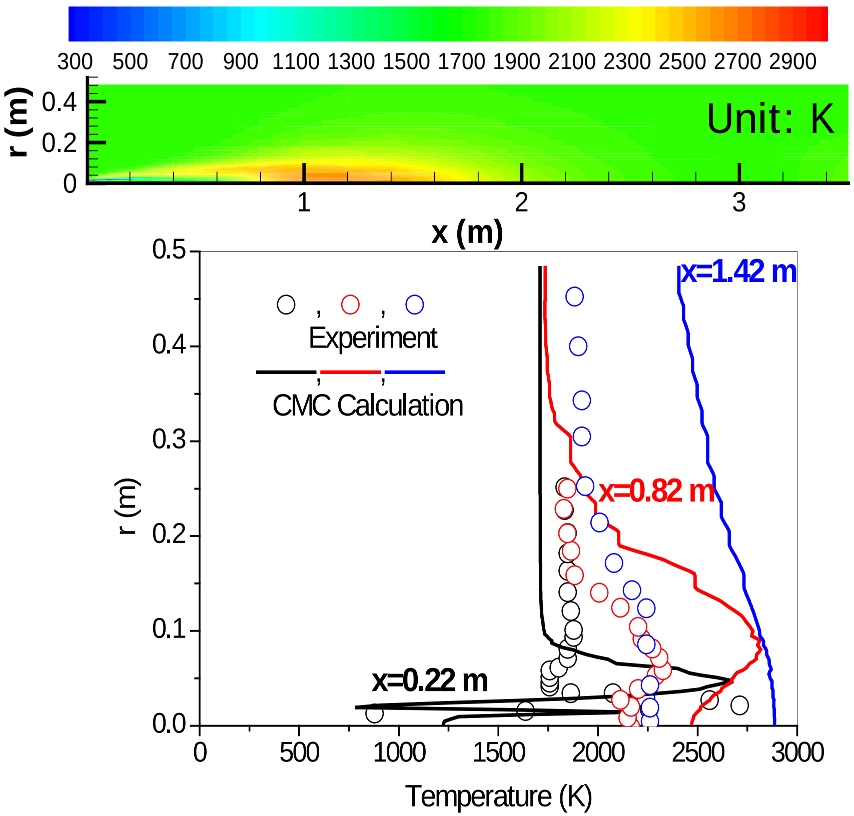
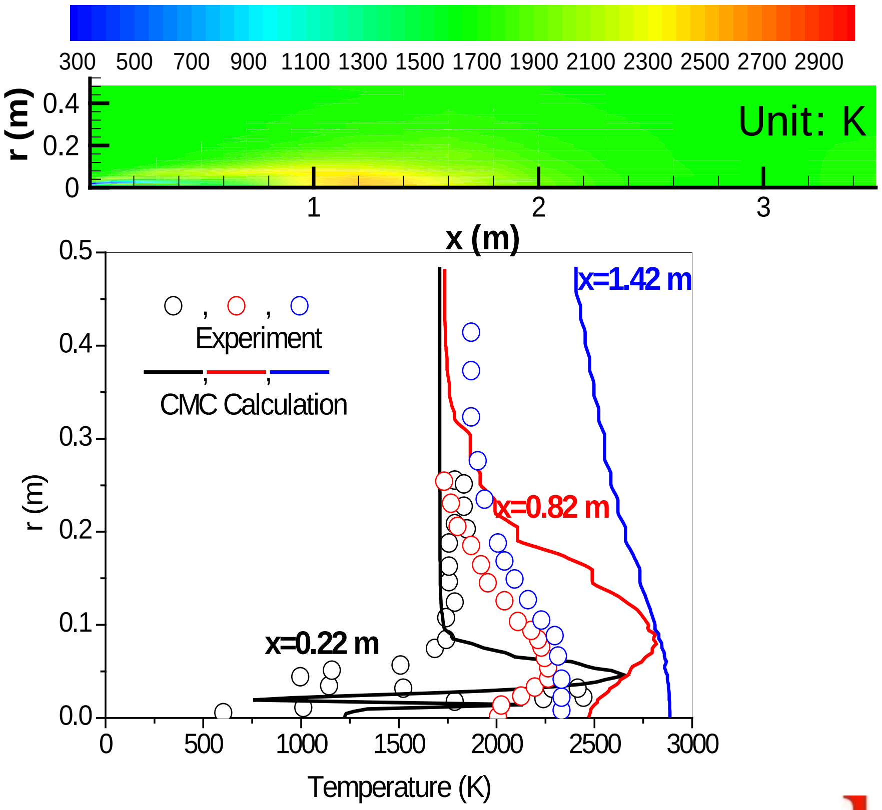
CMC Calculation Results

Temperature Fields

IFRF-Burner A



IFRF-Burner B



Inaccuracies in the Boundary Condition & Conditioned Moments

Difficulties in Numerical Modelling

Limited Benchmarking Data

- No Turbulent Flame Structure Data
  - **Lack of DNS Data & Optical Visualization or Measurements**
- Limited Industrial Furnace Measurement
  - **Incomplete Bench Marking Data from IFRF**

Choice of Model

- Flame Thickness ➔ Chemistry Closure (Flamelet or CMC)
- Strong Turbulence ➔ Inaccuracy of Conditioned Moments

Yet Premature for Parametric Studies

Technical Challenges

OFC in Industrial Furnaces

- Most Technical Problems Are Solved or Solvable.

Gasification

- Occurrence of Partial Combustion
- Extremely Difficult for Numerical Modelling

OFC for CCS

- Uncertainties in the Retrofit Routes
- High CCS Cost ➔ Increase in your electricity bill
  - Low Efficiency ➔ High Fuel Cost
  - More Equipment ➔ High Initial Investment

Difficulties in Gasification

- ❖ Consulting Inquiry from Samsung-BP
  - ➢ Gasification of HFO to Produce CO
  - ➢ Gasifier from GE-Energy (← Chevron-Texaco)
- ❖ Problems
  - ➢ Higher CO_2 Concentration ? → Yes !
  - ➢ Higher Soot Formation ? → Yes !
  - ➢ Flame Instability ? → Yes !
    - ◆ Burner Tip Was Damaged
- ❖ Cause
  - ➢ Burner Tip Damage → Loss of Stability
  - → Partial Quenching of Fuel Decomposition Layer
  - → Partial Combustion (CO2 & Soot Formation)
  - → More Heat Loss → More Partial Combustion
  - → Failure of Partial Oxidation

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Samsung-BP Case

- What Do They Want ?
  - **Numerical Simulation of Unsatisfactory Gasification & Find a Remedy**
- My Answer
  - No Way to do the Correct Numerical Simulation
  - **No Subgrid Model for Partial Combustion**
    - Partial Quenching of Thin Fuel-Decomposition Layer
- They Are Still Looking for Someone Who Can Do the Numerical Work.
- BAD Example Not to Follow
  - Numerical Modelling (?) without Physical Understanding

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Samsung-BP Case

- How to Solve the Problem
- Fuel Preparation
  - Preheating to Improve Atomization
  - Steam Injection : Adding H & O
- Burner Design
  - Better Thermal Cooling for the Tip
    - Increase Injection Speed (Smaller Diameter ?)
  - **Cheap Burner Design: Easy to Exchange**
- Optimize the Burner & Furnace Shapes

Oxy-PC Modelling Issue

Combustion with FGR

- Similar to Air Combustion : N_2 ➔ CO_2
- Doable with the Current Numerical Model

Radiative Heat Transfer

- **New Castle Group** : Stronger Radiation by CO_2
- **Utah Group** : No Significant Modification for Radiation
  - Radiation Dominated by Particles
- Others
  - <u>We Need More Research</u> to Figure Out Who's Correct.

CCS Cost (Retrofitting)

Coal Power Generation Cost		
Base COE (before CCS)		5¢/kWh
CCS Investment Cost	+1¢/kWh	6¢/kWh
CCS Energy Consumption ➢Efficiency : 40% → 30% ➔Less Electricity to Sell	**X 4/3**	8¢/kWh

- ❖ Over 50% Electricity Whole Sale Price Increase
- ❖ More Power Plants & Coal Consumption are Needed
- ❖ **Higher Cost Rise for Lower Efficiency Plants**
- ❖ There are Other Hidden Costs too.
- ❖ **Likely Double the COE**

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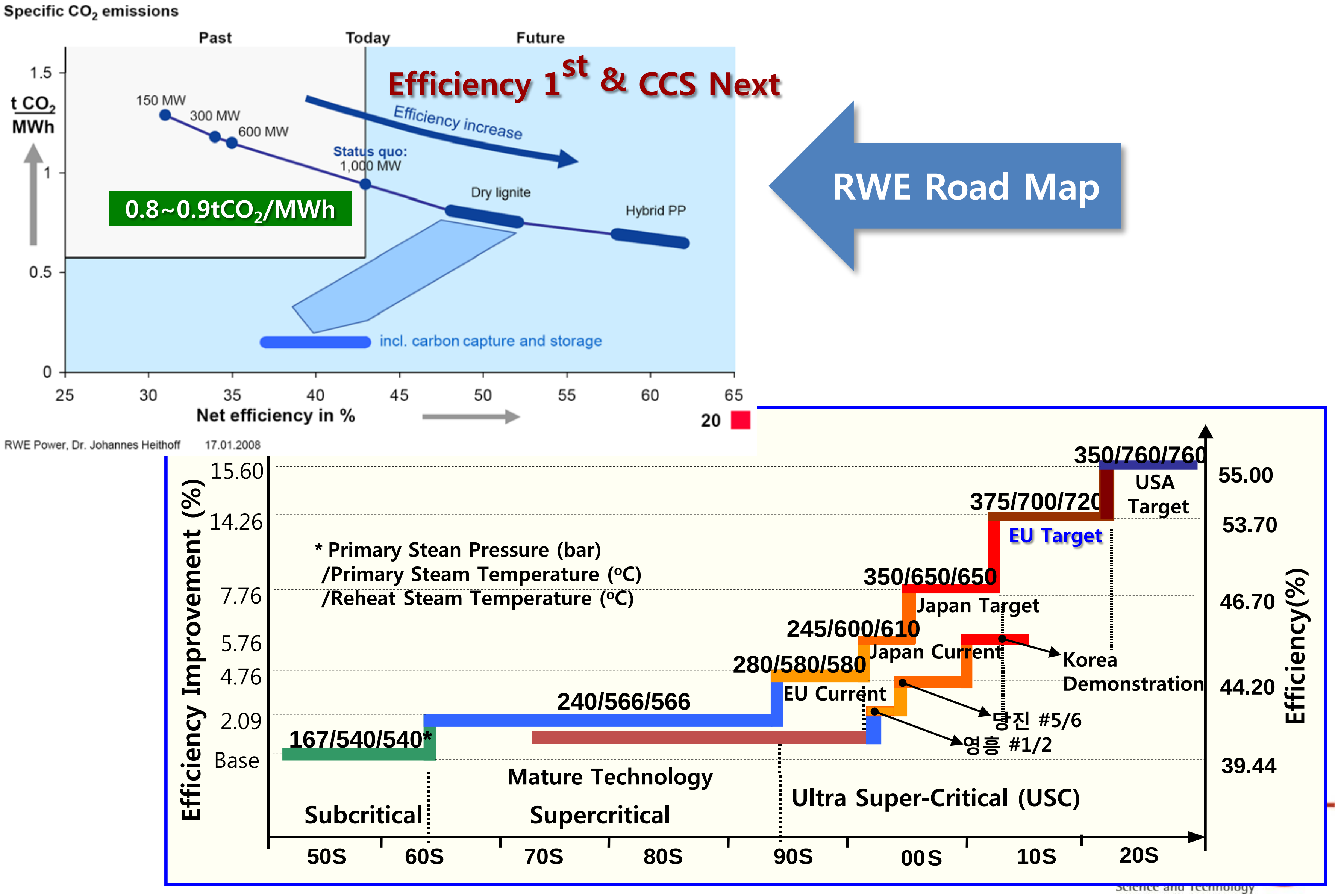
CCS Cost

- How to Reduce the CCS Cost
  - Improve Power Plant Efficiency
  - Reduce Fuel Cost
  - Reduce Equipment Cost

CCS @ Power Industry



Efficiency 1^{st} & CCS Next

RWE Road Map

Future CCS Technology

Placement

- Another Dark Age of Nuclear Power ?
- **More PC Power Demand (Base Load Coverage)**
- Sorry! Renewable Energy Cannot Meet the Baseline Power Demand.
- ➔ CCS Becomes the Primary Route to Reduce CO_2 Emission

Basic Requirements

- High Efficiency : 700+℃ Steam Temperature➔ $\eta > 50\%$
- Low Plant Cost : Simple & Compact Power Plant Design
- Fuel Flexibility : Lower Fuel Cost
- Easy CO_2 Capture

Basic Requirements

High Efficiency

- Hyper Super-Critical Cycle : Efficiency Target with CCS $\eta_{CCS} > 45\%$
- Material Development Needed for Higher Steam Temperature
- New Boiler Design & Turbine Development

Low Cost

- Low Flow Rate
- ➔ Compact Design for Furnace, Boiler, Environmental Equipments, …
- Large Capacity Possible : 1GWe

Near Zero Emission

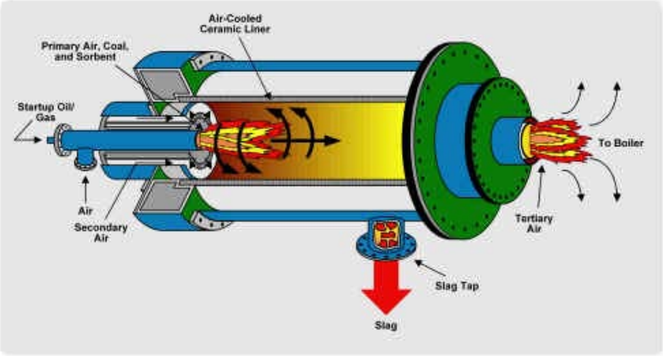
- Ultra Low PM, NOx & SOx Emission
- Overall CCS Efficiency > 90%

Fuel Quality

- Handling Low-Grade Coal, Coal Drying & Latent Heat Recovery
- Fuel Mixing with Biomass & RDF
- Slagging Resistance

Possibilities

- **Cyclone Furnace Oxy-Coal Combustion**
  - Recommended by KT, BL



- CFBC ?
  - Flow Rate may be too Low
  - Any Possibilities ?
- IGCC ?
  - Economically Competitive ?
  - Unlikely Against Oxy-Coal
- Any Likely Option for PCC Route ?
  - PCC = Post-Combustion Capture

Theoretical Challenges

- **Need to Verify the Two-Zone Structure for Turbulent Oxy-Fuel Flames**
  - **By DNS**
  - **& Optical Diagnostics**
- Chemistry Modelling
  - Thin Flame or Distributed Reaction ?
- Transport Modelling
  - Handling of the High Turbulence by High-Speed Injection.
- Industrial Simulation
  - Need Good Benchmark Data for Code Tuning

Technological Challenges

- Oxy-Fuel Combustion in General
  - Robust Flame ➔ Less Technical Difficulties
- **Gasification or Fuel Reforming**
  - Insufficient Understanding of Reaction Zone Structure
  - Prevention of Partial Combustion
  - How to Maintain the Integrity of the Fuel-Decomposition Reaction Front
- **Oxy-PC for CCS**
  - **Development of High Efficiency CCS-Ready Power Plant**
  - **Technological Doable**
  - **Financially Doable ?**

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